1 Differentiation Revisited

Every student knows what differentiation is, or does she? The essence of differentiation is the study of linear response. Many elementary properties of derivatives can be understood naturally from this point of view. Furthermore, this interpretation frees us from the elementary definition of derivatives, and paves the way to variational calculus and functional differentiation. However, these topics are postponed to **5** and **6**. In this section, we review differentiation.

Key words: differentiation, chain rule, derivative as susceptibility, strong derivative, differentiation of complex function, partial differentiation, d'Alembert's solution to wave equation, moving coordinates.

Summary:
(1) To compute (strong) derivatives is to study linear responses (**1.1**, **1.4**, **1.8**).
(2) The reader must be able to change freely the independent variables in PDE (**1.11**, **1.15**).
(3) 1D wave equation in free space can be solved via change of variables. The result is the famous d'Alembert's solution (**1.12**).

1.A Elementary Review

1.1 What is differentiation? Let f be a function defined on an (open) interval I, and $a \in I$. If the following limit, denoted by $f'(a)$, exists, we say f is *differentiable* at a:

$$f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}. \tag{1.1}$$

$f'(a)$ is called the *differential coefficient* of f at a. If f is differentiable

at $x = a$, then we have[1]

$$\delta f(a) \equiv f(a + \delta a) - f(a) \simeq f'(a)\delta a. \tag{1.2}$$

That is, we study the response of f against a small change of its variable. If a linear approximation of the response is reasonable for sufficiently small δa, we say f is differentiable. In other words, the essence of differentiation is the study of the linear response of f to a small perturbation of independent variables. This point of view will be exploited later (→**1.4**, **2.9**), but we must note two immediate consequences of linearity, **1.2** and **1.3**.

Exercise. Perhaps, we should check our working knowledge of elementary calculus first. if you are confident about your capability, you may use, e.g., Mathematica to do the menial work.
(A) Discuss whether the following statements are true.[2] If correct, prove the statement.
(1) P_m is a (multi-variable) polynomial in the following formula:

$$\frac{d^m}{dx^m}\left(\frac{1}{f}\right) = \frac{1}{f^{m+1}} P_m(f, f', \cdots, f^{(m)}), \tag{1.3}$$

where m is a positive integer.
(2) Let f be a differentiable function. If $f'(0) = 1$, then f is monotone in a sufficiently small neighborhood of 0.
(3) Let f be a C^∞ function with $\lim_{x\to\infty} f(x) = 0$. Then, $\lim_{x\to\infty} f'(x) = 0$.
(B) Elementary differentiation questions:
(1) Let $x = e^t \cos t$ and $y = e^t \sin t$. Compute d^2y/dx^2 as a function of t.
(2) Compute the limits

$$\lim_{x\to 0}\left(\frac{1}{x} - \frac{x}{\sin^2 x}\right), \tag{1.4}$$

$$\lim_{x\to 0}\frac{(1+x)^{1/x} - e}{x}. \tag{1.5}$$

(3) Compute $d^m(e^{-1/x^2})/dx^m$ at $x = 0$ for all positive integers m.
(C) How many times are the following functions differentiable?
(1)

$$f(x) = x^{9/4} \text{ for } x \geq 0,\ 0 \text{ for } x < 0 \tag{1.6}$$

(2)

$$f(x) = x^3 \text{ for } x \geq 0,\ 0 \text{ for } x < 0 \tag{1.7}$$

(3)

$$f(x) = |x|^3. \tag{1.8}$$

[1] $\simeq$ is used informally, but in these notes accurate meaning can always be attached. In the present case, $\simeq$ means equality ignoring $o[\delta a]$.

[2] B. R. Gelbaum and J. M. Olmsted, *Counterexamples in Analysis* (Holden-Day, 1964) is a useful book when you wish to think a delicate thing.

(4)

$$y = e^{-1/x(1-x)} \text{ for } x \in [0,1],\ 0 \text{ otherwise} \tag{1.9}$$

(5)

$$f(x) = x^n \sin\frac{1}{x} \ (\text{with } f(0) = 0), \tag{1.10}$$

where n is a positive integer.

(D) **Orthogonal polynomials**

They will be discussed in a unified way in **XX**, but here, let us check some formulas related to them (generalized Rodrigues' formulas →**??**)

(1) Demonstrate that $P_n^{(\alpha,\beta)}(x)$ defined as follows is an n-th degree polynomial (called *Jacobi's polynomial*→**??**) ($\alpha, \beta > -1$):

$$P_n^{(\alpha,\beta)}(x) = (1-x)^{-\alpha}(1+x)^{-\beta}\frac{(-1)^n}{2^n n!}\left(\frac{d}{dx}\right)^n \{(1-x)^{n+\alpha}(1+x)^{n+\beta}\}, \tag{1.11}$$

where $\alpha, \beta \in \boldsymbol{R}$.

In particular, $T_n(x) \equiv ((2n)!!/(2n-1)!!)P_n^{(-1/2,-1/2)}(x)$ are called the Chebychev polynomials (→**??**), and $P_n^{(0,0)}(x) \equiv P_n(x)$ are called the Legendre polynomials (→**??**).

(2)

$$H_n(x) = (-1)^n e^{x^2}\left(\frac{d}{dx}\right)^n e^{-x^2} \tag{1.12}$$

is an n-th degree polynomial called the Hermite polynomial (→**??**).

(3) $T_n(x) = \cos(n \arccos x)$ (Chebychev's polynomial) satisfies (→**??**)

$$(1-x^2)\frac{d^2u}{dx^2} - x\frac{du}{dx} + n^2 u = 0. \tag{1.13}$$

(4) Laguerr's polynomial

$$L_n^{(\alpha)}(x) = \sum_{r=0}^{n}(-1)^r\binom{n+\alpha}{n-r}\frac{x^r}{r!} \tag{1.14}$$

satisfies

$$x\frac{d^2u}{dx^2} + (\alpha + 1 - x)\frac{du}{dx} + nu = 0. \tag{1.15}$$

(E) The following is a collection of standard special functions. They will not be stressed in the book, but the reader should have enough analytical muscle to confirm the following assertions.

Γ is the Gamma function (→**XX**), but we only need

$$\Gamma(x+1) = x\Gamma(x) \tag{1.16}$$

for positive real x (→**??**).

(1)

$$J_m(x) = \left(\frac{x}{2}\right)^m \sum_{k=0}^{\infty}\frac{(-1)^k}{k!\Gamma(m+k+1)}\left(\frac{x}{2}\right)^{2k} \tag{1.17}$$

satisfies

$$\frac{d^2u}{dx^2} + \frac{1}{x}\frac{du}{dx} + \left(1 - \frac{m^2}{x^2}\right)u = 0. \tag{1.18}$$

J_m is called the Bessel function of order m (→**??**).[3]
(2)

$$I_\nu(x) = \left(\frac{x}{2}\right)^\nu \sum_{n=0}^{\infty} \frac{(x/2)^{2n}}{n!\Gamma(\nu + n + 1)} \tag{1.19}$$

satisfies

$$\frac{d^2u}{dx^2} + \frac{1}{x}\frac{du}{dx} - \left(1 + \frac{\nu^2}{x^2}\right)u = 0. \tag{1.20}$$

I_ν is called the *modified Bessel function* (of the first kind) (→**??**).
(3)

$$j_n(x) \equiv \sqrt{\frac{\pi}{2x}} J_{n+1/2}(x), \tag{1.21}$$

which is called the *spherical Bessel function* (→**??**), satisfies

$$\frac{d^2u}{dx^2} + \frac{2}{x}\frac{du}{dx} + \left(1 - \frac{n(n+1)}{x^2}\right)u = 0. \tag{1.22}$$

(4) Whitaker's function

$$M_{\kappa,\mu}(x) = x^{\mu+1/2}e^{-x/2} \sum_{n=0}^{\infty} \frac{\Gamma(2\mu+1)\Gamma(\mu-\kappa+n+1/2)x^n}{\Gamma(2\mu+n+1)\Gamma(\mu-\kappa+1/2)n!} \tag{1.23}$$

satisfies

$$\frac{d^2u}{dx^2} + \left(-\frac{1}{4} + \frac{\kappa}{x} - \frac{\mu^2 - (1/4)}{x^2}\right)u = 0. \tag{1.24}$$

(5) Kummer's confluent hypergeometric function

$$F(\alpha, \gamma, x) = \sum_{n=0}^{\infty} \frac{(\alpha)_n x^n}{(\gamma)_n n!} \tag{1.25}$$

satisfies

$$x\frac{d^2u}{dx^2} + (\gamma - x)\frac{du}{dx} - \alpha u = 0. \tag{1.26}$$

Here $(\alpha)_n = \alpha(\alpha+1)\cdots(\alpha+n-1)$, etc. with $(\alpha)_0 = 1$.
(6) (cf. **??**)

$$u(x) = J_\nu(e^x) \tag{1.27}$$

satisfies

$$\frac{d^2u}{dx^2} + (e^{2x} - \nu^2)u = 0. \tag{1.28}$$

[Hint: see Exercise (1) above or **??**.]

[3] Here, m can be any integer; if $m < 0$, terms with $m + k + 1 \leq 0$ are ignored. See **??**.

Discussion.
(A) A **convex function** is a function such that the set $\{(x, y) : y \geq f(x)\}$ is a convex set.[4] Any convex function can be written as

$$f(x) = \sup_{(a,b)\in A} \{ax + b\}, \tag{1.29}$$

where A is a subset of $\boldsymbol{R}^2$. A convex function must be a continuous function and have right and left derivatives. The concept of convex function is very important in physics, esp., in statistical physics. In 1873 Gibbs characterized the family of equilibrium states of a system which is compatible with thermodynamics as follows (in modern words): The totality of equilibrium states of a simple fluid is a once differentiable manifold, which is the graph of a convex function U (internal energy) of S (entropy) and V (volume).[5]
(1) If f is convex on $[a, b]$ (or $([b, a])$, then

$$f(pa + (1-p)b) \leq pf(a) + (1-p)f(b) \tag{1.30}$$

for any $p \in [0, 1]$. This property can be used to define the convexity. This is a simple case of *Jensen's inequality*: f is convex if and only if

$$f(\sum_i \lambda_i x_i) \leq \sum_i \lambda_i f(x_i), \tag{1.31}$$

where $\sum_i \lambda_i = 1$ and $\lambda_i \geq 0$. This can be proved with the aid of (1.29).
(2) Show that e^x, $-\log x$, x^q $(q \geq 1)$ are convex.
(3) Using the fact that $-\log x$ is convex and use Jensen's inequality, show

$$\prod_i a_i^{\lambda_i} \leq \sum_i \lambda_i a_i, \tag{1.32}$$

where λ_i are as in (1).
(4) A periodic convex function is a constant.
(5) Let f and g be convex, and g be monotone increasing. Then, $g \circ f$ is convex.[6] [Note that f and g need not be differentiable.]
(6) For $x > 0$ if $xf(x)$ is convex, so is $f(1/x)$. This is obvious, if $f''(x)$ exists. Is this true even if f is less smooth? [Hint. Use (5)]
(B) **Pathological continuous functions**.
(1) **Weierstrass function**. The first example of nowhere differentiable continuous

[4] A set A is a convex set if for any $x, y \in A$ the segment connecting x and y is inside A.

[5] R. T. Rockafeller, *Convex Analysis* (Princeton, UP, 1970) is the standard reference of the topic. Its use in statistical physics is explained in the introduction by A. S. Wightman in R. B. Israel, *Convexity in the Theory of Lattice Gases* (Princeton UP, 1979). Y. Takahashi, *Real functions and Fourier analysis I* (Iwanami) has a handy explanation of convex functions.

[6] $(g \circ f)(x) \equiv g(f(x))$, i.e., the composition is denoted by $\circ$.

function was given by Weierstrass (→**10.5**). An example is[7]

$$f(t) = \sum_{r=0}^{\infty} \frac{1}{r!} \sin((r!)^2 t). \tag{1.33}$$

The convergence is uniform, so that the limit must be a continuous function. To prove the nondifferentiability at any point, a detailed estimate is needed. See Körner Section 11. The lesson we should learn from such functions is that if we differentiate a function repeatedly many times, then we could encounter bizarre functions, because differentiation magnifies details (and generally reduces differentiability).
(2) **Takagi function**. Let $D(x)$ be the distance between x and the closest integer to it (That is, $D(x) = dist(x, \boldsymbol{Z})$).
(i) Illustrate the graph of $D(x)$.
(ii) Define

$$T(x) = \sum_{n=0}^{\infty} \frac{1}{2^n} D(2^n x). \tag{1.34}$$

This is called the *Takagi* function, which is continuous, but nowhere differentiable. The function has self-similarity.[8]
Is any curve (except lines) which is self-similar nowhere differentiable?
(3) **von Koch curve**. Many beautiful examples of bizarre curves can be found in B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, 1983). A simple example of nowhere differentiable (and consequently without length) curves is the von Koch curve constructed by a self-similar substitution as illustrated below.

1.2 Chain rule. Suppose the input to a system g (henceforth, a system and its response function are denoted by the same symbol) is x and we feed the output of g into another system f. Then the linear response of f to a small change in x must be the linear response of f

[7] The original Weierstrass' functions are

$$f(t) = \sum_{r}^{\infty} \frac{1}{a^r} \sin b^r t$$

with b being an integer and b/a and a sufficiently large.
[8] (To the instructor) Its Hausdorff dimension is 1.

to the 'linear response of g to the change of x.' This is the essence of the chain rule. Let $F = f \circ g$ (i.e., $F(x) = f(g(x))$). Then,

$$d(f \circ g)(x)/dx = f'(g(x))g'(x). \tag{1.35}$$

Exercise.
(1) Let F be a differentiable function, and define a sequence $\{x_n\}$ through $x_{n+1} = F(x_n)$. Compute dx_n/dx_1. In particular, if $F(x) = 2x$ for $x \in [0, 1/2]$ and $2(1-x)$ for $x \in (1/2, 1]$, then $|dx_n/dx_1| = 2^{n-1}$. This implies that x_n for large n (a long time asymptotic result) is extremely sensitive to a small change in the initial condition x_1. This is an important feature of deterministic chaos. Indeed, for this F, $\{x_n\}$ is a typical chaotic sequence.
(2) Demonstrate Leibniz' rule with the aid of the binomial theorem.

1.3 Linear responses can be superposed. If there are several parts to be changed by perturbation, then the overall perturbation effect is the superposition (→**3.2**) of all the responses of each part calculated as if other parts are intact. The simplest example is $d(fg)/dx = f'g + fg'$: the change of fg is the sum of the change of each part keeping the rest constant. Consider the following example:

$$\frac{d}{dt}\int_{f(t)}^{g(t)} h(x,t)dx, \tag{1.36}$$

where f, g and h are all well behaved. There are three places affected by the modification of the parameter t. Hence, the result should be the superposition of all three independent changes:

$$h(g(t),t)g'(t) - h(f(t),t)f'(t) + \int_{f(t)}^{g(t)} \frac{\partial h(x,t)}{\partial t}dx. \tag{1.37}$$

Exercise.
(A) Compute

$$\frac{d}{dt}\int_{\sin t}^{\log t} \cosh tx\, dx. \tag{1.38}$$

(B) Let f be a continuous function.
(1) Compute

$$\frac{d}{dx}\int_{-x^2/2}^{x^2/2} f(t)dt \tag{1.39}$$

(2) Find

$$\lim_{t\to 0}\frac{1}{2t}\int_{x-t}^{x+t} f(s)ds. \tag{1.40}$$

1.4 Generalization of differentiation, strong derivative. If we have a device to measure the size of the perturbation δa and the size of its effect δf (i.e., if we can reasonably say they are small (for example, if these quantities are vectors, we know how to evaluate their magnitudes[9]), then even if f is not an ordinary function and if a is not a number, we may be able to define the linear response. The relation between δf and δa should be linear. That is, if the response to $\delta_1 a$ of f is denoted by $\delta_1 f$ and that for $\delta_2 a$ $\delta_2 f$, then for any numbers α and β, the response of f to $\alpha\delta_1 a + \beta\delta_2 a$ is given by $\alpha\delta_1 f + \beta\delta_2 f$ (→**3.2**). If a relation between δa and δf satisfies this relation, we introduce a symbol Df (this is a linear operator →**3.2** whose domain is the set of possible perturbations) and write

$$\delta f = Df[a]\delta a. \tag{1.41}$$

Here the dependence of Df on a is denoted by $[a]$. If such Df exists, we say f is *strongly differentiable*, and $Df[a]$ is called the *strong derivative* of f (at a). Notice that the linear operator $Df[a]$ is independent of the choice of the perturbation δa. This independence characterizes the strong differentiability.

We write $Df[a] = f'(a)$ when f is an ordinary real scalar function on a real number set $\boldsymbol{R}$.

1.5 Differentiation of function on space. Consider a smooth function $f : \boldsymbol{R}^3 \to \boldsymbol{R}$. Changing $\boldsymbol{r} \in \boldsymbol{R}^3$ slightly, we can study the linear response of $f(\boldsymbol{r})$, which is a scalar δf and must be a linear function of $\delta\boldsymbol{r}$. The derivative Df must be a vector such that (cf. **1.6**)

$$\delta f \simeq Df \cdot \delta\boldsymbol{r}. \tag{1.42}$$

The vector Df is called the *gradient* of f at $\boldsymbol{r}$ (→**3.2**).

If f is a function of x and y, we can write

$$\delta f = (f_x, f_y)(\delta x, \delta y)^T. \tag{1.43}$$

Here ^{T} denotes the transposition of the vector. Thus, we may write

$$Df = (f_x, f_y)^T. \tag{1.44}$$

[9] We need a *norm* (→?? footnote, ??)

1.6 Warning. The existence of Df is much stronger than the condition for the existence of each f_x and f_y ($\rightarrow$**1.10**).

1.7 Differentiation of vector valued function. Let $f = (f_1, f_2, f_3)^T$.[10] Then, $D\boldsymbol{f}$ must be a 3×3 matrix whose each row is $grad\, f_i$ ($i = x, y,$ or z):

$$D\boldsymbol{f} = \frac{d\boldsymbol{f}}{d\boldsymbol{x}} = \begin{pmatrix} \frac{\partial f_x}{\partial x} & \frac{\partial f_x}{\partial y} & \frac{\partial f_x}{\partial z} \\ \frac{\partial f_y}{\partial x} & \frac{\partial f_y}{\partial y} & \frac{\partial f_y}{\partial z} \\ \frac{\partial f_z}{\partial x} & \frac{\partial f_z}{\partial y} & \frac{\partial f_z}{\partial z} \end{pmatrix} \tag{1.45}$$

Componentwisely, we can write

$$(D\boldsymbol{f})_{ij} = \frac{\partial f_i}{\partial x_j} \equiv f_{i,j}. \tag{1.46}$$

This is, of course, consistent with the formal expression

$$d\boldsymbol{f} = \frac{d\boldsymbol{f}}{d\boldsymbol{x}} d\boldsymbol{x}. \tag{1.47}$$

As we will see, the trace of $D\boldsymbol{f}$ is called $div\, f$ ($\rightarrow$**3.5**).

Discussion: Hessian. Let $f(x_1, \cdots x_n)$ be a twice differentiable function. The matrix

$$Hess(f) = Matr.\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right) \tag{1.48}$$

is called the *Hessian* of f at $(x_1, \cdots, x_n)$. If the point is a critical point (= the point where the derivative vanishes), then the Hessian determines its nature.

Exercise.
(A) Compute $D\boldsymbol{v}$ for the following vector fields on $\boldsymbol{R}^3$:
(1) $\boldsymbol{v} = (e^y - x\cos(xz), 0, z\cos(xz))$.
(2) $\boldsymbol{v} = (y^2 \sin z, 2xy \sin z, xy^2 \cos z)$.
(B) If we superpose the two Coulomb electric fields due to point charges of $+q$ and $-q$ at the origin and at $(d, 0, 0)$, respectively, we can get the electric field created by an appropriate dipole moment. Find the matrix A such that the electric field

[10] Whenever the components are written, we interpret the vectors to be column vectors.

due to the dipole moment $\boldsymbol{p}$ located at the origin is given by $A\boldsymbol{p}$. (Note that $\boldsymbol{p} = q(d, 0, 0)^T$.]

1.8 Differentiation of complex functions. A map from $\boldsymbol{C}$ to itself is usually called a *complex function*. If the following limit exists[11]

$$\lim_{h \to 0} \frac{f(z+h) - f(z)}{h}, \tag{1.49}$$

we say f is *differentiable* at z. The limit is written as $f'(z)$ or df/dz and is called the *derivative* of f at z. Notice that this is a strong derivative (→**1.4**). The condition that the limit does not depend on the direction along which the point $z+h$ reaches z is exactly the linearity requirement of the response.

Exercise.
(1) Show that $f(z) = \overline{z}$ is not strongly differentiable. In complex analysis, we simply say f is not differentiable.
(2) $z^n \overline{z}^m$ is strongly differentiable only when $m = 0$.

1.B Partial Differentiation Revisited

1.9 Partial differentiation. We have already used $\partial/\partial t$, etc., in **1**. For simplicity, let $f(x, y)$ be a real-valued function defined in a region $D \subset \boldsymbol{R}^2$, and $(a, b) \in D$. If $f(x, b)$ is differentiable at a with respect to x, we say that $f(x, y)$ is *partially differentiable* with respect to x at (a, b), and the derivative is denoted by $f_x(a, b)$. More generally, if f is partial differentiable in D with respect to x, we may define $f_x(x, y)$:

$$f_x(x, y) = \lim_{h \to 0} \frac{f(x+h, y) - f(x, y)}{h} = \frac{\partial f}{\partial x} = \partial_x f.$$

[11] This means that the limit does not depend on how the origin is approached on the complex plane.

If we write $z = f(x, y)$, $f_x(x, y)$ is written as $\partial z/\partial x$. $f_x(x, y)$ is called the *partial derivative* of f with respect to x. Usually, we do not explicitly write the variables kept constant (in this case y). We can analogously define $\partial f(x, y)/\partial y$.

Discussion [**Hadamard's notation**]. Hadamard introduced a convenient set of notations to facilitate analysis of multivariable functions of $x = (x_1, \cdots, x_n)$. Let $\alpha = (\alpha_1, \alpha_2, \cdots, \alpha_n)$. We write

$$|\alpha| \equiv \sum_i \alpha_i. \tag{1.50}$$

For $N = (N_1, \cdots, N_n)$,

$$x^N \equiv \prod_i x_i^{N_i}, \tag{1.51}$$

$$N! \equiv \prod_i N_i!. \tag{1.52}$$

Then, the partial differential operator is written as follows:

$$D^\alpha f(x) = \prod_i \frac{\partial^{\alpha_i}}{\partial x_i^{\alpha_i}} f(x) = \frac{\partial^\alpha f(x)}{\partial x^\alpha}. \tag{1.53}$$

(1) The multinomial theorem reads

$$|x|^n = \sum_N \frac{n!}{N!} x^N, \tag{1.54}$$

where the summation is over all N such that $|N| = n$ (The components of N must be non-negative).
(2) Taylor expansion reads

$$f(x + y) = \sum_N \frac{x^N}{N!} f^{(N)}(y). \tag{1.55}$$

Of course, $f^{(N)} \equiv D^N f$. For example,

$$e^{|x|} = \sum_N \frac{x^N}{N!}. \tag{1.56}$$

1.10 Warning. Even if f_x and f_y exist at a point, f need not be continuous at the point.

Exercise.

(1) Make or sketch such an example.
(2) If f_{xy} is not continuous, then $f_{xy} = f_{yx}$ is not guaranteed. Compute f_{xy} and f_{yx} at the origin for

$$f(x,y) = \frac{xy(x^2-y^2)}{x^2+y^2} \text{ for } (x,y) \neq (0,0) \tag{1.57}$$

with $f(0,0) = 0$. If you wish, use Mathematica for this problem and report what you find.

1.11 Change of variables. Suppose f is a well behaved function of x and t satisfying

$$\frac{\partial^2\psi}{\partial t^2} - c^2\frac{\partial^2\psi}{\partial x^2} = 0, \tag{1.58}$$

where c is a positive constant. This is a 1D wave equation (→**1.4**, **2.27**). In this formula, $\partial/\partial x$ is the partial differentiation with t being kept constant, which is not explicitly written. We wish to change the variables from (x,t) to (X,Y) such that $X = x + ct$ and $Y = x - ct$. Now, Y is kept constant, when we write $\partial/\partial X$. With the aid of the chain rule

$$\frac{\partial}{\partial x} = \frac{\partial X}{\partial x}\frac{\partial}{\partial X} + \frac{\partial Y}{\partial x}\frac{\partial}{\partial Y} = \frac{\partial}{\partial X} + \frac{\partial}{\partial Y}, \tag{1.59}$$

and

$$\frac{\partial}{\partial t} = \frac{\partial X}{\partial t}\frac{\partial}{\partial X} + \frac{\partial Y}{\partial t}\frac{\partial}{\partial Y} = c\frac{\partial}{\partial X} - c\frac{\partial}{\partial Y}. \tag{1.60}$$

Or

$$\frac{\partial}{\partial X} = \frac{1}{2}\left\{\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}\right\},\ \frac{\partial}{\partial Y} = -\frac{1}{2}\left\{\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}\right\}. \tag{1.61}$$

That is, we can rewrite the wave equation in the following form:

$$\frac{\partial^2\psi}{\partial X\partial Y} = 0. \tag{1.62}$$

This implies that $\partial\psi/\partial Y$ is a function of Y alone:[12]

$$\frac{\partial\psi}{\partial Y} = \phi(Y). \tag{1.63}$$

[12] We assume well-behavedness of functions as much as we need to avoid technical complications.

Hence, ψ must be a sum of the function of Y only and X only. In other words, the most general solution of (1.58) is given by

$$\psi(x,t) = F(x+ct) + G(x-ct), \tag{1.64}$$

where F and G are differentiable functions. Notice that $F(x+ct)$ denotes a wave propagating in the $-x$-direction with speed c without changing its shape. We have found a general solution to the wave equation:

1.12 D'Alembert's solution for 1-space wave equation. Consider (1.58) on the whole 1-space $\boldsymbol{R}$ and for all time $t \in (0, +\infty)$ with the initial condition $u(x,0) = f(x)$, and $\partial_t u(x,0) = g(x)$, where f is C^2 and g is C^1.[13] Then

$$u(t,x) = \frac{1}{2}[f(x+ct) + f(x-ct)] + \frac{1}{2c}\int_{x-ct}^{x+ct} g(s)ds. \tag{1.65}$$

This is called *d'Alembert's formula* and is a C^2-function. This is actually the unique solution of the problem.
[Demo] From (1.64) the functions F and G in the general solution are determined as follows:

$$\begin{aligned} F(x) + G(x) &= f(x), & (1.66)\\ cF'(x) - cG'(x) &= g(x). & (1.67) \end{aligned}$$

From (1.67) we get

$$F(x) - G(x) = \frac{1}{c}\int_{x_0}^{x} g(\zeta)d\zeta + const, \tag{1.68}$$

where x_0 is an arbitrary base point. From (1.67) and (1.68), we can solve F and G as

$$\begin{aligned} F(x) &= \frac{1}{2}\left[f(x) + \frac{1}{c}\int_{x_0}^{x} g(\zeta)d\zeta\right], & (1.69)\\ G(x) &= \frac{1}{2}\left[f(x) - \frac{1}{c}\int_{x_0}^{x} g(\zeta)d\zeta\right]. & (1.70) \end{aligned}$$

Here the integration constant in (1.68) is absorbed into the choice of x_0. This gives the desired formula.

Discussion.

[13] C^m denotes m-times continuously differentiable functions.

(A) Formally apply the method to derive d'Alembert's formula to the initial value problem $u(x,0) = f(x)$ and $\partial_y u(x,0) = g(x)$ of the Laplace equation to derive

$$u(x,y) = \frac{1}{2}[f(x+iy) + f(x-iy)] - \frac{i}{2}\int_{x-iy}^{x+iy} g(s)ds \tag{1.71}$$

The formula tells us that the fate of the solution is determined by the behavior of the functions on the complex plane. For example, if $f(x) = 1/(1+x^2)$, then singularities appear in the solution which cannot be controlled by the initial condition (not well posed →**??**).

(B) Solve the forced 1D wave equation on $\boldsymbol{R}$

$$\left(\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) u = Q(x,t) \tag{1.72}$$

with the initial condition $u = f(x)$ and $\partial_t u = 0$ (Use $x \pm t$).

Exercise.
(A) For a 1D wave equation, if the initial condition is nonzero only on a compact subset of $\boldsymbol{R}$, then so is the solution for any $t > 0$ (→**??**).
(B) All the spherically symmetric solutions to the 3-wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0 \tag{1.73}$$

in the whole space-time have the following form (see **3.31** for Δ, esp., (3.83); the solution must be non-singular at the origin.):

$$u(\boldsymbol{x},t) = \frac{F(|\boldsymbol{x}| - ct) + F(|\boldsymbol{x}| + ct)}{|\boldsymbol{x}|}. \tag{1.74}$$

(C)
(1) Find the solution to the 1-space wave equation ($c = 1$) on $\boldsymbol{R}$ with the following initial data:

$$u_{t=0} = \cosh^{-2} x, \quad \partial_t u_{t=0} = \cosh^{-2} x \tanh x. \tag{1.75}$$

(2) Find the solution to the 1-space wave equation ($c = 1$) on $\boldsymbol{R}$ with the initial condition

$$u_{t=0} = 0, \ \partial_t u|_{t=0} = A \operatorname{sech} x. \tag{1.76}$$

Write A in terms of the total energy (→**2.28** or **??**).
(3) Illustrate the solution of the wave equation for the following initial displacement with zero initial velocity.

(D) Obtain the solution under the Cauchy condition given on the line $x = at$ as $u(x, x/a) = f(x)$ and $\partial_t u(x, x/a) = g(x)$. What happens if $a = \pm c$?
(E) Find the general solution to
(1)

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \sin x \cos t. \tag{1.77}$$

(2)

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \sin(x - t). \tag{1.78}$$

these problems can also be solved by adding a particular solution for the in homogeneous equation to the general solution to the homogeneous equation.

1.13 Who was d'Alembert (1717-1783) ?.[14] He was born as an illegitimate son of a salon hostess and a cavalry officer, abandoned on the steps of the Saint Jean-Le-Rond in Paris by his mother, but was quickly located by his father, who found him a home with a humble glazier, named Rousseau. His father, though never revealed his identity, provided an annual annuity of 1200 livres and also helped him to enroll a prestigious school, Collége de Quatre-Nations, where he developed an aversion for religions. He started his mathematical study in ca 1738. He learned mathematics largely by himself, later writing that mathematics was the only occupation really interested him.

In 1739, he started submitting papers to Paris Academy of Science, and was elected a member in 1741. In 1743, he published his most famous scientific work, *Traité de Dynamique*, in which he formulated his principle. From 1744 for three years he developed partial differential equations as a branch of calculus, inventing the wave equation (→**1.4**, **XX**). His study of fluid dynamics is also a breakthrough (e.g., d'Alembert's paradox). However, d'Alembert's quickly written papers were poorly understood. When Euler (→**2.4**) refined these ideas and wrote masterful expositions that did not give d'Alembert ample credit, he was furious.

After 1750, his interest turned increasingly beyond mathematics, and served as the science editor of *Encyclopédie* for seven years, but he resigned in 1758, due to his article on Genevan pastors who "no longer believe in the divinity of Jesus Christ, $\cdots$." He was accepted to the French Academy in 1754. He worked zealously to enhance its dignity

[14] Mainly based on p479- of R. Calinger, *Classics of Mathematics* (Prentice-Hall, 1995). Read the original for his much more colorful private life, etc.

and was made perpetual secretary in 1772. As his scientific and literary fame spread, Friedrich the Great wanted him to be the president of the Berlin Academy in 1764. d'Alembert recommended Euler for the position. This healed a rift that had developed for more than a decade. He subsequently declined the offer of Catherine the Great as well, refusing to leave the cultural capitol, Paris.

D'Alembert, though himself discouraged about the future of mathematics, helped encourage Lagrange (→**2.7**) and Laplace (→**13.3**) to launch their careers.

He stressed the importance of continuity, which led him to the considerations of limits. Almost alone in his time, he understood derivatives as ratios of limits of quotients of increments. He clearly recognized that all the complex numbers can be written as the sum of real and imaginary parts.

1.14 Wave equation with boundary condition. Consider the *initial value problem* for 1-space wave equation on $[0, L]$

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right) u = 0, \quad x \in (0, L),\ t \in (0, \infty). \tag{1.79}$$

The initial condition is

$$u = f(x), \quad \frac{\partial u}{\partial t} = g(x), \quad \text{for } t = 0,\ x \in [0, L], \tag{1.80}$$

where f is a twice and g is a once differentiable function, and the boundary condition is $u = 0$ at $x = 0$ and $x = L$ for all $t > 0$. In this case the boundary condition implies from (1.64) $F(-ct) + G(ct) = 0$ and $F(L-ct)+G(L+ct) = 0$ for all $t > 0$. Thus $F(x) = -G(-x)$ and $F(x + L) = -G(-x + L)$.[15] Following **??**, we get

$$u(t, x) = \frac{1}{2}\left[f(x + ct) - f(-x + ct) + \frac{1}{c}\int_{-x+ct}^{x+ct} g(\zeta)d\zeta\right]. \tag{1.81}$$

We notice that $F(x) = F(x + 2L)$. That is, F must be a periodic function of period $2L$. This is the source of Daniel Bernoulli's idea.

See the following example.

[15] $F(x) = -G(-x + 2L) = F(x + 2L)$.

1.15 Moving coordinates. Consider the following equation

$$\frac{\partial \psi}{\partial t} + c\frac{\partial \psi}{\partial x} = D\frac{\partial^2 \psi}{\partial x^2}, \tag{1.82}$$

where c and D are positive constants. If $c = 0$, the equation is 2D diffusion equation, which should describe the relaxation of ψ back to 'equilibrium.' Let us rewrite this equation with the aid of the moving coordinate $X = x - ct$. To do so, the easiest way is to rewrite the equation in terms of t and X as the new independent variables. It is advantageous to introduce new time $T = t$ to minimize confusion. We get

$$\frac{\partial \psi}{\partial T} = D\frac{\partial^2 \psi}{\partial X^2}. \tag{1.83}$$

Thus, we understand the meaning of (1.82): it is a diffusion process advected by the flow of constant speed c to the positive x-direction.

Exercise.
(A) Rewrite the following equation with the aid of the moving coordinate $X = x - vt$, and find the general solution

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = F(x - vt), \tag{1.84}$$

where F is a well-behaved function.
(B) Consider the following (original) Fisher equation:

$$\frac{\partial \psi}{\partial t} = D\frac{\partial^2 \psi}{\partial x^2} + \psi(1 - \psi). \tag{1.85}$$

(1) Rewrite the equation as seen from the moving coordinate with velocity v.
(2) Find the equation for a steady moving front propagating with speed v.
(3) How can you show that there is such a wave front for sufficiently large v?. [Hint: interpret the equation obtained in (2) as an equation of motion of a particle moving in a potential with a damping term.]

2 Calculus of Variation

Variational calculus is the study of linear response of a functional (a map which maps a function to another object, say, a number). We discuss the classical Euler-Lagrange theory, and then reconsider the theory from the functional differentiation point of view. A necessary and sufficient condition for a functional to have a minimum and direct methods to variational calculus are briefly discussed.

Keywoods: functional, Euler-Lagrange equation, Lagrange multiplier, variable end point case, functional derivative, delta function, second variation, Legendre's condition, Noether's theorem, Vainberg's theorem, direct method.

Summary
(1) Calculus of variation is the calculus on a function space (**2.1**, **2.9**).
(2) Euler-Lagrange equation is a necessary condition for extremity (**2.2**). A sufficient condition for extremity is more involved than the ordinary calculus case (**2.16**).
(3) In terms of functional derivative (**2.9-2.11**), the parallelism between the ordinary calculus and variational calculus becomes explicit (**2.12-2.15**).
(4) Variational principle is practically useful (**2.21**, **2.22**), so remember that there is a way to costruct a variational functional (if any) for a given equation (**2.19**).

2.1 Variational calculus The study of the linear response (→**1.3**, **1.4**) of a functional (a map which maps a function to another function or to a number is called a *functional*) is called *variational calculus*. The essence of calculus of variation is the differential calculus of functionals. This point will be made more explicit later through the introduction of functional derivatives (→**2.9-2.11**). A typical problem of variational calculus is to extremize a given functional.

The best introductory book of calculus of variation is: I. M. Gel'fand and S. V. Fomin, *Calculus of Variation* (Englewood Cliffs, 1963).

An early example of variational problems was the following which tries to solve the Dirichlet problem for the Laplace equation. Find a C^1 function u on D such that

$$u = f \tag{2.1}$$

on ∂D, where D is a bounded region, and f is continuous, and minimize

$$I[u] = \int_D |\nabla u|^2 d\boldsymbol{x}. \tag{2.2}$$

This is the variational formulation of the Lapalce equation boundary value problem.

Initially, it was believed that any extremum problem had a solution. Riemann relied on a variational formulation of the Laplace equation to demonstrate the fundamental theorem of conformal transformation. However, soon later Weierstrass (→**10.5**) pointed out that it is not always the case. Weierstrass' counter example is the following: Find the C^1 function $\varphi : [0, 1] \to \boldsymbol{R}$, satisfying the end conditions $\varphi(0) = a$ and $\varphi(1) = b(\neq a)$, that gives the smallest value of

$$J[\varphi] = \int_0^1 (x\varphi'(x))^2 dx. \tag{2.3}$$

The infimum of J is obviously zero. However, there is no C^1-function which can give this value.

2.2 Theorem [Euler]. Let $S[f]$ be a functional on the set of C^1-functions on $[a, b]$ such that $f(a) = A$, $f(b) = B$ (fixed) defined as

$$S[f] = \int_a^b dx L(f, f', x), \tag{2.4}$$

where L is a C^2-function of its variables. A necessary condition for g to give an extremal value of S is that g satisfies *Euler's equation* (or the Euler-Lagrange equation)(→**2.7**, for a sufficient condition see **2.16**):

$$\frac{\partial L}{\partial f} - \frac{d}{dx}\left(\frac{\partial L}{\partial f'}\right) = 0. \tag{2.5}$$

□

2.3 Proof of Euler-Lagrange equation. A necessary condition for

f to give an extremal value with respect to the small change[16] of f is

$$\delta S[f] \equiv S[f+\delta f] - S[f] = \int_a^b dx \left[\frac{\partial L}{\partial f}\delta f + \frac{\partial L}{\partial f'}\delta f'\right] = 0 \qquad (2.6)$$

for any small δf (see the above footnote). Integrating this by parts, we get (note that $\delta f = 0$ at the boundaries)

$$\int_a^b dx \left[\frac{\partial L}{\partial f} - \frac{d}{dx}\frac{\partial L}{\partial f'}\right] \delta f = 0. \qquad (2.7)$$

Thus, the quantity in the square brackets must vanish.[17]

2.4 Who was Euler?[18] Euler's analysis textbook *Introductio in analysin infinitorum* (1748) was extremely influential beyond 1800, so that his notations such as sin, cos, e, π, i, $\sum$, etc., became conventional. He, not Newton, wrote down the so-called Newton's equation of motion for the first time, and laid the foundations of continuum mechanics including fluid dynamics (but see d'alembert **??**).

Leonhardt Euler was born in Basel, Switzerland, on April 15, 1707. He revealed a photographic memory by reciting *Aeneid* page by page by heart. In 1720 he enrolled at the University of Basel and graduated with first honors two years later. His master's thesis in 1724 compared the natural philosophies of Descartes and Newton. Euler convinced Johann Bernoulli to tutor him in mathematics and natural philosophy for one hour on Saturday afternoons. Bernoulli quickly recognized Euler's genius and helped convince his father to allow his son to concentrate on mathematics. After failing to get a physics position at Basel, he joined

[16] This statement is actually tricky. We must fix a method to evaluate the size of a function, or we must be able to tell whether a function f and g are close or not. We measure the size of f in the present context in terms of the *norm* $\|f\|$ (→**??**) which is the sum of the largest value of $|f|$ in the relevant domain and that of $|f'|$. This is called the C^1-norm. $\delta S = 0$ in (2.6) means, more precisely, that $\|\delta S\|$ is much smaller than $\|\delta f\|$, or $\|\delta S\| = o\|\delta f\|$.

[17] More precisely: if continuous functions α and β satisfy

$$\int_a^b [\alpha(x)h(x) + \beta(x)h'(x)]dx = 0$$

for any C^1-function on $[a,b]$ such that $h(a) = h(b) = 0$, β is differentiable and $\alpha - \beta' = 0$. See Gel'fand and Fomin, Lemma 3 in Section 3.

[18] This entry is mainly based on p486– of R. Calinger, *Classics of Mathematics* (Prentice-Hall, 1995).

the St. Petersburg Academy of Sciences in 1727, boarding at Daniel Bernoulli's home.

He became the first professor of mathematics, succeeding D. Bernoulli in 1733, who returned to Switzerland. From 1733 to 1741, Euler immersed himself in research with enthusiasm despite hostility from the Russian nobility and from the Orthodox Church which opposed Copernican astronomy. He precisely computed $\zeta(2) = \sum(1/n^2) = \pi^2/6$ (see Discussion below). He gained an European-wide reputation with this and with his first book *Mechanica* (1736). During this period he found $e^{ix} = \cos x + i \sin x$ and $e^{i\pi} + 1 = 0$. He also introduced beta and gamma functions (→**??**).

In 1741 he accepted the invitation of Friedrich the Great to join the Brandenburg Society (Berlin Academy of Sciences after 1744) (→**1.13**). He was the director of its mathematical section from 1744 to 1765. He was at the peak of his career during this period. In the mid-1750s Euler tutored Lagrange (→**2.7**) by correspondence and selflessly withheld from publication the part of his work on the calculus of variations (→**2.2**-**2.3**) so that Lagrange might receive due credit for his contribution to the subject.

After disagreeing with the king over academic freedom, Euler returned to Russia in 1766, where Catherine the Great made him a generous offer. A cataract and its maltreatment made him totally blind by 1771 (he had lost his right eye sight in 1735), but his productivity at least in number of pages increased; he dictated books to a small group of collaborators, doing calculations in his head involving as many as 50 decimal places. He died of a brain hemorrhage in 1784.

Euler was chiefly responsible for differential equations, and calculus of variation with Lagrange. He pioneered differential geometry and topology (Euler's polyhedral formula: $v - e + f = 2$). His colleagues dubbed him "analysis incarnate." His disciplinary intuition never failed when he used infinite series, even though its general theory was to be created by Cauchy (→**??**). Euler found the prime number theorem in 1752, although he could not prove it, which was to be rediscovered and proved by Gauss (→**3.14**). Most of his number theoretic results appeared in his correspondence with his best friend in St. Petersburg, Christian Goldbach (famous for his conjecture: every even number is a sum of two prime numbers. This is mentioned in Hilbert's 8th problem (→**??**), and is still open).

Discussion.

(1) Euler often used 'algebraic formalism' (the belief that algebraic expressions are always correct whatever numbers replace the symbols in them) to obtain nontrivial results. The following illustrates his approach to compute $\zeta(2)$, etc. [An example of the 'modern version' of 'algebraic formalism' is illustrated in **10.4** Discussion.]

Euler tried to extend the factorization of polynomials to more general func-

tions. Sine has zeros at $n\pi$ for all $n \in \boldsymbol{Z}$. Therefore, he guessed

$$\sin z \propto z\left(1-\frac{z^2}{\pi^2}\right)\left(1-\frac{z^2}{4\pi^2}\right)\cdots. \tag{2.8}$$

We know $\sin z \simeq z$ for small z, so that the proportionality constant should be 1:

$$\sin z = z\left(1-\frac{z^2}{\pi^2}\right)\left(1-\frac{z^2}{4\pi^2}\right)\cdots. \tag{2.9}$$

Admitting this relation (which is actually correct) and expanding the both sides in the Taylor series, we obtain

$$z-\frac{z^3}{3!}+\cdots = z\left\{1-\left(\frac{1}{\pi^2}+\frac{1}{4\pi^2}+\frac{1}{9\pi^2}+\cdots\right)z^2+\cdots\right\}. \tag{2.10}$$

Comparing the coefficients on both sides, Euler obtained

$$\zeta(2) \equiv 1+\frac{1}{2^2}+\frac{1}{3^2}+\cdots = \frac{\pi^2}{6}. \tag{2.11}$$

In this way the value of the zeta function for even positive integers can be obtained. Obtain $\zeta(4) = \pi^4/90$.
(2) Show

$$\int_0^\infty \frac{\log(1-x)}{x}dx = -\frac{\pi^2}{6}. \tag{2.12}$$

2.5 Remark on differentiability. For the action integral to be meaningful, we have only to assume that f is differentiable. However, the Euler equation is a second order differential equation. The interesting and important point is that the stationary f becomes twice differentiable even if it is not assumed so. This is due to the following theorem:
Theorem [essentially due to P. du Bois-Reymond]. Let f be a continuous function and φ be a sufficiently smooth function vanishing at the ends of the interval $[a, b]$. If

$$\int_a^b f(x)\varphi^{(m)}(x)dx = 0, \tag{2.13}$$

then f is m times differentiable and $f^{(m)}(x) = 0$.

2.6 Conditional extremum, Lagrange multiplier. Let $S[f]$ be a functional. We wish to extremize this under the condition that $G[f] =$

0, where G is another functional. A necessary condition for $S[f]$ to be extremal is as follows. Define $I[f,\lambda] = S[f]+\lambda G[f]$. Extremize I w.r.t. f and λ. This condition would give f as a function(al) of λ. Insert this into S, and fix λ with the auxiliary condition. The result gives the extremal value of S under $G = 0$.

$$\frac{\delta I}{\delta f} = 0, \quad \frac{\partial I}{\partial \lambda} = 0. \tag{2.14}$$

The parameter λ is called the *Lagrange multiplier*.

Discussion [Canonical distribution].
The canonical distribution function

$$\rho = \frac{1}{Z} e^{-\beta H} \tag{2.15}$$

of statistical mechanics can be obtained as the solution to the following conditional maximization problem: Maximize entropy

$$S = -\int \rho \ln \rho \, d\Gamma \tag{2.16}$$

under the condition

$$E = \int H \rho \, d\Gamma, \quad 1 = \int \rho d\Gamma. \tag{2.17}$$

Here, H is the system Hamiltonian, and $d\Gamma$ is the phase volume element (the Liouville measure). Z and β are introduced as the Lagrange multipliers.

The above formulation is for classical cases, but with the replacement of $\int d\Gamma$ with Tr, we can easily obtain the quantum counterpart. The formula for the entropy was first given by Gibbs. Later, the same formula was used to define information by Shannon.

The reader might be tempted to conclude that in this way we can found statistical mechanics on the Baysian statistics, and can dispense with the principle of equal probability. However, the principle is already implicit in (2.16) in the choice of the volume.

2.7 Who was Lagrange ?[19] Lagrange was born in Turin in 1736, where he stayed until 1766. In the mid-1750s he began to establish his reputation, and began his correspondence with Euler (→**2.4**), who became his tutor praising his work on variational calculus, and with

[19] Mainly based on R Calinger, *Classics of Mathematics* (Prentice Hall, 1982, 1995).

d'Alembert, who became his political counselor. As a poorly paid professor of the Royal Artillery School at Turin from 1755-66, he worked relentlessly to the extent to harm his health, sustained by his association with Euler and d'Alembert (→**1.13**). He brought the calculus of variation to maturity and applied it to mechanics.

In 1766, Lagrange succeeded Euler as director of the mathematical section of the Berlin Academy. The years in Berlin were extremely productive for Lagrange. He contributed to the three-body problem, various number theoretical problems, and his 1770 memoir opened a new era in algebra (group theory).

When Friedrich the Great died in 1787, he accepted an invitation of Louis XVI to join the Paris Academy of Science. A year later he published his classic, *Mécanique analytique*. This was the first book of mechanics without any geometrical argument.

Shy, diplomatic, and amenable, Lagrange not only survived the Revolution but was treated throughout with honor and respect. In 1790 he served on the committee which proposed the metric system. In 1794 he helped to establish Ecole Polytechnique. He taught elementary mathematics at Ecole Normale (with Laplace (→**13.3**) as his assistant).

He was the last great mathematician of the 18th century. He opened the abstract mathematics of the 19th century. He tried to give a sound foundation to calculus, which was to be given by Cauchy (→**??**), Weierstrass (→**10.5**), and others. To denote derivatives with $'$ was due to Lagrange.

2.8 Variable end points, transversality. Consider

$$S[f] = \int_a^b dx L(f, f', x) dx, \tag{2.18}$$

but now with the unspecified end point values of f. An elementary calculation gives

$$\delta S = \int_a^b dt \left(L_f - \frac{d}{dt} L_{f'} \right) \delta f(t) + L_{f'} \delta f(t) |_a^b + (L - L_{f'} f')_{t=b} \delta b - (L - L_{f'} f')_{t=a} \delta a. \tag{2.19}$$

The first order variations must be killed to be extremal, so f must obey the Euler-Lagrange equation (→**2.2**).

We still have first order terms at the end points. A realistic situation is that the end points are constrained on prescribed curves c_a and c_b. Hence $\delta f|_{t=a} = c_a'(a)\delta a$ and $\delta f|_{t=b} = c_b'(b)\delta b$. Putting these

conditions into (2.19), we get the following so-called *transversality conditions*:

$$[L + L_{f'}(c'_a - f')]_{t=a} = 0, \quad [L + L_{f'}(c'_b - f')]_{t=b} = 0. \tag{2.20}$$

These equations give the boundary conditions for the Euler-Lagrange equation to single out its solution.

2.9 Functional derivative. As we noted in **2.1**, calculus of variation is essentially the differential calculus on a function space.[20] As a preliminary step, let us review the differentiation of a scalar valued function of a vector $S(\boldsymbol{f})$. Its (strong) derivative ($\rightarrow$**1.4**) is the gradient of S and is a vector $gradS = (\partial S/\partial f_1, \cdots, \partial S/\partial f_n)$. We have

$$\delta S = \sum_{i=1}^{n} \frac{\partial S}{\partial f_i} \delta f_i. \tag{2.21}$$

Compare this with the formula (2.6). The parallelism becomes almost perfect, if we regard the value $f(a)$ of f at $x = a$ as the 'a-component of a vector f'. In this case a is a continuous parameter, so that the summation in (2.21) must be replaced by an integration over the parameter, and we have the form, something like:

$$\delta S = \int dx \frac{\delta S}{\delta f(x)} \delta f(x). \tag{2.22}$$

Here the integration kernel $\delta S/\delta f(x)$ is called by physicists the *functional derivative* of S with respect to f. Its functional form can be read off by comparing this formula and the standard variational formula such as (2.6). Hence, the calculation in the proof of Euler's theorem tells us that

$$\frac{\delta S}{\delta f(x)} = \frac{\partial L}{\partial f(x)} - \frac{d}{dx} \frac{\partial L}{\partial f'(x)}. \tag{2.23}$$

for S given in **2.2**.

[20] A set with a certain structure is often called a space. In the case of functional analysis, it is often a linear space. That is, linear combinations of the elements in the space are again in the space.

2.10 Delta function. We ought to be able to differentiate any (well-behaved) functional of f w.r.t. f. For example f itself is a functional of f just as the indentity map maps a vector $\boldsymbol{v}$ to itself. Because $\partial v_i/\partial v_j = \delta_{ij}$ (the identity matrix), we expect the functional derivative of f w.r.t. f itself should be an identity operator (or the integration kernel corresponding to the identity). We introduce δ as follows

$$\frac{\delta f(x)}{\delta f(y)} = \delta(x-y). \tag{2.24}$$

For any (integrable) variation δf, (2.6) in the present case reads[21]

$$\delta f(x) = \int dy \delta(x-y)\delta f(y). \tag{2.25}$$

$\delta(x-y)$ is called the *delta function*,[22] and later mathematically rationalized by Schwartz as a generalized function (→**7.4**). We will encounter this object later in many other contexts.

2.11 Formal rules of functional differentiation. With respect to the functional differentiation, the ordinary integration and differentiation just correspond to procedures to make linear combinations of the components of the vectors, so that we may freely change the order as

$$\frac{\delta f'(x)}{\delta f(y)} = \frac{d}{dx}\delta(x-y), \tag{2.26}$$

or

$$\frac{\delta}{\delta f(y)}\int_a^b dx f(x) = \int_a^b dx \delta(x-y). \tag{2.27}$$

Furthermore, the chain rule holds as

$$\frac{\delta F(f(x))}{\delta f(y)} = F'(f(x))\delta(x-y), \tag{2.28}$$

where F is a function. Hence, we can obtain Euler's equation **2.2** quite mechanically as follows:

$$\frac{\delta S[f]}{\delta f(y)} = \int dx \left[\frac{\partial L}{\partial f(x)}\delta(x-y) + \frac{\partial L}{\partial f'(x)}\frac{d}{dx}\delta(x-y)\right] = \frac{\partial L}{\partial f(y)} - \frac{d}{dy}\frac{\partial L}{\partial f'(y)}. \tag{2.29}$$

[21] The reader must remember that the definition of the delta 'function' is inseparable from the definition of the integral being used (→**??**).

[22] Physicists seem to believe that this was introduced by Dirac, but actually, this has been used for more than 100 years.

Here integration by parts has been used.

2.12 Intuitive introduction to minimization of functional I. Suppose we wish to minimize a well-behaved functional $S[f]$. **2.11** tells us that the essence of Euler's theorem **2.2** is that the necessary condition is

$$\frac{\delta S}{\delta f} = 0. \tag{2.30}$$

This is quite parallel to the ordinary calculus. Therefore, it is tempting to seek more parallelisms. To this end we need an analogue of the second derivative.

2.13 Second variation. If the change of $S[f]$ can be written as

$$S[f+h] = S[f] + \varphi_1[h] + \varphi_2[h] + o[\|h\|^2], \tag{2.31}$$

where φ_1 is a linear functional and φ_2 is a bilinear form, we say S has the *second variation*. In physicists' way, we can write

$$\varphi_2[h] = \frac{1}{2}\int dxdy \frac{\delta^2 S}{\delta f(x)\delta f(y)} h(x)h(y). \tag{2.32}$$

Actually, we can formally compute the second functional derivative as explained in **2.11**.

2.14 Legendre's condition. If we can write

$$S[f] = \int_a^b dx L(f(x), f'(x), x), \tag{2.33}$$

then the second variation can be written as (after integration by parts, taking into account $h(a) = h(b) = 0$)

$$\varphi_2[h] = \int_a^b (Qh^2 + Ph'^2)dx, \tag{2.34}$$

where

$$Q = \frac{1}{2}\left(L_{ff} - \frac{d}{dx}L_{ff'}\right), \quad P = \frac{1}{2}L_{f'f'}. \tag{2.35}$$

A necessary condition for φ_2 to be nonnegative is

$$P \geq 0. \tag{2.36}$$

2.15 Intuitive introduction to minimization of functional II. Legendre wished to establish a necessary and sufficient condition for the minimization of $S[f]$. Naturally, he guessed that the nonnegativity of the second variation as a sufficient condition. Therefore, he wished to claim that $P \geq 0$ in **2.14** was a sufficient condition, but failed to prove the assertion. Actually, the assertion is false, because the condition is only local. That is, if we change f only locally in space, indeed $P \geq 0$ implies the positivity of the second variation. However, a small change of f need not be spatially locally confined, and for such changes $P \geq 0$ does not guarantee the positivity of the second variation. We need a supplementary global condition. The final form of a sufficient condition reads:

2.16 Theorem [Sufficient condition for minimum w.r.t. C^1-norm][23] A sufficient condition for g to give a minimum of (2.4) is (1)+(2)+(3) below:
(1) g satisfies Euler's equation (2.5).
(2) $\partial^2 L/\partial f'^2(g, g', x) > 0$.
(3) The interval $[a, b]$ does not contain the conjugate point[24] of a.□
We need (3) to exclude the global pathology. (To understand the meaning of (3) consider the shortest distance between the points on a great circle of a 2-sphere.) The global condition cannot be derived easily by a formal consideration alone.

[23] Gel'fand and Fomin, Section 24 Theorem.

[24] Let g and $\tilde{g}$ be two solutions of (2.5) starting from point a. The *conjugate point* of a is the crossing point of g and $\tilde{g}$ in the limit of $\tilde{g} \to g$ in the C^1-norm (→**2.3** footnote).

Discussion. Discuss the relation between the conjugate point and focus in geometrical optics.

2.17 Noether's theorem.[25] Let the functional S in **2.2** be invariant under the following one to one map $g_\alpha : (x, f) \to (x^*, f^*)$, where $x^* = \varphi(x, f, \alpha)$ and $f^* = \psi(x, f, \alpha)$ such that $x = x^*$ and $f = f^*$ for $\alpha = 0$.[26] That is, $S[f] = S[f^*]$. We assume the transformation is differentiable with respect to α. Then, along each stationary curve, the following quantity is constant:

$$\hat{\psi} F_{f'} + (F - f' F_{f'})\hat{\phi} = \text{const.} \tag{2.37}$$

Here $\hat{}$ denotes the partial derivative w.r.t. α evaluated at $\alpha = 0$.□
This should be easily demonstrated, if we look at the calculation in **2.8**.

2.18 Usefulness of variational principle. As we see in **2.21**, if we could cast a (partial) differential equation in the variational principle form (i.e., if we know the variational functional whose Euler's equation (→**2.2**) is the desired equation), then there is a means to get its solution numerically, at least approximately. Hence, to construct a variational principle (if any) is of practical importance. The following Vainberg's theorem tells us when we can expect a variational principle.

2.19 Vainberg's theorem. Suppose
(1) N is an operator from a Hilbert space (→**??**) into its conjugate space,
(2) N has a linear Gâteaux[27] derivative $DN(u, h)$ at every point of the

[25] The theorem can be restated as: If a system is invariant under a continuous symmetry operation, then the corresponding generator of the symmetry operation is an integral of motion.

[26] That is, $\{g_\alpha\}$ is a one parameter transformation group, and $\alpha = 0$ corresponds to the unit element.

[27] A functional $N[f]$ is said to be Gâteaux differentiable if there is a linear operator Q such that for a function f, g and for sufficiently small λ $N[f+\lambda g] \simeq N[f]+\lambda Q[f]g$. This is a much weaker condition than the strong differentiability (→**1.4**).

ball $\|u - u_0\| < \epsilon$[28] for some positive ϵ,
(3) The scalar product $\langle h_1, DN(u, h_2)\rangle$ is continuous at every point of D.
Then, a necessary and sufficient condition for $N(u) = 0$ to be the Euler-Lagrange equation of a variational functional in the ball D is the symmetry

$$\langle h_1, DN(u, h_2)\rangle = \langle h_2, DN(u, h_1)\rangle. \tag{2.38}$$

A desired variational functional is given by

$$F(u) = -\int dt \int_0^1 d\lambda u N(\lambda u). \tag{2.39}$$

Here $-$ is only cosmetic. $\Box$[29]

2.20 Remark. This theorem is not quite general, because there are cases that the equation itself cannot be directly obtained by a variati onal principle, but the equation timessome function may well be derivable as an Euler-Lagrange equation. The case is well illustrated in A. K. Raycha udhuri, *Classical Mechanics* (Oxford UP, Calucutta, 1983).[30]

2.21 Direct method. The Euler-Lagrange equation often becomes a complicated partial differential equation, so a method to use approximation sequence directly in the variational functional was conceived.[31] For a functional $S[f]$, let us assume that it has an infimum $\inf_f S[f] = \mu > -\infty$. Then, due to the definition of infimum, there is a sequence $\{f_n\}$ such that $S[f_n] \to \mu$. Such a sequence is called a *minimization sequence*.

[28] $\|\ \|$ is the C^1 norm we discussed in the footnote of **2.3**.
[29] Actual applications can be seen in: R. W. Atherton and G. M. Homsy, "On the existence and formulation of variational principles for nonlinear differential equations", *Studies Appl. Math.* **LIV**, 31-60 (1975), and the references cited therein. For ODE see I. A. Anderson and G. Thompson, *The inverse problem of the calculus of variations for ordinary differential equations*, Memoirs of Am. Math. Soc. **98**, Number 473 (1991).
[30] Thi s book was kindly informed by Akash Bandyopadhyay.
[31] Already Euler used it.

Theorem.[32] If this sequence has a limit $\hat{f}$, and S is lower semicontinuous,[33] then

$$\lim_n S[f_n] = S[\hat{f}]. \tag{2.40}$$

□

2.22 Ritz's method. To construct a minimization sequence, Ritz used a complete function set (practically an orthonormal basis →**??**) $\{u_n\}$:

$$f_n = \sum_{j=1}^{n} c_j u_j. \tag{2.41}$$

Let μ_n be the minimum of $S[f_n]$ obtained by varying the coefficients in f_n. Then, obviously $\{\mu_n\}$ is a monotonically decreasing sequence.

Theorem. If $S[f]$ is continuous, and the function set $\{u_n\}$ is complete,[34] then μ_n converges to the desired minimum μ.

2.23 Why variational principle? The study of variational calculus was initiated to understand or to organize classical mechanics. The fundamental equation of motion is given as Newton's equation of motion. But why is this the form chosen by Creator? Under the strong influence of Christianity they thought the equation had to be a special one, for example, characterized by a sort of maximum or minimum principle. Thus a variational principle was pursued. Such a reasoning may sound irrational, but all the creative activities must have irrational components. We should not forget that Newton was a serious student of alchemy (his hair contains large amount of mercury, because he tasted reaction products) and the Bible chronology; his research was almost a religious activity to glorify God; he was a devout Unitarian. John Keynes wrote that Newton was the last magician.

[32] Gel'fand and Fomin, Section 36.

[33] That is, for $\epsilon > 0$ there is $\delta > 0$ such that for any h such that $|h| < \delta$ $S[f + h] - S[f] > -\epsilon$.

[34] Roughly speaking, this means that any function can be described as a linear combination of this set of functions (→**10.3**).

2.24 Hamilton-Jacobi's equation, Jacobi's theorem, etc. These are best understood in the context of classical mechanics, so they will not be covered here. Although there is no balanced modern textbook of classical mechanics, read the first and the last chapters of Landau-Lifshitz, *Classical Mechanics* to start with. For a more serious student, V I Arnol'd, *Mathematical Methods of Classical Mechanics* (Springer, 1979) is recommended. Especially read all the appendices.

3 Review of Vector Analysis

We will review vector analysis as intuitively as possible. Also coordinate free definitions of gradient, divergence and curl are stressed. As a technical topic, expressions of these operators in various cruvilinear coordinates are summarized.

Key words: gradient, nabla, divergence, curl, Laplacian, Gauss-Stokes-Green's theorem, Poincaré's lemma, converse of Poincaré's lemma, Helmholtz-Hodge's theorem, Helmholtz-Stokes-Blumental's theorem, curvilinear coordinates, metric tensor.

Summary:
(1) Geometrical meanings of *grad*, *div* and *curl* (**3.1**, **3.5**, **3.8**) as well as their coordinate-free definitions must be understood clearly (**1.5**, **3.6**, **3.9**).
(2) Gauss-Stokes-Green's theorem **3.13**, Poincaré's lemma **3.15**, and its converse (when the domain is *singly connected*) **3.17** are crucial.
(3) If *curl* and *div* both vanish, the vector field is (essentially) constant. This can be shown by the Helmholtz-Hodge decomposition **3.18**.
(4) The reader should be able to demonstrate various formulas of vector calculus (**3.20**).
(5) Differential operators in orthogonal curvilinear coordinates **3.24** must be understood without difficulty (**3.28**, **3.30**, **3.31**).
(6) Do not use ∇ as a simple operator except in the Cartesian coordinate system (**3.12**).

3.A Vector Analysis Revisited

3.1 Gradient. Suppose we have a sufficiently smooth function $f : D \to \boldsymbol{R}$, where $D \subset \boldsymbol{R}^2$ is a region. We may imagine that $f(P)$ for $P \in D$ is the altitude of the point P on the island D. Since we assume the landscape to be sufficiently smooth, at each point on D there is a well defined direction $\boldsymbol{n}$ of the steepest ascent and the slope (magnitude) $s(\geq 0)$. That is, at each point on D, we may define the *gradient vector* $s\boldsymbol{n}$, which will be denoted by a vector $grad\, f$.

Exercise.

(A) Demonstrate $Df = gradf$ (Hint. Compute the slope of f along that line in the direction $\boldsymbol{n}$ passing through $\boldsymbol{r}$: $(d/dt)f(t\boldsymbol{n}+\boldsymbol{r})$ with the aid of the chain rule.)
(B) Compute the following gradients. (1) $grad(r)$.
(2) $grad(r^{-2})$.

3.2 Coordinate expression of $grad\, f$. Although $grad\, f$ is meaningful without any specific coordinate system (i.e., the concept is coordinate-free), in actual calculations, introduction of a coordinate system is often useful. The 3-space version of gradient reads as follows. Choose a Cartesian coordinate system O-xyz.

$$grad\, f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right), \tag{3.1}$$

or

$$grad\, f = \boldsymbol{i}\frac{\partial f}{\partial x} + \boldsymbol{j}\frac{\partial f}{\partial y} + \boldsymbol{k}\frac{\partial f}{\partial z}. \tag{3.2}$$

3.3 Remark. Note that to represent $grad\, f$ (in 3-space) in terms of numbers, we need two devices: one is a coordinate system to specify the point in D with three numbers, which allow us to describe f as a function of three independent variables; the other device is the basis vectors spanning the three dimensional vector '$grad\, f$' at each point on D (i.e., spanning the tangent space at each point of D). In principle, any choice is fine, but practically, it is wise to choose these base vectors to be parallel to the coordinate directions at each point. In the choice of **3.2**, the coordinate system has globally the same coordinate directions at every point on D, and the basis vectors of the tangent space are chosen to be parallel to these directions, so again globally uniformly chosen. Nonuniformity of the choice of the base vectors causes complications. We must be very careful (→**3.7**, **3.12** for a warning), especially when we formally use operators explained below.

3.4 Nabla or del. (3.2) suggests that $grad$ is a map which maps f to the gradient vector at each point in its domain (if f is differentiable). We often write this linear operator (→**3.2**) as ∇, which is called *nabla*,[35] but is often read 'del' in the US. We write $grad\, f = \nabla f$. ∇ has the following expression if we use the Cartesian coordinates

$$\nabla \equiv \sum_{k=1}^{n} \boldsymbol{e}_k \frac{\partial}{\partial x_k}, \tag{3.3}$$

where x_k is the k-th coordinate and $\boldsymbol{e}_k$ is the unit directional vector in the k-th coordinate direction.

[35] 'Nabla' is a kind of harp (Assyrian harp).

3.5 Divergence. Suppose we have a flow field (velocity field) $\boldsymbol{u}$ on a region $D \in \boldsymbol{R}^3$. Let us consider a region $V \subset \boldsymbol{R}^3$ whose boundary ∂V is sufficiently smooth. V may be imagined to be covered by *area elements* $d\boldsymbol{S}$ which can be identified with a vector whose magnitude $|d\boldsymbol{S}|$ is the area of the area element, and whose direction is parallel to the outward normal direction of the area element. Then $\boldsymbol{u} \cdot d\boldsymbol{S}$ is the rate of the volume of fluid going out through the area element in the unit time (cf. **2.5**). The area integral

$$\int_{\partial V} d\boldsymbol{S} \cdot \boldsymbol{u} \tag{3.4}$$

is the total amount of the volume of the fluid lost from the region V. The following limit, if exists, is called the *divergence* of the vector field $\boldsymbol{u}$ at point P and is written as $div\, \boldsymbol{u}$:

$$div\, \boldsymbol{u} \equiv \lim_{|V| \to 0} \frac{\int_{\partial V} \boldsymbol{u} \cdot d\boldsymbol{S}}{|V|}, \tag{3.5}$$

where the limit is taken over a concentric spheres (or cubes) converging to a unique point P.[36] $div\, \boldsymbol{u}$ is the rate of loss of the quantity carried by the flow field $\boldsymbol{u}$ per unit volume (i.e., the loss rate density).

Discussion

(1) A precise version of (3.5) in terms of a generator producing a flow should have been mentioned at least in the discussion. However, to this end, we must discuss the flow T_t induced by a vector field $\boldsymbol{a}(\boldsymbol{x})$, where T_t is the solution semigroup (this concept should be explained in the elementary part of ODE) of

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{a}(\boldsymbol{x}). \tag{3.6}$$

Let D be a bounded region. $T_t(D)$ denotes the region after time t if the region is passively advected by the flow whose velocity field is given by $\boldsymbol{a}$. Then a precise version of (3.5) is

$$\left.\frac{d}{dt}\right|_{t=0} \int_{T_t(D)} d\boldsymbol{x} = \int_D div \boldsymbol{a}(\boldsymbol{x}) d\boldsymbol{x}. \tag{3.7}$$

The proof of this reduces to a calculation of the Jacobian $\partial(T_t\boldsymbol{x})/\partial(\boldsymbol{x})$ for very small t, or to calculate the determinant of the following matrix,

$$\frac{\partial(T_t\boldsymbol{x})}{\partial(\boldsymbol{x})} = 1 + t\frac{\partial(\boldsymbol{a})}{\partial(\boldsymbol{x})} + o[t]. \tag{3.8}$$

(2) The electric displacement satisfies $div\, \boldsymbol{D} = \rho$ ($\rightarrow$**2.49**), where ρ is the charge density. At the boundary of two media I and II is a surface charge of density σ. Let $\boldsymbol{n}$ be the unit normal vector of the interface pointing from I to II. Show

$$(\boldsymbol{D}_I - \boldsymbol{D}_{II}) \cdot \boldsymbol{n} = \sigma. \tag{3.9}$$

[36] Here the volume can have more general shapes, but our definition is usually enough.

See Section 1.5 of Jackson, *Classical Electrodynamics* (Wiley, 1975) for similar examples.

3.6 Cartesian expression of *div*. From (3.5) assuming the existence of the limit, we may easily derive the Cartesian expression for *div*. Choose as V a tiny cube whose surfaces are perpendicular to the Cartesian coordinates of O-xyz. We immediately get

$$div\, \boldsymbol{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}. \tag{3.10}$$

div has the following coordinate-free definition:

$$div\, \boldsymbol{u} = Tr(D\boldsymbol{u}), \tag{3.11}$$

where D denotes the strong derivative (see discussion (1) in **3.5**).

3.7 Operator *div*. (3.10) again suggests that *div* is a linear operator (→**3.2**) which maps a vector field to a scalar field. Comparing (3.3) and (3.10) allows us to write

$$div\, \boldsymbol{u} = \nabla \cdot \boldsymbol{u}. \tag{3.12}$$

This 'abuse' of nabla is allowed only in the Cartesian coordinates (why? →**3.3**). Generalization to n-space is straightforward.

Exercise. Compute $div(\boldsymbol{r}/r)$.

3.8 Curl. Let $\boldsymbol{u}$ be a vector field as in **3.5**. Take a singly connected[37] compact smooth surface S in $\boldsymbol{R}^3$ whose boundary is smooth.[38] to the existence of what we need is the existence of length, area and so on of the object The boundary closed curve with the orientation according to

[37] A region is *singly connected*, if, for any given pair of points in the region, any two curves connecting them are homotopic. That is, they can be smoothly deformed into each other without going out the region.

[38] Around here the word 'smooth' is used often to avoid pathological cases. Practical physicists may understand 'smoothness' as the existence of strong derivatives to any order needed. Often the smoothness assumption may be weakened; for example smoothness of the surface may be replaced by the existence of its area or smoothness of a curve with the existence of its length. Therefore, fractal surfaces and curves are usually excluded.

the right-hand rule is denoted by ∂S (see Fig.). Consider the following line integral along ∂S:

$$\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l}, \tag{3.13}$$

where $d\boldsymbol{l}$ is the line element along the boundary curve. Let us imagine a straight vortex line and take S to be a disc perpendicular to the line such that its center is on the line. Immediately we see that this integral is the strength of the vortex whose center (singular point) goes through S. Therefore, the following limit, if exists, describes the 'area' density of the $\boldsymbol{n}$-component of the vortex (as in the case of angular velocity, the direction of vortex is the direction of the axis of rotation with the right-hand rule):

$$\boldsymbol{n} \cdot curl\, \boldsymbol{u} = \lim_{|S| \to 0} \frac{\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l}}{|S|}, \tag{3.14}$$

where the limit is over the sequence of nested[39] smooth surfaces which converges to point P with its orientation in the $\boldsymbol{n}$-direction. If the limit exists, then obviously there is a vector $curl\, \boldsymbol{u}$ called *curl* of the vector field $\boldsymbol{u}$.

3.9 Cartesian expression of curl. If we assume the existence of the limit (3.14), we can easily derive the Cartesian expression for $curl\, \boldsymbol{u}$. We have

$$curl\, \boldsymbol{u} = \left(\frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z}, \frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x}, \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \right), \tag{3.15}$$

or

$$curl\, \boldsymbol{u} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ \partial_x & \partial_y & \partial_z \\ u_x & u_y & u_z \end{vmatrix} = \nabla \times \boldsymbol{u}. \tag{3.16}$$

This 'abuse' of the nabla symbol is admissible only with the Cartesian coordinates (→**3.3**).

Componentwisely, we can write (with the summation convention)

$$(curl\, \boldsymbol{u})_i = \epsilon_{ijk} \partial_j u_k, \tag{3.17}$$

where ϵ_{ijk} is defined as $\epsilon_{123} = 1$ and $\epsilon_{ijk} = sgn(ijk)$, where $sgn(ijk)$ is the sign of the permutation: if (ijk) is obtained from (123) with even number of exchanges of symbols, it is $+1$, and otherwise -1.[40] Notice that

$$(\boldsymbol{a} \times \boldsymbol{b})_i = \epsilon_{ijk} a_j b_k. \tag{3.18}$$

[39] They need not be nested, but for simplicity let us assume this.

[40] e.g., $(213) = -1$, and $(312) = +1$.

A useful formula is

$$\epsilon_{ijk}\epsilon_{abk} = \delta_{ia}\delta_{jb} - \delta_{ib}\delta_{ja}. \tag{3.19}$$

(The summation convention is implied.) The easiest way to demonstrate this equation is to start with the following general form

$$\epsilon_{ijk}\epsilon_{abk} = A_{ijab}\delta_{ij}\delta_{ab} + A_{iajb}\delta_{ia}\delta_{jb} + A_{ibja}\delta_{ib}\delta_{ja}, \tag{3.20}$$

and fix the coefficients. There is no term of other forms.

Exercise.
(1) Let $\boldsymbol{v} = (x^2z, -xy^3z^2, xy^2z)$. Compute $div\,\boldsymbol{v}$ and $curl\,\boldsymbol{v}$.
(2) Show

$$div(f\boldsymbol{v}) = grad\,f\cdot\boldsymbol{v} + f div\,\boldsymbol{v}, \tag{3.21}$$
$$curl(f\boldsymbol{v}) = gradf\times\boldsymbol{v} + f curl\boldsymbol{v}. \tag{3.22}$$

(3) Compute

$$curl\left(\boldsymbol{\mu}\times\boldsymbol{r}/r^3\right). \tag{3.23}$$

(4) Show

$$curl\,curl\,\boldsymbol{u} = grad\,div\boldsymbol{u} - \sum\frac{\partial^2}{\partial x_i^2}\boldsymbol{u}. \tag{3.24}$$

See **3.12** about the Laplacian applied to a vector.

The coordinate free definition can be written as follows. Compute the strong derivative $d\boldsymbol{u}/d\boldsymbol{x}$ ($\rightarrow$**1.4**). Denote its skew symmetric part[41] as $(d\boldsymbol{u}/d\boldsymbol{x})_-$.[42] Then

$$\left(\frac{d\boldsymbol{u}}{d\boldsymbol{x}}\right)_-\boldsymbol{v} = \frac{1}{2}curl\,\boldsymbol{u}\times\boldsymbol{v}, \tag{3.25}$$

where $\boldsymbol{v}$ is an arbitrary 3-vector. See **2.23**.

Discussion
Let us study the motion of a small vector $\boldsymbol{e}$ near the origin flowing with a flow field specified by $\boldsymbol{v}$. We have

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{v}. \tag{3.26}$$

[41] Let A be a square matrix. $A_- \equiv A - A^T$ is called its skew symmetric part.
[42]

$$\left(\frac{d\boldsymbol{u}}{d\boldsymbol{x}}\right)_- = \begin{pmatrix} 0 & \partial_y u_x - \partial_x u_y & \partial_z u_x - \partial_x u_z \\ \partial_x u_y - \partial_y u_x & 0 & \partial_z u_y - \partial_y u_z \\ \partial_x u_z - \partial_z u_x & \partial_y u_z - \partial_z u_y & 0 \end{pmatrix}.$$

If $\boldsymbol{e}$ is small, its deformation is governed by

$$\frac{d\boldsymbol{e}}{dt} = \boldsymbol{v}(\boldsymbol{e}) - \boldsymbol{v}(0) = \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_0 \boldsymbol{e}, \tag{3.27}$$

where the (strong) derivative of the velocity field is evaluated at the origin. For a very small time δt, we can solve this equation as

$$\boldsymbol{e}(\delta t) = \left(1 + \delta t \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_0\right) \boldsymbol{e}(0). \tag{3.28}$$

We can separate the velocity derivative into the symmetric (+) and anti (or skew) symmetric part (−) as

$$\left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_0 = \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_+ + \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_-, \tag{3.29}$$

where

$$\left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_\pm \equiv \frac{1}{2}\left[\left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_0 \pm \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_0^T\right]. \tag{3.30}$$

Ignoring higher order terms, we can rewrite (3.28) as

$$\boldsymbol{e}(\delta t) = \left(1 + \delta t \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_+\right)\left(1 + \delta t \left(\frac{d\boldsymbol{v}}{d\boldsymbol{r}}\right)_-\right) \boldsymbol{e}(0). \tag{3.31}$$

This tells us that we may separately study the effects of the symmetric and of the skew symmetric parts.
(1) Demonstrate that the symmetric part changes the volume of a (small) cube C spanned by $\boldsymbol{e}_x$, $\boldsymbol{e}_y$, and $\boldsymbol{e}_z$. The changing rate of the volume is given by $div\,\boldsymbol{v}$ (→**3.6**).
(2) Demonstrate that the skew part does not change the volume of the cube C. It rotates the cube with the angular velocity $curl\,\boldsymbol{v}/2$. This is (3.25) above.

3.10 Potential field, potential, solenoidal field, irrotational field. If a vector field $\boldsymbol{u}$ allows an expression $\boldsymbol{u} = grad\,\phi$, then the field is called a *potential field* and ϕ is called its *potential*. A field without divergence, $div\,\boldsymbol{u} = 0$, is called a divergenceless or *solenoidal field*. The field without curl, $curl\,\boldsymbol{u} = 0$, is called an *irrotational field*.

3.11 Laplacian, harmonic function. The operator Δ defined by

$$\Delta f \equiv div\,grad\,f \tag{3.32}$$

is called the *Laplacian*, and is often written as ∇^2. Δ is defined for a scalar function. A function f satisfying $\Delta f = 0$ in a region D is called

a *harmonic function* in D. According to our understanding of the Laplacian (→**1.8**) a harmonic function is a function which is invariant under the spatial moving average (→**??**-**??**). Hence, intuitively, no local extrema should exist. Graphs of harmonic functions.

3.12 Laplacian for vector fields. If we formally calculate $curl\, curl\, \boldsymbol{u}$ in the Cartesian coordinates, then we have (→(3.24)

$$curl\, curl\, \boldsymbol{u} = grad\, div\, \boldsymbol{u} - \nabla^2 \boldsymbol{u}. \tag{3.33}$$

Since the formal calculation treating ∇ as a vector is legitimate only in the Cartesian coordinate system (cf. **3.3**), this calculation is meaningful only in the Cartesian system. In particular, $\nabla^2 \boldsymbol{u} = (\Delta u_x, \Delta u_y, \Delta u_z)$ is meaningful only in this coordinate system. However, the other two terms in the above equality are coordinate-free. Hence, we *define* $\Delta \boldsymbol{u}$ as

$$\Delta \boldsymbol{u} \equiv grad\, div\, \boldsymbol{u} - curl\, curl\, \boldsymbol{u}. \tag{3.34}$$

3.13 Theorem [Gauss-Stokes-Green's theorem]. From our definitions of divergence and curl (→**3.5**, **3.8**), we have[43]

(1) Gauss' theorem.

$$\int_{\partial V} \boldsymbol{u} \cdot d\boldsymbol{S} = \int_V div\, \boldsymbol{u}\, d\tau, \tag{3.35}$$

[43] Here the boundaries ∂V, ∂S and ∂D below must be sufficiently smooth, and the vector field must be (piecewise) C^1.

where V is a region in the 3-space and $d\tau$ is the volume element.
(2) Stokes' theorem.[44]

$$\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l} = \int_S curl\, \boldsymbol{u} \cdot d\boldsymbol{S}, \tag{3.36}$$

where S is a compact surface in 3-space.
(3) In 2-space, Stokes' theorem reduces to *Green's theorem*

$$\int_{\partial D} (udx + vdy) = \int_D \left(-\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) dxdy, \tag{3.37}$$

where u and v are differentiable functions of x and y.

Exercise.[45]
(A)
(1) Let $S = \{(x, y, z) \,|\, 4x^2 + y^2 + z = 1, -3 \leq z\}$ and $\boldsymbol{v}(x, y, z) = (3xy + 7y + x, y, z + 3)$. What is $\int_S \boldsymbol{v} \cdot d\boldsymbol{S}$?
(2) Let $S = \{(x, y, z) \,|\, x^2 + y^2 + 4z^6 = 4, 0 \leq z\}$ and $\boldsymbol{v}(x, y, z) = (e^y, z, x^2)$. What is $\int_S \boldsymbol{v} \cdot d\boldsymbol{S}$?
(3) Compute

$$\int_S \boldsymbol{v} \cdot d\boldsymbol{S} \tag{3.38}$$

for $S = \{(x, y, z) \,|\, x^2 + y^2 + 4z^6 = 4, 0 \leq z\}$ and $\boldsymbol{v}(x, y, z) = (e^y, z, x^2 + \cos y)$ (this is not a misprint).
(B) Prove Green's formula (3.37).

3.14 Who was Gauss?[46] Carl Friedrich Gauss was born on April 30, 1777 in Braunschweig. Although he studied at University of Göttingen from 1795 to 98, he was already the first rate mathematician, and completed his number theory masterpiece (*Disquisitiones Arithmeticae*) when he was 20 (the printing of this famous book, which Dirichlet carried wherever he went, started in April, 1798, but was interrupted several times, and was published only in 1801).

He obtained his PhD in 1799 from University of Helmstedt with the thesis on the existence of the roots of algebraic equations. This was his favorite topic, which he proved several times with different methods in his life. The thesis avoided the use of imaginary numbers, because he was afraid that he might not get PhD due to conventional professors. Therefore, the statement was that any algebraic equation can be

[44] George Gabriel Stokes, 1819-1903.
[45] From K Fukaya, *Electromagnetic Fields and Vector Analysis* (Iwanami, 1995), p98.
[46] heavily relying on T. Takagi, *Kinsei Suugaku Shidan* (Tales from Modern Mathematics History) (Kyoritu, 1933). See also W. K. Bühler, *Gauss, a biographical sketch* (Springer, 1981). All of his offsprings seem to be in the US.

factorized into first or second order factors.

After his PhD, from 1799 to 1807, he was fully supported by Prince Ferdinand of Braunschweig, and could concentrate on mathematics until he was 30. Almost all his great accomplishments started during this 'happiest time of my life' (according to old Gauss in his 70s,"for mathematics unhindered and uninterrupted time is mandatory").

After 1807, he was a professor and the chief astronomer at Göttingen, and 'could not have any time to do big work.' "When my head is completely occupied by the effort to grasp a shadow of the spirit floating in the air comes the time to give a lecture. I must jump up and switch my attention to a completely different world. The pain is beyond any expression $\cdots$." In his memoir mixed with the calculations on elliptic functions one finds, "Der Tod ist mir lieber als ein solches Leben."[47]

From 1816 he participated in the field work to make the map of Hannover. It is a famous story that he attempted to check the flatness of the space. In 1828 Gauss invited Wilhelm Weber to Göttingen, and for a few tens of years they collaborated on the study of electromagnetism. He died on May 22, 1855 in Göttingen. His monument carries 'Mathematicorum princeps.'

Gauss had already known the main part of complex function theory by 1811, but he never published it. He should have known elliptic function theory, but he did not publish it. Later Abel and Jacobi constructed the theory, expecting that Gauss should have known most results. Gauss knew non-Euclidean geometry, but he did not publish it. He avoided debate and argument with reactionary conservatives (recall what he did in his thesis). His seal had one tree with a couple of fruits with the motto 'pauca sed matura.'[48]

Gauss wrote in his diary on January 8, 1797 that he started to study lemniscate in conjunction to

$$u = \int_0^x \frac{dx}{\sqrt{1-x^4}}. \tag{3.39}$$

He was trying to generalize trigonometric functions for some time using the analogy

$$\text{arc sin}x = \int_0^x \frac{dx}{\sqrt{1-x^2}}. \tag{3.40}$$

This was the starting point of his study of elliptic functions. In this study (and in many others) he did a lot of experimental mathematics using numerical studies. He loved numbers; for example, when one of his acquaintances died, he computed the life span of the deceased in days on the back of the notice. In one of his note he gave $e^{-\pi}$ up to 50

[47] Death is dearer than such a life.

[48] cf., paucity, maturity.

decimal places. His computations were extremely elegant and clever, often exploiting number theory. His mathematics was inductive; he was an explorer of the universe of numbers.

He developed fast Fourier transform (→**12.26**), one of the best numerical integration schemes (1814 →**17A** needed to perform perturbation calculation), the least square approximation method (1821-3 in order to study the motion of planetoids), etc. His theory of curved surfaces (1827) was during his map making activity, and his potential theory (1839-40) was related to his electromagnetism study.

His pure and applied mathematics were inseparably intertwined, that is, his applied mathematics was the true applied mathematics; we saw such examples recently in Kolmogorov.

3.15 Poincaré's lemma.[49]
(1) $div\, curl \boldsymbol{A} = 0$,
(2) $curl\, grad\, \phi = 0$.
[Demo] Let V be a compact region of $\boldsymbol{R}^3$ whose boundary ∂V is sufficiently smooth. Notice that $\partial^2 V = \emptyset$. With the aid of the Gauss-Stokes-Green theorem (→**3.13**), we have

$$\int_V d\tau\, div\, curl\, \boldsymbol{A} = \int_{\partial V} curl\, \boldsymbol{A} \cdot d\boldsymbol{S} = \int_{\partial^2 V} \boldsymbol{A} \cdot d\boldsymbol{\ell} = 0. \tag{3.41}$$

To demonstrate (2), take a surface S whose boundary ∂S is sufficiently smooth. Then, Stokes' theorem and the definition of *grad* tell us

$$\int_S curl\, grad\, \phi \cdot d\boldsymbol{S} = \int_{\partial S} grad\, \phi \cdot d\boldsymbol{\ell} = 0. \tag{3.42}$$

3.16 Remark: differential forms. Notice that these relations are due to the topologically trivial fact that the boundary of a boundary is an empty set ($\partial^2 V = \emptyset$). These are examples of the general formula $d^2\omega = 0$, where ω is a *differential form*. I. M. Singer and J. A. Thorpe, *Lecture Notes on Elementary Topology and Geometry* (Scott, Foresman and Company, 1967) is strongly recommended. B. Schutz, *Geometrical Methods of Mathematical Physics* (Cambridge UP, 1980) is less modern, but may still be good for physicists who are not interested in elegance and depth of mathematical ideas. The Gauss-Stokes-Green theorem has the following unified expression

$$\int_M d\omega = \int_{\partial M} \omega, \tag{3.43}$$

[49] Henri Poincaré, 1854-1912.

where M is an orientable[50] n-manifold (which must be sufficiently smooth), and ω is a differential form. Notice that this is a natural extension of the fundamental theorem of calculus:

$$\int_{[a,b]} df = f(b) - f(a) \, (= \int_{[a],[b]} f). \tag{3.44}$$

Poincaré's lemma $d^2\omega = 0$ follows from $\partial^2 M = \emptyset$. d and ∂ are, in a certain sense, dual (Good symbols reveal deep relations. This duality is the duality between cohomology and homology. The references cited above will tell the reader about this a bit.).

3.17 Converse of Poincaré's lemma holds.

(1) If a vector field $\boldsymbol{F}$ is *irrotational* (i.e., $curl\, \boldsymbol{F} = 0$) in a singly connected orientable region, there is a potential function ϕ such that $\boldsymbol{F} = grad\, \phi$.
(2) If a vector field $\boldsymbol{F}$ is *solenoidal* (i.e., $div\, \boldsymbol{F} = 0$) in a singly connected orientable region, then there is a vector field (called a *vector potential*) $\boldsymbol{A}$ such that $\boldsymbol{F} = curl\, \boldsymbol{A}$. □
In the language of differential forms, the converse of Poincaré's lemma can be written as: if $d\omega = 0 \Rightarrow$ there is a differential form ϕ such that $\omega = d\phi$. (1) can be demonstrated easily by calculation. Do not overlook the importance of the shape of the region.
[Demo of (1)] Define

$$\phi(x) \overset{\text{def}}{=} \int_0^1 dt \boldsymbol{F}(t\boldsymbol{x} + (1-t)\boldsymbol{x}_0) \cdot (\boldsymbol{x} - \boldsymbol{x}_0). \tag{3.45}$$

The assumption of (1) implies that for any closed curve C in the region $\int_C \boldsymbol{F} \cdot d\boldsymbol{\ell} = 0$. That is, the line integral of $\boldsymbol{F}$ along a smooth curve in the region D connecting two points $\boldsymbol{x}_0 \in D$ and $\boldsymbol{x} \in D$ does not depend on smooth paths connecting these two points. Hence ϕ is a well-defined function of $\boldsymbol{x}$. Check that actually $grad\, \phi = \boldsymbol{F}$.
Perhaps the clearest way to demonstrate (2) is to use the Helmholtz-Hodge theorem **3.18** below. The condition of (2) with the aid of **3.15** implies that $\boldsymbol{F}$ can be written as (3.48) with $\Delta\phi = 0$ such that $\phi \to 0$ at infinity. We will see later that only $\phi \equiv 0$ satisfies this condition (→Liouville's theorem **??**).

Exercise
(A) Hint: There is no clever method. Guess.
(1) Show that the following 3-vector field has a vector potential and construct it.

$$\boldsymbol{v} = (e^y - x\cos(xz), 0, z\cos(xz)). \tag{3.46}$$

(2) Show that the following 3-vector field has a scalar potential and find it

$$\boldsymbol{v} = (y^2 \sin z, 2xy \sin z, xy^2 \cos z). \tag{3.47}$$

[50] A n-manifold is orientable, if an atlas can be chosen which is with a consistent handedness.

(3) Find the vector potential of $\boldsymbol{v} = (-y/(x^2+y^2), x/(x^2+y^2), 0)$.
(4) Find a potential for $\boldsymbol{v} = f(r)\boldsymbol{r}$.
(B) Construct an example of an irrotational vector field on an appropriate domain which does not have any scalar potential.

3.18 Theorem [Helmholtz-Hodge]. Let $\boldsymbol{F}$ be a vector field which is once differentiable, and its first order derivatives vanish at infinity. Then, there is a scalar field ϕ and a solenoidal (i.e., $div\,\boldsymbol{A} = 0$) vector field $\boldsymbol{A}$ such that[51]

$$\boldsymbol{F} = grad\,\phi + curl\,\boldsymbol{A}. \tag{3.48}$$

□
This can be rewritten with the aid of **3.15** as

3.19 Theorem [Helmholtz-Stokes-Blumental]. Let $\boldsymbol{F}$ be a vector field which is once differentiable, and its first order derivatives vanish at infinity. Then, there is the following decomposition of $\boldsymbol{F}$:

$$\boldsymbol{F} = \boldsymbol{U} + \boldsymbol{V},\ \ curl\,\boldsymbol{U} = 0,\ div\,\boldsymbol{V} = 0. \tag{3.49}$$

□

Discussion.
Check the following formal result: Let

$$\phi(\boldsymbol{r}) = -\frac{1}{4\pi}\int_V \frac{div\boldsymbol{F}}{r}d\tau, \tag{3.50}$$

$$\boldsymbol{A}(\boldsymbol{r}) = \frac{1}{4\pi}\int_V \frac{curl\boldsymbol{F}}{r}d\tau, \tag{3.51}$$

where r is the distance between the volume element $d\tau$ and $\boldsymbol{r}$. Furthermore, V is the finite domain containing the supports of $curl\boldsymbol{F}$ and $div\boldsymbol{F}$. Then

$$\boldsymbol{F} = grad\,\phi + curl\boldsymbol{A}. \tag{3.52}$$

3.20 Formulas of vector calculus.
(1) $grad\,\boldsymbol{A}\cdot\boldsymbol{B} = (\boldsymbol{B}\cdot\nabla)\boldsymbol{A} + (\boldsymbol{A}\cdot\nabla)\boldsymbol{B} + \boldsymbol{B}\times curl\,\boldsymbol{A} + \boldsymbol{A}\times curl\,\boldsymbol{B}$.
(2) $div\,(\boldsymbol{A}\times\boldsymbol{B}) = curl\,\boldsymbol{A}\cdot\boldsymbol{B} - curl\,\boldsymbol{B}\cdot\boldsymbol{A}$.
(3) $curl(\boldsymbol{A}\times\boldsymbol{B}) = (div\,\boldsymbol{B})\boldsymbol{A} - (div\,\boldsymbol{A})\boldsymbol{B} + (\boldsymbol{B}\cdot\nabla)\boldsymbol{A} - (\boldsymbol{A}\cdot\nabla)\boldsymbol{B}$.

[51] We need a condition to control the 'size' of $\boldsymbol{F}$ near infinity: For example, $|\boldsymbol{F}| \sim 1/r^2$ is a good condition. Such a condition is needed because we must solve the Poisson equation to find ϕ and $\boldsymbol{A}$ (cf. **??**).

In particular, $curl(\boldsymbol{A} \times \boldsymbol{r}/2) = \boldsymbol{A}$, if $\boldsymbol{A}$ is constant.
(4) $(\boldsymbol{C} \cdot \nabla)(\boldsymbol{A} \times \boldsymbol{B}) = \boldsymbol{A} \times (\boldsymbol{C} \cdot \nabla)\boldsymbol{B} - \boldsymbol{B} \times (\boldsymbol{C} \cdot \nabla)\boldsymbol{A}$.
(5) $\boldsymbol{C} \cdot grad\,(\boldsymbol{A} \cdot \boldsymbol{B}) = \boldsymbol{A} \cdot (\boldsymbol{C} \cdot \nabla)\boldsymbol{B} + \boldsymbol{B} \cdot (\boldsymbol{C} \cdot \nabla)\boldsymbol{A}$.
(6) $div(grad\, f \times grad\, g) = 0$.

Exercise.
Demonstrate all the formulas. In $curl(\boldsymbol{A} \times \boldsymbol{r}/2) = \boldsymbol{A}$, $\boldsymbol{A}$ must be constant. If not, what is the result? [Perhaps, the componentwise demonstration is the easiest.]

3.B Curvilinear Coordinates

3.21 Curvilinear coordinates, metric tensor. The role of a coordinate system in 3-space is to assign uniquely a numerical vector (q^1, q^2, q^3) to each point in $\boldsymbol{R}^3$. Thus the Cartesian coordinates of the point x^1, x^2, x^3 are unique functions of (q^1, q^2, q^3). Let $(q^1 + dq^1, q^2 + dq^2, q^3 + dq^3)$ be a point an infinitesimal distance away from (q^1, q^2, q^3). The distance between these two points ds can be written as the following quadratic form:

$$ds^2 = \sum_{i,j} g_{ij} dq^i dq^j, \tag{3.53}$$

where

$$g_{ij} \equiv \sum_k \frac{\partial x^k}{\partial q^i} \frac{\partial x^k}{\partial q^j}, \tag{3.54}$$

which is called the *metric tensor*.

3.22 Riemann geometry. The Riemann geometry (→**3.23**) is the geometry determined by the metric tensor. M. Spivac, *Comprehensive Introduction to Differential Geometry* (Publish or Perish, Inc., Berkeley, 1979), vol. II, Chapter 4 contains Riemann's epoch-making inaugural lecture (English translation) with a detailed mathematical paraphrase of the lecture, "What did Riemann say?". According to Dedekind,[52] Gauss (→**3.14**) sat at the lecture which surpassed all his expectations, in the greatest astonishment, and on the way back from the faculty meeting he spoke to Wilhelm Weber (Riemann's lifelong patron), with the greatest appreciation, and with an excitement rare for him, about the depth of the idea presented by Riemann.

Read for a nice introduction to Riemann geometry an overview by Kazdan in Bull. Amer. Math. Soc. **33**, 339 (1996).

[52] Julius Wilhelm Richard Dedekind, 1831-1916.

3.23 Who was Riemann?[53] Georg Friedrich Bernhard Riemann was born on September 17, 1826 in a small village on the Elbe near Lüneburg. He was the second of six children of a poor pastor. He was educated by his father before he entered the gymnasium. When he was fourteen, he lived with his grandmother in Hanover and entered the third grade of the gymnasium there. After his grandmother died, he transferred to the second grade of a gymnasium in Lüneburg in April, 1842. The principal of the school recognized his mathematical genius and lent his math books. Riemann always returned the books within a couple of days, so the principal was surprised but found that Rieman understood them. He became familiar with Euler's work in those days.

He entered University of Göttingen in April, 1846 as a Linguistics and Theology major to get a job as quickly as possible to support his parents and siblings. He also attended Gauss' (→**3.14**) lectures on the least square method. His desire to study mathematics became irrepressible, and he finally asked for his father's permission to switch his major. In those days Gauss was about 70, and gave only a few applied mathematics courses, so he was disappointed and moved to the University of Berlin in 1847.

In Berlin, Jacobi (algebra and analytical mechanics), Dirichlet (number theory, integration theory, PDE), Steiner, and other professors gave lectures on their new results. Dirichlet aimed at logical rigor and avoided calculations as much as possible. This style met Riemann's taste.

In the spring of 1849, he returned to Göttingen, and was attracted to Weber's experimental physics course. Weber recognized his genius and became his patron. Riemann did not get any direct instruction from Gauss, but was strongly influenced by the atmosphere created by the great mathematician. For example, Riemann accepted the idea of 'ether' which Gauss also had.

In November 1851, he submitted his thesis entitled, The foundation of general theory of functions of one complex variable. He defined holomorphic functions in terms of the Cauchy-Riemann equation. The idea of conformal maps was also conceived. He also introduced Riemann surfaces. Gauss praised the thesis: Mr. Riemann's thesis clearly tells us that his study is thorough, that he has a sharp brain, and that he has a magnificent and rich creativity. From every point, the thesis is a precious accompishment and far surpasses the standard of doctoral theses. When Riemann visited Gauss after the exam, Gauss told him that he had similar thoughts (→**3.14**), and that he had a similar aim.

He next started preparation for the Habilitation paper. He chose to study Fourier series (→**9**), but this was not an easy task. Fortu-

[53] Mainly based on K. Kobori, *Great Mathematicians of the 19th Century* (Kobundon, 1940).

nately, Dirichlet visited Göttingen, who checked Riemann's manuscript together, and "Professor Dirichlet gave me detailed suggestions with kindness I could not imagine when I took into account the difference of our social statuses. I pray Professor will remember me forever."(from a letter to his father). He submitted his paper, The expressibility of functions by trigonometric series, in December 1853. The Riemann integration appeared for the first time in this paper (→**10.22**(3)). In those days he was an assistant of Weber.

The famous Habilitations exam was held on June 10, 1854. He introduced (1) the concept of manifold, (2) a new definition of distance through the quadratic form, and (3) the concept of curvature.[54]

He became a lecturer in 1854. His first lecture was on PDE and its applications to physics. He had eight students ("I am glad that I have so many students."(from a letter to his father)). In 1855, Dirichlet succeeded Gauss. Dirichlet made effort to make Riemann an associate professor, but failed. He finished his study of elliptic functions which was started in ca. 1851. His lecture on elliptic functions attracted only three participants including Dedekind. He became an associate professor on January 9, 1857.

In 1857 he completed "On the number of prime numbers less than a given number." He introduced the zeta function

$$\zeta(s) = \sum_{i=1}^{\infty} \frac{1}{n^s}, \tag{3.55}$$

and conjectured that all the zeros in the strip $0 < Re\, s < 1$ are on $Re\, s = 1/2$ (the Riemann conjecture). With Dedekind, he is the founder of analytic number theory. Dirichlet died on March 9, 1859. Riemann became a full professor on July 30, 1859. He got married on June 3, 1863 with his sister's friend Elise Koch, but this was his last happy period. He became ill in August. Weber persuaded the government to support his stay in Italy to recover his health. He had a wonderful time in Italy, befriending Italian mathematicians, Betti, Beltrami, and others.

His health never recovered fully, and in June 15, 1866, he went on his third Italian trip to rest at Selasca on Lake Maggiore. He died there in July, 1866.

3.24 Orthogonal curvilinear coordinate system. At each point (q^1, q^2, q^3), call the direction of the tangent to the i-th coordinate the i-th coordinate direction at (q^1, q^2, q^3) [e.g., the direction of the tangent

[54] This is a generalization of Gauss's curvature, but the new aspect was to write it in terms of the metric tensor.

to the second coordinate is the direction parallel to $(q^1, q^2 + dq^2, q^3) - (q^1, q^2, q^3)]$. If at every point all the coordinate directions are orthogonal to each other, we call the coordinate system an *orthogonal curvilinear coordinate system*. In this case, the metric tensor is always diagonal at every point:

$$g_{ij} = \begin{pmatrix} h_1^2 & 0 & 0 \\ 0 & h_2^2 & 0 \\ 0 & 0 & h_3^2 \end{pmatrix}, \tag{3.56}$$

where

$$h_i = \sqrt{\sum_k \left(\frac{\partial x_k}{\partial q^i}\right)^2}. \tag{3.57}$$

3.25 Cylindrical coordinates. $(q^1, q^2, q^3) = (r, \varphi, z)$, and

$$\begin{aligned} x &= r\cos\varphi, \\ y &= r\sin\varphi, \\ z &= z. \end{aligned} \tag{3.58}$$

From (3.57) we have $h_1 = 1$, $h_2 = r$, and $h_3 = 1$.

3.26 Spherical coordinates. $(q^1, q^2, q^3) = (r, \theta, \varphi)$, and

$$\begin{aligned} x &= r\sin\theta\cos\varphi, \\ y &= r\sin\theta\sin\varphi, \\ z &= r\cos\theta. \end{aligned} \tag{3.59}$$

From (3.57) we have $h_1 = 1$, $h_2 = r$, and $h_3 = r\sin\theta$.

3.27 Elliptic cylindrical coordinates.[55] $(q^1, q^2, q^3) = (\xi, \eta, \varphi)$, and for some positive real c

$$\begin{aligned} x &= c\sqrt{(\xi^2 - 1)(1 - \eta^2)}\cos\varphi, \\ y &= c\sqrt{(\xi^2 - 1)(1 - \eta^2)}\sin\varphi, \\ z &= c\xi\eta. \end{aligned} \tag{3.60}$$

[55] This is a natural coordinate system for the Schrödinger equation for H_2^+ molecular ion.

From (3.57) we have

$$h_1 = c\sqrt{\frac{\xi^2-\eta^2}{\xi^2-1}},\ h_2 = c\sqrt{\frac{\xi^2-\eta^2}{1-\eta^2}},\ h_3 = c\sqrt{(\xi^2-1)(1-\eta^2)}, \quad (3.61)$$

where ξ and η can also be defined as

$$\xi = \frac{r_1+r_2}{2c},\ \eta = \frac{r_1-r_2}{2c}. \quad (3.62)$$

Discussion.
(A) Compute h_i ($\rightarrow$**3.24**) for the toroidal coordinates (α, β, φ) where

$$x = \frac{c\sinh\alpha\cos\varphi}{\cosh\alpha-\cosh\beta},\ y = \frac{c\sinh\alpha\sin\varphi}{\cosh\alpha-\cosh\beta},\ z = \frac{c\sin\beta}{\cosh\alpha-\cosh\beta}. \quad (3.63)$$

Here $\alpha \in [0,\infty)$, $\beta, \varphi \in (-\pi, \pi]$. What is the general shape of $\beta =$ constant surface?
(B) Introduce u and v variables that are related to ρ and z as

$$\rho = F_1(u,v),\ z = F_2(u,v) \quad (3.64)$$

such that u =const. and v =const. curves are orthogonal on the (ρ, z)-plane, and $\rho = 0$ is among such curves. Rotating the plane around the z-axis, we can make surfaces orthogonal to each other. Therefore, if we introduce the rotation angle φ, (u, v, φ) is a orthogonal curvilinear coordinate system in 3-space. Its relation to the usual Cartesian system is given by $\rho = \sqrt{x^2+y^2}$ and $\varphi = \tan^{-1}(x/y)$.

$$x = F_1(u,v)\cos\varphi, \quad (3.65)$$
$$y = F_1(u,v)\sin\varphi, \quad (3.66)$$
$$z = F_2(u,v). \quad (3.67)$$

(1) For this system show that

$$h_1 = \sqrt{\left(\frac{\partial F_1}{\partial u}\right)^2+\left(\frac{\partial F_2}{\partial u}\right)^2},\ h_2 = \sqrt{\left(\frac{\partial F_1}{\partial v}\right)^2+\left(\frac{\partial F_2}{\partial v}\right)^2},\ h_3 = \rho. \quad (3.68)$$

(2) For elliptic cylindrical coordinates, the choice is

$$\rho = a\sqrt{(u^2-1)(1-v^2)},\ z = auv \quad (3.69)$$

3.28 Gradient in orthogonal curvilinear coordinates. Consider an infinitesimal cube whose apices are at $(q^1+\theta_1 dq^1, q^2+\theta_2 dq^2, q^3+\theta_3 dq^3)$, where $\theta_i = 0$ or 1. The lengths of the edges of the cube are

$|h_1 dq^1|$, $|h_2 dq^2|$, and $|h_3 dq^3|$. From the geometrical definition of *grad* (→**3.1**), we have

$$(grad\,\phi)_1 = \frac{1}{h_1}\frac{\partial\phi}{\partial q^1},\ (grad\,\phi)_2 = \frac{1}{h_2}\frac{\partial\phi}{\partial q^2},\ (grad\,\phi)_3 = \frac{1}{h_3}\frac{\partial\phi}{\partial q^3}. \quad (3.70)$$

Here, 1, 2 and 3 denote the components of the vector in the 1, 2 and 3 coordinate directions, respectively.

Exercise.
(A) Find the velocity and acceleration components along the coordinate directions of a particle in
(1) spherical coordinates,
(2) elliptical cylindrical coordinates.
[Hint. Find the relation between the unit vectors of the curvilinear and Cartesian coordinates.]
(B) Demonstrate for the spherical coordinate system

$$\frac{\partial}{\partial x} = \sin\theta\cos\varphi\frac{\partial}{\partial r} + \cos\theta\cos\varphi\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\sin\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}, \quad (3.71)$$

$$\frac{\partial}{\partial y} = \sin\theta\sin\varphi\frac{\partial}{\partial r} + \cos\theta\sin\varphi\frac{1}{r}\frac{\partial}{\partial\theta} - \frac{\cos\varphi}{r\sin\theta}\frac{\partial}{\partial\varphi}, \quad (3.72)$$

$$\frac{\partial}{\partial z} = \cos\theta\frac{\partial}{\partial r} - \sin\theta\frac{1}{r}\frac{\partial}{\partial\theta}. \quad (3.73)$$

3.29 Volume element in orthogonal curvilinear coordinates. From the consideration above obviously the volume element $d\tau$ is given by

$$d\tau = h_1 h_2 h_3 dq^1 dq^2 dq^3. \quad (3.74)$$

Exercise. Compute the volume element for the elliptic cylindrical coordinates.

3.30 Divergence and curl in orthogonal curvilinear coordinates. From the geometrical definitions of these quantities (→**3.5**, **3.8**), we get

$$div\,\boldsymbol{A} = \frac{1}{h_1 h_2 h_2}\left[\frac{\partial}{\partial q^1}(h_2 h_3 A_1) + \frac{\partial}{\partial q^2}(h_3 h_1 A_2) + \frac{\partial}{\partial q^3}(h_1 h_2 A_3)\right], \quad (3.75)$$

$$(curl\,\boldsymbol{A})_1 = \frac{1}{h_2 h_3}\left[\frac{\partial}{\partial q_2}(h_3 A_3) - \frac{\partial}{\partial q_3}(h_2 A_2)\right]. \quad (3.76)$$

$(curl\ \boldsymbol{A})_2$ and $(curl\ \boldsymbol{A})_3$ are obtained from (3.76) by cyclic permutations of the indices. Notice that in these formulas A_i are the actual projection of the vector $\boldsymbol{A}$ on the i-th coordinate direction.

Exercise.
(1) Compute *curl* and *div* of $\boldsymbol{A} = r^2\boldsymbol{e}_r$, where $\boldsymbol{e}_r$ is the unit coordinate vector parallel to the radius in the spherical coordinates. How about if $\boldsymbol{e}_r$ is the unit vector parallel to the radius in the cylindrical coordinates?
(2) Show in the spherical coordinates that

$$curl\left(\frac{\cot\theta\boldsymbol{e}_\varphi}{r}\right) = -\frac{\boldsymbol{e}_r}{r^2}. \tag{3.77}$$

3.31 Laplacian in orthogonal curvilinear coordinates. Combining (3.70) and (3.75), we get for the Laplacian ($\Delta \equiv div\, grad$)

$$\Delta = \frac{1}{h_1h_2h_3}\left[\frac{\partial}{\partial q_1}\frac{h_2h_3}{h_1}\frac{\partial}{\partial q_1} + \frac{\partial}{\partial q_2}\frac{h_3h_1}{h_2}\frac{\partial}{\partial q_2} + \frac{\partial}{\partial q_3}\frac{h_1h_2}{h_3}\frac{\partial}{\partial q_3}\right]. \tag{3.78}$$

For the cylindrical coordinates, we have

$$\Delta = \frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2} + \frac{\partial^2}{\partial z^2}. \tag{3.79}$$

Notice that

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r}. \tag{3.80}$$

For the spherical coordinates, we have

$$\Delta = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \frac{1}{r^2}L^2 \tag{3.81}$$

with

$$L^2 \equiv \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{3.82}$$

Notice that

$$\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} = \frac{1}{r}\frac{\partial^2}{\partial r^2}r. \tag{3.83}$$

Exercise. Derive the formula for the Laplacian in the elliptic cylindrical coordinates.

4 Ordinary Differential Equation: General

The general theory of ordinary differential equations (ODE) is outlined with precise statements. In the second half of the section, elementary analytical techniques to solve ODE are summarized for convenience.

Key words: general solution, particular solution, singular solution, normal form, Cauchy-Peano's theorem, Lipshitz condition, Cauchy-Lipshitz' theorem, separation of variables, perfect differential equation, integrating factor, Bernoulli equation, Riccati equation, Lagrange's method.

Summary
(1) Any (normal form) ODE can be converted to a first order vector ODE (**4.4**-**4.6**).
(2) For simple first order ODE, look up representative examples first. Some representative examples are in **7B**.
(3) For linear ODE, although a general theory will be given in the following sections (**8**, **XX**), simple second order constant coefficient equations can be solved without any difficulty (**4.26**-**4.28**).

4.A General Theory

4.1 Practical advice. See, for example, Schaum's outline series *Differential Equations* by R. Bronson for elementary methods and practice. To learn the theoretical side, V. I. Arnold, *Ordinary differential equations* (MIT Press 1973; there is a new version from Springer) is highly recommended. E. A. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, (McGraw-Hill, 1955) is a standard classic reference. I cannot recommend D. Zwillinger, *Handbook of Differential Equations* (Academic Press, 1989). This book may be useful, but the organization should be more intelligent.

Exercise. If you do not have any problem with the following ODE, then you can skip Subsection **B**.
Find the general solutions of the following ODE.
(1) (→**4.20**)

$$x\frac{dy}{dx} + 2y = \sin x. \tag{4.1}$$

(2) (→**4.21**)

$$\frac{dy}{dx} + \frac{y}{x} = x^2 y^3. \tag{4.2}$$

(3) (→**4.22**, $y = x$ is a solution.)

$$\frac{dy}{dx} = y^2 - xy + 1. \tag{4.3}$$

(4) (→**4.25**-**4.28**)

$$\frac{d^2y}{dx^2} + 2\frac{dy}{dx} + 2y = xe^{-2x}. \tag{4.4}$$

Discussion [**Calogero-Moser equation**]. Let

$$\frac{dq_i}{dt} = p_i, \quad \frac{dp_i}{dt} = -\sum_{j \neq i} (q_i - q_j)^{-3}, \tag{4.5}$$

where $i \in \{1, \cdots, n\}$. For a solution to these equations, define a s quare matrix $L = \mathrm{Matr}(L_{ij})$ as follows:

$$L_{ii} = p_i, \;\; L_{ij} = (q_i - q_j)^{-1} \text{ for } i \neq j. \tag{4.6}$$

(1) Show that if for some square matrix B,

$$\frac{dL}{dt} = BL - LB = [B, L], \tag{4.7}$$

which is called a *Lax relation*, then $tr(L^m)$ is independent of t for all positive integers m.
(2) Let the square matrix B be defined as

$$b_{ii} = \sum_{k \neq i} (q_k - q_i)^{-2}, \;\; b_{ij} = (q_i - q_j)^{-2}, \tag{4.8}$$

then show (1) holds.
Hence, we have proved that for all positive integers m, $tr(L^m)$ are constants of motion. Lax relation implies that the system is completely integrable (that is, the flow is on a $2n$-dimensional torus).□

4.2 Ordinary differential equation. Let y be a n-times differentiable function of $x \in \boldsymbol{R}$. A functional relation

$$f(x, y(x), y'(x), \cdots, y^{(n)}(x)) = 0 \tag{4.9}$$

among x, $y(x)$, $y'(x)$, $\cdots$, $y^{(n)}(x)$ is called an *ordinary differential equation* (ODE) for $y(x)$, and n is called its *order*, where the domain of f is assumed to be appropriate. Such $y(x)$ that satisfies $f = 0$ is called a *solution* to the ODE.

Discussion.
Which is more general (or more powerful as a descriptive means), (normal form→**4.5**) ODE or (normal form) difference equations:

$$y_{k+n} = F(x, y_k, y_{k+1}, \cdots, y_{k+n-1}) \tag{4.10}$$

?[56]

[Hint: look up the following technical terms, suspension, and Poincaré section in a standard dynamical systems textbook.]

4.3 General solution, particular solution, singular solution. The solution $y = \varphi(x, c_1, c_2, \cdots, c_n)$ to $f = 0$ in **4.2** which contains n arbitrary constants c_1, $\cdots$, c_n (which are called *integral constants*) is called the *general solution* of $f = 0$. A solution which can be obtained from this by specifying finite values for the arbitrary constants is called a *particular solution*. A solution which cannot be obtained as a particular solution is called a *singular solution*. For example, the envelope curve[57] of the general solutions is a singular solution.

Discussion.
(A) Consider the following equation called *Clairaut's equation*:

$$y = x\frac{dy}{dx} + f\left(\frac{dy}{dx}\right). \tag{4.11}$$

(1) Show that its general solution is

$$y = Cx + f(C), \tag{4.12}$$

where C is a constant. [Hint. Differentiate (4.11) and factor out the second derivative. See **4.31**.]
(2) The envelope curve of the family of lines defined by (4.12) is also a solution of (4.11). This is a singular solution.
(B) In **4.12** $x \equiv 0$ is a singular solution to (4.33).

4.4 Normal form. If the highest order derivative of y is explicitly solved as

$$y^{(n)}(x) = F(x, y, y', \cdots, y^{(n-1)}) \tag{4.13}$$

from $f = 0$, we say the ODE is in the *normal form*.[58]

[56] This can alway be written in terms of differences $\Delta_1(k) \equiv y_{k+1} - y_k$, and higher order differences $\Delta_2(k) = \Delta_1(k+1) - \Delta_1(k)$, etc. Therefore, (4.10) may be considered as an n-th order difference equation. If the equation is linear with constant coefficients, then there is a general method to solve it (→**XX**).

[57] The envelop curve of a smooth family of curves $\{F(x, \alpha) = 0\}$, where α is a parameter, is a curve tangent to all the members of the family, and is given by the conditions $F(x, \alpha) = 0$ and $\partial F(x, \alpha)/\partial\alpha = 0$.

[58] Notice that not normal ODE's may have many pathological phenomena, but we will not pay any attention to the non-normal form case henceforth in this book.

4.5 Normal form ODE is essentially first order. Let $y_j \equiv y^{(j-1)}$ $(j = 1, \cdots, n)$. Then (4.13) can be rewritten as

$$\begin{aligned} \frac{dy_1}{dx} &= y_2, && (4.14)\\ \frac{dy_2}{dx} &= y_3, && (4.15)\\ &\cdots && (4.16)\\ \frac{dy_{n-1}}{dx} &= y_n, && (4.17)\\ \frac{dy_n}{dx} &= F(x, y_1, y_2, \cdots, y_n). && (4.18) \end{aligned}$$

That is, (4.13) has been converted into a first order ODE for a vector $\boldsymbol{y} = (y_1, y_2, \cdots, y_n)^T$. Any normal form n-th order scalar ODE can be converted into the n-vector first order ODE of the form

$$\frac{d\boldsymbol{y}}{dx} = \boldsymbol{v}(x, \boldsymbol{y}). \tag{4.19}$$

Any solution $\boldsymbol{y}(x)$ can be understood as an orbit parametrized with 'time' x in the n-space (= phase space) in which $\boldsymbol{y}$ lives.

4.6 Nonautonomous equation is not special. In (4.13) if F does not depend on x explicitly, we say the ODE is *autonomous*. If not, it is called *nonautonomous*. Parallelly, if $\boldsymbol{v}$ does not depend on x explicitly, we say (4.19) is autonomous; otherwise, nonautonomous. If we introduce one more variable t such that $dx/dt = 1$, then the set of equations in **4.5** becomes autonomous:

$$\begin{aligned} \frac{d\boldsymbol{y}}{dt} &= \boldsymbol{v}(x, \boldsymbol{y}),\\ \frac{dx}{dt} &= 1. && (4.20) \end{aligned}$$

Hence, there is no fundamental difference as to the basic theory between autonomous and nonautonomous cases.[59] Thus to understand ODE, we have only to understand first order autonomous vector ODE.

4.7 Initial value problem for first order ODE. To solve

$$\frac{d\boldsymbol{y}}{dx} = \boldsymbol{v}(\boldsymbol{y}) \tag{4.21}$$

[59] Of course, the dimension of the phase space is increased by one, and this could cause a tremendous qualitative difference.

under the condition that $\boldsymbol{y}(0) = \boldsymbol{y}_0$ is called an *initial value problem*, where $\boldsymbol{y}(0)$ is called the *initial data*. The vector field $\boldsymbol{v}$ defining an ODE may be considered to be a flow velocity field on an n-space. Hence, the initial value problem is geometrically a problem to find an orbit passing through $\boldsymbol{y}_0$ at 'time' $x = 0$.

We summarize the standard theorems in the following. The general idea can be understood intuitively. A point where $\boldsymbol{v} = 0$ is called a *critical point*. Not near a critical point, the essence of the unique existence of the solution is given by the *rectification*. That is, the flow can be transformed to a constant flow parallel to the first coordinate (by a one-to-one continuous map $\equiv$ homeomorphism):

$$\frac{d\boldsymbol{y}}{dx} = \boldsymbol{e}_1. \tag{4.22}$$

This should be ituitively easy to understand through imagining the vector field being drawn on a rubber sheet.[60] From (4.22) the unique existence of a local solution is obvious.

Discussion

(1) [Glass patterns]. An interesting method to make and visualize simple vector field is the Glass patterns. Make a random dot pattern more or less uniformly distributed on a sheet of paper, and make its transparency copy (it could be slightly scaled, or warped, so generating the points on computer may be advantageous). Then, superpose it on the original. If the displacements of the points are small, the reader will recognize a clear pattern, because her brain is a good detector of spatial correlation. The random dot moiré patterns are called *Glass patterns* after its discoverer L. Glass.[61] Applications of dynamical systems (= qualitative studies of differential equations) to cognitive psychology can be found in J. A. Scott Kelso, *Dynamic Patterns, the self-organization of brain and behavior* (MIT Press, 1995).

(2) [**Time change**]. Let $\boldsymbol{a}$ be a continuous vector field on $\mathbf{R}^d$, and μ be a nonzero

[60] Read the introductory part of the book review by P. Holmes, Bull. Amer. Math. Soc. **22**, 339 (1990).

[61] L. Glass, Nature, **223**, 578 (1960); L. Glass and R. Perez, Nature **246**, 3603 (1971).

continuous real function. Let the flows determined by the following ODEs be T_t and S_t, respectively:

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{a}, \qquad \frac{d\boldsymbol{x}}{dt} = \mu\boldsymbol{a}. \tag{4.23}$$

Then, there is a function $\tau(t, \boldsymbol{x})$ such that

$$S_t\boldsymbol{x} = T_{\tau(t,\boldsymbol{x})}\boldsymbol{x}. \tag{4.24}$$

Furthermore,

$$\tau(t+s, \boldsymbol{x}) = \tau(t, \boldsymbol{x}) + \tau(s, T_t\boldsymbol{x}). \tag{4.25}$$

S_t is called a *time change* of T_t. The above equality guarantees that S_t is a semigroup when T_t is, and is called the *cocyle condition*.

4.8 Theorem [Cauchy-Peano]. If for (4.21) $\boldsymbol{v}$ is continuous on a region $D \subset \boldsymbol{R}^n$, then for any $\boldsymbol{y}_0 \in D$ there is a solution $\boldsymbol{y}(x)$ of (4.21) passing through this point whose domain is an open interval (α, ω) $(-\infty \leq \alpha < \omega \leq \infty)$. □

4.9 Who was Cauchy?[62] Augustin-Louis Cauchy was born in Paris in the year the Revolution began (Aug. 21, 1789). His father, a barrister and police lieutenant escaped the Reign of Terror (1793-4) to live in Arceuil, as the neighbors of Laplace (→**13.3**) and Berthollet. Lagrange (→**2.7**) reportedly forecast the scientific genius of the boy. Cauchy thought pure mathematics was over, and the remaining task was applied mathematics. He worked as a military engineer at Cherbourg for two years from 1811, but resigned due to ill-health. Lagrange and Laplace persuaded him to leave engineering and to turn exclusively to mathematics in 1813.

Cauchy was a politically ultraconservative royalist, and after Restoration in 1814, he was appointed a member of the Paris Academy after Monge and 'regicide' Carnot (father of Sadi Carnot) were expelled.

Spurred by Fourier's work on Fourier series (→**10.22**), Cauchy tried to rationalize analysis. His results were published in Cour d'Analyse (1821) and Résumé des Lecons sur le Calcul infinitésimal (1823). In the former, he introduced the concept of functions as maps. He proved for the first time that continuous functions have primitive functions. The proof itself is important, but the recognition that a proof is needed was novel and more important. His course is almost the same as we teach now in the introductory calculus courses (for example, ϵ-δ).[63]

[62] See also B. Belhost, *Augustin-Louis Cauchy, a biography* (Springer, 1991).

[63] It is a famous story that Lagrange hurried home, and checked his celestial mechanics book, when Cauchy published his work on convergence in 1820, which he started around 1814, but after 1818 when he knew Fourier's work (→**3.4**) he was convinced that his program to rationalize calculus was meaningful.

He tried to unify methods to calculate definite integrals in 1825 (14 years after Gauss's letter to Bessel revealing Gauss' full knowledge of complex analysis.). Even in the proof of the residue theorem, Cauchy did not denote complex numbers with single letters, but always wrote in the two real number form, $x + iy$. Although this paper of 1825 is now regarded as the historic starting point of complex function theory, Cauchy did not recognize so at least for a very long time, because his main purpose was to unify and streamline the methods of calculating definite integrals (→**8**) with the aid of the changing of the order of double integration used extensively by Laplace, Legendre, and others.

His life was quiet until the July Revolution of 1830. He refused to take the oath of allegiance to the new king who replaced a Bourbon king, and went into a self-imposed exile of 8 years. In 1832 he realized the relation between complex analysis and power series. Especially, he realized the relation between the radius of convergence and the singularity (published in 1837). Now, there was a chance to relate his integration theory and the Taylor expansion theory, but it took for him for about 20 years to clearly recognize as a mathematical object 'analytic function.'

He returned to Paris in 1838 to resume his work at the Academy. In 1851, he introduced the concept of differentiability (strong differentiability in our terminology →**1.4**), which was Riemann's starting point in his thesis (1851) (→**3.23**).

Devoutly catholic, he was a social worker in the town of Sceaux (his house is still there on the corner next to Mary-Curie High School), and occasionally criticized scientists for research that he considered dangerous to religion – he was absolutely correct in this respect, because institutionalized religions and science cannot be compatible in a conscientious and at the same time intelligent person. Cauchy published 789 papers, and died in 1857.

Cauchy provided the first phase of rigorous foundation of calculus. He also gave an important contribution to group theory.

4.10 Lipschitz condition. Let $\boldsymbol{v}$ be a continuous vector function whose domain is a region $D \subset \boldsymbol{R}^n$. For any compact[64] set $K \subset D$, if for any $\boldsymbol{y}_1$ and $\boldsymbol{y}_2$ both in K there is a positive constant L_K (which is usually dependent on K) such that

$$|\boldsymbol{v}(\boldsymbol{y}_1) - \boldsymbol{v}(\boldsymbol{y}_2)| \leq L_K |\boldsymbol{y}_1 - \boldsymbol{y}_2|, \tag{4.26}$$

then $\boldsymbol{v}$ is said to satisfy a *Lipschitz condition* on D.
If a vector field is C^1, then it is Lipshitz.

Discussion.

[64] 'Compact' means in a finite dimensional space 'closed and bounded'.

(A) [**Hölder continuity**].
If a function f satisfies

$$|f(x) - f(y)| \le L|x - y|^{\alpha} \tag{4.27}$$

on its domain for constants L and $\alpha \in (0, 1)$, f is said to be *Hölder continuous* of order α. In particular, if $\alpha = 1$, f is said to be *Lipschitz continuous*. A C^1 function is Lipschitz continuous due to the mean value theorem.
(B) **Cantor set and Cantor function (devil's staircase)**. Let $x \in [0, 1]$ be written as

$$x = \sum_{n=1}^{\infty} \frac{a_n}{3^n}, \tag{4.28}$$

where $a_n \in \{0, 1, 2\}$. The function f is defined as follows:
(a) If $a_1, \cdots, a_{r-1}$ are not 1, but $a_r = 1$

$$f(x) = \sum_{n=1}^{r-1} \frac{a_n}{2^{n+1}} + \frac{1}{2^n}. \tag{4.29}$$

(b) Otherwise

$$f(x) = \sum_{n=1}^{\infty} \frac{a_n}{2^{n+1}}. \tag{4.30}$$

That is, $f(x)$ has the binary expansion $a_1/2 \cdots a_n/2$ ($a_i = 0$ or 2).
Sketch the function.

The function increases on the classical Cantor (→**10.23**) set:[65]

$$C \equiv \left\{ x = \sum_{n=1}^{\infty} \frac{a_n}{3^n} \middle| \, a_n \in \{0, 2\} \right\}. \tag{4.31}$$

(3) The Cantor function is Hölder continuous (see (A) above) of order $\log 2/\log 3$.
(4) What is the total length of C?
(5) Is C countable or uncountable? Is $[0, 1]\backslash C$ countable or uncountable? (→**10.22**(4)).

[65] More generally, a perfect (that is, there is no isolated point) nowhere dense set is called a *Cantor set*.

4.11 Theorem [Cauchy-Lipschitz uniqueness theorem]. For (4.21), if $\boldsymbol{v}$ satisfies a Lipschitz condition on D, and if there is a solution passing through $\boldsymbol{y}_0 \in D$, it is unique. □

Discussion.
(A) **Why is the unique existence theorem important?** Physicists almost always ignore the existence theorem and the uniqueness theorem. However, they are very crucial even from the physics point of view. According to the Newton-Laplace determinacy (an empitrical fact), the motion of a point mass is completely determined by its initial position and velocity. Therefore, if the motion obeys a differential equation at all, it is easy to guess that the equation must be a second order equation. If we demand that there must be time reversal symmetry, we arrive at Newton's equation of motion (without the first order derivatives).[66] Is this guess really correct? If f is reasonable, yes. This affirmative answer is supplied by the unique existence theorem.
(B) Even if the Lipshitz condition is not satisfied: If the variables are separable as

$$\frac{dy}{dx} = \frac{Y(y)}{X(x)}, \tag{4.32}$$

and X and Y are continuous and not zero near (x_0, y_0), then the solution near this point is unique. However, the condition is important as we see in the next.

4.12 Importance of being more than continuous. If the initial condition is given at a critical point of the vector field (i.e., where $\boldsymbol{v} = 0$), then the solution need not be unique. However, if the vector field is differentiable, then uniqueness still holds in this case. Consider for some positive integer n the following equation with the initial condition $x = 0$:

$$\frac{dx}{dt} = x^{1-1/n}. \tag{4.33}$$

$x \equiv 0$ is obviously a solution, but this is not the unique solution (Find the other). However, if we consider $dx/dt = x$, then $x \equiv 0$ is the only solution.

Exercise.
Find all the solutions such that $x = 0$ at $t = 0$ for (4.33). [Hint. Infinitely many].

4.13 Continuous dependence on initial conditions. If the vector field is Lipschitz continuous (→**4.10**), then the solution at time t depends on the initial condition continuously.

[66] This is the way Arnold introduces Newton's equation of motion in his book, *Mathematical Methods of Classical Mechanics* (Springer, 1979).

4.14 Smooth dependence on parameter. If the vector field is smooth, then the solution at finite time is as smooth as the vector field. If the vector field is holomorphic, then the solution is also holomorphic. Then, we can use perturbation theory to obtain the solution in powers of the parameter. This was the idea of Poincaré.

4.B Elementary Solution Methods

4.15 Method of quadrature. To solve an ODE by a finite number of indefinite integrals is called the *method of quadrature*. Representative examples are given in this subsection. In practice, consult any elementary textbook of ODE or outline series.

4.16 Separation of variables. The first order equation of the following form

$$\frac{dy}{dx} = p(x)q(y), \tag{4.34}$$

where p and q are continuous functions, is solvable by the separation of variables: Let $Q(y)$ be a primitive function of $1/q(y)$ and P that of p. Then $Q(y) = P(x) + C$ is the general solution, where C is the integration constant (→**4.11** Discussion (A)).

Exercise.
Show that

$$\frac{dy}{dx} = f(ax + by + c) \tag{4.35}$$

can be separated with the new dependent variable $u = ax + by + c$.

4.17 Perfect differential equation. Consider the first order ODE of the following form

$$\frac{dy}{dx} = -\frac{P(x, y)}{Q(x, y)}, \tag{4.36}$$

where $Q \neq 0$. If there is a function Φ such that $\Phi_x = P$ and $\Phi_y = Q$, then (4.36) is equivalent to

$$d\Phi = \Phi_x dx + \Phi_y dy = 0, \tag{4.37}$$

so that $\Phi(x, y) = C$, C being the integral constant, is the general solution.

Exercise.

(A) Show that the separable case (→**4.16**) is a special case of perfect differential equations.
(B) Solve the following differential equation:
(1) $(x^2 + \log y)dx + \frac{x}{y}dy = 0$.
(2)

$$\frac{dy}{dx} = \frac{2 + ye^{xy}}{2y - xe^{xy}}.$$

4.18 Integrating factor. Even if P and Q may not have such a 'potential' Φ, P and Q times some common function factor $I(x, y)$ called *integrating factor* may have a 'potential' Ψ:

$$d\Psi = IPdx + IQdy. \tag{4.38}$$

Then $\Psi = C$, C being the integral constant, is the general solution to (4.36).

It is generally not easy to find an integrating factor. However, we can easily check whether there is an integrating factor dependent on x alone or y alone. In such cases we can explicitly construct an integrating factor.

A necessary and sufficient condition for (4.36) to have an integrating factor dependent only on x is that

$$\frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) \tag{4.39}$$

is a function of x alone. An integrating factor can be obtained in this case as

$$I(x) = \exp\left(\int_{x_0}^{x} \frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) dx\right). \tag{4.40}$$

Exercise.
(1) Guess a necessary and sufficient condtion for (4.36) to have an integraing factor depedent only on y, and demonstrate your guess.
(2) Show that

$$I(x) = \exp\left(\int_{x_0}^{x} p(s)ds\right) \tag{4.41}$$

is an integrating factor for (4.36) in **4.17**.

The existence problem of the integrating factor is crucial to thermodynamics. The second law, in essence, asserts that the heat form $\omega = dE - \sum x_i dX_i$, where E is the internal energy, X_i is an extensive variable, and x_i its conjugate intensive quantity, has an integrating factor called the absolute temperature (or its reciprocal).

Notice that if the number of independent variables (x and y in (4.36), E and X_i in thermodynamics) is two, then locally always intergrating factors do exist. See Discussion in (B) below.

Discussion.
(A) If there is one integrating factor, then there are infinitely many. Suppose λ is an integrating factor of $Pdx + Qdy$ such that $du = \lambda(Pdx + Qdy)$. Show that any $\mu = \lambda\psi(u)$, where $\psi(u)$ is any differentiable function of u, is an integrating factor.
(B) **Incompleteness of elementary exposition of thermodynamics**. Born[67] pointed out that

$$dQ = Xdx + Ydy \tag{4.42}$$

always has an integrating factor. His argument is as follows. $dQ = 0$ means

$$\frac{dy}{dx} = -\frac{X}{Y} \tag{4.43}$$

so that it has (at least locally) a solution $\varphi(x, y) = C$ (Notice that this integration is generally impossible, if there are more than two variables). Hence,

$$\varphi_x dx + \varphi_y dy = \left(\varphi_x - \varphi_y \frac{X}{Y}\right) dx = 0. \tag{4.44}$$

for any dx. This implies that $\varphi_x/\varphi_y = X/Y$, so that there must be an integrating factor.

This observation has a grave consequence on elementary exposition of thermodynamics, because if a system is described in terms of E and V (as is customarily done in the Carnot cycle), then we do not need the second law to assert that there is an integrating factor for the heat form $\omega = dE + pdV$. The elementary introduction is, if not incorrect, grossly incomplete. This was first recognized by Born and motivated Caratheodory to study the mathematical foundation of thermodynamics.
(C)Notice that the proposition that any 2 dimensional 1-form has an integrating factor is equivalent to the proposition that 2-dimensional space time is always conformally flat.
(D) Demonstrate that

$$dQ = -ydx + zdy + kdz, \tag{4.45}$$

where k is a constant, has no integrating factor.[Hint. This is related to a perfect differential.]

4.19 Homogeneous equation. The following type of ODE is called a *homogeneous equation*:

$$\frac{dy}{dx} = f\left(\frac{y}{x}\right). \tag{4.46}$$

[67] Read M. Born, Physik Z. **22**, 218, 249, 282 (1922), if you can read German. The lecturer recommends this review article to every serious (statistical) physicist.

If we introduce $w = y/x$, this reduces to the separable case **4.16**:

$$\frac{dw}{dx} = \frac{f(w) - w}{x}. \tag{4.47}$$

Exercise.
(1)

$$\frac{dy}{dx} = f\left(\frac{ax + by + c}{a'x + b'y + c'}\right) \tag{4.48}$$

can be converted to the homogeneous form ($a'b - ab' \neq 0$ is assumed). How can you do this? What happens if $a'b - ab' = 0$?
(2) Solve

$$\frac{dy}{dx} = \frac{y^4 + x^4}{xy^3}. \tag{4.49}$$

(3) Solve

$$\frac{dy}{dx} = \frac{x^2 + y^2}{xy} \tag{4.50}$$

4.20 Linear first order equation, variation of constants. The first order equation

$$\frac{dy}{dx} = p(x)y + q(x) \tag{4.51}$$

is called a *linear equation*. The equation can be solved by the method of variation of constants. Let

$$y(x) = C(x)e^{\int^x p(s)ds}. \tag{4.52}$$

Then, the equation for C can be integrated easily. As we will see in **4.28**, the method of variation of constants *always* works for linear equations (Lagrange's method).

Exercise. Solve

$$\frac{dy}{dx} = x(x + y). \tag{4.53}$$

4.21 Bernoulli equation. The first order equation of the following form is called a *Bernoulli equation*:

$$\frac{dy}{dx} = P(x)y + Q(x)y^n, \tag{4.54}$$

where n is a real number. Introducing the new variable $z(x) = y(x)^{1-n}$, we can reduce this equation to the case **4.20** for $z(x)$.

Exercise.
Solve
(1)

$$\frac{dy}{dx} + xy - xy^2 = 0. \tag{4.55}$$

(2)

$$\frac{dy}{dx} + y - y^{-2} = 0. \tag{4.56}$$

4.22 Riccati's equation. The first order equation of the following form is called a *Riccati's equation*:

$$\frac{dy}{dx} = R(x)y^2 + P(x)y + Q(x). \tag{4.57}$$

If $R = 0$, then it is linear (→**4.20**); if $Q = 0$, then it is a Bernoulli equation (→**4.21**). Otherwise, there is no general way to solve this equation by quadrature. However, if we know one solution $y = y_1(x)$ for this equation, the function $v(x) = y(x) - y_1(x)$ obeys the following Bernoulli equation,

$$\frac{dv}{dx} = [P(x) + 2R(x)y_1(x)]v(x) + R(x)u^2(x), \tag{4.58}$$

so we can obtain the general solution for (4.57) as $v + y_1$ in terms of the general solution v to this Bernoulli equation.

Exercise. Let $(x(t), y(t))$ be a parametric representation of a plane smooth curve (say, C^2). The differential equation $dp(t)/dt$, where $p(t)$ is the slope of the tangent(i.e., $p(t) = dy/dx$), has the form of Riccati' s equation. Demonstrate this claim and determine R, P and Q.
Discussion.[68]
Riccati discussed

$$\frac{dy}{dx} + ay^2 = bx^\alpha, \tag{4.59}$$

where a, b and α are constant. To avoid trivial cases, we assume all of them are non-zero. Liouville demonstrated that this equation can be solved in terms of elementray functions (trigonometric, exponetial, algebraic functions and their elementary combinations) only in the following cases:

[68] K Yosida,*Solution Methods for Differential Equations* , second ed. (Iwanami, 1978) p20–.

(i) $\alpha = -2$,
(ii) $\alpha = -4n/(2n-1)$ for $n = 1, 2, \cdots$.
(iii) $\alpha = -4n/(2n+1)$ for $n = 1, 2, \cdots$.

4.23 Second order ODE. This has the following form[69]

$$\frac{d^2y}{dx^2} = f\left(x, \frac{dy}{dx}\right). \tag{4.60}$$

If it is autonomous (→**4.6**), it can be reduced to a first order PDE by introducing $p = dy/dx$ as the new unknown function, and y as the independent variable:

$$p\frac{dp}{dy} = f(y, p). \tag{4.61}$$

If f does not depend on p, then this is **4.16**, so p can be obtained. The resultant solution is interpreted as the first order ODE for y

$$\frac{1}{2}\left(\frac{dy}{dx}\right)^2 = \int^y dz\, f(z) + const., \tag{4.62}$$

which is again separable. This is a well-known method to solve 1D autonomous classical mechanical system.

4.24 Method of reducing of order.

$$\frac{d^2y}{dx^2} + a(x)\frac{dy}{dx} + b(x)y = 0 \tag{4.63}$$

can be converted to Riccati's equation by introducing

$$z = \frac{1}{y}\frac{dy}{dx}. \tag{4.64}$$

The result is

$$\frac{dz}{dx} + z^2 + a(x)z + b(x) = 0. \tag{4.65}$$

This method is due to d'Alembert (→**1.13**) and is called the *method of lowering the order*. (4.64) is called *d'Alembert's transformation*. This technique allows us to reduce n-th order linear ODE to $n-1$-th order (generally nonlinear) ODE in general.

[69] We consider only the normal forms (→**4.4**).

4.25 Standard form of linear second order ODE. If $a = 0$ in (4.63), the equation is said to be in the *standard form*. If $a \neq 0$, then we introduce

$$z = y \exp\left(\frac{1}{2}\int^x a(x')dx'\right). \tag{4.66}$$

We have

$$\frac{d^2z}{dx^2} = -\left(b - \frac{a^2}{4} - \frac{a'(x)}{2}\right) z. \tag{4.67}$$

This form is a useful starting point for approximate solutions.

Discussion.
The following equation:

$$\mathcal{L}_{ST}u \equiv \left[\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] u = 0 \tag{4.68}$$

is called a Sturm-Liouville equation (→**8.4**), and

$$\frac{1}{w(x)}\mathcal{L}_{ST}u = \lambda u \tag{4.69}$$

with appropriate boundary conditions is called a Sturm-Liouville eigenvalue problem (→**XX**). Any second order linear ODE can be converted to the Sturm-Liouville form.
(1) Demonstrate that

$$p_2(x)\frac{d^2u}{dx^2} + p_1(x)\frac{du}{dx} + p_0(x)u - \lambda u = 0 \tag{4.70}$$

can be converted to the Sturm-Liouville form with the following relations

$$w(x) = \frac{1}{p_2(x)} \exp\left[\int^x \frac{p_1(t)}{p_2(t)}dt\right], \tag{4.71}$$

$$p(x) = w(x)p_2(x), \tag{4.72}$$

$$q(x) = w(x)p_0(x). \tag{4.73}$$

(2) Convert Bessel's equation (→(1.18)) to the Sturm-Liouville form:

$$\frac{d}{dx}\left(x\frac{du}{dx}\right) + \left(1 - \frac{m^2}{x^2}\right) u = 0. \tag{4.74}$$

(3) By the following *Liouville transformation*

$$u(x) = v(t)[p(x)w(x)]^{-1/4} \tag{4.75}$$

with

$$t = \int^x \sqrt{\frac{w(s)}{p(s)}}ds \tag{4.76}$$

the above Sturm-Liouville equation can be converted to the Schrödinger form:

$$-\frac{d^2v}{dt^2} + V(t)v = \lambda v, \tag{4.77}$$

where the potential is given by[70]

$$V(t) = \frac{q(x)}{w(x)} + [p(x)w(x)]^{-1/4}\frac{d^2}{dt^2}[p(x)w(x)]^{1/4}. \tag{4.78}$$

In this formula x is understood as the function of t as defined by (4.76). This form is a good starting point to study asymptotic behaviors of the solutions.
(4) Convert Bessel's equation into the Schrödinger form:

$$\frac{d^2v}{dt^2} + \left[k^2 - \frac{m^2 - 1/4}{t^2}\right] v = 0. \tag{4.79}$$

Compare this result with (4.67).

4.26 Linear second order ODE with constant coefficients. Consider

$$\frac{d^2y}{dx^2} + a\frac{dy}{dx} + by = 0, \tag{4.80}$$

where a and b are constants.

$$P(\lambda) = \lambda^2 + a\lambda + b \tag{4.81}$$

is called its *characteristic polynomial*, and its roots are called *characteristic roots*. We will discuss the general theory in the next section (→**5.5**), but in this simple second order case the general conclusion is the following:

4.27 Theorem [General solution to (4.80)]. If the characteristic roots of (4.80) are α and β ($\neq \alpha$), then its general solution is the linear combination of $\varphi_1(x) = e^{\alpha x}$ and $\varphi_2(x) = e^{\beta x}$. If $\alpha = \beta$, then the general solution is the linear combination of $\varphi_1(x) = e^{\alpha x}$ and $\varphi_2(x) = xe^{\alpha x}$ (the characteristic roots need not be real.) □
$\varphi_1(x)$ and $\varphi_2(x)$ are called *fundamental solutions* and $\{\varphi_1(x), \varphi_2(x)\}$ is called a *system of fundamental solutions* for (4.80). A set of solutions is a fundamental system, if it spans (is a basis set of) the totality of the solution set of the ODE. See **XX** for more general statements.

Exercise.

[70] d/dt in the following formula acts only in $V(t)$; it is NOT an operator acting even outside the formula.

Study the qualitative behavior of the following equation when the (bifurcation parameter) ϵ changes its sign:

$$\frac{d^2x}{dt^2} + 2\epsilon\frac{dx}{dt} + \omega^2 x = 0. \tag{4.82}$$

4.28 Inhomogeneous equation, Lagrange's method of variation of constants. An ODE

$$\frac{d^2y}{dx^2} + a\frac{dy}{dx} + by = f(x) \tag{4.83}$$

with nonzero f is called an *inhomogeneous* ODE (the one without f is called a *homogeneous* equation). The general solution is given by the sum of the general solution to the corresponding homogeneous equation and one particular solution to the inhomogeneous problem. A method to find a particular solution to (4.83) is *Lagrange's method of variation of constants*. Let $\varphi_i(x)$ be the fundamental solutions. We determine the functions $C_i(x)$ to satisfy (4.83):

$$u(x) = C_1(x)\varphi_1(x) + C_2(x)\varphi_2(x). \tag{4.84}$$

One solution can be obtained from

$$\frac{dC_1}{dx} = -\frac{f(x)\varphi_2(x)}{W(x)}, \quad \frac{dC_2}{dx} = \frac{f(x)\varphi_1(x)}{W(x)}, \tag{4.85}$$

where $W(x) = \varphi_1(x)\varphi_2'(x) - \varphi_2(x)\varphi_1'(x)$, the Wronskian (→**??**) of the fundamental system $\{\varphi_1, \varphi_2\}$. □
If the two characteristic roots (→**4.26**) α and β are distinct, then such a u is given by

$$u(x) = \frac{1}{\alpha - \beta}\left(\int_0^t ds f(s)e^{\alpha(t-s)} - \int_0^t ds f(s)e^{\beta(t-s)}\right). \tag{4.86}$$

Lagrange's method can be generalized to n-th order linear ODEs.

Discussion
Consider the relation of Lagrange's method and Green's function (→**X15**). Riemann introduced Green's functions to solve linear ODE, so it is often called Riemann's function as well.

Exercise.
Solve
(1)

$$\frac{d^2y}{dt^2} - 2\frac{dy}{dt} + 2y = \sin t. \tag{4.87}$$

(2)

$$\frac{d^2x}{dt^2} + 4x = \cos^2 2t, \tag{4.88}$$

(3)

$$\frac{d^2x}{dt^2} + x = \sin t. \tag{4.89}$$

4.29 Equidimensional equation: invariance under scaling. If an ODE is invariant under the scaling of the independent variable $x \to ax$, then we call the equation an *equidimensional equation* (in x). Explicit appearance of x in the equation can be removed by introducing $t = \ln x$ as the new independent variable. That is, the equation becomes an autonomous equation (→**4.6**) in t (→**4.30** Discussion).

If the equation is linear, then the general solution is given by the linear combination of the power of x, whose exponent can be determined by introducing x^μ (this is understood as $\log x$ if $\mu = 0$) into the equation. For example, the general solution to

$$\frac{d^2}{dr^2} rR = \frac{R}{r}\ell(1+\ell) \tag{4.90}$$

is given by $R(r) = Ar^\ell + Br^{-\ell-1}$. The equation appears when we separate the variable of the Laplace equation (or, e.g., the Schrödinger equation in spherical infinite potential well) in the spherical coordinates (→**??**).

Exercise.
Show that the following Euler's differential equation

$$x^n \frac{d^n y}{dx^n} + a_1 x^{n-1} \frac{d^{n-1} y}{dx^{n-1}} + \cdots + a_n y = 0 \tag{4.91}$$

can be transformed to a constant coefficient linear ODE with the introduction of new independent variable t as $x = e^t$.

4.30 Scale invariant equation. If an ODE is invariant under the scaling $x \to ax$ and $y \to a^p y$ for some p, we call the equation *scale invariant*. In this case, $v \equiv y/x^p$ obeys an equidimensional ODE, so that we can use the trick in **4.29**.

Discussion.
The following equation is called the *Thomas-Fermi equation*

$$\frac{d^2\varphi}{dx^2} = \frac{1}{\sqrt{x}}\varphi^{3/2}. \tag{4.92}$$

This is a scale invariant equation under $x \to ax$ and $\varphi \to a^{-3}\varphi$. In the physical situation, the equation is solved under the boundary condition $\varphi(0) = 1$ and $\lim_{x\to\infty} \varphi(x) = 0$, so that such a simple scaling invariance does not hold. Still, if one wishes to get an asymptotic form for large x, this should be a good strategy.
(1) Show that in this asymptotic limit

$$\varphi(x) \simeq \frac{144}{x^3} \tag{4.93}$$

is a reasonable approximation.
(2) To obtain the correction to this solution, let us write

$$\varphi(x) = \frac{144}{x^3} + \psi, \tag{4.94}$$

and solve the equation to first order in ψ. The equation for ψ to this order becomes

$$\frac{d^2\psi}{dx^2} = \frac{18}{x^2}\psi, \tag{4.95}$$

(3) This is an equidimensional equation (→**??**), so we can obtain the solution in the power form. The result is

$$\psi \propto x^{-\beta} \tag{4.96}$$

with $\beta = (-1 + \sqrt{73})/2 \simeq 3.77$. If we obey the instruction above, we introduce $t = \ln x$ to convert the equation into

$$\left(\frac{d^2}{dt^2} - \frac{d}{dt}\right)\psi = 18\psi. \tag{4.97}$$

This is easy to solve (→**5.5**(A))).
(4) In this case the following amazing solution can be constructed. Using both the asymptotic solution and the correction we computed, we can construct

$$\varphi = \frac{144}{x^3(1 + Cx^{-0.77})^n}, \tag{4.98}$$

where C and n are adjustable parameters. To make $\varphi(0)$ finite, we must choose $3 - 0.77n = 0$ or $n = 3.9$. Now, we can impose the boundary condition at 0. $C = 144^{0.77/3}$. Hence,

$$\varphi(x) = \left[1 + \left(\frac{x}{12^{2/3}}\right)^{0.77}\right]^{-3.90}. \tag{4.99}$$

According to Migdal, this solution agrees well with the numerical result.

4.31 Clairaut's differential equation. The following differential equation is called *Clairaut's differential equation*

$$y = px + f(p), \tag{4.100}$$

where $p = dy/dx$ and f is a C^1-function. Its general solution is

$$y = Cx + f(C), \tag{4.101}$$

where C is a constant. The equation has a singular solution (→**4.3**), which is the envelop curve of (4.101).
Let us assume that (4.100) has a solution $y = y(x)$ which is not exhausted by (4.101). Put this in (4.100), and differentiate it with x. We obtain

$$\frac{dp}{dx}\left(x + \frac{df(p)}{dp}\right) = 0. \tag{4.102}$$

This implies $p = C$, or

$$x + \frac{df(p)}{dp} = 0. \tag{4.103}$$

This is the equation obtained from the derivative of (4.101) with respect to C and (4.100).

Exercise.
Solve

$$y = px + p - p^2. \tag{4.104}$$

5 Constant Coefficient Linear ODE

A practical method is outlined to solve constant coefficient linear ODE explicitly (constructively). A method to analyze the stability of a fixed point is also explained. A useful theorem to locate eigenvalues of a matrix is Gershgorin's theorem.

Key words: Exponential of matrix, stability, hyperbolic fixed point, Hartman-Grobman theorem, Gershgorin's theorem.

Summary
(1) Practice calculating e^A when A is not diagonalizable (**5.2**, **5.5**).
(2) Linear stability analysis: the stability around a hyperbolic fixed point is completely determined by the linearized equation (**5.8**-**5.10**).
(3) There is a useful theorem to restrict the locations of eigenvalues of a (complex) square matrix on the complex plane (Gershgorin's theorem) (**5.10**).

5.1 General form. n-th order ODE with constant coefficients can always be written in the form (→**4.4**-**4.6**)

$$\frac{d\boldsymbol{u}}{dx} = A\boldsymbol{u}, \tag{5.1}$$

where A is a $n\times n$ constant matrix, and $\boldsymbol{u}$ consists of $u, u_1 \equiv du/dx, u_2 \equiv d^2u/dx^2, \cdots, u_{n-1} \equiv d^{n-1}u/dx^{n-1}$. We have only to solve the constant coefficient first order equation (5.1). For non-constant coefficient cases, see **X**.

5.2 Exponential function of matrix. Consider the following formal series

$$f(t) = 1 + At + \frac{1}{2!}A^2t^2 + \frac{1}{3!}A^3t^3 + \cdots + \frac{1}{n!}A^nt^n + \cdots, \tag{5.2}$$

where 1 is the $n \times n$ unit matrix. If this series is truncated at some finite order, the result should be an $n \times n$ matrix. We say the series converges if $f(t)$ applied to any finite vector $\boldsymbol{v}$ converges.[71] We define the *norm* of the matrix by

$$\|A\| \equiv \sup_{\boldsymbol{v}} |A\boldsymbol{v}|/|\boldsymbol{v}|. \tag{5.3}$$

[71] This is equivalent to the componentwise convergence of the matrix series.

We can obtain

$$\|f(t)\| \leq \exp(\|A\|t). \tag{5.4}$$

Hence, if the components of A are finite, then the series is absolutely convergent and consequently $f(t)$ is well defined.[72] The series is also uniformly (in t) convergent. Therefore, we may termwisely differentiate it to get a matrix relation

$$\frac{df(t)}{dt} = Af(t). \tag{5.5}$$

Hence, $f(t)$ is written as $f(t) = e^{tA}$ ($f(0) = I$ is the initial condition, where I is the unit matrix).

5.3 General solution to (5.1). The general solution to (5.1) is

$$\boldsymbol{u}(t) = e^{tA}\boldsymbol{u}_0, \tag{5.6}$$

where $\boldsymbol{u}_0$ is a constant n-vector (the initial condition vector). For an orthonormal basis $\{\boldsymbol{e}_1, \cdots, \boldsymbol{e}_n\}$, $\{e^{At}\boldsymbol{e}_1, \cdots, e^{At}\boldsymbol{e}_n\}$ is a fundamental system of solutions of (5.1). Since e^{At} is nonsingular for any A, the dimension of the space spanned by the initial data and that of the solutions at any time t are identical. That is, $\boldsymbol{u}(0)$ and $\boldsymbol{u}(t)$ are one-to-one correspondent. Theoretically, the formal solution may be enough, but we must be able to calculate the matrix e^{tA} explicitly.

5.4 Diagonalizable cases. Since our equation is linear, *complexification* is always helpful. That is, we interpret the equation to be on $\boldsymbol{C}^n$ instead of $\boldsymbol{R}^n$, and take the real part of the solution to obtain the real solution to the original problem. If the matrix A is normal (i.e., $A^*A = AA^*$), then A is diagonalizable by a similarity transformation.[73] In this case there is a unitary matrix U such that $U^*AU = \Lambda$, which is a diagonal matrix $\lambda_1 \oplus \lambda_2 \oplus \cdots \oplus \lambda_n$. It is easy to demonstrate (return to the definitioin **5.2**) that

$$U^*e^{tA}U = e^{\Lambda t}. \tag{5.7}$$

Therefore, the general solution[74] to (5.1) reads

$$\boldsymbol{u}(t) = c_1\boldsymbol{p}_1e^{\lambda_1 t} + c_2\boldsymbol{p}_2e^{\lambda_2 t} + \cdots + c_n\boldsymbol{p}_ne^{\lambda_n t}, \tag{5.8}$$

[72] If we interpret $|\boldsymbol{v}|$ to be the ordinary Euclidean length, then the norm defined here is equal to the maximum of the square root of the eigenvalues of A^*A.

[73] This is only true in general when the vector space is considered on the field $\boldsymbol{C}$. This is why we need complexification.

[74] Here, 'general' means that a solution from any initial data can be obtained.

where c_i are arbitrary constants and $\boldsymbol{p}_i$ is a normalized eigenvector belonging to the eigenvalue λ_i (here all the eigenvalues are multiply taken into account according to their multiplicity). This should be obvious from (5.6), (5.7) and the structure of the unitary matrix $U = (\boldsymbol{p}_1, \boldsymbol{p}_2, \cdots, \boldsymbol{p}_n)$, if we interpret $\boldsymbol{p}_i$ to be column vectors.
If the matrix cannot be diagonalized by a similarity transformation, then polynomials of t appears in place of constants. All the cases including this nondiagonalizable case can be solved constructively[75] as follows:

5.5 Practical procedure.
(A) In the above the most general approach is described to solve (5.1). To solve a constant coefficient n-th order linear ODE

$$a_n \frac{d^n u}{dt^n} + a_{n-1} \frac{d^{n-1} u}{dt^{n-1}} + \cdots + a_1 \frac{du}{dt} + a_0 u = 0, \tag{5.9}$$

we need not consider the general matrix, but a very special form which can be guessed from **4.5**. Let its characteristic roots, i.e., the roots of

$$a_n \lambda^n + a_{n-1} \lambda^{n-1} + \cdots + a_1 \lambda + a_0 = 0, \tag{5.10}$$

be $\lambda_1, \cdots, \lambda_r$ with the multiplicity $m_1, \cdots, m_r$, respectively. Then, the general solution for (5.9) is given by a linear combination of

$$\{e^{\lambda_1 t}, te^{\lambda_1 t}, \cdots, t^{m_1 - 1} e^{\lambda_1 t}, e^{\lambda_2 t}, \cdots, t^{m_2 - 1} e^{\lambda_2 t}, \cdots, t^{m_r - 1} e^{\lambda_r t}\}. \tag{5.11}$$

A set of solutions which can span the totality of the solution space of an ODE is called its *fundamental system of solutions*. (5.11) is a fundamental system for (5.9).
(B) A general procedure to compute e^{tA} is as follows:
(1) Find the characteristic polynomial $f(x) = det(xI - A)$, and eigenvalues (the zeros of f). Let

$$f(x) = (x - \lambda_1)^{\mu_1} (x - \lambda_2)^{\mu_2} \cdots (x - \lambda_k)^{\mu_k} \tag{5.12}$$

(2) Compute the partial fraction expansion

$$\frac{1}{f(x)} = \frac{g_1(x)}{(x - \lambda_1)^{\mu_1}} + \frac{g_2(x)}{(x - \lambda_2)^{\mu_2}} + \cdots + \frac{g_k(x)}{(x - \lambda_k)^{\mu_k}}. \tag{5.13}$$

(3) Compute

$$f_j(x) \rightleftharpoons f(x)/(x - \lambda_j)^{\mu_j}. \tag{5.14}$$

[75] 'Constructive' means that an explicit procedure to obtain a solution is given.

Then make the following matrix (this is a projection operator →**??**)

$$P_j = f_j(A)g_j(A). \tag{5.15}$$

(4) e^{At} is given by

$$e^{At} = e^{At}(P_1 + P_2 + \cdots + P_k). \tag{5.16}$$

Each term can be computed as follows:

$$\begin{aligned} e^{At}P_j &= e^{\lambda_j t}e^{(A-\lambda_j I)t}P_j, & (5.17)\\ &= e^{\lambda_j t}\sum_{m=0}^{\nu_j-1}\frac{t^m}{m!}(A-\lambda_j I)^m P_j. & (5.18) \end{aligned}$$

In this calculation, we need not actually know what ν_j are. Simply calculate (5.18) until one gets the vanishing factor. Notice that ν_j does not exceed the multiplicity μ_j.[76]

A theoretical explanation why this procedure works is given in Appendix **8A**.[77]

Exercise.
(A) Solve the following linear ODEs:
(1)

$$\frac{d\boldsymbol{u}}{dt} = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}\boldsymbol{u}. \tag{5.19}$$

(2)

$$\frac{d\boldsymbol{u}}{dt} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}\boldsymbol{u}. \tag{5.20}$$

(3)

$$\frac{d\boldsymbol{u}}{dt} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & -2 & -5 \\ 0 & 1 & 2 \end{pmatrix}\boldsymbol{u}. \tag{5.21}$$

In this case the matrix can be diagonalized, but still the general method is useful.
(B) Construct the projection operators for eigenspaces of the following matrices

$$A = \begin{pmatrix} 1 & 9 \\ 1 & 1 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & -1 & 2 \end{pmatrix}. \tag{5.22}$$

[76] μ_j is the usual multiplicity (=algebraic multiplicity) of the eigenvalue λ_j. The number of eigenvectors (i.e., the dimension of the eigenspace for λ_j) need not be the same as μ_j. This dimension is the number ν_j.

[77] Y. Takahashi, *Dynamical systems and differential equation* (Iwanami, 1996) Section 2.3 contains a complete proof.

5.6 Inhomogeneous case. The general solution to the following inhomogeneous equation

$$\frac{d\boldsymbol{u}}{dx} = A\boldsymbol{u} + \boldsymbol{f} \tag{5.23}$$

is given by (use the method of variation of constants →**4.20**, **4.28**)

$$\boldsymbol{u}(x) = e^{xA}\boldsymbol{u}_0 + \int_0^x e^{(x-y)A}\boldsymbol{f}(y)dy. \tag{5.24}$$

This has the usual form (→**4.28**): sum of the general solution to the homogeneous equation (the first term) and a special solution for the inhomogeneous equation (the second term).

The equation of motion of a charged particle whose charge-mass ratio is unity may be written as

$$\frac{d\boldsymbol{v}}{ddt} = \boldsymbol{v} \times \boldsymbol{B} + \boldsymbol{E}, \tag{5.25}$$

where B is the magnetic field and E is the electric field (the first term is the Lorentz force).

(1) Rewrite this equation in the form of (5.23).

(2) Solve the eqution.

(3) What is the trajectory of the particle? Sketch it.

5.7 Stability question of fixed point. Suppose we have a vector ODE

$$\frac{d\boldsymbol{x}}{dt} = \boldsymbol{v}(\boldsymbol{x}) \tag{5.26}$$

for which $\boldsymbol{x} = 0$ is a fixed point (i.e., $\boldsymbol{v}(0) = 0$). An important question is whether this solution is stable or not. That is, if we perturb the solution slightly $0 \to \delta\boldsymbol{x}$, does $|\delta\boldsymbol{x}|$ grow in time? If yes, then the solution cannot be stable. On the other hand, if this quantity goes to zero eventually for any small displacement, we may conclude that the fixed point is stable. The following theorem is a fundamental theorem (stated for the present case):

5.8 Theorem [Hartman-Grobman]. If 0 is a *hyperbolic fixed point*, that is, $d\boldsymbol{v}/d\boldsymbol{x}$ at $\boldsymbol{x} = 0$ does not have any pure imaginary eigenvalue, then for sufficiently small neighborhood of 0 the orbits of (5.26) and those of

$$\frac{d\boldsymbol{x}}{dt} = A\boldsymbol{x}, \tag{5.27}$$

where $A = d\boldsymbol{v}/d\boldsymbol{x}|_{\boldsymbol{x}=0}$, can be related one to one.[78] In particular, the stability (or instability) of 0 for (5.26) is equivalent to the stability (or instability) of 0 for (5.27).

5.9 Stability analysis of fixed point. **5.8** tells us that the stability of the fixed point of (5.26) is completely determined by the eigenvalues of the derivative $d\boldsymbol{v}/d\boldsymbol{x}$ evaluated at the fixed point, (if the fixed point is hyperbolic; if not, we must pay attention to the higher order terms; that is, linearization is not enough). If there is no eigenvalue whose real part is non-negative, then the fixed point is *linearly stable*. Thus the linear stability problem boils down to the eigenvalue problem. Sometimes the following theorem **5.10** is useful, which can give some information about the location of the eigenvalues on the complex plain.[79]

Discussion [Logical sloppiness].
Let

$$\frac{d\boldsymbol{x}}{dt} = A\boldsymbol{x} + g(\boldsymbol{x}),$$

where A is a constant matrix whose eigenvalues are all on the left half complex plane, and $g(0) = 0$, and $\|g(\boldsymbol{x})\| \leq C\|\boldsymbol{x}\|$ for some positive constant C. Then, there is a positive number δ such that

$$\|\boldsymbol{x}(0)\| < \delta \Rightarrow \lim_{t\to\infty} \boldsymbol{x}(t) = 0.$$

Its proof is not very trivial.[80]
Physicists often argue as follows. "Linearize the equation around the point of interest and make an equation for the small displacement δx. Since we find it shrinks to zero, we conclude that the point is stable." The reader might think what all the fuss is about of the above proof. What we must demonstrate is that if the displacement is small initially, then linearization is OK for all $t > 0$. If the reader assumes this, then the argument is perfectly all right, but the argument sounds almost circular.

Exercise.
(1) Find the fixed point (equilibrium point) of

$$\frac{dx}{dt} = x - xy, \tag{5.28}$$

$$\frac{dy}{dt} = -y + xy. \tag{5.29}$$

[78] More precisely, the orbits are homeomorphic. That is, there is a continuous map which maps any orbit of (5.26) to that of (5.27) one to one continuously (but not generally diffeomorphic) in both ways.

[79] For the stability only, we do not need such a strong theorem as the Hartman-Grobman theorem as can be seen in Takahashi, ibid., Section 4.2. However, practically to remember the Hartman-Gromman-theorem is useful.

[80] See Takahashi, ibid., p110-111.

Show that the fixed point is not hyperbolic. Change the local coordinates around the fixed point to the polar coordinates, and demonstrate that the point is actually stable (i.e., the perturbation does not grow indefinitely).
(2) Study the stability of the origin of the following Lorenz equation.[81]

$$\dot{x} = -10(x-y), \tag{5.30}$$
$$\dot{y} = rx - y - xz, \tag{5.31}$$
$$\dot{z} = -\frac{8}{3}z + xy. \tag{5.32}$$

Here r is a positive bifurcation parameter which controls the behavior of the system.
(3) Demonstrate that $x = 0$ is a stable solution (stable fixed point) of

$$\frac{dx}{dt} = Ax, \tag{5.33}$$

where

$$A = \begin{pmatrix} -1 & 0 & 1/2 & -1/3 \\ 1/4 & -1/2 & 1/5 & 0 \\ 1/4 & 0 & -1 & 1/2 \\ 1/4 & 1/3 & 4 & -5 \end{pmatrix}. \tag{5.34}$$

5.10 Gershgorin's theorem. Let $A = Matr\{a_{ij}\}$ be an $n \times n$ complex matrix. Its eigenvalues are all in the union $D = \cup_{i=1}^{n} C_i$, where C_i are discs called Gershgorin's disks:

$$C_i \equiv \{z \in \boldsymbol{C} | \, |z - a_{ii}| \leq \sum_{j \neq i} |a_{ij}|\} \tag{5.35}$$

for $i = 1, \cdots, n$ (here no summation convention). The number of eigenvalues contained in each connected component of D is equal to the number of disks making each connected component. □
Remark. Since the eigenvalues of A and its transposition A^T are identical, you can apply the theorem to columns. However, you cannot mix both. That is, if you decide to use raws, then you must use summation over j's in (5.35).
[Demo] Let λ be an eigenvalue of A and $\boldsymbol{x} = (x_1, \cdots, x_n)^T$ a corresponding eigenvector. We have

$$\sum_{j=1}^{n} a_{ij} x_j = \lambda x_i, \quad (i = 1, \cdots, n). \tag{5.36}$$

Since $\boldsymbol{x} \neq 0$, there must be x_k such that $|x_k| = \max_i |x_i| \neq 0$. For $i = k$ (5.36) reads

$$(\lambda - a_{kk}) x_k = \sum_{j \neq k} a_{kj} x_j. \tag{5.37}$$

[81] See, for example, E. A. Jackson, *Perspective of Nonlinear Dynamics*, vol.2 Sections 7.3-5. M. Viana, "What's new on Lorenz strange attractors?", *Math Intelligencer*, **22**(3) 6 (2000).

In other words,

$$|\lambda - a_{kk}| \leq \sum_{j \neq k} |a_{kj}| \frac{|x_j|}{|x_k|} \leq \sum_{j \neq k} |a_{kj}| = r_k. \tag{5.38}$$

This implies that $\lambda \in C_k$ which is obviously in D.

To prove the last part, we note the fact that the eigenvalues are continuously dependent on the matrix components. Let us split A into its diagonal part A_D and the off-diagonal part A_0: $A = A_D + A_O$. We make $A(t) = A_D + tA_O$. The second part of the theorem is trivially true for $A(0)$. The Gershgorin disks $C_i(t)$ for $A(t)$ depends on t continuously. The eigenvalues of $A(t)$ is also continuous functions of t. Hence, for any t (particularly for $t = 1$) the theorem must be true.

Discussion.
Study the trajectories of the eigenvalues of the following matrix $A(t)$ for $t \in [0, 1]$, and discuss their relation with the Gershgorin disks:[82]

$$A(t) = \begin{pmatrix} 0 & 3t \\ -7t & 8 \end{pmatrix}. \tag{5.39}$$

Notice that the eigenvalues do not move under the similarity transformation, but the matrix elements are altered, so that the estimate can be made better or worse with an application of a similarity transformation before applying the theorem. See the next example.

5.11 Application of Gershgorin's theorem.[83] Find the location of the eigenvalues of A.

$$A = \begin{pmatrix} 1 & \epsilon & 0 \\ \epsilon & 2 & \epsilon \\ 0 & \epsilon & 3 \end{pmatrix}. \tag{5.40}$$

If we apply the similarity transformation $A \to D^{-1}AD$, where

$$D = \begin{pmatrix} 1/4 & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{pmatrix}, \tag{5.41}$$

then the eigenvalue close to 1 can be located within the order of ϵ^2 instead of ϵ. This demonstrates the usefulness of similarity transformations applied before the estimation. It is not hard to find similar transformations allowing us to estimate the other eigenvalues with the same order of accuracy.

[82] Iri 1995

[83] From M. Iri, *Linear Algebra II* (Iwanami, 1994) p218. This is the best linear algebra textbook currently available, but in Japanese.

5.12 Linear difference equation. Our knowledge about linear ODE allows us to guess the following theorem:
Theorem Any solution of the following constant (complex) coefficient linear difference equation (of order p)

$$x_{n+p} + c_1 x_{n+p-1} + \cdots + c_p x_n = 0 \tag{5.42}$$

has the following form

$$u_n = \sum_{j=1}^{k} \sum_{m=0}^{m_j - 1} C_{j,m} n^m \lambda_j^n, \tag{5.43}$$

where $C_{j,m}$ ($j = 1, 2, \cdots, k$ and $m = 1, \cdots, m_{j-1}$) are complex constants, and λ_j is the m_j-tuple zero of the *characteristic polynomial* of the difference equation:

$$P(z) = z^p + c_1 z^{p-1} + \cdots + c_p. \tag{5.44}$$

□
The coefficients are determined by the auxiliary conditions such as the boundary conditions. See the following examples.

Examples
(1) Fibonacci sequence.

$$x_{n+1} = x_n + x_{n-1} \tag{5.45}$$

with $x_0 = x_1 = 1$ determines the Fibonacci sequence, 1, 1, 2, 3, 5, 8, 13, $\cdots$. The general solution to (5.45) is given by

$$x_n = C_1 \left(\frac{1+\sqrt{5}}{2} \right)^n + C_2 \left(\frac{1-\sqrt{5}}{2} \right)^n. \tag{5.46}$$

Therefore, the Fibonacci sequence has the following general term

$$x_n = \frac{5+\sqrt{5}}{10} \left(\frac{1+\sqrt{5}}{2} \right)^n + \frac{5-\sqrt{5}}{10} \left(\frac{1-\sqrt{5}}{2} \right)^n. \tag{5.47}$$

(It is interesting to notice that to describe integer sequences we need irrational numbers.)
(2) Polyenes in the Hückel molecular orbital approximation. Suppose a chain or a ring of carbon atoms is made (through the so-called σ- bonds), and on this chain is a single extra electron. Let the probability amplitude of the wave function of this electron at the j-th carbon be c_j. Then, the energy E of this wave function is given by the following discrete version of the Schrödinger equation:

$$\beta c_{i+1} + \alpha c_i + \beta c_{i-1} = E c_i. \tag{5.48}$$

(Here β, which is usually negative, is called the overlap integral describing how easily an electron can jump from one carbon atom to its neighboring carbon atoms; α is

called the Coulomb integral describing how strongly an atom attracts an electron.) It is convenient to rewrite the equation with the aid of its linearity as

$$c_{i+1} + xc_i + c_{i-1} = 0, \tag{5.49}$$

where $x = (\alpha - E)/\beta$.
(i) Linear polyene. If the carbon chain consisting of N carbons is linear, then we can use (5.49) for $i = 1, \cdots, N$ with the boundary conditions $c_0 = c_{N+1} = 0$. The characteristic equation is

$$\lambda^2 + x\lambda + 1 = 0. \tag{5.50}$$

Let the roots be λ_1 and λ_2. Then $\lambda_1\lambda_2 = 1$, and $\lambda_1 + \lambda_2 = -x$. To satisfy the boundary condition, c_n should not exponentially grow in the increasing nor decreasing direction of n. Hence, $|\lambda_1| = |\lambda_2| = 1$ is required (see the general form of the solution in the theorem). That is, λ_1 and λ_2 must be complex conjugate and must be on the unit circle. Let $\lambda_1 = e^{-\theta}$. Then, $x = -2\cos\theta$. The general solution to (5.49) is given by

$$c_n = Ae^{in\theta} + Be^{-in\theta}. \tag{5.51}$$

Therefore, the boundary conditions imply

$$A + B = 0, \quad Ae^{i(N+1)\theta} + Be^{-i(N+1)\theta} = 0. \tag{5.52}$$

That is,

$$e^{2i(N+1)\theta} = 1. \tag{5.53}$$

From this we obtain $\theta = \pi k/(N+1)$ and $\theta = \pi k/(N+1) + \pi$ $(k = 0, 1, \cdots, N)$. However, $k = 0$ implies $c_n = 0$. Furthermore, these two sets of angles give exactly the same set of cosine values. Hence,

$$x = 2\cos\left(\frac{\pi k}{N+1}\right), \quad k = 1, 2, \cdots, N. \tag{5.54}$$

In other words,

$$E = \alpha + 2\beta\cos\left(\frac{\pi k}{N+1}\right), \quad k = 1, 2, \cdots, N. \tag{5.55}$$

That is, the energy allowed to the electron on the carbon chain is determined as an eigenvalue problem (as in the usual quantum mechanical problems).
(ii) Cyclic polyene. The difference equation for the coefficients (5.49) is the same. The only difference from the linear case is the boundary condition. This time, we must impose a cyclic boundary condition. If the ring contains N carbon atoms, we extend the chain by one carbon at the ends and $c_0 = c_N$ and $c_1 = c_{N+1}$ are imposed. From (5.51), the boundary condition becomes

$$Ae^{i(N+1)\theta} + Be^{-i(N+1)\theta} = Ae^{i\theta} + Be^{-i\theta}, \tag{5.56}$$

$$Ae^{iN\theta} + Be^{-iN\theta} = A + B. \tag{5.57}$$

This requires

$$e^{iN\theta} = 1. \tag{5.58}$$

That is, the energies of the cyclic polyene orbitals are given by

$$E = \alpha + 2\beta \cos\left(\frac{2\pi k}{N}\right),\ k = 0, 1, \cdots, N-1. \tag{5.59}$$

APPENDIX 8A Decomposition of e^{At}

A theoretical basis of the practical method **??** is outlined here. Conventionally, the Jordan canonical form is used to compute e^{At}, but to make the Jordan canonical form may not be very easy.[84]
(1) Let $f(x)$ be the characteristic polynomial: $f(x) = det\,(xI - A)$. If

$$f(x) = (x - \lambda_1)^{\mu_1}(x - \lambda_2)^{\mu_2} \cdots (x - \lambda_k)^{\mu_k} \tag{5.60}$$

λ_j is an eigenvalue and μ_j is called its *multiplicity*.
(2) The lowest order polynomial $\varphi(x)$ satisfying $\varphi(A) = 0$ is called the *minimal polynomial* of A. φ must divide f and has the following form:

$$\varphi(x) = (x - \lambda_1)^{\nu_1}(x - \lambda_2)^{\nu_2} \cdots (x - \lambda_k)^{\nu_k}. \tag{5.61}$$

$0 < \nu_j \leq \mu_j$. A necessary and sufficient condition for A to be diagonalizable is $\nu_j = 1$ for all j.
(3) **Theorem [Frobenius]**. Let $g(x)$ be the largest (highest order) common divisor of all the $(n-1)$-subdeterminant minors of $xI - A$. Then the minimal polynomial φ is given by $\varphi = f/g$, where f is the characteristic polynomial.
(4) $W_j \rightleftharpoons ker(\lambda_j I - A)$ (i.e., all the vectors satisfying $A\boldsymbol{p} = \lambda_j \boldsymbol{p}$) is called the *eigenspace* of A belonging to λ_j. $\tilde{W}_j \rightleftharpoons ker(\lambda_j I - A)^{\nu_j}$ (i.e., all the vectors satisfying $(\lambda_j I - A)^{\nu_j}\boldsymbol{p} = 0$) is called the *generalized eigenspace* of A belonging to λ_j. If A is diagonalizable, then $W_j = \tilde{W}_j$ for all j.
(5) $\tilde{W}_1 \oplus \tilde{W}_2 \oplus \cdots \oplus \tilde{W}_k = \boldsymbol{C}^n$. That is, the vector space on which A is acting is decomposed into the direct sum of generalized eigenspaces.
(6) The projection operator P_j for the generalized eigenspace $\tilde{W}_j$ can be constructed as follows: Let f be the characteristic polynomial. Compute the partial fraction expansion

$$\frac{1}{f(x)} = \frac{g_1(x)}{(x - \lambda_1)^{\mu_1}} + \frac{g_2(x)}{(x - \lambda_2)^{\mu_2}} + \cdots + \frac{g_k(x)}{(x - \lambda_k)^{\mu_k}}. \tag{5.62}$$

Here $g_j(x)$ is a polynomial of order not larger than $\mu_j - 1$. Then

$$P_j = f_j(A)g_j(A), \tag{5.63}$$

where

$$f_j(x) \rightleftharpoons f(x)/(x - \lambda_j)^{\mu_j}. \tag{5.64}$$

(7) $(A - \lambda_j I)^q P_j = 0$ for $q \geq \nu_j$.
(8) Now we can decompose e^{At} as follows: $e^{At}(P_1 + P_2 + \cdots + P_k)$. Here

$$e^{At}P_j = e^{\lambda_j t}e^{(A-\lambda_j I)t}P_j, \tag{5.65}$$

$$= e^{\lambda_j t}\sum_{m=0}^{\nu_j - 1}\frac{t^m}{m!}(A - \lambda_j I)^m P_j, \tag{5.66}$$

where we have used (7) after expanding the exponential function.

[84] For this approach see M. W. Hirsch and S. Smale, *Differential Equations, Dynamical Systems, and Linear Algebra* (Academic Press 1974).

6 Quasilinear First Order PDE

Quasilinear first order PDE has become increasingly important in recent years in physics in conjunction to renormalization group theory. Subsection A discusses how to solve general quasilinear first order PDE analytically in terms of characteristics. In Subsection B, as an application, we discuss homogeneous functions that are important in statistical mechanics and mechanics. In the last subsection C, the method outlined in A is applied to constant coefficient linear PDE including wave and diffusion equations.

Key words: quasilinearity, characteristic equation, characteristic curve, (generalized) homogeneous function

Summary:
(1) Quasilinear first order PDE can be solved with the aid of a system of ODE called characteristic equations, which can be written down easily (**6.4**).
(2) Homogeneous functions (**6.8**), their derivatives (**6.10**) and the PDE they obey (**6.9**) must be clearly understood.
(3) Constant coefficient cases may be solved by several standard tricks (**6.16-6.19**).

6.A General Theory

6.1 Quasilinear first order PDE. Let f_i $(i = 1, \cdots, n)$ and g be continuous functions of $x_1, \cdots, x_n$ and u.

$$\sum_{i=1}^{n} f_i \frac{\partial u}{\partial x_i} = g \tag{6.1}$$

is called a *quasilinear first order partial differential equation*. It is called linear, because it is a linear combination of partial derivatives. It is called 'quasilinear', because f_i and g are allowed to depend on u. It is clearly nonlinear in the physicists' sense, if f_i depends on u.

6.2 Typical example. Suppose a flow field (i.e., the velocity field $\boldsymbol{v}$) of an incompressible fluid is given. The continuity equation (the mass

conservation) reads (→**2.33**)

$$\frac{\partial \rho}{\partial t} = -div\, \rho \boldsymbol{v} = -\boldsymbol{v} \cdot grad\, \rho. \tag{6.2}$$

This is a typical quasilinear first order PDE. From its meaning, if $\rho_{t=0}(\boldsymbol{r}) = f(\boldsymbol{r})$, then $\rho(t, \boldsymbol{r}) = f(\boldsymbol{r}(t))$, where $\boldsymbol{r}(t)$ is the particle trajectory starting from $\boldsymbol{r}$ at $t = 0$; that is, the solution to

$$\frac{d\boldsymbol{r}}{dt} = \boldsymbol{v} \tag{6.3}$$

with the initial condition $\boldsymbol{r}(0) = \boldsymbol{r}$. This is an example of the characteristic curve in the next entry.

6.3 Two variable case. Consider

$$f(x, y, z)\frac{\partial z}{\partial x} + g(x, y, z)\frac{\partial z}{\partial y} = h(x, y, z), \tag{6.4}$$

where f, g and h are well-behaved functions[85] of x, y and z. To solve the equation is to find a relation among x, y and z so that (6.4) is true. We wish to find a 2-surface S given by $z = H(x, y)$ on which (6.4) holds. Suppose (x, y, z) and $(x + dx, y + dy, z + dz)$ are both on this surface. Then

$$\left(\frac{\partial H}{\partial x}, \frac{\partial H}{\partial y}, -1\right) \cdot (dx, dy, dz) = 0, \tag{6.5}$$

i.e., $\boldsymbol{n} = (\partial z/\partial x, \partial z/\partial y, -1)$ is a normal vector of the surface S. (6.4) implies that $\boldsymbol{n}$ and the vector (f, g, h) are orthogonal. That is, to solve (6.4) is to determine a surface $z = H(x, y)$ whose tangent vectors are (f, g, h). The equation of a curve whose tangent is (f, g, h) is given by

$$\frac{dx}{f} = \frac{dy}{g} = \frac{dz}{h}. \tag{6.6}$$

This is called the *characteristic differential equation* for (6.4) (cf. (6.3)). The solutions to (6.6) are called *characteristic curves*.

In the present case (6.6) is actually two ODE so that the general solution to (6.6) is given by two equations

$$F_1(x, y, z) = c_1, \quad F_2(x, y, z) = c_2, \tag{6.7}$$

[85] 'Well-behaved' means that the relevant quantities are with sufficiently good properties, say smoothness, to allow us to ignore inessential technical details.

where c_1 and c_2 are integration constants. These equations describe surfaces, so their intersection is generically a curve we are looking for. It can be parametrized by these two parameters c_1 and c_2. If we change c_1 and c_2, the curve moves in space. If there is a functional relation between c_1 and c_2, then changing, say, c_1 (c_2 is slaved to c_1) produces a surface. Hence the general formula for the surface whose tangent vectors are given by (f, g, h) is given by

$$G(F_1, F_2) = 0, \tag{6.8}$$

where G is a (well-behaved) function which must be determined by auxiliary conditions. This is the general solution we have been looking for.

6.4 How to solve quasilinear first ODE: method of characteristic equation. The characteristic equation for (6.1) is

$$\frac{dx_1}{f_1} = \frac{dx_2}{f_2} = \cdots = \frac{dx_n}{f_n} = \frac{du}{g}. \tag{6.9}$$

Solving this (actually n ordinary differential equations), we get n solutions corresponding to (6.7) (any convenient combinations can be chosen)

$$F_i(x_1, x_2, \cdots, x_n, u) = c_i \ \ (i = 1, 2, \cdots, n), \tag{6.10}$$

from which we can get the general solution to (6.1) as

$$G(F_1, F_2, \cdots, F_n) = 0, \tag{6.11}$$

where G is a well-behaved function.

Historically, the method (and consequently the relation between the PDE and the ODE) was stated for the first time by Leibniz in his letter to l'Hospital in November, 1695.[86]

6.5 Homogeneous case. If $g = 0$ in (6.1), then $du/g = du/0$ in (6.9) is interpreted as $u = const.$ That is, one of the equations in (6.10) is $u =$ const. In this case the general solution can be written as

$$u = G(F_1, F_2, \cdots, F_{n-1}), \tag{6.12}$$

where $F_1, \cdots, F_{n-1}$ are the remaining $n - 1$ relations of (6.10).

Discussion. [Complete integral].
A solution of a first order PDE is called a *complete integral*, if it has the same number

[86] K. Okamoto, Butsuri, Jan. 1996.

of arbitrary constants as the number of independent variables.[87] If we have such a solution, we can make a solution which is dependent on a single arbitrary function w as follows: Let $a_n = w(a_1, \cdots, a_{n-1})$, and construct the envelope surface of $u(\boldsymbol{x}, a_1, \cdots, a_{n-1}, w(a_1, \cdots, a_{n-1}))$: that is, we make the following equations:

$$u_{a_1} + u_{a_n} w_{a_1} = 0, \tag{6.13}$$

$$\cdots \quad , \tag{6.14}$$

$$u_{a_{n-1}} + u_{a_n} w_{a_{n-1}} = 0. \tag{6.15}$$

From these equations we solve $n-1$ parameters as a function of $\boldsymbol{x}$. Then put these solutions into u. This is the desired solution. However, there is NO guarantee that the method can exhaust all the solutions constructed by the characteristic curve method.
(2) For example,

$$u = ax + by + \sqrt{1 - a^2 - b^2} z + c \tag{6.16}$$

is a complete integral of $(grad\, u)^2 = 1$.

6.6 Examples.

(1) For (6.2), the characteristic equation reads

$$\frac{dt}{1} = \frac{dx}{v_x} = \frac{dy}{v_y} = \frac{dz}{v_z} = \frac{d\rho}{0}, \tag{6.17}$$

or (6.3) and $d\rho = 0$ ($\rightarrow$**6.5**). Hence, $\rho(t, \boldsymbol{r}) = f(\boldsymbol{r}(t))$ in **6.2** is justified.
(2)

$$(bx - ay)\frac{\partial f}{\partial x} + (ax + by - 1)\frac{\partial f}{\partial y} = 0. \tag{6.18}$$

The characteristic equation ($\rightarrow$**6.4**) is

$$\frac{dx}{bx - ay} = \frac{dy}{ax + by - 1} = \frac{df}{0}. \tag{6.19}$$

Solving this ($\rightarrow$**4.19**), the general solution is given by (cf. **6.5**)

$$f(x, y) = G\left(\frac{b}{a} \arctan \frac{y - \beta}{x - \alpha} - \frac{1}{2} \log \left[1 + \left(\frac{y - \beta}{x - \alpha}\right)^2\right] - \log(x - \alpha)\right) \tag{6.20}$$

with $\alpha \equiv a/(a^2 + b^2)$ and $\beta \equiv b/(a^2 + b^2)$.
(3)

$$\frac{\partial f}{\partial x} - \frac{\partial f}{\partial y} = (x - y) f. \tag{6.21}$$

[87] More precisely, the matrix $\partial^2 u / \partial_{x_i} \partial_{a_j}$ must be non-singular, where $u(x_i, a_j)$ is a complete solution.

Its general solution is given by

$$f = e^{-xy} G(x+y). \tag{6.22}$$

Exercise.
(A) Solve the following quasilinear first order PDE.
(1)

$$(y^2+z^2-x^2)\frac{\partial z}{\partial x} - 2xy\frac{\partial z}{\partial y} + 2xz = 0. \tag{6.23}$$

(2)

$$(bz-cy)\frac{\partial z}{\partial x} + (cx-az)\frac{\partial z}{\partial y} = ay - bx. \tag{6.24}$$

(3)[88]

$$\left[L\frac{\partial}{\partial L} + \frac{u}{\pi^2}\left(\frac{\epsilon\pi^2}{2} - u\right)\frac{\partial}{\partial u} + \frac{u}{(2\pi)^2}N\frac{\partial}{\partial N}\right] f = 0. \tag{6.25}$$

(4) Demonstrate that the solution to

$$-y\frac{\partial u}{\partial x} + x\frac{\partial u}{\partial y} = 0 \tag{6.26}$$

is rotationary symmetric.
(B) Find the solution of $z(\partial z/\partial x) + \partial z/\partial y = 1$ passing through the curves $y = 2z$ and $x = z^2$.
(C) Solve

$$x\frac{\partial z}{\partial x} - y\frac{\partial z}{\partial y} = z, \tag{6.27}$$

and

$$x^2\frac{\partial z}{\partial x} - y^2\frac{\partial z}{\partial y} = y^2 - x^2. \tag{6.28}$$

Find the particular solution to the above equations going through $x = y = z$.

6.7 Dilation parameter. It is often technically convenient to introduce a parameter λ (called *dilation parameter*) to solve the characteristic equation (6.9)

$$\frac{dx_1}{f_1} = \frac{dx_2}{f_2} = \cdots = \frac{dx_n}{f_n} = \frac{du}{g} = \frac{d\lambda}{\lambda}$$

This gives a parametric representation of characteristic curves.

[88] This is the renormalization group equation for the mean square end-to-end distance of a self-avoiding walk calculated by the ϵ-expansion method. What do you expect to happen in the $N \to \infty$ limit? Here, N is the number of steps.

6.B Homogeneous Functions

6.8 Homogeneous function of degree p. Let u be a well behaved real-valued function defined on a region in $\boldsymbol{R}^n$. If

$$u(\lambda x_1, \lambda x_2, \cdots, \lambda x_n) = \lambda^p u(x_1, x_2, \cdots, x_n) \tag{6.29}$$

for any real λ, u is called a *homogeneous function of degree* p, where p can be any real number. Since λ can be any number, $\lambda = x_1^{-1}$ is admissible, for example. This implies that a homogeneous function of degree p can be rewritten, for example, as

$$u(x_1, \cdots, x_n) = x_1^p f\left(\frac{x_2}{x_1}, \cdots, \frac{x_n}{x_1}\right). \tag{6.30}$$

Discussion.
More generally, a functional $f(\boldsymbol{r})$ is called a homogeneous function, if

$$f(\lambda \boldsymbol{r}) = g(\lambda) f(\boldsymbol{r}), \tag{6.31}$$

where g is a function of λ only. Show that

$$g(\lambda\mu) = g(\lambda) g(\mu). \tag{6.32}$$

If g is continuous at a point, then the following form is the only nontrivial solution to this functional equation: $g(x) = x^p$. Its proof is not easy.

6.9 Theorem [Necessary and sufficient condition for homogeneity]. A necessary and sufficient condition for u to be a once-differentiable homogeneous function of degree p is

$$\sum_{i=1}^{n} x_i \frac{\partial u}{\partial x_i} = pu. \tag{6.33}$$

[Demo] Necessity follows easily from the chain rule. To prove sufficiency, construct the general solution of (6.33) (→**6.4**) and explicitly demonstrate that it is indeed homogeneous of degree p. Actually, we can easily get the form like (6.30).

6.10 Theorem [Derivative of homogeneous functions are homogeneous]. Let u be a differentiable homogeneous function of degree $p \in \boldsymbol{R}$. Then, for any x_i, $\partial u/\partial x_i$ is a homogeneous function of degree $p - 1$. □
This follows trivially from the definition of homogeneous functions.

6.11 Green's theorem and homogeneous function. Let $f(x, y)$ be a continuously differentiable homogeneous function of order p on a compact domain $\Omega \subset \boldsymbol{R}^2$. Then,

$$(p+2)\int_\Omega f(x,y)dxdy = \int_{\partial\Omega} f(x,y)(xdy - ydx). \tag{6.34}$$

[Demo] Let $u = -yf$ and $v = xf$.

$$\frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} = 2f + x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y} = (2+p)f \tag{6.35}$$

thanks to the homogeneity of order p of f ($\rightarrow$**6.9**). Therefore, Green's theorem ($\rightarrow$**3.13**) implies the above relation. □

This relation can be extended to $\boldsymbol{R}^n$ $(n > 2)$:[89]

$$(n+p)\int_\Omega d\tau = \int_{\partial\Omega} f(\boldsymbol{r})\boldsymbol{r}\cdot d\boldsymbol{S}. \tag{6.36}$$

6.12 Example from thermodynamics. *Extensive quantities* in thermodynamics such as the Gibbs free energy, magnetization, entropy are homogeneous functions of degree 1 of the masses of the constituents (chemical species) of the system. **6.10** implies that *intensive quantities* such as temperature, chemical potential, pressure are homogeneous functions of degree 0. From, for example, $dE = TdS - pdV + \mu dN$ $E = TS - pV + \mu N$ follows according to Theorem **6.9**.[90]

??.
Let x be the extensive quantity X per unit mass. Show

$$de = Tds - pdv + \mu dn. \tag{6.37}$$

6.13 Kepler's third law. Consider an n-body conservative system with the potential energy given by $U(\boldsymbol{r}_1, \cdots, \boldsymbol{r}_2)$ which is a homogeneous function of degree p. This implies that the force is a homogeneous

[89] See J. B. Lasserre, *Integration and homogeneous functions*, Proc. Amer. Math. Soc. **127**, 813 (1999). This contains much more general results.

[90] The best thermodynamics textbook (introductory) for physicists is: H. B. Callen, *Thermodynamics* (Wiley, 1960); R. Kubo, *Thermodynamics* (North-Holland; translation of the first part of *Daigaku Enshu: Netsugaku·Tokerikigaku*, (Shokabo)); There recent books in Japanese by S. Sasa and H. Tazaki; these books are under the influence of E. Lieb and J. Yngvason, *The physics and mathematics of the second law of thermodynamics*, Phys. Rep., **340**, 1-96 (1999).

(vector-valued) function of degree $p-1$ (→**6.10**). Newton's equation of motion

$$m_i \frac{d^2 \boldsymbol{r}_i}{dt^2} = -\frac{\partial U}{\partial \boldsymbol{r}_i}, \tag{6.38}$$

where m_i is the math of the i-th body, has the following scaling property: Scaling $\boldsymbol{r}_i \to \lambda \boldsymbol{r}_i$ and $t \to \mu t$ gives

$$m_i \frac{d^2 \boldsymbol{r}_i}{dt^2} = -\lambda^{p-2} \mu^2 \frac{\partial U}{\partial \boldsymbol{r}_i}. \tag{6.39}$$

Therefore, if $\mu = \lambda^{1-p/2}$, the equation of motion is invariant. For gravity, $p = -1$, so that this implies Kepler's third law ($T^2 = a^3$).[91]

6.14 Generalized homogeneous function. If a function f satisfies

$$f(\lambda^a x, \lambda^b y) = \lambda^p f(x, y) \tag{6.40}$$

for any real λ and for some real numbers a, b and p, f is called a *generalized homogeneous function*. This is important in understanding critical phenomena. For example, the static scaling hypothesis (due to Widom) asserts that the Helmholtz free energy $F(T - T_c, H)$ of a magnet, where T_c is the critical temperature, and H the magnetic field, is a generalized homogeneous function for $\tau \equiv |T - T_c| \simeq 0$ and $H \simeq 0$:[92]

$$F = \tau^{2-\alpha} f(\tau / H^{1/\beta\delta}), \tag{6.41}$$

where α, β and δ are called *critical exponents*. These exponents and the functional form of f are universal for a class of materials.[93]

6.C Application to Constant Coefficient Linear PDE

6.15 Constant coefficient linear PDE. Introduce the notation $\partial_i \equiv \partial/\partial x_i$, and write collectively $\{\partial_i\}$. Let $P(\{x_i\})$ be a constant coefficient polynomial.

$$P(\{\partial_i\})u = g, \tag{6.42}$$

[91] For other examples, see J. M. Smith, *Mathematical Ideas in Biology* (Cambridge UP).

[92] See, for example, H. E. Stanley, *Introduction to Phase Transition and Critical Phenomena* (Oxford UP, 1971), Chapter 11, 12 and 15.

[93] See N. Goldenfeld, *Lectures on Phase Transitions and the Renormalization Group* (Addison Wesley, 1992).

where g is a function of $\{x_i\}$, is called a constant coefficient linear partial differential equation. The general solution to (6.42) is the sum of the general solution[94] to the homogeneous problem $Pu = 0$ and a solution for $Pu = g$.

6.16 Theorem [Malgrange-Ehrenpreis]. If g is C^∞ in a region $D \subset \boldsymbol{R}^n$, then (6.42) has a C^∞ solution in D. □[95]

6.17 Factorization 'theorem'. If P is factorized into two mutually prime factors as $P = P_1P_2$, then the general solution to $Pu = 0$ is the sum of the general solutions to $P_1u = 0$ and $P_2u = 0$. □[96]

This should be obvious from $P(f_1 + f_2) = P_2P_1f_1 + P_1P_2f_2$. Here we assume the function f is sufficiently smooth.

Since P is a polynomial of many variables, there is no guarantee that we can factorize this into distinct first order factors of the form $\sum a_i\partial_i$. If we can, we can exploit our knowledge of first order linear PDE (→**6.5**). If we cannot factorize P into first order operators, there is no general way to solve the PDE (however, see **6.22**).

From now on we study only two independent variable cases.

6.18 How to solve inhomogeneous equation. As is stated in **6.15** we have only to find one solution to $Pu = g$ by whatever means we can use. Useful observations are:
(1) If $P = P_1P_2$, then $Pu = g$ can be solved step by step. First find u_1 such that $P_1u_1 = g$, and then solve $P_2u = u_1$.
(2) $P(\partial_x, \partial_y)e^{ax+by}u = e^{ax+by}P(\partial_x+a, \partial_y+b)u$. [This can easily be seen from, e.g., $\partial_x^n e^{ax+by}u = \partial_x^{n-1}e^{ax+by}(\partial_x + a)u$.]

6.19 Lemma. The general solution to

$$(a\partial_x + b\partial_y + c)^n u = 0 \tag{6.43}$$

is

$$u = e^{-cx/a}\sum_{i=0}^{n-1} x^i\phi_i(bx - ay), \tag{6.44}$$

[94] By "general solution" we mean a solution containing m arbitrary functions for a m-th order PDE in the linear case.

[95] For a proof, see G. B. Folland, *Introduction to Partial Differential Equation*, p84-7.

[96] Practically, the 'theorem' is very useful as we see below, but precisely speaking, the theorem cannot be true, because the smoothness of the solution to a lower order PDE need not be as large as the original higher order PDE. Hence, the 'theorem' is useful only when we look for sufficiently smooth solutions.

where ϕ_i are arbitrary functions. (If $a = 0$, then replace $e^{-cx/a}$ with $e^{-cy/b}$ and x^i with y^i). □

To demonstrate this use (1) and (2) of **6.18**. Also it is useful to remember the following standard trick. Let L be a linear first order differential operator and we wish to solve $L^2u = 0$. If we know the solution to $Lv = 0$, then introduce w as $u = wv$. The equation for w is usually easier to solve.

6.20 Examples. Find the general solutions (Review **1.11**).
(1) 1-space wave equation:

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \tag{6.45}$$

For this equation

$$P(\partial_t, \partial_x) = \partial_t^2 - c^2\partial_x^2 = (\partial_t - c\partial_x)(\partial_t + c\partial_x). \tag{6.46}$$

Hence, the factorization theorem **6.17** implies that the general solution to the wave equation is the sum of the general solution to $(\partial_t - c\partial_x)u = 0$ and $(\partial_t + c\partial_x)u = 0$. These can be solved easily by the standard method **6.18**, so that the general solution to (6.45) is

$$u(t, x) = F(x - ct) + G(x + ct), \tag{6.47}$$

where F and G are arbitrary twice differentiable functions.[97] That is, the general solution is a superposition of right and left propagating waves as we have already seen in **1.11**.
(2) 2-space Laplace equation:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0. \tag{6.48}$$

This is the case with $c = i$ of (6.45). Hence, its general solution can be written as $F(x + iy) + G(x - iy)$. We are looking for real solutions. If $F(z) + G(\overline{z})$ is real, then it must be a real part of some analytic function.[98] Hence, the general solution is a real part of any analytic function.
(3)

$$\frac{\partial^2 u}{\partial x \partial y} + 2\frac{\partial^2 u}{\partial y^2} - \frac{\partial u}{\partial x} - 2\frac{\partial u}{\partial y} = 0. \tag{6.49}$$

[97] See the footnote of **6.16**.

[98] Notice first that $G(\overline{z})$ may be considered as the complex conjugate of some analytic function $H(z)$. Hence, $F(z) + \overline{H(z)}$ is real. We know $F(z) + \overline{F(z)}$ is also real for all z, so that $F(z) - H(z)$ must be real for all z. However, such an analytic function must be a real constant. Hence, we may identify H and F.

Its general solution reads

$$u(x,y) = F(2x-y) + e^y G(x), \tag{6.50}$$

where F and G are twice differentiable functions.

6.21 Examples of inhomogeneous equations. Find general solutions:
(1)

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = x. \tag{6.51}$$

Use **6.18**(1), or by inspection $u = x^3/6$ is a solution. Thus the general solution to this equation reads (→**6.20**)

$$u(x,y) = F(x+iy) + G(x-iy) + \frac{x^3}{6}. \tag{6.52}$$

(2)

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \sin(x+at) \quad (a \neq \pm 1). \tag{6.53}$$

We use **6.18**(2). Use the linearity of the equation and the fact that $Im\, e^{i(x+at)} = \sin(x+at)$. That is, get a solution to $(\partial_t^2 - \partial_x^2)u = e^{i(x+at)}$:

$$u = \frac{1}{2i(1-a^2)} e^{i(x+at)} \tag{6.54}$$

Its imaginary part is the desired solution. Hence, the general solution to (6.53) is (→**6.20**(1))

$$u = F(x-t) + G(x+t) + \frac{1}{a^2-1}\sin(x+at). \tag{6.55}$$

If $a = \pm 1$ (resonant case), then introduce v as $u = e^{i(x+at)}v$, and make the equation for v. This is a standard method to solve resonant problems.[99]

Exercise.
(1) Find the solution of $z(\partial z/\partial x) + \partial z/\partial y = 1$ passing through the curves $y = 2z$ and $x = z^2$.
(2) Consider the following *telegraph equation*:

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} + (a+b)\frac{\partial u}{\partial t} + abu = 0, \tag{6.56}$$

[99] This is the general trick we considered in **6.19**.

where a and b are constants. The standard way to remove the first order derivative term is to introduce

$$v = e^{(a+b)t/2}u. \tag{6.57}$$

We have

$$\frac{\partial^2 v}{\partial t^2} - \left(\frac{a-b}{2}\right)^2 v - c^2\frac{\partial^2 v}{\partial x^2} = 0. \tag{6.58}$$

If $a = b$, then the cable can propagate a wave without distorting the wave form, although the signal strength decays.

6.22 Application to diffusion equation. For a diffusion equation in 1-space, the differential operator $P = (\partial_t - D\partial_x^2)$, so that we cannot factorize this into first order factors. However, if $P(a, b) = 0$, then $\exp(at + bx)$ is a solution. Hence, for example

$$e^{ikx - Dk^2 t} \tag{6.59}$$

is a solution. Since the equation is linear, if the integral

$$u(x,t) = \int_{-\infty}^{\infty} dk f(k) e^{ikx - Dk^2 t} \tag{6.60}$$

converges, then this turns out to be the general solution, where f is an appropriate function of k. For example, if f is in L_2 (→**??**(2)), the integral converges, and $u(x, t)$ is at least meaningful as a weak solution (a solution in the generalized function sense →**10**).

6.18(2) is also useful to find a special solution to inhomogeneous diffusion equations. For example, consider

$$\partial_x^2 u - \partial_t u = \sin(ax + bt). \tag{6.61}$$

$$\tilde{u} = \frac{1}{a^4 + b^2}\left[-a^2 \sin(ax + bt) + b\cos(ax + bt)\right] \tag{6.62}$$

is a solution.

7 Generalized Function

The δ-function is not an ordinary function, and is meaningful only inside the integral. The theory of distribution in the sense of Sobolev and Schwartz rationalizes such objects like the δ-function. Rudiments of the theory is outlined from the practitioner's point of view. Calculation of Green's functions may be facilitated by the theory of generalized functions which justifies apparent abuses of classical analysis.

Key words: generalized function, distribution, test function, Schwartz class, regular distribution, convolution, δ-function, differentiation of δ-function, Heaviside step function, Cauchy principal part.

Summary:
(1) Generalized functions are defined by their outcome when they are applied to test functions (**7.4**, **7.8**). Whenever, the reader feels intuition is doubtful, use test functions.
(2) Understand the definition of differentiation of generalized functions (**7.14**). All the elementary rules of calculus survive for generalized functions; besides, the order of limit and differentiation can always be exchanged (**7.19**).
(3) Change of the variables in δ-function should not cause any problem (**7.12-7.14**).
(4) Be familiar with convolution (**7.23**).

7.1 Green's function and delta-function. The fundamental idea of Green was introduced at **3.6**, where we realized that it is very convenient to introduce an object δ_a which has weight 1 at point a but zero elsewhere. If we consider the mass density distribution $\rho(x)$ corresponding to this weight distribution, then we need $\rho(x)$ which is $+\infty$ at $x = a$ but zero elsewhere. The symbol $\delta(x - a)$ was introduced for such an object in **??** in conjunction to functional derivative. Basically, to implement Green's idea we have to solve, for example,

$$-\Delta\psi = \delta(x - a) \tag{7.1}$$

under an appropriate boundary condition. We need a systematic theory of such "density functions."

7.2 Green's function and fundamental solution. Let L be a linear differential operator.[100] Any solution to

$$L\psi(x) = \delta(x - y) \tag{7.2}$$

is called a *fundamental solution*. If it satisfies, further, the auxiliary conditions of the problem, we say the solution is the *Green's function* for the problem. As we will see later (→**9.17** for an example), we have only to consider homogeneous auxiliary conditions, so when we say $G(x|y)$ is the Green's function of a problem which is described by the linear differential operator L and linear auxiliary conditions (→**3.3**) $A\psi = f$, we mean

$$LG(x|y) = \delta(x - y) \tag{7.3}$$

with the corresponding homogeneous auxiliary condition $AG(x|y) = 0$.

7.3 Motivation of theory: Delta function as linear functional. Let $\mathcal{D}$ be a set of real-valued functions on $\boldsymbol{R}$. Let us define a map $T_\delta : \mathcal{D} \to \boldsymbol{R}$ as $T_\delta(f) = f(0)$. Recall that T_δ is exactly the 'integral' of f times δ over $\boldsymbol{R}$ in the original 'definition' of δ (→**??**). The most obvious and important property of T_δ is its linearity:

$$T_\delta(af + bg) = aT_\delta(f) + bT_\delta(g), \tag{7.4}$$

where a and b are reals. Therefore, we are tempted to write T_δ in terms of integral with some integration kernel δ: $T_\delta(f) = \int dx\, \delta(x)f(x)$ as in the original 'definition.' However, for T_δ there is no ordinary function δ satisfying this equality, because its 'value' at 0 cannot be finite. Still, T_δ is well-defined. Therefore, we define δ through T_δ:

7.4 Generalized function. Let T_q be a linear functional defined on a set $\mathcal{D}$ of real-valued functions on $\boldsymbol{R}$. The formal symbol $q(x)$ such that for $f \in \mathcal{D}$

$$T_q(f) = \int dx\, q(x)f(x) \tag{7.5}$$

is called a *generalized function*. The following notation, reminding us of the inner product (→**??**), is also often used for convenience:

$$T_q(f) = \langle q, f \rangle. \tag{7.6}$$

The definition must include the following rule for changing the independent variable. The rule is exactly the same as in the case of ordinary functions:

$$\int dx q(x)f(x) = \int ds \varphi'(s) q(\varphi(s))f(\varphi(s)), \tag{7.7}$$

[100] A linear operator L is called a *differential operator*, if $Lf(x)$ depends on $f(x)$ and its derivatives at x. For example, $-d^2/dx^2 + V(x)$, where V is a function, is a linear differential operator.

where q is a generalized function, f is a test function, and $x = \varphi(s)$ defines the change of variable.

7.5 δ-function: an official definition.[101] The symbol $\delta(x)$ such that

$$T_\delta(f) = \int \delta(x) f(x) dx = f(0) \tag{7.8}$$

is called the *δ-function*. Since the variable x in δ transforms as the usual x in the ordinary functions, the symbol for the map $f(x) \to f(a)$ is written as $\delta(x-a)$ (as we already noted in **7.1**):

$$\int \delta(x-a) f(x) dx = \int \delta(y) f(y+a) dy = f(a). \tag{7.9}$$

Exercise.
(A)
Evaluate
(1)

$$\int_{-5}^{5} \cos x \, \delta(x) dx. \tag{7.10}$$

(2)

$$\int_{-5}^{10} \delta(x) \log \Gamma(x+5) dx. \tag{7.11}$$

(B) A mass M is located at $x = 0$ on an infinite string: that is the density of the string is $\rho(x) = \rho + M\delta(x)$. Write down the equation of motion for the string under uniform tension τ (→**2.27**). We wish to consider the effect of the point mass on the incident wave. The wave $F(t - x/c)$ is incident from $x = -\infty$. The displacement is written as

$$u(x,t) = \begin{cases} F(t-x/c) + R(t+x/c) \text{ for } x < 0, \\ T(t-x/c) \text{ for } x > 0. \end{cases} \tag{7.12}$$

Show that

$$T'' + \gamma T' = \gamma F, \tag{7.13}$$

where $\gamma = \tau/Mc$. Find T in terms of F.[102]

7.6 Value of generalized function at each point is meaningless. The value of a generalized function at a point is totally meaningless, because changing the value of a function at a point does not affect its

[101] It is often called the Dirac δ-function, ignoring the fact that this type of functions have been used for well over a hundred years.
[102] See G L Lamb, Jr. *Introductory Applications of Parital Differential Equations* (Wiley, 1995).

integral (→**??**, **??**). Therefore, although δ-function was originally 'defined' such that $\delta(x) = 0$ for $x \neq 0$, according to our official definition, we cannot mention anything about the value of $\delta(x)$ for any $x \in \boldsymbol{R}$. Consequently, the product of delta functions containing common variables is a very dangerous concept.

Discussion.
However,
(A) **Localization theorem of generalized functions**. The value of a generalized function g at each point does not make sense, but it is possible to make such statement as $g = 0$ meaningful in a neighborhood of a point. To this end, we must define $g = 0$ on an open set U.

We say $g = 0$ on U, if $\langle \phi, g \rangle = 0$ for any $\phi \in C_0^\infty(U)$ (= the set of all the C^∞ functions whose support is in U, that is, $\phi = 0$ outside U). Two generalized functions f and g are equal on U if $f - g = 0$ on U.
Theorem [**Localization theorem**]. For any x if there is its neighborhood on which $g = 0$, then $g = 0$ in the sense of generalized functions.
Theorem[**Localization of derivatives**]. If $f = g$ on U, then their derivatives are identical on U.
About the local properties, Section 3.2 of R. D. Richtmeyer, *Principles of Advanced Mathematical Physics* vol.1 (Springer, 1978) may be accessible.
(B) Of course, $f(g)$ does not usually make any sense for generalized functions f and g.

7.7 Multidimensional delta funcion. The definition of generalized functions on multidimensional space should be obvious (→**??** for curvilinear coordinate cases).

Exercise.
Let $d\tau$ be the volume element in 3-space, and r be the radial coordinate of the spherical coordinates. $\boldsymbol{r}$ is the position vector. Evaluate

$$\int d\tau e^{-r^2} \delta(r). \tag{7.14}$$

Here r must be considered as a function of $\boldsymbol{r}$. What is its difference from

$$\int d\tau e^{-r^2} \delta(\boldsymbol{r})\,? \tag{7.15}$$

7.8 Test functions. Since we cannot evaluate generalized functions pointwisely, the only way to study the property of a generalized function is to apply it to functions in an appropriate function set $\mathcal{D}$. The set $\mathcal{D}$ is called the set of *test functions*.

Discussion.
The choice of the test function set $\mathcal{D}$ is a matter of convenience, but the set must satisfy some obvious conditions such as its closedness: if $f_n \to f$ and $f_n \in \mathcal{D}$, then f should also be in $\mathcal{D}$. If the set $\mathcal{D}$ is very poor, then many generalized functions become indistinguishable. On the other hand, if $\mathcal{D}$ is too large, then we must meticulously pay attention to minute details of the generalized functions. From the practitioner's point of view, we need not pay much attention to $\mathcal{D}$, but should remember that very often $\mathcal{D}$ is the set of all the C^∞-functions with compact domains (i.e., C_0^∞) or the set of all the *functions of rapid decay* (or rapidly decreasing functions, *Schwartz-class functions*):

$$\mathcal{D} = \{f : \boldsymbol{R} \to \boldsymbol{C},\ C^\infty \text{ such that } x^n f^{(r)}(x) \to 0 \text{ as } |x| \to \infty \text{ for } \forall n, r \in \boldsymbol{N}\}.$$

(In words, $\mathcal{D}$ consists of infinite times differentiable functions whose any derivative decays faster than any inverse power.) The generalized functions defined on this $\mathcal{D}$ is called *generalized functions of slow growth*.

7.9 Equality of generalized functions. Two generalized functions p and q are said to be equal,[103] if no test function can discriminate them:

$$T_p(f) = T_q(f) \text{ for all the test functions } f \iff p = q. \tag{7.16}$$

7.10 Regular distribution. Let $\mathcal{D}$ be an appropriate test function set (see the footnote in **7.8**). If a generalized function q is equal to some ordinary function, we say q is a *regular distribution*.

7.11 $\boldsymbol{\delta(ax) = |a|^{\ 1}\delta(x)}$. To demonstrate an equality of generalized functions, the surest way is to return to the definition of the equality **7.9**.

$$\int \delta(ax) f(x) d(x) = \int \delta(y) f(y/a) |a|^{-1} dy = |a|^{-1} f(0/a) = \int |a|^{-1} \delta(x) f(x) dx \tag{7.17}$$

for any test function, so that we may conclude the desired relation.

7.12 $\boldsymbol{\delta(g(x))}$. Let g be a differentiable function. If $g \neq 0$ at x, then a sufficiently small neighborhood of x does not contribute to $\int dx \delta(g) f$. If $g(x_0) = 0$, then $g(x) \simeq g'(x_0)(x - x_0)$ locally, so we may replace

[103] This equality is consistent with the equality discussed in **7.6** Discussion (A).

$\delta(g(x))$ with $|g'(x_0)|^{-1}\delta(x-x_0)$ locally (→**7.11**). In this way we have the following general formula for differentiable g:

$$\delta(g(x)) = \sum_i |g'(x_i)|^{-1}\delta(x-x_i), \tag{7.18}$$

where the summation is over all the real zeros $\{x_i\}$ of g.

Exercise.
Evaluate
(1)

$$\int_{-5}^{5} \delta(3x)\cos x dx, \tag{7.19}$$

(2)

$$\int_{0}^{4} \delta(1-5x)\sin x dx, \tag{7.20}$$

(3)

$$\int_{-\infty}^{\infty} \delta(x^2-5x+6)x^2 dx, \tag{7.21}$$

(4)

$$\int_{-\infty}^{\infty} \delta(\sin 2\pi x)2^{-|x|} dx \tag{7.22}$$

7.13 Convergence of generalized function. A sequence of generalized functions q_n is said to converge to q, if

$$\langle q_n, f\rangle \to \langle q, f\rangle \text{ for all } f \in \mathcal{D}, \tag{7.23}$$

and is written as $\lim_{n\to\infty} q_n = q$. If we use the integral form, we have

$$\lim_{n\to\infty} \int dx q_n(x)f(x) = \int dx \lim_{n\to\infty} q_n(x)f(x). \tag{7.24}$$

That is, limit and integration can be freely interchanged, if we interpret an ordinary function as a regular distribution (→**7.10**). Consequently, termwise integration of series can be performed freely. If we never take the result outside the integral symbol, then we need not worry whether the final result is again a regular distribution or not. Recall that Green's functions (→**3.6**, **7.1**, **X**) always appear inside the integral symbol in practice. Hence, calculus of generalized function becomes a powerful tool especially when we construct and use Green's functions.

Discussion.
We have learned that if the limit of a sequence $\{\varphi_n\}$ converges weakly, then the

limit is a generalized function.
(A) Let $G(x,t|y,0)$ be the Green's function for the diffusion equation in the free space (→**??**) Show that for a continuous f

$$\lim_{t\to 0}\int_{\boldsymbol{R}^3} dyG(x,t|y,0)f(y) = f(x). \tag{7.25}$$

We write this as

$$w\text{-}\lim_{t\to 0} G(x,t|y) = \delta(x-y), \tag{7.26}$$

where w-lim denotes the *weak limit* which is meaningful only inside the integration. This is a possible definition of Dirac's δ-function.
(B) This observation allows us to introduce generalized functions in a different way (due to Korevaar). We prepare a weakly convergent[104] sequence (called *D-fundamental series*[105]) of sufficiently smooth functions $\{\varphi_n\}$ and declare its weak limit to be a generalized function.[106]

Take a positive number sequence ϵ_n such that $\lim_n \epsilon_n = 0$. Consider an arbitrary sequence of non-negative continuous functions $\{\varphi_n\}$ such that $\varphi_n(x) = 0$ for $|x| \geq \epsilon_n$ and

$$\int_{-\infty}^{\infty} \varphi_n(x)dx = 1. \tag{7.27}$$

The D-fundamental sequence $\{\varphi_n\}$ defines the $\delta(x)$.
(C) Demonstrate that indeed the sequence in (B) weakly converges to the δ-function in the $n \to \infty$ limit.
(D) The following sequences are examples of D-fundamental sequences for the delta function:

$$\varphi_n(x) = \frac{n}{\sqrt{\pi}}e^{-n^2x^2}, \tag{7.28}$$

$$\varphi_n(x) = \frac{n}{\pi}\frac{1}{1+n^2x^2} = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ikx-|k|/n}dk, \tag{7.29}$$

$$\varphi_n(x) = \frac{\sin nx}{\pi x} = \frac{1}{2\pi}\int_{-n}^{n} e^{ikx}dk = \frac{1}{\pi}\int_0^n \cos(xk)dk, \tag{7.30}$$

$$\varphi_n(x) = \frac{1}{2\pi}\frac{\sin[(n+1/2)x]}{\sin(x/2)} \text{ (the Dirichlet kernel)}, \tag{7.31}$$

$$\varphi_n(x) = n[\Theta(x+1/2n) - \Theta(x-1/2n)], \text{ (Θ is the Heaviside step function)}, \tag{7.32}$$

$$\varphi_n(x) = 0 \text{ for } |x| \geq 1/n \text{ and } n - n^2|x|, \text{ otherwise }, \tag{7.33}$$

$$\varphi_n(x) = \frac{1}{2n\pi}\left[\frac{\sin(nx/2)}{\sin(x/2)}\right]^2 \text{ (due to Fejer →**??**)} \tag{7.34}$$

[104] w.r.t. a test function set
[105] D for distribution.
[106] A precise definition in the original paper: J. Korevaar, Indagationes Math., **17**, 1955, is much more elaborate, because he wished to construct a theory equivalent to the one due to Schwartz. Here, the lecturer only wishes to make a subclass, so only a grossly simplified version of the original is given.

$$\varphi_n(x) \quad = \quad \sum_{j=-n}^{n} e^{2j\pi ix} \quad \text{for } x \in (-2\pi, 2\pi). \tag{7.35}$$

7.14 Differentiation of generalized functions. If q is an ordinary differentiable function, then for $f \in \mathcal{D}$

$$\int q'(x)f(x)dx = -\int q(x)f'(x)dx. \tag{7.36}$$

The right hand side makes sense, if f is differentiable. Our test function (→**7.8**) is always infinite times differentiable, so that we may regard (7.36) as the definition of q': the derivative q' of a generalized function q is defined as the generalized function satisfying

$$\langle q', f\rangle = -\langle q, f'\rangle. \tag{7.37}$$

By definition, generalized functions are infinite times differentiable.

Discussion.
(1) Derivatives of generalized functions are given by the derivatives of its D-fundamental sequence (if it is differentiable →**7.19**). As we can see in **8.7** some are differentiable many or infinite times but some are not. We may choose convenient differentiable sequences without any contradiction.
(2) L_p-derivative. (T220)

Exercise.
(A) Show

$$x\delta'(x) = -\delta(x). \tag{7.38}$$

(B) Let $\Theta(x, y)$ be 1 when $x > 0$ and $y > 0$, and 0, otherwise. Then,

$$\frac{\partial^2\Theta(x, y)}{\partial x\partial y} = \delta(x)\delta(y). \tag{7.39}$$

(C) Evaluate
(1)

$$\int_{-5}^{5} \delta'(5x)\cosh x dx. \tag{7.40}$$

(Here $\delta'(f(x))$ is interpreted as the $\delta'(z)$ whose variable z is replaced by $f(x)$.) (2)

$$\int_{-\infty}^{\infty} \delta'(x^2 - 1)\cos x dx. \tag{7.41}$$

7.15 Structural theorem. A version of the structural theorem of generalized functions: A generalized function is obtained by differentia ting a continuous function finitely many times.

7.16 Examples.
(1)

$$\frac{d|x|}{dx} = sgn(x) \rightleftharpoons \begin{cases} 1 \text{ for } x \geq 0, \\ -1 \text{ for } x < 0. \end{cases} \tag{7.42}$$

The reader may conclude this by intuition.[107] A standard demonstration may be to start with, for a test function f,

$$\begin{aligned} -\int dx|x|f'(x) &= -\int_0^\infty dx\, xf'(x) + \int_{-\infty}^0 dx\, xf'(x) \\ &= \int_0^\infty dx f(x) - \int_{-\infty}^0 dx f(x) = \int sgn(x)f(x)dx. \end{aligned} \tag{7.43}$$

(2)

$$\frac{dsgn(x)}{dx} = 2\delta(x). \tag{7.44}$$

(3) The *Heaviside step function* $\Theta(x)$ is defined by $\Theta(x) = (1+sgn(x))/2$.

$$\frac{d\Theta(x)}{dx} = \delta(x). \tag{7.45}$$

7.17 All the ordinary rules for differentiation survive. For example, the chain rule is applicable.
When the reader feels uneasy in some use or abuse of generalized functions, always return to the definition **7.4**: operate the generalized function to test functions. See the next example.

7.18 Cauchy principal value $P(1/x)$. $P(1/x)$ is defined by

$$\int_{-\infty}^{\infty} P\frac{1}{x} f(x)dx \rightleftharpoons P\int_{-\infty}^{\infty} \frac{f(x)}{x}dx, \tag{7.46}$$

where P is defined as $\lim_{\epsilon\to 0}(\int_{-\infty}^{-\epsilon} + \int_{\epsilon}^{\infty})$.
(1) We have

$$\frac{d\ln|x|}{dx} = P\frac{1}{x}. \tag{7.47}$$

[107] The value at $x = 0$ does not matter.

(2) Note that

$$xf = 1 \Rightarrow f = P\frac{1}{x} + c\delta(x), \tag{7.48}$$

where c is a constant. A demonstration follows. Note that obviously $xP(1/x) = 1$. Let $\phi \in \mathcal{D}$.

$$\begin{aligned}
\int f(x)\phi(x)dx &= \int f(x)\left[P\frac{1}{x}(\phi(x) - \phi(0))x + \phi(0)\right]dx \\
&= \int \left[P\frac{1}{x}(\phi(x) - \phi(0)) + f(x)\phi(0)\right]dx \\
&= \int P\frac{1}{x}\phi(x)dx + \int \left(f(x) - P\frac{1}{x}\right)\phi(0)dx \\
&= P\int \frac{\phi}{x}dx + const. \times \phi(0).
\end{aligned} \tag{7.49}$$

Exercise.
Compute

$$P\int_{-1}^{1} \operatorname{cosec} x\, dx. \tag{7.50}$$

7.19 Theorem [Differentiation and limit always commute].

$$q_n \to q \Rightarrow q_n' \to q'. \tag{7.51}$$

□
This is a remarkably simple result. Termwise differentiation of series is allowed. To demonstrate the theorem is easy: For $f \in \mathcal{D}$

$$\langle q_n', f\rangle = -\langle q_n, f'\rangle \to -\langle q, f'\rangle = \langle q', f\rangle. \tag{7.52}$$

Compare this with the situation of the ordinary calculus (→**??**(4)); we need uniform convergence of termwisely differentiated series.

Exercise.
From

$$\tanh\left(\frac{x}{\epsilon}\right) \to \operatorname{sgn} x \tag{7.53}$$

show

$$1/\left[\epsilon \cosh^2(x/\epsilon)\right] \to 2\delta(x). \tag{7.54}$$

7.20 Example.

$$\frac{n}{\pi(1+n^2x^2)} \to \delta(x) \Rightarrow -\frac{2n^3x}{\pi(1+n^2x^2)^2} \to \delta'(x). \tag{7.55}$$

7.21 Example: Coulomb potential. In 3-space we have

$$\Delta\frac{1}{|\boldsymbol{x}|} = -4\pi\delta(\boldsymbol{x}). \tag{7.56}$$

Let us take a test function (→**??**) f and compute

$$\left\langle \Delta\frac{1}{|\boldsymbol{x}|}, f \right\rangle = \left\langle \frac{1}{|\boldsymbol{x}|}, \Delta f \right\rangle = 4\pi\int_0^\infty dr\, r^2\frac{1}{r}\overline{\Delta f} = 4\pi\int_0^\infty r\Delta\overline{f}dr, \tag{7.57}$$

where overline implies the average over directions (over θ and φ). Since (→**??**) $\overline{f}$ is spherically symmetric, we have $\Delta\overline{f} = r^{-1}d^2(r\overline{f})/dr^2$ (→**??**). Hence,

$$\left\langle \Delta\frac{1}{|\boldsymbol{x}|}, f \right\rangle = 4\pi\int_0^\infty \frac{d^2}{dr^2}r\overline{f}dr = 4\pi[r\overline{f}' + \overline{f}]_0^\infty = -4\pi f(0). \tag{7.58}$$

7.22 Integral of generalized functions. A generalized function F is an *integral* of f, if $F' = f$. That is, $\langle F, \phi\rangle = -\langle f, \Phi\rangle$, where $\Phi' = \phi \in \mathcal{D}$.[108] Just as the ordinary calculus, we have a
Theorem. The integral of a generalized function is unique up to an additive constant. □
In summary, all the ordinary calculus rules survive.

Discussion.
The following integrals are sometimes useful (→**32C** also):

$$|u| = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{1-\cos ku}{k^2}dk, \tag{7.59}$$

$$\pi\delta(x) \pm iP\frac{1}{x} = \int_0^\infty e^{\pm ixk}dx, \tag{7.60}$$

$$\frac{\pi}{2}\min(a,b) = \int_0^\infty \frac{\sin ax \sin bx}{x^2}dx. \tag{7.61}$$

[108] There is a technical difficulty in this definition, since Φ may not be in $\mathcal{D}$. This problem can be overcome. See, for example, D. H. Griffel, *Applied Functional Analysis* (Ellis Harwood LTD, 1981), p. 38 Theorem 2.2.

7.23 Convolution. The *convolution* $p*q$ of two generalized functions p and q is defined as

$$\langle p*q, f\rangle \equiv \int dx \int dy\, p(x)q(y)f(x+y). \tag{7.62}$$

We use the following notation as well which is consistent with the above formula.

$$p*q(x) = \int p(y)q(x-y)dy. \tag{7.63}$$

Notice that $*$ is commutative, that is, $p*q = q*p$, and associative, that is, $q_1*(q_2*q_3) = (q_1*q_2)*q_3$. Therefore, we may define $q_1*q_2*q_3*\cdots$.

Exercise.
Compute $\delta'*|x|$. See **7.24**(2).

7.24 Example.
(1) $\delta*q = q$. That is, the delta function serves as the unit element for $*$-product.
(2) $\delta'*q = q'$. More generally, $\delta^{(n)}*q = q^{(n)}$. For example, $(\Delta\delta)*q = \Delta q$.
(3) $(p*q)' = p'*q = p*q'$. This can be demonstrated easily with the aid of (2) and associativity of $*$-product.
(4) The solution to Poisson's equation (→**1.7**)

$$\Delta\phi = -\frac{\rho}{\epsilon_0} \text{ with } \phi \to 0 \quad (|x| \to \infty) \tag{7.64}$$

is given by $\rho*(1/4\pi\epsilon_0|x|)$ (→**7.21**). This is an implementation of Green's idea (→**3.6**).

8 Green's Functions for ODE

Green's functions for second order linear ODE are constructed explicitly. Symmetry of the Green's function can be demonstrated clearly.

Key words: δ-function, Green's operator, fundamental solution, Green's function, Sturm-Liouville problem.

Summary:
(1) Understand the method to construct a fundamental solution in **8.2**.
(2) If we can obtain a fundamental system of solutions, we can construct the Green's function for a regular Sturm-Liouville problem (**8.6**-**8.7**).

8.1 Fundamental solution exists for ODE. Let

$$\mathcal{L} \equiv \sum_{i=0}^{n} a_i(x) \left(\frac{d}{dx}\right)^{n-i}, \tag{8.1}$$

where $a_0(x) \neq 0$ and $a_0, \cdots, a_n$ are smooth functions. Then $\mathcal{L}u = 0$ has a fundamental solution ($\rightarrow$**7.2**). The difference of any two fundamental solutions is a solution to the homogeneous equation $\mathcal{L}u = 0$ ($\rightarrow$**4.28**). □
We will demonstrate this for $n = 2$ below through explicitly constructing a fundamental solution.

8.2 Proof of 8.1 for $n = 2$. We wish to find a solution to

$$\left(a_0 \frac{d^2}{dx^2} + a_1 \frac{d}{dx} + a_2\right) w(x|y) = \delta(x - y). \tag{8.2}$$

Regard x as the time variable. and assume that $w(x|y) \to 0$ as $x \to -\infty$. Then, causality implies that $w(x|y) = 0$ for $x < y$. d^2w/dx^2 cannot have a singularity worse than $\delta(x - y)$, so that dw/dx is at worst discontinuous at $x = y$, and w is continuous at $x = y$ ($\rightarrow$**??**). Hence, we may assume $w(y + 0|y) = 0$. Since (8.2) is a second order ODE, we can construct its solution uniquely with one more condition. Integrate (8.2) from $x = y - \epsilon$ to $y + \epsilon$ for infinitesimal $\epsilon > 0$. We get ($w^{(1)} \equiv dw/dx$)

$$a_0(y)[w^{(1)}(y + 0|y) - w^{(1)}(y - 0|y)] = 1. \tag{8.3}$$

Here we have used the continuity of a_0 and w. We have already assumed that w is zero for $x < y$, so that this equation implies

$$a_0(y)w^{(1)}(y+0|y) = 1. \tag{8.4}$$

This is the needed second condition. In this way, we can construct a solution to (8.2).

8.3 Example: damped oscillator under impact. Find a fundamental solution to[109]

$$\frac{d^2x}{dt^2} + 2k\frac{dx}{dt} + \omega^2 x = \delta(t-s). \tag{8.5}$$

The fundamental solution constructed in **??** reads for this case

$$w(t|s) = (\omega^2 - k^2)^{-1/2} e^{-k(t-s)} \sin\left[\sqrt{\omega^2 - k^2}(t-s)\right] \Theta(t-s). \tag{8.6}$$

8.4 Regular Sturm-Liouville problem.

$$\mathcal{L}_{ST}u \equiv \left[\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right] u = 0 \tag{8.7}$$

under the following boundary condition is called a *regular Sturm-Liouville problem* (cf. **17.7**), if p is of constant sign:

$$B_a[u] \equiv Ap(a)u'(a) - Bu(a) = 0, \tag{8.8}$$
$$B_b[u] \equiv Cp(b)u'(b) - Du(b) = 0, \tag{8.9}$$

where A, B, C and D are constants (cf. **??**).

8.5 Theorem [Green's function exists for recular Sturm-Liouville problem]. The Green's function for a regular Sturm-Liouville problem

$$\mathcal{L}_{ST}u = \delta(x-y) \tag{8.10}$$

under the above boundary condition exists, if the operator does not possess zero eigenvalue. The Green's function, when it exists, is a symmetric function of x and y. □

[109] The best way to solve this under the condition $x = 0$ for $t < s$ and $x'(s+0) = 1$ (this corresponds to (8.4)) is to use the Laplace transformation (→**33**).

Exercise.
Under what condition does the following operator with the boundary condition: $u(0)$ bounded and $u(a) = 0$, not have the Green's function?

$$Lu = u'' + \frac{1}{x}u' + \left(k^2 - \frac{16}{x^2}\right)u. \tag{8.11}$$

The symmetry of the Green's function is proved by explicitly constructing the required Green's function as follows:

8.6 Explicit form of Green's function. The Green's function for a regular Sturm-Liouville problem in **??** is given by

$$G(x|y) = \begin{cases} Ku_1(x)u_2(y) & \text{for } x < y, \\ Ku_2(x)u_1(y) & \text{for } x > y, \end{cases} \tag{8.12}$$

where $K^{-1} = p(x)(u_1u_2' - u_2u_1')$ (which is actually a constant); u_1 is a nontrivial solution to $\mathcal{L}_{ST}u = 0$ with $B_a[u] = 0$, and u_2 is a nontrivial solution to $\mathcal{L}_{ST}u = 0$ with $B_b[u] = 0$.□
Indeed, $G(x|y) = G(y|x)$ (→**??**, cf. **9.16**). As we will see soon, $\{u_1, u_2\}$ is a fundamental system of solutions (→**??**) for $\mathcal{L}_{ST}u = 0$.
Exercise. Demosntrate the symmetry $G(x|y) = G(y|x)$.

8.7 Construction of Green's function. From $\mathcal{L}_{ST}G = \delta(x - y)$, we see that $G(y + 0|y) = G(y - 0|y)$, and

$$p(y)\left[\frac{\partial}{\partial x}G(x|y)\,|_{x=y+0} - \frac{\partial}{\partial x}G(x|y)\,|_{x=y-0}\right] = 1. \tag{8.13}$$

See (8.3) in **8.2**. We can always construct u_1 and u_2 as stated above. Let us construct G in the following form:

$$G(x|y) = \begin{cases} c_1(y)u_1(x) & \text{for } x < y, \\ c_2(y)u_2(x) & \text{for } x > y. \end{cases} \tag{8.14}$$

To satisfy the conditions at $x = y$, we get

$$c_1(y)u_1(y) = c_2(y)u_2(y), \tag{8.15}$$
$$c_1(y)u_1'(y) - c_2(y)u_2'(y) = -1/p(y). \tag{8.16}$$

We can solve this for c_1 and c_2 only if $u_1u_2' - u_1'u_2 \neq 0$ (that is, the Wronskian (→**??**) of u_1 and u_2 is nonzero), but this is guaranteed.[110]

[110] Notice that this condition is the condition that the Sturm-Liouville eigenvalue problem (→**??**) does not have zero eigenvalues. $u_1u_2' - u_1'u_2 = 0$ implies that $d(u_1/u_2)/dx = 0$ or $u_1 \propto u_2$. That is, u_1 satisfies $\mathcal{L}_{ST}u_1 = 0$ and $B_a[u_1] = B_b[u_1] = 0$, and $u_1 \not\equiv 0$. Hence, u_1 is an eigenfunction belonging to 0.

Since u_1 and u_2 satisfy $\mathcal{L}_{ST}u = 0$,

$$\frac{d}{dx}[p(x)(u_1u_2' - u_1'u_2)] = u_1\mathcal{L}_{ST}u_2 - u_2\mathcal{L}_{ST}u_1 = 0. \tag{8.17}$$

Hence

$$p(x)(u_1u_2' - u_2u_1') \equiv K^{-1} \tag{8.18}$$

is a nonzero constant. Using this constant, we can solve as $c_1 = Ku_2$ and $c_2 = Ku_1$.

8.8 Remark. If we know a fundamental solution $w(x|y)$ to $\mathcal{L}u = \delta(x-y)$, then the general solution to this inhomogeneous equation can be written as (→**4.28**)

$$G(x|y) = w(x|y) + A(y)u_1(x) + B(y)u_2(x). \tag{8.19}$$

A and B can be determined to satisfy the boundary conditions (they can depend on y).

8.9 Examples. The following examples can be solved either by the method of **8.7** or **8.8**.
(1) $u'' = 0$ with the boundary conditions $B_0[u] = u'(0) - u(0) = 0$ and $B_1[u] \equiv u'(1) = 0$. The Green's function for this is $G(x|y) = (x-y)\Theta(x-y) - (x+1)$.[111]
(2) $(d^2/dx^2 + k^2)u = 0$ with the boundary condition $B_0[u] \equiv u(0) = 0$ and $B_1[u] \equiv u(1) = 0$ (assume $\sin k \neq 0$). The Green's function for this is

$$G(x|y) = \begin{cases} \sin kx \sin k(y-1)/k \sin k & \text{for } x < y, \\ \sin ky \sin k(x-1)/k \sin k & \text{for } x > y. \end{cases} \tag{8.20}$$

Exercise.
(A) Obtain the Green's function with a Dirichlet condition of the equation

$$\sqrt{x}\frac{d}{dx}\left(\sqrt{x}\frac{du}{dx}\right) + a^2u = 0 \tag{8.21}$$

on $[0, L]$, knowing that the general solution to this equation is given by

$$u(x) = A\sin(2a\sqrt{x}) + B\cos(2a\sqrt{x}). \tag{8.22}$$

(Calculation of K is messy, so you may forget about it.)
(B) Determine the Green's function for

$$L = \frac{d}{dx}x\frac{d}{dx} - \frac{1}{x} \tag{8.23}$$

[111] The definition of $\Theta(x-y)$ at $x = y$ does not matter. That is, we may interpret Θ as a generalized function (→**7.4**).

with the homogeneous boundary conditions $u(0) = u(1) = 0$.[112]
(C) Consider the following 1-Schrödinger problem

$$(-\Delta + V)\psi = E\psi, \tag{8.24}$$

where V vanishes at infinity. If this equation has a bound state (i.e., a solution in L_2-space $\rightarrow$**??**, in otherwise normalizable as a wave function), it cannot be degenerate. In particular, the lowest energy bound state (ground state) cannot be degenerate. Prove this showing or answering the following:
(1) Degeneracy implies that there are two independent solutions for a given energy. What must be their Wronskian?
(2) The Wronskian for localized state is zero.

(D) Show that the Green's function for the following operator

$$\left[\frac{d}{dx}(1-x^2)\frac{d}{dx} - \frac{n^2}{1-x^2}\right] \tag{8.25}$$

with the boundary condition that the solution is bounded at $x = \pm 1$, where $n \in \boldsymbol{N}$, is given by

$$G(x|y) = \frac{1}{2n}\left(\frac{1+x)(1-y)}{(1-x)(1+y)}\right)^{n/2} \tag{8.26}$$

for $x \leq y$.

8.10 Theorem [Inhomogeneous boundary condition]. The solution to the following inhomogeneous boundary value problem:

$$\begin{aligned} \mathcal{L}u(x) &= \varphi(x), & (8.27)\\ B_a[u] &= \alpha, \quad B_b[u] = \beta, & (8.28) \end{aligned}$$

where $\mathcal{L}$, B_a and B_b are the same as in **8.4**, and $BD \neq 0$, is given by

$$u(x) = \int_a^b dy G(x|y)\varphi(y) + p(a)B^{-1}\alpha\left(\frac{\partial G}{\partial y}\right)_{y=a} - p(b)D^{-1}\beta\left(\frac{\partial G}{\partial y}\right)_{y=b}. \tag{8.29}$$

[Demo] First, we note an analogue of Green's formula ($\rightarrow$**??**, cf. **??**)

$$\int_a^b dx u\mathcal{L}v - \int_a^b dx v\mathcal{L}u = p(uv' - u'v)|_a^b. \tag{8.30}$$

Let $v(x) \equiv G(x|y)$, and u be the solution to the problem. Then, (8.30) implies

$$u(y) = \int_a^b dx G(x|y)\varphi(x) + \left\{p(x)[u(x)\frac{\partial G}{\partial x} - Gu'(x)]\right\}_{x=a}^{x=b}. \tag{8.31}$$

[112] Hint: The equation is equidimensional ($\rightarrow$**??**).

Exchanging x and y in this formula, and using the symmetry of the Green's function (→**8.6**, **??**), we get (note $B_b[u] = \beta$ and $B_b[G] = 0$)

$$Du(b)\partial_y G(x|y)|_{y=b} - Du'(b)G(x|b) = -\beta\partial_y G(x|b) \tag{8.32}$$

An analogous formula holds at the other end of the region. These relations allow us to rewrite the second term of (8.31) as desired.
Exercise.
Use the Green's function to solve

$$\left(\frac{d^2}{dx^2} + k^2\right) u = \sin kx \tag{8.33}$$

on $[0, 1]$ with the boundary condition $u(0) = u(1) = 1$.

8.11 Another method to solve inhomogeneous case. Practically, the following (usual) splitting method is also very useful: Separate the problem (8.27) + (8.28) as
(I) $\mathcal{L}u_1 = 0$ with the inhomogeneous boundary condition $B_a[u_1] = \alpha$, $B_b[u_1] = \beta$.
(II) $\mathcal{L}u_2 = \varphi$ with the homogeneous boundary condition $B_a[u_2] = 0$, $B_b[u_2] = 0$.
The solution we want is given by $u_1 + u_2$. (I) can be solved as usual (→XX), and (II) can be solved with the aid of the Green's function as $u_2 = \int dy G(x|y)\varphi(y)$.

9 Green's Function for PDE – Elementary Approach

Green's idea is illustrated with simple (but representative) examples. We first construct free space Green's functions. With the aid of the image source method, we construct Green's functions for simple domains as well. Dirichlet boundary value problems for the Laplacian are discussed toward the end.

Key words: free space Green's function, method of descent, method of images, reflection principle, image source, conformal map, Green's theorem

Summary:
(1) Free space Green's functions can be constructed as spherically symmetric solutions (**??**-**??**, **9.22**, **??**).
(2) Inhomogeneous equations can be solved with the aid of Green's functions (**9.17**, **9.39**).
(3) Green's functions for simple domains may be constructed with the aid of the method of images (**9.3**-**9.13**, **9.27**, **9.34**).
(4) In 2-space, conformal maps can be fully exploited to construct Green's function for the Laplace equation. Neumann problems can be reduced to Dirichlet problems (→**??**), and the latter can be mapped on a Dirichlet problem on the unit disk (**??**, **9.41**, **9.42**). Look up 'stylebooks' of conformal maps.

9.1 Method of descent. In d-space, if we assume that the system is translationally symmetric along one coordinate direction, then the cross-section of this solution perpendicular to this direction should be indistinguishable from the $(d-1)$-space result. That is, averaging over one direction of d-space results gives $(d-1)$-space results. This method to obtain lower dimensional results is called the *method of descent*.

Since

$$-\Delta_d\varphi = -\left(\Delta_{(d-1)} - \frac{d^2}{dx_d^2}\right)\varphi = \delta_{d-1}(\boldsymbol{x}' - \boldsymbol{y}')\delta(x_d - y_d), \qquad (9.1)$$

Integrating this w.r.t. x_d, we get from the d-problem the desired $(d-1)$-problem. If we integrate the d-Coulomb potential (**??**) over x_d, then we should get the $(d-1)$-Coulomb potential, because $\int dx_d \delta_d(\boldsymbol{x} - \boldsymbol{y}) = \delta_{d-1}(\boldsymbol{x}' - \boldsymbol{y}')$, where $\boldsymbol{x}'$ is $\boldsymbol{x}$ with its x_d-component suppressed. The best way to demonstrate this is to use the exponentiation trick

explained in **14.9** and to integrate over x_d:

$$\int_{-\infty}^{+\infty} dx_d \frac{1}{(a^2+x_d^2)^{(d-2)/2}} = \int_0^{+\infty} dt \int_{-\infty}^{+\infty} dx_d \frac{1}{\Gamma((d-2)/2)} t^{(d-2)/2-1} e^{-(a^2+x_d^2)t}, \tag{9.2}$$

$$= \frac{\sqrt{\pi}}{\Gamma((d-2)/2)} \int_0^{+\infty} dt\, t^{(d-3)/2-1} e^{-a^2 t} \tag{9.3}$$

$$= \frac{\sqrt{\pi}}{\Gamma((d-2)/2)} \Gamma\left(\frac{d-3}{2}\right) \frac{1}{a^{d-3}}, \tag{9.4}$$

where $a^2 = x_1^2 + \cdots + x_{d-1}^2$. With the aid of this and the fundamental functional relation **??** of the Gamma function, we eventually obtain the $(d-1)$-Coulomb potential. This is a good exercise.

9.2 Green's function in (semi)bounded space. If the domain of the equation is (semi)bounded, then to satisfy the boundary conditions is nontrivial in general. However, if the domain enjoys nice symmetries, there is a clever way – method of image sources. Basically, we tessellate the space by the copy of the domain with appropriate sign change of the source terms (called *image sources*).

9.3 Method of images I. Half space. The Green's function $G(x,y,z|x',y',z')$ for 3-Laplace equation is the electrostatic potential at (x,y,z) due to a point charge at (x',y',z') with a suitable potential values specified on the boundary of the region. The Green's function for the Laplace equation on the $x>0$ half space with a (homogeneous) Dirichlet boundary condition is given by

$$G_D(x,y,z;x',y',z') = \frac{1}{4\pi}\left[\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}} - \frac{1}{\sqrt{(x+x')^2+(y-y')^2+(z-z')^2}}\right]. \tag{9.5}$$

Here the source term is at (x',y',z'), and its image source is at $(-x',y',z')$. To maintain the zero potential condition at $x=0$, the effects of the both sources must cancel exactly on the yz-plane. Hence, the image source must be -1.
If the boundary condition is the homogeneous Neumann condition at $x=0$, then to kill the gradient on the yz-plane, the image charge

must be +1. Hence, the Neumann function (= Green's function with a Neumann condition) for semiinfinite space reads

$$G_N(x,y,z;x',y',z') = \frac{1}{4\pi}\left[\frac{1}{\sqrt{(x-x')^2+(y-y')^2+(z-z')^2}} + \frac{1}{\sqrt{(x+x')^2+(y-y')^2+(z-z')^2}}\right]. \quad (9.6)$$

9.4 Method of images II. More complicated cases. As we have seen the locations of image sources and their signs are what we need. Several examples are illustrated.

Warning. If the region under consideration is bounded (i.e., enclosed in a finite sphere whose center is located at the origin), then the Neumann condition Green's function (Neumann's function) for the Laplace equation requires an extra care (→**1.22**(3)), so we will NOT discuss this case here. See **??** and **??**.

Exercise.
(1) Find the Green's function for the Laplace equation on the infinite strip $(-\infty,+\infty)\times[0,\pi]$ with a homogeneous Dirichlet condition. [The reader must impose a further condition to single out the solution (→**1.22** Discussion (2)).
(2) Find the Green's function for the Laplace equation on the half 3-space defined by $x > a$, where a is a constant.
(3) Find the electric potential in 3-space with $x = 0$ and $y = 0$ maintained at zero potential and the charge Q placed at $(x', y', 0)$.

9.5 Harmonicity and symmetry. Green's functions for the Laplace equation are harmonic (→**3.11**) except at their singularities. If we study the method of images, the keys are

(1) harmonicity is preserved by reflection,
(2) charges are mirrored onto charges.
Hence, the essence of the method of images is that there are special symmetry operations preserving harmonicity.

9.6 Reflection principle. Let D be a region such that if $(x_1, x_2, \cdots, x_{d-1}, x_d) \in D$, then $(x_1, x_2, \cdots, x_{d-1}, -x_d) \in D$. Write D^+ for the subset of D for $x_d > 0$ and $D^- = D \setminus D^+$. If u is harmonic ($\rightarrow$**3.11**) on D^+ and $u = 0$ for $x_d = 0$ (that is, on the boundary between D^+ and D^-), then the function g defined as

$$\begin{aligned} g(x_1, \cdots x_{d-1}, x_d) &= u(x_1, \cdots x_{d-1}, x_d) \quad \text{on } D^+ && (9.7) \\ &= -u(x_1, \cdots x_{d-1}, -x_d) \quad \text{on } D^- && (9.8) \end{aligned}$$

is a harmonic function on the whole D. □
[Demo] Inside D^- g is obviously harmonic. Therefore, we have only to take care of g near the boundary between D^+ and D^-. This is easy to show if we use the converse of the mean-value theorem **??**.

9.7 Conformal mapping. A *conformal transform* (*Kelvin transform*) $\hat{u}$ of a function u is given in d-space by

$$\hat{u}(\boldsymbol{x}) = |\boldsymbol{x} - \boldsymbol{a}|^{2-d} u((\boldsymbol{x} - \boldsymbol{a})/|\boldsymbol{x} - \boldsymbol{a}|^2), \tag{9.9}$$

where $\boldsymbol{a}$ is a constant. This is the composition of translation $\boldsymbol{x} \to \boldsymbol{x} - \boldsymbol{a}$ and inversion $\boldsymbol{x} \to \boldsymbol{x}/|\boldsymbol{x}|^2$. Notice that this transformation makes the universe 'inside out'; big scales become small and vice versa, and keeps the unit sphere centered at $\boldsymbol{a}$ intact.[113] That is, the Kelvin transformation makes the universe inside out.

9.8 Harmonicity is conformal invariant. Let $\hat{D} \subset \boldsymbol{R}^d \setminus \{\boldsymbol{a}\}$ and $D = \{\boldsymbol{x} \,|\, \boldsymbol{x} = (\boldsymbol{y} - \boldsymbol{a})/|\boldsymbol{y} - \boldsymbol{a}|^2, \boldsymbol{y} \in \hat{D}\}$. If u is harmonic on D, then $\hat{u}$ given by (9.9) is again harmonic on $\hat{D}$. □
Note that the Kelvin transformation transforms a harmonic function on a ball centered at $\boldsymbol{a}$ to a harmonic function defined on the domain outside the ball. Remember that a half space can be interpreted as a sphere with an infinite radius.

[113] Actually, the definition of conformal maps should be more general, but if n is not even, then the combination of the Kelvin transformation and affine transformations exhaust the conformal transformation.

9.9 Demonstration of conformal invariance of harmonicity. To show **9.8** we have only to demonstrate $\Delta\hat{u}(x) = 0$ honestly. However, a clever organization of calculation is desirable. We may set $\boldsymbol{a} = 0$ without any loss of generality. First, notice that

$$\frac{\partial^2}{\partial x_i^2} fg = \frac{\partial^2 f}{\partial x_i^2} g + 2\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial x_i} + f\frac{\partial^2 g}{\partial x_i^2}, \tag{9.10}$$

and

$$\frac{\partial}{\partial x_i} u\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|^2}\right) = u_j\left(\frac{\boldsymbol{x}}{|\boldsymbol{x}|^2}\right)\left(\frac{\delta_{ij}}{|\boldsymbol{x}|^2} - 2\frac{x_i x_j}{|\boldsymbol{x}|^4}\right), \tag{9.11}$$

where $u_j = \partial u/\partial x_j$. We have only to show the formula for $\boldsymbol{x} \neq 0$. Note that $\partial_i^2 |\boldsymbol{x}|^{2-d} = 0$. The rest is left for the reader.

9.10 Method of images III General case. The conformal invariance **9.8** and the reflection principle **9.7** provide a special method to solve Poisson's equation; actually, we have already used the reflection principle repeatedly (→**9.25**, **9.4**). It is often easier to solve a problem without boundary conditions at finite distance. Use **9.7** and **??** to extend the domain with boundary conditions to the whole space. An important point is that a singularity is conformally mapped to a singularity. That is, the images of charges must be charges (*image charge*).

9.11 Sphere, Dirichlet condition. Physically this is the problem of finding electric potential in the sphere surrounded by a grounded conducting sphere. A charge of q is at $(r, 0, 0)$ $(a > r > 0$, that is, inside the sphere) and a grounded sphere of radius a is centered at the origin. We use the conformal invariance of harmonicity (→**9.8**). Consider the conformal map which makes the sphere inside out:

$$\boldsymbol{r} \to a^2\boldsymbol{r}/r^2. \tag{9.12}$$

The image of $(r, 0, 0)$ due to this map is at $(a^2/r, 0, 0)$. Therefore the mapped field must have a singularity at this point. This means that there is a charge (image charge) q' there. This is determined by the fact that at $(a, 0, 0)$ the field must be zero:

$$\frac{q}{a^2/r - a} + \frac{q'}{a - r} = 0. \tag{9.13}$$

That is, $q' = -aq/r$. Thus, we have, inside the sphere

$$\phi = \frac{q}{4\pi\epsilon_0}\left(\frac{1}{\sqrt{(x-r)^2 + y^2 + z^2}} - \frac{a}{r\sqrt{(x - a/r)^2 + y^2 + z^2}}\right). \tag{9.14}$$

From this the Green's function for the sphere under the Dirichlet condition is obtained.

Exercise.
Construct the Green's function for a disk with a Dirichlet condition. Then, compare the result with the one obtained with the aid of conformal maps (→**??**, **9.41**).

9.12 Charge outside conducting sphere, not grounded. Suppose the charge is outside the sphere. In this case the net charge induced on the sphere must be zero due to charge conservation. If we put q' given in **9.11** at a^2/r and $-q'$ at the origin, all the boundary conditions are satisfied (See also Jackson, Section 2.6).

9.13 Method of images for dielectric materials. Method of images can be generalized to the cases with dielectric materials, but only for the cases with plane surfaces (not applicable to dielectric spheres). See Jackson.

9.14 How to use Green's function (homogeneous Laplace case). If the boundary condition is homogeneous, then linear inhomogeneous PDE can be solved in terms of its Green's function as outlined in **3.6**. A typical problem is to solve Poisson's equation under homogeneous boundary condition

$$-\Delta\psi = f(\boldsymbol{x}), \tag{9.15}$$

which is solved as

$$\psi(\boldsymbol{x}) = \int_D d\boldsymbol{y} G(\boldsymbol{x}|\boldsymbol{y}) f(\boldsymbol{y}), \tag{9.16}$$

where D is the domain of the problem.

9.15 Green's formula. Let $D \subset \boldsymbol{R}^d$ be a bounded region, and u and v be C^2-functions defined on the closure of D. Then,

$$\int_D (v\Delta u + grad\, u \cdot grad\, v) d\tau = \int_{\partial D} v\, grad\, u \cdot d\boldsymbol{S}, \tag{9.17}$$

and

$$\int_D (v\Delta u - u\Delta v) d\tau = \int_{\partial D} (v\, grad\, u - u\, grad\, v) \cdot d\boldsymbol{S}. \tag{9.18}$$

[Demo] (9.17) follows immediately from $div(u\, grad\, v) = grad\, u \cdot grad\, v + u\Delta v$, and Gauss' theorem (→**3.13**). The second formula (9.18) is obvious from (9.17).

Exercise.
Let $D \subset \boldsymbol{R}^d$ be a region on which u is harmonic. Show

$$\int_{\partial D} grad\, u \cdot d\boldsymbol{S} = 0. \tag{9.19}$$

9.16 Symmetry of Green's function. (See **??** and **6.17** also) Let $G(\boldsymbol{x}|\boldsymbol{y})$ be the Green's function on the domain D with the homogeneous Dirichlet condition. Then,

$$G(\boldsymbol{x}|\boldsymbol{y}) = G(\boldsymbol{y}|\boldsymbol{x}). \tag{9.20}$$

To demonstrate this set $u = G(\boldsymbol{z}|\boldsymbol{x})$ and $v = G(\boldsymbol{z}|\boldsymbol{y})$ in Green's formula (the integration is over

9.17 Solution to Dirichlet problem in terms of Green's function. (See the warning in **9.4**.) The solution to the following Dirichlet problem on an open region D

$$-\Delta u = \varphi, \quad u|_{\partial D} = f, \tag{9.21}$$

where φ and f are integrable functions, is given by

$$u(x) = \int_D G(x|y)\varphi(y)dy - \int_{\partial D} f(y)\partial_{n(y)}G(x|y)d\sigma(y). \tag{9.22}$$

Here $\partial_{n(y)}$ is the outward normal derivative at y, τ is the volume element, and σ is the surface volume element.

The formula easily follows from Green's formula in **9.15** with u being the solution and v being the Green's function for the problem. In this way with the Green's functions we can solve inhomogeneous boundary condition problems.

Discussion.
(A) The second term in (9.22) is understood as the electric potential made by an electrical double layer.
(B) The surface integral in (9.22) can be written in the following remarkable form

$$\frac{1}{2\pi}\int_{\partial\Omega} d\omega f(y), \tag{9.23}$$

where ω is the solid angle of the surface element (at y) seen from x.[114]
(C) Derive the following *Kirchhoff's formula*: For $x \in D$

$$u(x) = \int_D G_0(x|y)\varphi(y)dy - \int_{\partial D} d\sigma(y)\left[u(y)\partial_{n(y)}G(x|y) - \partial_{n(y)}u(y)G_0(x|y)\right], \tag{9.24}$$

[114] B130.

where G_0 is the free space Green's function given in **??**. This formula is meaningful even when x is outside D. Show that this is zero if $x \notin D$. Because the first term in the formula is smooth, the discontinuity comes from the surface integral. The formula cannot be used to obtain the solution because we usually do not know u and its derivative on the surface simultaneously. Recall that the Cauchy problem of the Laplace equation is generally not well posed (→**??** for well-posedness).

9.18 Green's function for more general domain. We will discuss this in **XX** and **XX**.

9.A Green's Function for Diffusion Equation

9.19 Fundamental solution of diffusion equation. A fundamental solution (→**7.2**) of a diffusion equation is a solution to

$$\frac{\partial \psi}{\partial t} - D\Delta\psi = \delta(t-s)\delta(\boldsymbol{x}-\boldsymbol{y}). \tag{9.25}$$

It is easy to check by explicit calculation that in d-space

$$G(\boldsymbol{x},t|\boldsymbol{y},s) = \left(\frac{1}{4\pi D(t-s)}\right)^{d/2} \exp\left(-\frac{|\boldsymbol{x}-\boldsymbol{y}|^2}{4D(t-s)}\right) \tag{9.26}$$

is a solution. Hence, this is a fundamental solution of a diffusion equation (→**9.22**). This is also the Green's function (→**7.2**) for the diffusion equation (9.25) under the condition that the solution vanishes at infinity. This is often called the *diffusion kernel*. We can demonstrate (cf. **8.7**) that

$$w\text{-}\lim_{t\to s} G(\boldsymbol{x},t|\boldsymbol{y},s) = \delta(\boldsymbol{x}-\boldsymbol{y}). \tag{9.27}$$

Discussion.
(1) It is important to use the formal solution, or the integral equation form of PDE in terms of the Green's function, because it allows us to apply various approximation methods (→**??**). The formal solution of

$$\frac{\partial u}{\partial t} = D\Delta u + f(x,t)u \tag{9.28}$$

with an appropriate homogeneous boundary condition can be written as

$$u(x,t) = \int d\boldsymbol{y} G(\boldsymbol{x},t|\boldsymbol{y},0)u_0(\boldsymbol{y}) + \int_0^t ds \int d\boldsymbol{y} G(\boldsymbol{x},t|\boldsymbol{y},s)u(\boldsymbol{y},s)f(\boldsymbol{y},s), \tag{9.29}$$

where u_0 is the initial conditon, and G is the Green's function.
(2) Find the partial differential equation governing u satisfying the following integral equation

$$u(\boldsymbol{x},t) = \int d\boldsymbol{y} e^{-At} G(\boldsymbol{x},t|\boldsymbol{y},0) f(\boldsymbol{y}) - \int_0^t ds \int d\boldsymbol{y} e^{-A(t-s)} G(\boldsymbol{x},t|\boldsymbol{y},s) \{u(\boldsymbol{y},s)\}^3, \tag{9.30}$$

where G is given by (16.38), and f is a continuous function on the whole space. A is a constant, and the spatial integration range is the whole 3-space.

9.20 Scaling invariant solution of diffusion equation. Looking at the diffusion equation, we realize that the equation is invariant under the scaling transformation $(\boldsymbol{x},t) \to (\lambda\boldsymbol{x},\lambda^2 t)$.[115] If we demand that the solution keeps its total mass after scaling (we know the diffusion equation conserves the total mass →**2.9**)

$$\int \psi(\boldsymbol{x}) d\boldsymbol{x} = 1, \tag{9.31}$$

then, we conclude in d-space

$$\psi(\boldsymbol{x},t) = \lambda^d \psi(\lambda\boldsymbol{x},\lambda^2 t). \tag{9.32}$$

9.21 Dimensional analysis. Another way to obtain the scale invariant solution is to perform *dimensional analysis*. Dimensional analysis is a way to find combinations of variables that are invariant under change of units (i.e., change of scales). The dimension of a quantity Q is often denoted by $[Q]$. Let the dimension of length be L: $[\boldsymbol{x}] = L$, and that of time be T: $[t] = T$. Then $[D] = L^2/T$. Also from $\int dx\, u = 1$, we get $[u] = L^{-d}$. We can construct two dimensionless quantities (i.e., scale invariant quantities):

$$[\boldsymbol{x}/\sqrt{Dt}] = 1, \quad [(tD)^{d/2} u] = 1. \tag{9.33}$$

Therefore, $u(Dt)^{d/2}$ must be a function of $\boldsymbol{x}/\sqrt{Dt}$:

$$u(\boldsymbol{x},t) = (Dt)^{-d/2} f(\boldsymbol{x}/\sqrt{Dt}). \tag{9.34}$$

[115] This is actually the idea of dimensional analysis. See the next entry.

9.22 Scaling invariant spherically symmetric solution to diffusion equation. If we assume that the solution is spherically symmetric around $\boldsymbol{x} = 0$, then f in **9.21** depends on $r \equiv |\boldsymbol{x}|$. That is, there is a function h such that

$$\psi(\boldsymbol{x}, t) = t^{-d/2} h(r/\sqrt{Dt}). \tag{9.35}$$

Putting this into the diffusion equation, we get an ODE for h as a function of $x = r/\sqrt{Dt}$:

$$h'' + \left(\frac{d-1}{x} + \frac{x}{2}\right) h' + \frac{d}{2} h = 0. \tag{9.36}$$

Since the solution must be smooth at the origin, actually h must be a well-behaved function of x^2: $h(x) = g(x^2)$. g obeys the following equation:

$$\frac{d}{2}(g + 4g') + x^2 \frac{d}{dx}(g + 4g') = 0. \tag{9.37}$$

If we demand the boundedness of the solution, $g + 4g' = 0$ is the only choice. That is,

$$\psi(\boldsymbol{x}, t) = \frac{C}{t^{-d/2}} e^{-x^2/4Dt} \tag{9.38}$$

C is a constant determined by the normalization condition. We see (9.26) is obtained after shifting the source position in space time with the aid of the translational symmetry of the equation.

9.23 Initial trick for diffusion equation. Consider the following initial-boundary value problem for the diffusion equation on a region D:

$$\frac{\partial \psi}{\partial t} = D\Delta\psi, \quad \psi_{t=0} = \psi_0, \quad \psi|_{\partial D} = \varphi. \tag{9.39}$$

This problem can be converted to

$$\frac{\partial \psi}{\partial t} = D\Delta\psi + \delta(t)\psi_0, \quad \psi = 0 \text{ for } t \leq 0, \quad \psi|_{\partial D} = \varphi. \tag{9.40}$$

That is, the inhomogeneous initial condition is always converted to the source term ($\rightarrow$**2.7**) of the equation. This can be demonstrated by integrating the both sides of the equation (9.40) from $t = -\epsilon$ to $t = +\epsilon$ (cf. **8.2**), where $\epsilon > 0$ is taken to be 0 after integration with the assumption of the smoothness of the solution.

Exercise.
(A) Consider a uniform rod of length l with the thermal diffusion constant D (placed

along the x axis as $[0, l]$). The rod is thermally insulated except at the ends. The end temperatures are specified as

$$T(0,t) = g(t), \quad T(l,t) = h(t) \tag{9.41}$$

for $t > 0$,[116] and the initial condition is

$$T(x,0) = f(x). \tag{9.42}$$

Here f, g and h are assumed to be C^1 for simplicity.
(B) Consider a uniform rod of length l as above, but now the rod is not insulated. Heat is lost according to Newton's radiation law (→**1.21**) with the ambient temperature T_0. The end at $x = 0$ is maintained at the temperature A, and the other end is insulated. Let the initial temperature be uniform and A. The equation has the following form

$$\frac{\partial T}{\partial t} = D\frac{\partial^2 T}{\partial x^2} - c(T - T_0). \tag{9.43}$$

The standard trick to solve this is to introduce the new dependent variable $\tau = e^{-ct}(T - T_0)$.

9.24 Method of descent. Analogously to **9.1** we can obtain $(d-1)$-space Green's function from the d-space version. In the present case, this demonstration is easy with the aid of the Gaussian integral (→**??**).

9.25 Markovian property of diffusion kernel. The diffusion kernel (9.26) enjoys the following remarkable property called the *Markovian property*:

$$G(\boldsymbol{x}, t|\boldsymbol{y}, s) = \int d\boldsymbol{z} G(\boldsymbol{x}, t|\boldsymbol{z}, s')G(\boldsymbol{z}, s'|\boldsymbol{y}, s) \tag{9.44}$$

for any $s' \in (s, t)$. Notice that there is NO integration over the intermediate time s'. This can be demonstrated by direct integration. This can be more elegantly shown with the aid of Fourier and Laplace transform as we will see later (→**??**). A clever way may be touse the initial condition trick (9.40). This is the key to the Feynman-Kac path integral formula (→**??**, **??**).

9.26 —bf Random walk and heat kernel. Consider a walker whose n-th step is a vector $\boldsymbol{a}_n$. After N-steps, the position of the walker starting from the origin is $\boldsymbol{R} = \sum_{n=1}^{N} \boldsymbol{a}_n$. Each step vector is $\boldsymbol{e}_i$ or $-\boldsymbol{e}_i$ with equal probability $1/2d$, where $\boldsymbol{e}_i$ is the i-th the unit vector parallel to

[116] These conditions are compatible with any initial condition so long as $t = 0$ is excluded.

the i-th coordinate. The trajectory of the walker is a stochastic process called the random walk (on the simple cubic lattice, in this case). Let us compute the distribution function of the end position $\boldsymbol{R}$ after N steps. The density distribution is given by

$$f(\boldsymbol{R}, N) = \left\langle \delta \left(\boldsymbol{R} - \sum_{n=1}^{N} \boldsymbol{a}_n \right) \right\rangle , \tag{9.45}$$

where $\langle \ \ \rangle$ is the average over all the possible choices of all the steps. The best way to compute this average is to use its Fourier transform ($\rightarrow$**??**), or the generating function of $\boldsymbol{R}$:

$$\begin{aligned} \int_{-\infty}^{+\infty} f(\boldsymbol{R}, N) e^{i\boldsymbol{R}\cdot\boldsymbol{k}} d^d\boldsymbol{R} &= \left\langle \exp\left[\sum_{n=1}^{N} i\boldsymbol{k}\cdot\boldsymbol{a}_n \right] \right\rangle , & (9.46) \\ &= \langle \exp\left[i\boldsymbol{k}\cdot\boldsymbol{a}_1 \right] \rangle^N . & (9.47) \end{aligned}$$

Here the fact that all the steps obey the identical probability law has been used. From now on a physicist's approach is used.[117] We are interested in the large scale distribution, so we have only to study the above integral for small $\boldsymbol{k}$ only. We can approximate as

$$\int_{-\infty}^{+\infty} f(\boldsymbol{R}, N) e^{i\boldsymbol{R}\cdots\boldsymbol{k}} d^d\boldsymbol{R} = \left(1 - \frac{1}{2}k^2 + \cdots \right)^N \simeq e^{-Nk^2/2}. \tag{9.48}$$

Inverting this Fourier transform, we get

$$f(\boldsymbol{R}, N) = \sqrt{\frac{d}{2\pi N}} e^{-dR^2/2N}. \tag{9.49}$$

This is essentially the heat kernel. This implies that the diffusion equation describes the average behavior of the random walk, or the behavior of the ensemble of random walkers.

The Markovian property **9.25** can be interpreted as the sum of all the gate probabilities as shown in the figure.

[117] For a more respectable approach, see W Feller, *Introduction to Probability Theory and Its Applications* (Academic Press), for example.

9.27 Method of images for diffusion equation – image sources. We know the Green's function (9.26) for the diffusion equation in the infinite space $\boldsymbol{R}^3$ (→**16B.1**). Now, consider the equation on the half space $x > 0$ with the boundary condition that $u = 0$ on the yz-plane.
(1) **Dirichlet case**. The unit impulsive source is placed at time $t = 0$ at $x = x' > 0$. Let G^- be the Green's function whose unit impulsive source at time $t = 0$ is placed at $x = -x'$. Then, $H \equiv G - G^-$ satisfies all the conditions of the problem. That is, H is the desired Green's function for the half space with a homogeneous Dirichlet condition at $x = 0$. This means that H is the solution to the whole space problem with +source at x' and −source at $-x'$. The latter is the *image source* for the current problem.
(2) **Neumann case**. If the boundary condition at the origin is a homogeneous Neumann condition, then $G+G^-$ should be the desired Green's function in the half space. That is, +source at $-x_0$ is the needed image source to make the problem a whole space problem. More complicated cases discussed in **9.4** can be treated analogously. In the case of diffusion equation, there is no difficulty for the Neumann problem on a bounded region.

Exercise.
(A) Find the solution of the diffusion equation on $[0, 1]$ with a homogeneous Dirichlet condition at $x = 0$ and a homogeneous Neumann condition at $x = 1$ with a unit impulsive source placed at $x = x_0$ at time $t = 0$.
(B) **Diffusion equation to defend God?** Kelvin accepted organic evolution advocated by Darwin, but he could not swallow the logical consequence of Darwinism: no design or in this case no divine intervention at the beginning of life. He used heat conduction to destroy Darwinism:
The temperature gradient in the Earth near its surface is roughly $v = 0.035$K/m at the present time. He assumed that the Earth was a homogeneous sphere of radius $R \simeq 6400$km. The evolution of the temperature $T(\boldsymbol{r}, t)$ at position $\boldsymbol{r}$ at time t obeys Fourier's law

$$\frac{\partial T}{\partial t} = \kappa \nabla^2 T.$$

At time $t = 0$ he assumed that the Earth was at its melting temperature which was $T_0 = 3000$K above the surface temperature for $|\boldsymbol{r}| < R$. Its surface temperature must have been close to the present temperature for all $t > 0$ to allow life. Let us choose this to be the zero point of temperature for all $t > 0$.
(1) Using the numbers v, T_0 and R, give an argument that the thickness of the transition layer over which the temperature differs significantly from T_0 is much smaller than the Earth's radius at the present time.
(2) Hence, the full sphere problem simplifies to the 1-d problem:

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$

under the condition that $T(x, 0) = T_0$ for all $x > 0$, and $T(0, t) = 0$ for all $t > 0$. Find the solution.

(3) Using the value of v, compute the age (in years) of the Earth, assuming that the thermal diffusivity is $\kappa = 0.7 \times 10^{-6}\mathrm{m}^2/\mathrm{s}$.[118]
(4) Read the following to be a bit wiser as a physicist:
C. Darwin, *The Origin of Species* (Sixth edition Jan, 1872) Chapter X, " Sir W Thompson concludes that the consolidation of the crust can hardly have occurred less than 20 or more than 400 millions years ago, but probably not less than 98 or more than 200 millions years."
Ibid., Chapter XV, "$\cdots$ and this objection, as urged by Sir William Thompson, is probably one of the gravest as yet advanced, I can only say firstly, that we do not know at what rate species change as measured by years, and secondly, that many philosophers are not as yet willing to admit that we know enough of the constitution of the universe $\cdots$"

Now we know Darwin was perfectly right. Thompson did not know the radioactivity. In a certain sense, in retrospect at least, Darwin pointed out the existence of unknown physics.

Later, Huxley commented: Mathematics may be compared to a mill of exquisite workmanship, which grinds your stuff of any degree of fineness; but nevertheless. what you get out depends what you put in; and as the grandest mill in the world will not extract wheat-flour from peascods, so pages of formulae will not get a definite result out of loose data. However, in this case the defect of the theory was much more serious. In any case Darwin did not have much respect of mathematics; Boltzmann was strongly influenced by Darwin, and he suggested that the 19th century may be called the century of Darwin.

It is said that Fourier had a dream to explore the interior of the earth thr ough the studyof heat conduction, and then to study the formation process of the earth and the solar system. Kelvin seems to have realized a nightmare.

9.28 How to use Green's function: homogeneous boundary problems. In the case of the diffusion equation (with a source term),

$$\frac{\partial \psi}{\partial t} - D\Delta\psi = \sigma(\boldsymbol{x}, t), \tag{9.50}$$

even if the boundary condition is homogeneous, we must take into account the initial condition (→**??**):

$$\psi(\boldsymbol{x}, 0) = f(\boldsymbol{x}). \tag{9.51}$$

We already know that the nitial condition can be absorbed into the source term (→**9.23**), so that

$$\frac{\partial \psi}{\partial t} - D\Delta\psi = \sigma(\boldsymbol{x}, t) + f(\boldsymbol{x})\delta(t). \tag{9.52}$$

[118] The number obtained here is ridiculously short (although much longer than some beliefs based on the wrong reading of the Bible).

Thus the solution to (9.50) + (9.51) with a homogeneous boundary condition can be written in terms of the Green's function as

$$\psi(\boldsymbol{x},t) = \int_D d\boldsymbol{y} \int_0^t ds G(\boldsymbol{x},t|\boldsymbol{y},s)\sigma(\boldsymbol{y},s) + \int_D d\boldsymbol{y} G(\boldsymbol{x},t|\boldsymbol{y},0)f(\boldsymbol{y}). \tag{9.53}$$

Here D is the domain of the problem (cf. **??**).

To solve inhomogeneous boundary value problems, we can use **9.29**, but there is a clever trick. See **??**.

Discussion.
Solve the following semilinear parabolic equation to order ϵ in free 1-space:

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2} - \epsilon u^3 \tag{9.54}$$

with the initial condition

$$u(0) = \frac{1}{\sqrt{2\pi\delta}} e^{-x^2/2\delta}. \tag{9.55}$$

Here δ is a small positive constant. Demonstrate that the order ϵ term is asymptotically (for $t/\delta \gg 1$) proportional to $\ln(t/\delta)$.[119]

9.29 Analogue of Green's formula for diffusion equation. We have a formula analogous to Green's formula (→**9.15**) for diffusion equation. This generalization will be postponed to **XX**.

9.B Green's Function for Wave Equation

9.30 Free-space Green's function for 3-wave equation. We wish to solve

$$\left(\frac{\partial^2}{\partial t^2} - c^2\Delta\right)\psi = \delta(t)\delta(\boldsymbol{x}). \tag{9.56}$$

It is not hard to guess (from physics) a spherical symmetric solution as

$$\psi(\boldsymbol{x},t) = \frac{\delta(|\boldsymbol{x}| - ct)}{4\pi c|\boldsymbol{x}|}\Theta(t), \tag{9.57}$$

where the step function Θ is put to satisfy the causality. Check that this is indeed the solution.

[119] If the reader is familiar with the renormalization group theory, it is immediate from this observation that the problem has a renormalization group structure governing the long-time behavior.

The following calculation may be helpful. Under spherical symmetry, the wave equation reads for $|\boldsymbol{x}| > 0$

$$\left(\frac{\partial^2}{\partial t^2} - \frac{1}{r}\frac{\partial^2}{\partial r^2}r\right)\psi = 0 \tag{9.58}$$

It is worth remembering that if we introduce $r\psi = F$, then F obeys a 1d wave equation.

The topic of this section naturally continues to section 39.Now with the aid of space-time translational symmetry, we obtain the Green's function for the free space as

$$G(\boldsymbol{x}, t|\boldsymbol{y}, s) = \frac{\delta(|\boldsymbol{x} - \boldsymbol{y}| - c(t-s))}{4\pi c|\boldsymbol{x} - \boldsymbol{y}|}\Theta(t-s), \tag{9.59}$$

(9.59) is called the *retarded Green's function*.

Exercise.
(1) One way to obtain the Green's function for the wave equation is to use its temporal Fourier transformation (the Helmholtz equation):

$$(k^2 - \Delta)\psi_\omega(x) = \delta(\boldsymbol{x}). \tag{9.60}$$

Here $k = \omega/c$. Obtain

$$\psi_\omega(\boldsymbol{x}) = \frac{i}{2k}e^{ik|\boldsymbol{x}|}. \tag{9.61}$$

(2) There is a point source of wave at the origin. Describe the wave radiated from this source (respecting causality). That is, solve

$$(c^{-2}\partial_t^2 - \Delta)u(x,t) = Q\cos\omega t\delta(x) \tag{9.62}$$

in 3-space, respecting the radiation condition (i.e., there is no incoming wave).
(3) The same as (2) but with a point (oscillating) dipole at the origin. That is, solve the wave equation with the source

$$\rho(x,t) = -\boldsymbol{p}\cdot\nabla\delta(x)\cos\omega t, \tag{9.63}$$

where $\boldsymbol{p}$ is the dipole strength. Again respect causality.

9.31 Retarded and advanced Green's functions. Since the wave equation is time reversal symmetric,

$$\psi(\boldsymbol{x}, t) = \frac{\delta(|\boldsymbol{x}| + ct)}{4\pi c|\boldsymbol{x}|}\Theta(-t), \tag{9.64}$$

must also be a solution. This is a strange 'anti-causal' solution, and is called the *advanced Green's function* in contrast to (9.59).

9.32 Method of descent for wave equation. Applying this method explained in **9.1** to the retarded Green's function (9.59), we can construct the retarded Green's function for 2-space as

$$G(\boldsymbol{x}|\boldsymbol{y}) = \frac{\Theta(ct - |\boldsymbol{x}-\boldsymbol{y}|)}{2\pi c\sqrt{c^2t - |\boldsymbol{x}-\boldsymbol{y}|^2}}\Theta(t). \tag{9.65}$$

The reason why the step function shows up is that for the δ-function to contribute,the function inside the *delta*-function must have real zeros. The step function specifiesthe condition.

Exercise.

Apply the method of descent to the Green's function (9.61) of the Helmholtz equation.

9.33 Afterglow. Notice that the 2-space Green's function for the wave equation is not zero for $|\boldsymbol{x}-\boldsymbol{y}| < ct$. This implies that for an observer in 2-space a flash of a lamp at a distance brightens up the world slightly even after the first pulse arrived to the observer (*afterglow effect*) (see also **??**). We will see this is a feature of even dimensional space (→**12.51**).

The difference between odd and even dimensional spaces also appears in the spherical wave as follows:

$$\phi(r,t) = u(r)e^{-i\omega t}. \tag{9.66}$$

Then, u obeys the Helmholtz equation (→**??**, **X**)

$$\frac{\partial^2 u}{\partial r^2} + \frac{d-1}{r}\frac{\partial u}{\partial r} + k^2 u = 0, \tag{9.67}$$

where $k = \omega/c$. The general solution for this can be written in terms of

$$u(r) = \frac{1}{r^{d/2-1}}J_{\pm(d/2-1)}(kr). \tag{9.68}$$

The Bessel functions with half odd orders are written in terms of trigonometric functions, but not elementary otherwise (→**??**).

9.34 Method of images for wave equation. This is almost a repetition of what we have seen in **9.25** and **9.27**. If we assume that the boundary condition is Dirichlet, then the corresponding Green's function reads

$$G(\boldsymbol{x},t|\boldsymbol{y},s) = \frac{\delta(|\boldsymbol{x}-\boldsymbol{y}| - c(t-s))}{4\pi c|\boldsymbol{x}-\boldsymbol{y}|}\Theta(t-s) - \frac{\delta(|\boldsymbol{x}-\boldsymbol{y}\,| - c(t-s))}{4\pi c|\boldsymbol{x}-\boldsymbol{y}\,|}\Theta(t-s), \tag{9.69}$$

where $\boldsymbol{y}'$ is the position mirror symmetric to $\boldsymbol{y}$ with respect to the yz-plane. This is an idealized reflection from a hard wall. Consider the Neumann case.

Exercise.
With the aid of the method of images, write down the solution to the 1 dimensional wave equation

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)u = 0 \tag{9.70}$$

on the half line $[0, +\infty)$ with the fixed end condition at $x = 0$ and the initial condition

$$u|_{t=0} = f(x), \quad \left.\frac{\partial u}{\partial t}\right|_{t=0} = g(x), \tag{9.71}$$

where $f(0) = g(0) = 0$. [This is NOT a Green's function problem.]

9.C Laplace Equation in 2-Space

9.35 What do we know from complex analysis?
(1) The real and imaginary parts of a holomorphic function are harmonic functions. $\log|f|$ is harmonic on the region where f is holomorphic and nonzero.
(2) Let u be a harmonic function on a simply connected region D. Then, there is a holomorphic function ψ on D such that its real part is u. ψ is unique up to a pure imaginary additive constant.
The uniqueness follows from the Cauchy-Riemann equation; suppose there are two holomorphic functions f_1 and f_2 such that $\Re f_1 = \Re f_2 = u$ and$\Im f_1 = v_1$ and $\Re f_2 = v_2$. Then partial derivatives of $v_1 - v_2$ vanish, so it must be a constant. But since real part of f has no freedom of choice, the constant must be real.
(3) Harmonicity is conformal invariant. □

9.36 Neumann problem can be reduced to Dirichlet problem:
The Neumann problem:

$$\Delta V = 0 \text{ (in } D), \quad \frac{\partial V}{\partial n}(s) = g(s) \text{ (on } \partial D) \tag{9.72}$$

is converted to the problem to solve its conjugate harmonic function U (→**??**), which is the solution to the Dirichlet problem:

$$\Delta U = 0 \text{ (in } D), \quad U(s) = -\int_a^s g(s)ds \equiv h(s) \text{ (on } \partial D), \tag{9.73}$$

where a is any point on ∂D. □

Notice that the Neumann problem (9.72) is meaningful only when (→**??**)

$$\int_{\partial D} g(s)ds = 0. \tag{9.74}$$

[Demo] Let U and V be conjugate harmonic functions. Then, we have

$$\frac{\partial U}{\partial n} = \frac{\partial V}{\partial s}, \quad \frac{\partial U}{\partial s} = -\frac{\partial V}{\partial n}, \tag{9.75}$$

where n is the outward normal and s is the arc length parameter (the positive direction = orientation of s in the standard way. They are disguised Cauchy-Riemann equations.

From the second equation in (9.75), we get the condition for the Dirichlet problem (9.73). Thanks to (9.74) $h(s)$ is a univalent function on the boundary. □

9.37 Green's function solves Dirichlet problem: Let D be a region with ∂D being sufficiently smooth. Let G be the Green's function for this region, and u be a harmonic function on D and continuous on the closure of D. Then, for $z \in D$

$$u(z) = \int_{\partial D} u(\zeta)\frac{\partial G(\zeta, z)}{\partial n}ds. \tag{9.76}$$

Here $\partial/\partial n$ is the outward normal derivative at ζ, and s is the contour length coordinate of ζ along the boundary curve. □
This is a familiar formula (→**9.17**).

9.38 Poisson's formula: If u is harmonic on $|z| < R$ and continuous on $|z| \leq R$, then on $|z| \leq R$

$$u(r, \theta) = \frac{1}{2\pi}\int_0^{2\pi} u(R, \phi)\frac{R^2 - r^2}{R^2 - 2Rr\cos(\theta - \phi) + r^2}d\phi. \tag{9.77}$$

□
The formula can be obtained easily, if we use complex function theory, but here we will derive it later with the aid of Fourier expansion (→**11.6**).

9.39 Solution to Dirichlet problem on disk: Schwarz' theorem: Let $f(\phi)$ $(0 \le \phi < 2\pi)$ be integrable.[120] Then

$$u(r,\theta) = \frac{1}{2\pi}\int_0^{2\pi} f(\phi)\frac{R^2-r^2}{R^2-2Rr\cos(\theta-\phi)+r^2}d\phi \tag{9.78}$$

is harmonic on $|z| < R$. □
The first half is essentially **9.38**, but explicitly we can apply (→**??**) the Laplacian to (9.78):

$$\Delta u(r,\theta) = \frac{1}{2\pi}\int_0^{2\pi} d\phi f(\phi)\Delta\Re\left(\frac{Re^{i\phi}+z}{Re^{i\phi}-z}\right) = 0. \tag{9.79}$$

9.40 Fourier expansion of harmonic function on the disk: Under the same assumptions in **9.38**, u can be Fourier-expanded in $|z| < R$ as

$$u(r,\theta) = \frac{a_0}{2} + \sum_{n=1}^{\infty}(a_n\cos n\theta + b_n\sin n\theta)\left(\frac{r}{R}\right)^n, \tag{9.80}$$

where the coefficients are given by

$$a_n = \frac{1}{\pi}\int_0^{2\pi} u(R,\theta)\cos n\theta d\theta, \ (\text{for } n = 0,1,\cdots) \tag{9.81}$$

$$b_n = \frac{1}{\pi}\int_0^{2\pi} u(R,\theta)\sin n\theta d\theta, \ (\text{for } n = 1,2,\cdots). \tag{9.82}$$

□
[Demo] The integral kernel in the Poisson formula can be Fourier-expanded as

$$\frac{R^2-r^2}{R^2-2Rr\cos(\theta-\phi)+r^2} = 1 + 2\sum_{n=1}^{\infty}\left(\frac{r}{R}\right)^n\cos n(\theta-\phi). \tag{9.83}$$

This follows easily from $(\zeta+z)/(\zeta-z) = 1+2\sum(z/\zeta)^n$ with $\zeta = Re^{i\phi}$ and $z = re^{i\theta}$. This is uniformly convergent, so we may integrate the expansion of the integrand of the Poisson integral formula termwisely. The result is the one we wanted. □
The 3-space version of this formula is the spherical harmonics expansion.

9.41 Conformal mapping and Green's function: Let Δ be a region on the w-plane whose Green's function is $G_\Delta(w,w_0)$. If a conformal map $w = f(z)$ maps a region D on the z-plane onto Δ, then

$$G_D(z,z_0) \equiv G_\Delta(f(z),f(z_0)) \tag{9.84}$$

[120] i.e., Lebesgue integrable (→**??**), so this theorem is distinct from Poisson's formula.

is the Green's function for the region D with the pole at z_0 such that $w_0 = f(z_0)$. □
This theorem with **9.39** and the Riemann mapping theorem together demonstrate that for any singly connected region, there is a Green's function.
[Demo] We have only to check **??**. Thanks to the mapping theorem $G_D(z, z_0)$ is harmonic on D except at z_0. f is continuous on the closure of Δ,[121] so G_D vanishes when z approaches ∂D from inside. Now we have

$$2\pi G_D(z,z_0)+\log|z-z_0| = 2\pi G_\Delta(f(z),f(z_0))+\log|f(z)-f(z_0)|-\log\left|\frac{f(z)-f(z_0)}{z-z_0}\right|. \tag{9.85}$$

$G_\Delta(w, w_0) + (1/2\pi)\log|w - w_0|$ is harmonic near w_0 and f is holomorphic near z_0, so the last term is harmonic. □

9.42 Green's function for a region D: Let $w = f(z)$ be a conformal map which maps the region D on the z-plane onto the unit disk. Then the Green's function of D with the pole at $z_0 \in D$ is given by (→**??**)

$$G(z,z_0) = \log\left|\frac{1-\overline{f(z_0)}f(z)}{f(z)-f(z_0)}\right|. \tag{9.86}$$

□

9.43 Harmonic function on the half plane: Let $f(x)$ $(-\infty < x < \infty)$ be integrable. Then

$$u(x,y) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{yf(\eta)}{y^2+(x-\eta)^2}d\eta \tag{9.87}$$

is harmonic on the upper half plane. If x_0 is a continuous point of f, then $u(x, y) \to f(x_0)$ when z approaches to x_0 from above. If f is uniformly continuous on $x_1 \le x \le x_2$, then the convergence of $u(x, y) \to f(x)$ is uniform. □
[Demo] The integral converges uniformly for $y > 0$, so we may exchange the order of differentiation and integration. Notice that the imaginary part of $1/(z - \eta)$ is harmonic, so the integral is also harmonic. The convergence result will not be proved here. □

[121] We must demonstrate this – Carathèodory's theorem.

10 Fourier Expansion

Fourier expansion and its salient features are summarized. We should pay due attention to the relation between the decay rate of the Fourier coefficients and the smoothness of the function. Impacts of Fourier's idea on Modern Mathematics is also briefly outlined.

Key words: Fourier expansion, periodic extension, Gibbs phenomenon, Riemann-Lebesgue lemma, countable.

Summary:
(1) Three basic facts (**10.7**) for piecewise smooth functions are worth memorizing as well as the formal expansion formulas in **10.1**.
(2) Fourier coefficients decay faster if the function is smoother. This is due to the Riemann-Lebesgue lemma (**10.13-10.15**).
(3) To use Fourier expansion to solve a boundary problem, a problem-adapted form should be looked for (**10.17-10.19**).
(4) Attempts to rationalize Fourier series almost dictated modern mathematics (**10.22**).

10.1 Fourier expansion of function with period 2ℓ: A formal statement. If f is a periodic function with period 2ℓ, then

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} \left[a_n \cos \frac{n\pi x}{\ell} + b_n \sin \frac{n\pi x}{\ell} \right] \text{ for } x \in [-\ell, \ell], \tag{10.1}$$

where

$$a_n = \frac{1}{\ell} \int_{-\ell}^{\ell} f(x) \cos \frac{n\pi x}{\ell} dx, \quad b_n = \frac{1}{\ell} \int_{-\ell}^{\ell} f(x) \sin \frac{n\pi x}{\ell} dx. \tag{10.2}$$

Or, we may write

$$f(x) = \sum_{n=-\infty}^{+\infty} c_n e^{in\pi x/\ell}, \tag{10.3}$$

where

$$c_n = \frac{1}{2\ell} \int_{-\ell}^{\ell} f(x) e^{-in\pi x/\ell}. \tag{10.4}$$

This is what Fourier asserted, but he could not convince mathematicians he admired (→**3.4**, **3.5**, **10.22**). The formal series (10.1) or (10.3) are called *Fourier series*. If we may freely exchange the order of summation and integration, then it is easy to check Fourier's claim (see also

??).
The real value condition of f in terms of its Fourier coefficients is $c_n = \overline{c_{-n}}$.
The best introductory book of Fourier analysis is E. Körner's *Fourier Analysis* (Cambridge, 1988). For solved problems, Schaum's outline series is useful as usual.

Discussion.
(A) **Fourier expansion as least square approximation**.
Let

$$g(x) = \frac{a_0}{2} + \sum_{n=1}^{N} \left[a_n \cos \frac{n\pi x}{\ell} + b_n \sin \frac{n\pi x}{\ell} \right], \tag{10.5}$$

where a_n and b_n are given by (10.3). The Fourier coefficients minimizes the following integral:

$$\int_{-\ell}^{\ell} |f(x) - g(x)|^2 dx. \tag{10.6}$$

We say g is the closest to f in the L_2-norm (→**??**). That is, the Fourier expansion is understood as the least square approximation of a function in terms of trigonometric functions up to a given wavelength (→**??**).
(B) **Acceleration of convergence**. The convergence of Fourier series can be accelerated. Consider in $(-\pi, \pi)$

$$f(x) = \sum_{n=2}^{\infty} (-1)^n \frac{n^3}{n^4 - 1} \sin nx \tag{10.7}$$

We know

$$\sum_{n=1}^{\infty} (-1)^n \frac{\sin nx}{n} = \frac{x}{2}. \tag{10.8}$$

Let us subtract this from f:

$$f(x) - \frac{x}{2} = \sin x + \sum_{n=2}^{\infty} (-1)^n \frac{\sin nx}{n^5 - n}. \tag{10.9}$$

The series should be faster convergent than the original one, so this subtraction trick is useful in numerical calculation.

Try a similar trick to

$$\sum_{n=1}^{\infty} \frac{\cos nx}{n + a}, \tag{10.10}$$

where $a > 0$.
(C) **Crystal periodicity**. Let $f(\boldsymbol{r})$ be a function defined on $\boldsymbol{R}^3$ with the following 'lattice structure':

$$f(\boldsymbol{r} + \boldsymbol{a}_i) = f(\boldsymbol{r}) \tag{10.11}$$

for three (linearly independent) vectors $\boldsymbol{a}_i$ $(i = 1, 2, 3)$ called the *crystal lattice vectors*. The parallelepiped spanned by these vectors is called the *unit cell*. Such a

function can be expanded as

$$f(\boldsymbol{r}) = \sum_{\boldsymbol{h}} A_{\boldsymbol{h}} \exp(2\pi i \boldsymbol{h} \cdot \boldsymbol{r}), \tag{10.12}$$

where the summation is over all the vectors $\boldsymbol{h}$ such that

$$\boldsymbol{h} = \sum_{i=1}^{3} h_i \boldsymbol{b}_i \tag{10.13}$$

for any integer h_i. The vectors $\boldsymbol{b}_i$ $(i = 1, 2, 3)$ called *reciprocal lattice vectors* are give by

$$\boldsymbol{b}_1 = \frac{\boldsymbol{a}_2 \times \boldsymbol{a}_3}{V_c}. \tag{10.14}$$

and cyclical permutations of the suffices, where V_c is the volume of the 'uint cell':

$$V_c = \boldsymbol{a}_1 \cdot \boldsymbol{a}_2 \times \boldsymbol{a}_3. \tag{10.15}$$

The expansion coefficient can be obtained by

$$A_{\boldsymbol{h}} = \frac{1}{V_c} \int_{\text{cell}} d\boldsymbol{r}\, f(\boldsymbol{r}) \exp(-2\pi i \boldsymbol{h} \cdot \boldsymbol{r}). \tag{10.16}$$

Exercise.
(1) Fourier-expand the following functions of x (here a is a real such that $a \in (-1, 1)$.

$$\frac{1 - a^2}{1 - 2a\cos x + a^2}. \tag{10.17}$$

and

$$\frac{a \sin x}{1 - 2a\cos x + a^2}. \tag{10.18}$$

See **9.40**.
(2) Fourier expand

$$f(x) = |\cos ax|. \tag{10.19}$$

(3) Find the Fourier expansions of the following graphically given periodic functions.

(4) Let $f(x) = Ax^2 + Bx + C$ in $(-\pi, \pi)$, where A, B, C are constants. Find its Fourier expansion, or show

$$Ax^2 + Bx + C = \frac{A\pi^2}{3} + C + 4A\sum_{n=1}^{\infty}(-1)^n\frac{\cos nx}{n^2} - 2B\sum_{n=1}^{\infty}(-1)^n\frac{\sin nx}{n}. \quad (10.20)$$

If the range is $(0, 2\pi)$, then

$$Ax^2 + Bx + C = \frac{4A\pi^2}{3} + B\pi + C + 4A\sum_{n=1}^{\infty}\frac{\cos nx}{n^2} - 2B\sum_{n=1}^{\infty}\frac{\sin nx}{n}. \quad (10.21)$$

With the aid of these expansions, we can compute the following series

$$\sum_{n=1}^{\infty}\frac{\sin nx}{n}, \ \sum_{n=1}^{\infty}(-1)^n\frac{\cos nx}{n^2}. \quad (10.22)$$

(5) **Exercise**. Let $f(t)$ be a periodic function. Show that the modul us of its Fouriercoefficients c_n does not change if $f(t)$ is displaced along the time axis. That is, the Fourier coefficients c'_n of $f(t + \tau)$ for any τ satisfies $|c_n| = |c'_n|$. [This is trivial, but worth noting .]

10.2 Periodic extension of function. If f is defined only on $[-\ell, \ell]$, or one is interested in f on this interval, f can be extended to a periodic function F defined on the whole $\boldsymbol{R}$, and we may use **10.1**. There are many ways to define a function which is a periodic extension of f

As we will discuss in detail later (→**10.17**-) we should, in practice,

make the extended function F to be as smooth as possible.

Any periodic function with period T can be written as a sum of a periodic even function and a periodic odd function with the same period T.

10.3 Theorem [Weierstrass]. Any continuous function on (a, b) can be approximated in the sup-norm sense[122] by a polynomial. More precisely, for a given continuous function f defined on (a, b), and for any specified positive ϵ there is a polynomial P such that $\|f - P\|_{sup} < \epsilon$. □

We say that the set of polynomials is *complete* in the set of continuous functions.

It is straightforward to generalize the theorem for multivariable functions.

Discussion: Theorem [Hausdorff] on the moment problem.
Let $[a, b]$ be a finite interval and let f, g be continuous functions. Then, if

$$\int_a^b x^n f(x)dx = \int_a^b x^n g(x)dx \tag{10.23}$$

for all $n \in \boldsymbol{N}$, $f = g$ on $[a, b]$. □
The condition is equivalent to

$$\int_a^b P(x)(f - g)dx = 0 \tag{10.24}$$

for any polynomial P. Weierstrass (→**10.5**) tells us that there is a sequence of polynomials P_n uniformly converging to $f - g$ on $[a, b]$. Hence, the condition implies $\int (f - g)^2 dx = 0$. Hence, $f = g$ follows.

If the domain is not bounded, then Hausdorff's theorem does not hold. That is, the knowledge about all the moments do not uniquely specify a distribution function.

10.4 Bernstein polynomial. A constructive demonstration of Weierstrass' theorem is the following in terms of the *Bernstein polynomial*. We study a continuous function f defined on $[0, 1]$. Let

$$B_n(x) = \sum_{k=0}^{n} \binom{n}{k} x^k (1 - x)^{n-k} f\left(\frac{k}{n}\right). \tag{10.25}$$

This uniformly converges to f as $n \to \infty$.

This tells us that any continuous function is approximated as a

[122] The sup-norm $\| \ \|_{sup}$ is defined by $\|f(x)\|_{sup} = \sup_{x \in (a,b)} |f(x)|$. That is, we measure the distance between two functions f and g by the widest possible separation of their graphs. See **??** for 'norm.'

linear combination of monomials $1, x, x^2, \cdots$. The set of monomials is *complete* in the space of continuous functions (= any continuous function is in the closure of the totality of the linear combination of monomials). [123]

Exercise.
(1) Demonstrate that for $f(t) = 1, t$, and t^2 $B_n(t)$ converges to the respective target functions uniformly.[124] [Hint: Use a generating function.]
(2) $\{1, \cos nt\}$ is complete on $[0, \pi]$ but not so on $[-\pi, \pi]$. The same is true for $\{\sin nt\}$.

Discussion. Here, a theoretical physicists' formal demonstration of the convergence of (10.25) is given. We first note that the Taylor expansion can be written as[125]

$$f(x+y) = \exp\left(y\frac{d}{dx}\right) f(x). \tag{10.26}$$

(10.25) can be rewritten as

$$\begin{aligned} B_n(x) &= \sum_{k=0}^{n} \binom{n}{k} x^k (1-x)^{n-k} \exp\left(\frac{k}{n}\frac{d}{dt}\right) f(t)\Big|_{t=0}, & (10.27)\\ &= \left(1 - x + x\exp\left(\frac{1}{n}\frac{d}{dt}\right)\right)^n f(t)\Big|_{t=0}. & (10.28) \end{aligned}$$

Here, we have used the binomial theorem. Now n is extremely large, so the exponent can be expanded to obtain

$$\begin{aligned} B_n(x) &= \left(1 - x + x\left(1 + \frac{1}{n}\frac{d}{dt} + \cdots\right)\right)^n f(t)\Big|_{t=0}, & (10.29)\\ &= \left(1 + \frac{x}{n}\frac{d}{dt} + \cdots\right)^n f(t)\Big|_{t=0}, & (10.30)\\ &\to \exp\left(x\frac{d}{dt}\right) f(t)\Big|_{t=0}, & (10.31)\\ &= f(x). & (10.32) \end{aligned}$$

[123] The good function principle (→**15.17**) can be restated as follows: If a relation among integrals on a finite closed interval is correct for polynomials, then it is correct for any integrable functions.
[124] This demonstrates that B_n converges uniformly to any continuous target function thanks to the Bohman-Korovin theorem:
Let L_n be a linear operator on $C[a, b]$ (continuous functions on $[a, b]$) which is monotonic (i.e., if $f \le g$, then $L_n f \le L_n g$). The following two conditions are equivalent:
(A) $L_n f \to f$ is uniform for any $f \in C[a, b]$,
(B) $L_n f \to f$ is uniform for $f = 1, x$ and x^2. □
The theorem is the shortest route to the Weierstrass approximation theorem.
[125] If the reader knows that the momentum operator is the generator of translation in quantum mechanics, the formula should be obvious.

Mathematically, this is not a proof (note that this works only for analytic functions); this is just the Euler style 'algebraic formalism' (→wweul Discussion), but it is not empty.

10.5 Who was Weierstrass? Karl Theodor Wilhelm Weierstrass was born on October 31, 1815 at Ostenfelde in Münsterland. His family was rather poor, but a very cultivated one. He was a student *cum laude* every year, good at German, Greek, Latin, and Math. His father wished him to be a politician, so he studied law and economics at the University of Bonn (from Fall of 1834). However, he soon realized that these were not true scholarly disciplines but only for bread, and began to feel them as a waste of his life. He studied Laplace' *Mechanique celeste*, Jacobi's *Fundamenta nova*, etc., but he could never patiently attend mathematics classes except the one by Plücker's geometry.[126] He studied only mathematics for four years without taking any exams in any subject. He also loved taverns and became an expert in fencing with his great physical strength and agility. Hence, when he returned home after four years, naturally he was treated very coldly.

Since he knew he could not go to a good university to learn mathematics, he decided to be a teacher, and enrolled in the Theological and Philosophical Academy at Münster on May 22, 1839, where Gudermann[127] was teaching mathematics. Weierstrass quit the Academy in the same Fall, and prepared for the exam to be a teacher. In the exam in 1840, he gave a new result on elliptic functions.

He became a teacher of Münster gymnasium in 1841. He wished to complete his work submitted as a part of the exam, but thought that he should first clarify the foundation of the theory of general functions. He completed a paper proving Cauchy's theorem without using double integrals (note that Gauss' letter (→**??** Discussion (A)) was not known until 1880). The paper also contained Laurent's theorem (**??**). In 1842, he completed a fundamental paper on analytic functions. There he introduced the idea of function elements (→**7.7**), analytic continuation

[126] Plücker was a professor of physics concentrating on analytical geometry. However, it was said that a non-physicist occupying a physics position was inappropriate, so after 1846 for about twenty years he concentrated on physics. However, he could not stop studying mathematics, so that he decided to return to math, and started to construct a new geometry (introducing the Plücker coordinate), but could not finish it.

[127] C. Gudermann (1798-1851). He stressed the importance of power series, and this gave a profound influence on Weierstrass, who always appreciated Gudermann in every possible opportunity (e.g., on his (=KW) seventieth and eightieth birthdays). Weierstrass never attended any class but Gudermann's. There were 13 students in the first class, but in the second class Weierstrass was the only student.

(→**??**), singularities (→**??**), natural boundary (→**??**), etc.[128] In the Fall of 1842, he moved to the Royal Catholic Gymnasium at Deutsch-Krone (West Prussia). He had to teach calligraphy, geography, and gymnastics. He published his first paper on the gamma function (→**9**, the infinite product formula) in the proceedings of the gymnasium. Of course, no one read it who could understand it. For the next six years, he stayed in the position without becoming desperate.

In 1848 fall, he was promoted to a teacher of an Obere-Gymnasium (high school) at Braunsberg on the Baltic. Fortunately, the principal, Mr F. Schurz, understood him. His research was at the second stage of completing the theory of elliptic functions. His work on Abel functions appeared in Crelle's journal[129] in 1854. It was a sensational paper, making him famous instantly. University of Königsberg decided to give him *Doctor honoris causa*, and they (including math Professor Richelot who proposed this) went to Braunsberg to hand the doctorate.[130]

In 1856, he became a professor of Geverbe-Institute in Berlin from July 1, and then from the Fall, thanks to the recommendation of Kummer, he was also an associate professor of the University of Berlin. Kronecker was also there. However, he had to give lectures 12 hours a week at the Institute, and also had to give a lecture on Gauss' theory on the dispersion of light, so he did not have enough time to do research. He and Kummer founded the first seminar in Germany devoted exclusively to pure mathematics in 1861. After 1862 he could lecture only while seated in a chair because of brain spasms and the onset of recurrent attacks of bronchitis and phlebitis. During his classes an advanced student assisted him by writing on the blackboard.

He became a full professor in 1864, and was already very well known all over the world (even in the US).[131] By the 1870s as many as 250 students attended his classes each year. This enrollment was exceptionally high for advanced mathematics courses in his time. He removed the requirement that doctoral dissertations be in Latin.

He tried hard to eliminate use of intuition as much as possible. He analyzed intuitive concepts and wished to reconstruct everything on the concept of integers. Also he made effort to find the shortest path from the very basic.

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[128] The paper was not published for a few tens of years.

[129] This is still the top-ranking mathematics journal.

[130] According to Mittag-Leffler, at his 80th birthday, Weierstrass recollected with tears in his eyes that it was his most delightful event that Professor Richelot came over in person to hand him the degree. 'However, I still regret that the day came too late for me.' He spent 15 years teaching boys.

[131] When Mittag-Leffler went to Paris to learn with Hermite, Hermite said,"You have made an error. You should have attended courses of Weierstrass in Berlin. He is our master of all." (in 1873 just after the Franco-Prussian war).

Sonia Kowalevskaya[132] became his private student from 1870 Fall, because she had an excellent recommendation from Königsberger, his former student. He became the Provost of University of Berlin in 1873, but he continued to teach her. She received her PhD in 1874 with the now famous work about PDE (Cauchy-Kowalevskaya theorem).

Kowalevskaya died in 1889; Kronecker died in the same year.[133] He retired in 1892. He chose as his successor Frobenius (→**24B**). He died on February 19, 1897 of aggravated influenza.

10.6 Set of trigonometric functions is complete.[134] Let $f(\theta)$ be a 2π-periodic function. Introduce

$$\varphi(x, y) = r f(\theta), \tag{10.33}$$

where $x = r\cos\theta$ and $y = r\sin\theta$. This agrees with $f(\theta)$ on the unit circle $x^2 + y^2 = 1$. φ can be uniformly approximated by a polynomial of x and y on $[0, 1] \times [0, 1]$. Setting $r = 1$ the resultant formula becomes a polynomial of $\cos\theta$ and $\sin\theta$. However, with the aid of the formulas of trigonometric functions, this can always be reduced to the form of the partial sum of Fourier series.

Discussion [Münz' theorem].
The set of powers $\{x^{\alpha_i}\}$ with $\alpha_i \to \infty$ is complete (w.r.t. the ordinary sup norm) on $[0, 1]$, if and only if $\sum_i (\alpha_i)^{-1}$ diverges. □[135]
From this we realize that $\{e^{-\alpha_i t}\}$ is a complete set on a finite interval $[0, s]$ for any $s > 0$ under the same condition. Thus we can approximate correlation functions $c(t)$ (→**12.22**) on any large time interval $[0, T]$ with the linear combination of exponentially decaying functions.[136]

10.7 Three basic facts for piecewise smooth functions.[137] Let f_N be the partial sum of (10.1) up to the $n = N$ terms. We assume f

[132] January 15, 1850 Moscow - February 10, 1889 Stockholm.
[133] Kronecker did not like Weierstrass' theory of irrational numbers. He aimed at arithmetization of mathematics, saying "Die ganze Zahl schuf der liebe Gott, alles Übriges is Menschenwerk." Needless to say, Kronecker hated Cantor (→**??**), but Weierstrass defended him.
[134] This smart proof is found in Courant-Hilbert (Chapter 2, Section 5.4).
[135] H. Münz, Festschrift H A Schwarz, p303 (1914); The lecturer has not read the original. This is quoted in Courant-Hilbert Chapter 2, Section 10.6. See P Borwein and T Erdelyi, "Polynomials and Polynomial Inequalities" (Springer, 1995) for detailed information about the theorem and the related topics.
[136] This implies that we can approximate any Gaussian process with a linear combination of Gauss-Markov processes.
[137] A function which is continuously differentiable except finitely many points (at most countably many points) is called a *piecewise smooth function*.

to be piecewisely smooth. Then, there are three basic facts:
(1) $\lim_{N\to\infty} f_N(x) = [f(x+0) + f(x-0)]/2$.
(2) On any closed interval $[a, b]$ which is in an open region where f is smooth,[138] the convergence is uniform:
$\lim_{N\to\infty} \max_{x\in[a,b]} |f(x) - f_N(x)| = 0$.
(3) At an isolated jump discontinuity at x_0, *Gibbs' phenomenon*[139] occurs: for sufficiently small $\delta > 0$:
$\lim_{N\to\infty}[\max_{|x-x_0|<\delta} f_N(x) - \min_{|x-x_0|<\delta} f_N(x)] = C|f(x_0+0) - f(x_0-0)|$, where C is a universal constant given by $C = \frac{2}{\pi}\int_0^\pi \frac{\sin x}{x} dx \simeq 1.17897974\cdots$ (i.e., there is about 18% overshooting).

Discussion.
(A) Intuitive understanding of the fundamental theorem of Fourier expansion.
Let f be a periodic function with period 2π. We have

$$f(t) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty}\int_{-\pi}^{\pi} ds f(s) e^{in(t-s)} \tag{10.34}$$

Truncate the sum as

$$f_N(t) = \frac{1}{2\pi}\sum_{n=-N}^{N}\int_{-\pi}^{\pi} ds f(s) e^{in(t-s)}. \tag{10.35}$$

This can be rewritten as

$$f_N(t) = \int_{-\pi}^{\pi} ds f(s)\Delta_N(t-s), \tag{10.36}$$

where

$$\Delta_N(z) = \frac{1}{2\pi}\frac{\sin\left(N+\frac{1}{2}\right)z}{\sin\frac{z}{2}} \tag{10.37}$$

This is called the Dirichlet kernel (→**??** Discussion (D)). Its graph looks like the ones in the figure below. The Gibbs phenomenon and the average value property can be seen from the following figures.[140]

[138] that is, f is continuous and piecewise C^1 (the so-called strong Dini condition).
[139] Read Körner, Section 17.
[140] Ezawa

(B) Dirichlet integral: Let $a < 0 < b$ and f be piecewise monotonic in $[a, b]$. Then,

$$\lim_{\lambda\to\infty} \int_a^b f(x) \frac{\sin \lambda x}{x} dx = \frac{\pi}{2}(f(+0) + f(-0)). \tag{10.38}$$

Discuss the relation of this to (2) above.

10.8 Gibbs phenomenon. The pathology called Gibbs' phenomenon occurs near the jump. Any jump could be used to check the assertion in **10.7**(3).[141] We may use the following sawtooth function

LOCALIZATION of singularity must be clearly mentioned.

$$f(x) = x \text{ for } x \in (-\pi, \pi) \text{ and } f(\pm\pi) = 0. \tag{10.39}$$

Let S_n be the partial sum up to the n-th term of its sine Fourier expansion formula (→**10.15**). Then, it is not hard to see

$$S_n(\pi - \pi/n) \to C\pi, \tag{10.40}$$

where C is given in **10.7**(3).

10.9 Dirichlet's sufficient condition for expandability: practical condition. The basic facts in **10.7** are for piecewise smooth functions. Much wilder functions can be written as Fourier series. A sufficient condition for **10.7**(1) is:
f is periodic with at most finite number of extremal points and discontinuities.
This is sufficiently general for practitioners, but an ultimate version is:

[141] However, this localization of pathology is only in 1-space. The multidimensional pathology is explained in M. A. Pinsky, "Pointwise Fourier inversion in severeal variables," Notices Amer. Math. Soc. **42**, 330 (1995). Anexample is:
Let f be the characteristic function of the unit ball centered at the orig in in the 3-cube$[-2, 2]^3$ (i.e., $f(x) = 1$ if $|x| < 1$, and zero, otherwise) . The Fourier expansion of thisdoes not converge at the origin even though the function is smooth there.

10.10 Theorem [Riemann-Lebesgue].[142] A necessary and sufficient condition for (10.1) to converge to f at x is that

$$\lim_{\lambda\to\infty}\int_0^\delta \frac{1}{2}[f(x+t)+f(x-t)-2f(x)]\frac{\sin\lambda t}{t}dt=0 \qquad (10.41)$$

for some $\delta\in(0,\pi)$. If this holds uniformly in $[a,b]$, then (10.1) uniformly converges to $f(x)$ on $[a,b]$.
Corollary [Dini]. If $|f(x+t)+f(x-t)-2f(x)|/t$ is integrable as a function of t on $(0,\delta)$ for some $\delta\in(0,\pi)$, then (10.1) converges to $f(x)$ at x. In other words, if for any $\delta>0$

$$\int_{-\delta}^{\delta}\frac{f(x+t)-f(x-t)}{t}dt \qquad (10.42)$$

exists, then (10.1) converges to f at x.

10.11 Advanced theorems.
Theorem[Dini]. If $f(x)$ is L_1 (Lebesgue integrable, →**??**), and is Hölder continuous,[143] then its Fourier series converges to $f(x)$ at x.
Theorem[Carlson] (1966). For any L_2-function (square Lebesgue integrable, →**??**), there is a convergent subsequence of its Fourier finite series such that it converges pointwisely to f for almost all (→**??**) points.

10.12 Remark.
(1) **Warning.** There exists continuous functions whose Fourier expansions do not converge at some point [duBois-Reymond].[144] Hence, continuity is not enough to ensure the convergence, although we know the Fourier series of a continuous function contains all the information needed to recover the original continuous function if summed according to Cesaro:[145]

[142] See Y. Katznelson, *An Introduction to Harmonic Analysis* (Dover, 1968), Section 5, II-2, p51-55.
[143] That is, there are positive numbers α and C such that for any $\epsilon>0$ there is $\delta>0$ such that

$$|x-y|<\delta \Rightarrow |f(x)-f(y)|<C|x-y|^\alpha.$$

[144] Paul David Gustave du Bois Reymond, 1831-1889.
[145] As seen here, even a divergent series can sometimes be used to reconstruct the original function. We will come to another example later in asymptotic expansions (→**??**-**??**).

Fejer'stheorem.[146] Let S_n be the partial sum of the Fourier series (10.1) up to the n-th (both sine and cosine) term. Define

$$\sigma_n \equiv \frac{1}{n+1}\sum_{k=0}^{n} S_k. \tag{10.43}$$

If f is 2ℓ-periodic continuous function, then σ_n uniformly converges to f. □
Fejer's theorem can be written as (→**8.7** Discussion (D))

$$f(x) = \lim_{n\to\infty} \frac{2}{\pi}\int_{-\pi}^{\pi} f(y)\left(\frac{\sin\frac{n(y-x)}{2}}{2\sin\frac{y-x}{2}}\right)^2 dy. \tag{10.44}$$

Note that the kernel of the integral does not change its sign in contrast to the Dirichlet kernel in Discussion (A) of **10.7**.
(2) There exists L_1-functions (i.e., Lebesgue integrable functions →**??**) whose Fourier series diverges everywhere.
(3) For any L_2-function (i.e., square Lebesgue integrable functions →**??**), the set on which its Fourier series diverges is measure zero (→**??**). This explains partially why Lebesgue integral is the most natural framework to treat Fourier analysis (→**XX**). See also **10.11**.

10.13 Theorem [Riemann-Lebesgue lemma]. Let f be integrable on $[a, b]$. Then,

$$\lim_{m\to\infty}\int_a^b f(x)e^{imx}dx = 0. \tag{10.45}$$

Here m need not be an integer. □[147]

Of course, this implies that sine and cosine Fourier coefficients also vanish in the $m \to \infty$ limit.

Physically, the essence of the lemma is that if the total energy carried by the wave is finite, then the energy carried by every high frequency modes must be sufficiently small to avoid any 'ultraviolet catastrophe,' because the total energy ought to be the sum of the energy carried by each mode.

10.14 Smoothness and decay rate. If f is a k-times differentiable periodic function and $f^{(k)}$ is integrable, then

$$\int_{-\pi}^{\pi} f(x)e^{inx}dx = o[n^{-k}] \text{ as } |n| \to \infty. \tag{10.46}$$

[146] Liót Fejér (1880-1959) proved this sensational theorem when he was 19.
[147] See Katznelson p13.

This follows easily from the Riemann-Lebesgue lemma through integration by parts (cf. **??**).
(1) This supports our intuition that smoother functions have less high-frequency components.
(2) If $f \in C^\infty$, then its Fourier coefficients must decay in the $n \to \infty$ limit faster than any negative power of n.[148]

A precise statement is as follows:[149]

Theorem. Let $k \in \boldsymbol{Z}$. If $\sum_{n=-\infty}^{\infty} |n^k g(n)| < \infty$, then $f(x) = \sum_{n=-\infty}^{\infty} g(n) e^{inx}$ is a C^k-function.

(3) **Theorem** [Paley-Wiener]. A necessary and sufficient condition for a real analytic periodic function $f(x)$ to be analytic on a strip $|Im\, z| < \sigma$ is that for any $a \in (0, \sigma)$ there is a positive constant C (which may depend on a) such that $|\hat{f}(n)| \leq Ce^{-a|n|}$, where $\hat{f}(n)$ is the Fourier coefficient.

Discussion.
Around a nonsmooth point the convergence is slow as shown in the figure.[150]

Exercise.
(1) Compute the Fourier expansion of $x|x|$ on $[-\pi, \pi]$. Then, discuss the relation of your result and the smoothness of the function.
(2) Let f be a periodic C^m function. Then, its cosine and sine Fourier coefficients have the following asymptotic property:

$$|a_n|,\ |b_n| = O[n^{-m}]. \tag{10.47}$$

[148] This property turns out to be crucial for the definition of the Fourier transforms of generalized functions (→**12.34**).
[149] K. Tanishima, *Buturisugaku nyumon* (Univ. Tokyo Press, 1994).
[150] Ezawa

10.15 Smoothness examples. If a function f is such that $f^{(k)}$ is continuous, but that $f^{(k+1)}$ is not, then $a_n \sim n^{-(k+2)}$: on $(-\pi, \pi)$:

$$x = \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \sin nx, \tag{10.48}$$

$$|x| = \frac{\pi}{2} - \frac{4}{\pi} \sum \frac{1}{(2n-1)^2} \cos(2n-1)x, \tag{10.49}$$

$$x(\pi^2 - x^2) = 12 \sum \frac{(-1)^{n+1}}{n^3} \sin nx, \tag{10.50}$$

$$x^2(2\pi^2 - x^2) = \frac{7\pi^4}{15} + 48 \sum \frac{(-1)^n)}{n^4} \cos nx. \tag{10.51}$$

10.16 Nontrivial numerical series obtained via Fourier expansion. Fourier expansions could be used to get the following series results. From $|x|$ we get

$$\frac{\pi^2}{8} = 1 + \frac{1}{3^2} + \frac{1}{5^2} + \cdots, \tag{10.52}$$

$$\frac{\pi^2}{6} = 1 + \frac{1}{2^2} + \frac{1}{3^2} + \cdots, \tag{10.53}$$

$$\frac{\pi^2}{12} = 1 - \frac{1}{2^2} + \frac{1}{3^2} - \cdots. \tag{10.54}$$

From x^3 we get, for example,

$$\frac{\pi^3}{12} = 1 - \frac{1}{3^3} + \frac{1}{5^3} - \cdots. \tag{10.55}$$

10.17 Importance of smoothness. We wish to use Fourier expansions to solve PDE. Therefore, the convergence property of the series is very important. We should be able to differentiate the series termwisely. For this to be allowed a sufficient condition is the uniform convergence of the termwisely differentiated series. Hence, we wish to have the Fourier coefficients to decay as fast as possible (see the next entry). The previous entry explains why we must pay careful attention to the smoothness of periodic extension (→**10.2**) of a function defined on an interval.

10.18 Sine and cosine Fourier expansion. If f is defined only on $[0, \ell]$, then f is extended periodically as a function of period ℓ to use Fourier expansion formulas (→**10.2**). It is often convenient to extend f as an even or odd function of period 2ℓ (or longer →**10.19**). When we extend the function, it is advantageous to make the extended function as smooth as possible to ensure the good converging property of the series as discussed above.
(1) If $f(0) = 0$, then f defined on $[0, \ell]$ should be *sine-Fourier* expanded as

$$f(x) = \sum_{n=1}^{\infty} b_n \sin \frac{n\pi x}{\ell} \text{ for } x \in [0, \ell], \tag{10.56}$$

where

$$b_n = \frac{2}{\ell} \int_0^{\ell} f(x) \sin \frac{n\pi x}{\ell} dx. \tag{10.57}$$

(2) If $f \neq 0$, then f defined on $[0, \ell]$ can be *cosine-Fourier* expanded as

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{\infty} a_n \cos \frac{n\pi x}{\ell} \text{ for } x \in [0, \ell], \tag{10.58}$$

where

$$a_n = \frac{2}{\ell} \int_0^{\ell} f(x) \cos \frac{n\pi x}{\ell} dx. \tag{10.59}$$

[In the latter case we can subtract $f(0)$ from f to apply the sine-Fourier expansion, too.]

Exercise.
Expand the following functions on $[0, \pi]$ in Fourier cosine series:
(1)

$$f(x) = \cos ax \tag{10.60}$$

(2)

$$f(x) = \Theta(b - x), \tag{10.61}$$

where $b \in (0, \pi)$.

10.19 More sophisticated extension. To pursue the smoothness of the function to be expanded, for example, we can use the following trick to extend the original function on $[0, \ell]$ into a periodic function of period 4ℓ:
The following set could be used to expand any function on $(0, \ell)$

$$\left\{ \sin \frac{(2n-1)\pi x}{2\ell} \right\}. \tag{10.62}$$

The formulas are

$$f(x) = \sum_{n=1}^{\infty} a_n \sin \frac{(2n-1)\pi x}{2\ell}, \tag{10.63}$$

with

$$a_n = \frac{2}{\ell} \int_0^{\ell} dx\, f(x) \sin \frac{(2n-1)\pi x}{2\ell}. \tag{10.64}$$

This expansion is particularly useful when $f(0) = 0$ and $f'(\ell) = 0$ Analogously, we could use the cosine counterpart.

10.20 Formal limit of Fourier expansion for infinite domain. Let us define

$$\hat{f}_\ell(k) \equiv \int_{-\ell}^{\ell} f(x) e^{-ikx} dx. \tag{10.65}$$

The complex Fourier coefficient (10.4) in **10.1** may be written as

$$c_n = \frac{1}{2\ell} \hat{f}_\ell(k_n), \tag{10.66}$$

where $k_n = \pi n/\ell$. (10.3) reads

$$f(x) = \sum_{n=-\infty}^{\infty} \frac{1}{2\ell} \hat{f}_\ell(k_n) e^{ik_n x}. \tag{10.67}$$

We wish to take the $\ell \to \infty$ limit. Let us assume that this limit exists for (10.65):

$$\hat{f}(k) = \lim_{\ell \to \infty} \int_{-\ell}^{\ell} f(x) e^{-ikx} de = \int_{-\infty}^{\infty} f(x) e^{-ikx} dx. \tag{10.68}$$

The summation over n may be written as (this sum may be understood as a Riemann sum) ($dk = \pi dn/\ell$)

$$\frac{1}{2\ell} \sum_{n=-\infty}^{\infty} \to \frac{1}{2\ell} \int_{-\infty}^{\infty} dn = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \tag{10.69}$$

so that (10.67) can be written in the $\ell \to \infty$ limit as

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dk. \tag{10.70}$$

This heuristic result may be more formally summarized as follows (Fourier used a similar logic).

10.21 Fourier transform preview. Let f be an absolutely integrable function on $\boldsymbol{R}$. If the following integral exists

$$\hat{f}(k) = \mathcal{F}(f)(k) \equiv \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \tag{10.71}$$

it is called the *Fourier transform* of f. Multidimensional cases can be treated similarly.

Theorem [**Fourier inversion**]. If $f : \boldsymbol{R} \to \boldsymbol{C}$ is continuous, and both f and $\hat{f}$ are absolutely integrable, then the inversion formula holds

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(k) e^{+ikx} dk \equiv \mathcal{F}^{-1}(\hat{f}). \tag{10.72}$$

□

(12.12) appears so often that we have a fairly standard abbreviation

$$\int_k \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk, \quad \int_{\boldsymbol{k}} \equiv \left(\frac{1}{2\pi}\right)^d \int d^d \boldsymbol{k}. \tag{10.73}$$

10.22 Impact of Fourier. The impact of Fourier's general assertion was not confined within applied mathematics. As we see below, it almost dictated Modern Mathematics.

In essence, if f is piecewise smooth function which can be Fourier-expanded, then the series can be termwisely differentiated to make the Fourier series for f'.

(1) Function concept had to be clarified. Fourier claimed that any function can be expanded into Fourier series (→**3.4**, **3.5**). In those days the idea of function was not very clear. For example, there was a dispute between d'Alembert (→**1.13**) and Euler (→**2.4**): Euler thought every hand-drawable function is a respectable function, but d'Alembert thought only analytically expressible functions are respectable. Therefore, to make sense out of Fourier's claim, the concept of function had to be clarified. Eventually, the modern concept of function as a map culminated through the work of Cauchy (→**??**) and Dirichlet: if a value $f(x)$ is uniquely specified for a given value of the independent variable x, then f is a respectable function. Then, inevitably, many strange functions began to be found (see. e.g., **1.1** Discussion (B)). Now, we know many examples such as fractal curves.[151] Nowhere continuous functions were also found. A famous example is the *Dirichlet function*: $D(x) = 1$ if x is rational, and 0 otherwise (→**??**).

(2) Convergence condition. The convergence condition of infinite

[151] B. B. Mandelbrot, *The Fractal Geometry of Nature* (Freeman, 1985).

series had to be considered. This spurred Cauchy to construct his theory of convergence.

(3) Concept of integration had to be sharpened. Fourier proposed an integral formula for the Fourier coefficients as summarized in **10.1**. However, if a function f is not continuous, then it was not clear how to interpret the integral. To clarify this point, Riemann invented the concept of Riemann integration with clear integrability condition (in 1853 →**3.23**).

(4) Set theory became necessary. Cantor (→**10.23**) found that even if the values of the function at infinitely many points were unknown, still the Fourier series was determined uniquely. He studied very carefully how large 'sets' of points could be removed without affecting the Fourier coefficients. Soon he had to characterize these collections of points. The first surprise he found was that infinity of the totality of real numbers and that of rational numbers are distinct.[152] To organize his theory of infinity, Cantor attempted to introduce the concept of 'set.' However, many antinomies ('paradoxes') were found.[153]

(5) Securing foundation required axiomatic set theory. Eventually, to secure the foundation of set theory a set of axioms[154] were introduced by Zermelo.[155] Hence, the currently most popular axiomatic system of mathematics (ZFC) is under almost the direct impact of Fourier's idea.

(6) Further sharpening of integration concept was required. According to Cantor the area of $D(x)$ for $x \in [0,1]$ must be zero (→**??**), but we cannot make any sense out of the Riemann integral of the Dirichlet function D (→**??**). A more powerful integral was needed, which was eventually provided by Lebesgue as the Lebesgue integration (→**??**).

Discussion.

The reader must know and be able to explain to her lay friend the argument showing

[152] Cantor's first important result (December, 1873). →**??**.

[153] Perhaps the most famous antinomy is the Russel paradox (1902). The Russel paradox is as follows. 'Sets' can be classified into two classes: 'sets' which contain themselves as their elements ($x \in x$) and 'sets' which do not contain themselves ($x \notin x$). Make the 'set' Z of all the 'sets' x such that $x \notin x$: $Z \rightleftharpoons \{x : x \notin x\}$. Is Z in Z or not? If $Z \notin Z$, then $Z \in Z$, but if $Z \in Z$, then $Z \notin Z$, a paradox.

[154] Y N. Moschovakis, *Notes on Set Theory* (Springer, 1994) and J. Winfried and M Weese, *Discovering Modern Set Theory I. the basics* (AMS, 1996) are recommended. P. Maddy, *Realism in Mathematics* (Oxford, 1990) may be used to understand the background of axiomatic set theories.

[155] Ernst Friedrichs Ferdinand Zermelo, 1871-1953. For physicists, Zermelo is famous for his discussion against Boltzmann: the 'Rückkehreinwand.' He was an assistant of Planck in those days and was against atomism (as his boss was). See G. H. Moore, *Zermelo's Axiom of Choice, its origins, development, and influence* (Springer, 1982). Perhaps this is more entertaining than many novels.

that $\boldsymbol{Q}$ is countable, but $[0,1]$ is not. Also she must be able to explain why $[0,1]^n$ for any $n \in \boldsymbol{N}$ has the same density as $[0,1]$ (i.e., there is a one-to-one correspondence between any dimensional cube and the interval $[0,1]$.

10.23 Who was Cantor? Georg Ferdinand Cantor was born in 1845 into a cosmopolitan merchant family in St. Petersburg. He was an artistically inclined child (a dessin is reproduced in his biography by Dauben[156]). He got his university education at Berlin (from 1863) from Weierstrass (→**10.5**), Kummer, Kronecker and others. His thesis solved a problem left unsettled by Gauss.

After briefly teaching at a Berlin's girls' school, he got his permanent job at Halle in 1869, where he became a junior colleague of Heine,[157] who urged Cantor to study the question about the uniqueness of the Fourier coefficients. Cantor quickly found what is outlined in **(4)** of **10.22**. In 1891, Cantor invented an entirely different proof of uncountability of reals, the so-called *diagonal method* (or method of diagonalization). This allowed him to make an ascending hierarchy of transfinite (=infinite) numbers. Cantor accepted the concept of actual infinity through his study of Plato, Aquinas, Spinoza and Leibniz. This put him at odds with a tradition stretching from Aristotle to Gauss that accepted only potential infinity. Most of his first papers were published in Acta Mathematica published by Mittag-Leffler.

To organize his theory of transfinite numbers, Cantor attempted to introduce the concept of 'set.' By a "set" he meant any collection M of definite, distinct objects m (called elements of M) which we can perceive or think. Cantor published his famous Beiträge[158] part I in 1895. This was the birth of set theory.

Cantor wished to move to a position more prestigious than Halle, but Kronecker hated his theory of transfinite numbers and opposed his appointment at Berlin. Mental illness afflicted his final decades of his life. Beginning in 1884 he suffered sporadically from depression. Although his studies in other fields than mathematics may look strange (to try to prove that Bacon wrote Shakespeare's plays, Freemasonry, etc), he continued to work actively in mathematics. In 1890 he founded the Association of German Mathematicians. He advocated international congress of mathematicians and made arrangements for

[156] J. W. Dauben, *Georg Cantor, His Mathematics and Philosophy of the Infinite* (Princeton UP, 1979) is a very informative and enjoyable book.

[157] Heinrich Eduard Heine, 1821-1881, well known for his covering theorem (Heine-Borel).

[158] which means 'contributions.' "Beiträge zur Begrundung der transfiniten Mengenlehre" Math. Ann. **46**, 481 (1895). A Dover translation is available: *Contribution to the founding of the theory of transfinite numbers* (Dover, 1955; the original translation by P E B Jourdain in 1915).

the first of these held in Zurich in 1897. He died in January 1918 at the University of Halle mental hospital.
Cantor showed a unique ability in the art of asking questions that opened vast new areas of mathematical inquiry, an ability that he considered more valuable than solving questions.

11 Separation of Variables –Rectangular Domain –

As the first section devoted to solve second order PDE explicitly, boundary value problems on rectangular regions are considered. The essence of separation of variables is the expansion of the solution into Fourier series.

Key words: separation of variables, eigenvalue problem, Poisson's formula.

Summary:
(1) How to construct appropriate eigenvalue problems is the key to separation of variable (**11.1-11.2**).

11.1 Separation of variables: general strategy.[159] Suppose we wish to solve a PDE of the form

$$(L_1(x) + L_2(y))u(x, y) = 0, \tag{11.1}$$

where L_1 and L_2 are linear differential operators (→**3.2**) such that $L_1(x)f(y) = L_2(y)g(x) = 0$ for any function f and g. If we assume

$$u(x, y) = X(x)Y(y), \tag{11.2}$$

then

$$YL_1X + XL_2Y = 0, \tag{11.3}$$

or we conclude that

$$(L_1X)/X = -(L_2Y)/Y. \tag{11.4}$$

(1) [**Splitting step**]. The LHS of (11.4) depends only on x and the RHS only on y, so this equality implies that both sides must be constant:

$$(L_1X)/X = -(L_2Y)/Y = \lambda \tag{11.5}$$

where λ is a constant (Sometimes called a *separation constant*.
(2) [**Eigenvalue problem**]. We must split the auxiliary conditions

[159] This method was first employed by Daniel Bernoulli around 1755 to solve the wave equation. A more abstract setting and a general theory will be given later (→**XX**).

accordingly to obtain two problems which depend only on one of the variables.
If the boundary condition is homogeneous for, say, x-direction, then $L_1X = \lambda X$ becomes an *eigenvalue problem*, because the nonzero solution usually exists only for very special values (eigenvalues) of λ. For each eigenvalue, we have a nontrivial solution denoted by $X_\lambda(x)$.
(3) [**Inhomogeneous boundary problem**]. For such λ, we must solve the second problem $L_2Y = -\lambda Y$ under appropriate auxiliary conditions, which are usually not homogeneous. Let us denote its solution by $Y_\lambda(y)$.
(4) [**Superposition**]. Since our problem is linear, the superposition principle (→**3.2**) tells us that $\sum_\lambda X_\lambda(x)Y_\lambda(y)$ is also a solution.
If any smooth function can be expanded as a linear combination of X_λ (i.e., if the set $\{X_\lambda\}$ is complete), then we will be able to solve the problem generally.[160] If $\{X_\lambda\}$ is the set of trigonometric functions, the theory of Fourier series (→**XX**) can be fully exploited as Fourier expected (→**3.4**). In summary, the essence of the separation of variables is to use a problem-adapted Fourier expansion.

11.2 Illustration: 2D Laplace, Dirichlet. Solve the following two-dimensional Laplace equation on $[0,1]\times[0,1]$:

$$\partial_x^2\psi + \partial_y^2\psi = 0 \text{ on } [0,1]\times[0,1] \tag{11.6}$$

with the inhomogeneous Dirichlet condition

$$\psi(0,y) = u_0(y),\ \ \psi(1,y) = u_1(y),\ \ \psi(x,0) = v_0(x),\ \ \psi(x,1) = v_1(x). \tag{11.7}$$

(1) [**Separating step**] We use the superposition principle (→**3.2**) to split the problem as

$$\partial_x^2\psi + \partial_y^2\psi = 0 \text{ on } [0,1]\times[0,1], \tag{11.8}$$

$$\psi(0,y) = u_0(y),\ \ \psi(1,y) = u_1(y),\ \ \psi(x,0) = 0,\ \ \psi(x,1) = 0. \tag{11.9}$$

[160] We must be able to show that the series converges uniformly, and we can freely exchange the order of the infinite summation and differentiation, etc. A condition for $\sum_{n=1}^\infty u_n(x)$ to be termwisely differentiable is:
(i) $u_n(x)$ is C^1,
(ii) the series is pointwise convergent,
(iii) $\sum_{n=1}^\infty u_n'(x)$ is uniformly convergent.
Physicists usually do not care about these things, believing that their solutions are always well-behaved (e.g., sufficiently smooth). Indeed, often they are right, and that is why physicists do not pay much attention to mathematicians' careful statements.

and

$$\partial_x^2\psi + \partial_y^2\psi = 0 \text{ on } [0,1]\times[0,1], \tag{11.10}$$

$$\psi(0,y) = 0, \quad \psi(1,y) = 0, \quad \psi(x,0) = v_0(x), \quad \psi(x,1) = v_1(x). \tag{11.11}$$

The separation of boundary conditions expects eigenvalue problems in all but one coordinate directions. (Further decomposition is possible, but usually there is no need or no merit.) Here we only solve the first set, since the second set is analogous. The solution to the original equation is the sum of the solutions to these split problems.

(2) [**Eigenvalue problem**] (11.8)+(11.9) has a homogeneous boundary condition perpendicular to the y direction (i.e., $\psi = 0$ at $y = 0$ and $y = 1$). Therefore, we should study the eigenvalue problem of ∂_y^2 under the homogeneous boundary condition. Solving the eigenvalue problem

$$\frac{d^2u}{dy^2} = -\mu u, \quad u(0) = u(1) = 0, \tag{11.12}$$

we get $\mu = \pi^2 n^2$ for $n = 1, 2, \cdots$ with the corresponding eigenfunction $\sin n\pi y$. We know the totality of such functions is a complete set according to **10.18**(1). Notice that the sign of the separation constant μ is dictated by the requirement that (11.12) becomes an eigenvalue problem (the solutions must be oscillatory).

(3) [**Inhomogeneous boundary problem**] Therefore, superposition principle tells us that the solution must have the following form:

$$\psi = \sum_{n=1}^{\infty} Q_n(x)\sin n\pi y, \tag{11.13}$$

where $A_n(x)$ satisfies

$$\frac{d^2Q_n(x)}{dx^2} = n^2\pi^2 Q_n(x). \tag{11.14}$$

(4) [**Superposition**] The general solution to (11.14) is $A_n \sinh n\pi x + B_n \cosh n\pi x$, so that the general form of the solution to our problem reads

$$\psi = \sum_{n=1}^{\infty}(A_n \sinh n\pi x + B_n \cosh n\pi x)\sin n\pi y. \tag{11.15}$$

The inhomogeneous boundary conditions at $x = 0$ and $x = 1$ requires

$$\sum_{n=1}^{\infty} B_n \sin n\pi y = u_0(y), \tag{11.16}$$

$$\sum_{n=1}^{\infty}(A_n \sinh n\pi + B_n \cosh n\pi)\sin n\pi y = u_1(y). \tag{11.17}$$

We can determine B_n and A_n from these equations, following **10.15**(1).[161]

Exercise.
(1) Consider

$$\frac{\partial^2 u}{\partial t^2} + a^2 \frac{\partial^4 u}{\partial x^4} = 0 \tag{11.18}$$

for $x \in [0, L]$ and $t \geq 0$.
(i) Discuss possible boundary conditions to single out the solution.
(ii) Assume that on the boundary u and $\partial_x^2 u$ vanish and the initial condition is $\partial_t u(x, 0) = 0$ and $u(x, 0) = f(x)$.
(2) Solve the Laplace equation for the following boundary conditions. Before solving these problems, you must be able to guess the approximate shapes of the solutions.

11.3 Laplace equation: Dirichlet condition.

$$\Delta\psi = 0 \text{ on } [0, a_x] \times [0, a_y] \times [0, a_z] \tag{11.19}$$

with the Dirichlet boundary condition

$$\begin{aligned} \psi(0, y, z) = f_x(y, z), \quad \psi(a_x, y, z) = g_x(y, z), \\ \psi(x, 0, z) = f_y(x, z), \quad \psi(x, a_y, z) = g_y(x, z), \\ \psi(x, y, 0) = f_z(x, y), \quad \psi(x, y, a_z) = g_z(x, y). \end{aligned} \tag{11.20}$$

Procedure **11.2**(1) gives, for example, the problem

$$\Delta\psi = 0, \text{ on } [0, a_x] \times [0, a_y] \times [0, a_z], \tag{11.21}$$

$$\psi(0, y, z) = \psi(a_x, y, z) = \psi(x, 0, z) = \psi(x, a_y, z) = 0, \tag{11.22}$$

$$\psi(x, y, 0) = f_z(x, y), \ \psi(x, y, a_z) = g_z(x, y). \tag{11.23}$$

[161] Of course, u_0 and u_1 must be Fourier-expandable.

(x, y, z in the boundary conditions must be in the domain of the problem, of course.) Thus the relevant eigenvalue problem analogous to that appearing in **11.2**(2) is

$$(\partial_x^2 + \partial_y^2)u = -\mu^2 u \tag{11.24}$$

with the homogeneous Dirichlet boundary condition $u(0, y) = u(a_x, y) = u(x, 0) = u(x, a_y) = 0$. This can be separated further, and the superposition principle asserts

$$\psi = \sum_{m,n} (A_{m,n} \sinh \mu_{m,n} z + B_{m,n} \cosh \mu_{m,n} z) \sin \frac{m\pi x}{a_x} \sin \frac{n\pi y}{a_y}. \tag{11.25}$$

where $\mu_{m,n}^2 = (m\pi)^2/a_x^2 + (n\pi)^2/a_y^2$. The unknown constants $A_{m,n}$ and $B_{m,n}$ are fixed with the aid of **10.18**(1).

If, for example, a_x is not finite, the summation over m in (11.25) becomes an integral (*Fourier sine transform*) (→**12.9**).

The full solution to our problem is obtained by summing all three solutions to inhomogeneous problems in the x, y and z directions resulted from the splitting.

Exercise.
Consider the Laplace equation on a square $[0, L] \times [0, L]$ with the boundary conditions

$$u(0, y) = 0, \;\; u(L, y) = A \sin(2\pi x/L), \;\; u(x, 0) = 0, \;\; u(x, L) = B \sin(2\pi x/L). \tag{11.26}$$

11.4 Laplace equation: Neumann condition.

$$\Delta\psi = 0 \text{ on } [0, a_x] \times [0, a_y] \times [0, a_z] \tag{11.27}$$

with the Neumann boundary condition

$$\begin{aligned} &\partial_x\psi(0, y, z) = f_x(y, z), \;\; \partial_x\psi(a_x, y, z) = g_x(y, z), \\ &\partial_y\psi(x, 0, z) = f_y(x, z), \;\; \partial_y\psi(x, a_y, z) = g_y(x, z), \\ &\partial_z\psi(x, y, 0) = f_z(x, y), \;\; \partial_z\psi(x, y, a_z) = g_z(x, y). \end{aligned} \tag{11.28}$$

11.2(1) gives, for example, the problem

$$\Delta\psi = 0 \text{ on } [0, a_x] \times [0, a_y] \times [0, a_z], \tag{11.29}$$

$$\partial_x\psi(0, y, z) = \partial_x\psi(a_x, y, z) = \partial_y\psi(x, 0, z) = \partial_y\psi(x, a_y, z) = 0, \tag{11.30}$$

$$\partial_z\psi(x, y, 0) = f_z(x, y), \;\; \partial_z\psi(x, y, a_z) = g_z(x, y). \tag{11.31}$$

Thus the relevant eigenvalue problem is

$$(\partial_x^2 + \partial_y^2)u = -\mu^2 u \tag{11.32}$$

with the homogeneous Neumann boundary condition $\partial_x u(0,y) = \partial_x u(a_x,y) = \partial_y u(x,0) = \partial_y u(x,a_y) = 0$. This can be separated further, and eventually we get

$$\psi = \sum_{m,n}(A_{m,n}\sinh\mu_{m,n}z + B_{m,n}\cosh\mu_{m,n}z)\cos\frac{m\pi x}{a_x}\cos\frac{n\pi y}{a_y}. \tag{11.33}$$

where $\mu_{m,n}^2 = (m\pi)^2/a_x^2 + (n\pi)^2/a_y^2$. The unknown constants $A_{m,n}$ and $B_{m,n}$ are fixed with the aid of **10.18**(2).

If the region is not bounded, then the summation over m and/or n becomes integration (*Fourier cosine transform*→**12.9**).

11.5 Diffusion equation. Consider

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{11.34}$$

for $x \in (0,l)$ and for $t > 0$ with the initial condition $u(x,0) = A$ for $x \in (0,l)$ and the boundary condition $u(0,t) = B$ and $u(l,t) = C$ for $t > 0$, where A, B, C are constants.[162]
A clever (and standard) trick is to convert the problem to a homogeneous boundary value problem by introducing

$$v = u - \left(\frac{C-B}{l}x + B\right). \tag{11.35}$$

We have

$$\frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial x^2} \tag{11.36}$$

for $x \in (0,l)$ and for $t > 0$ with the initial condition $v(x,0) = (B - C)x/l + A - B$ for $x \in (0,l)$ and the boundary condition $v(0,t) = 0$ and $v(l,t) = 0$ for $t > 0$. Thus we may assume the following solution

$$v(x,t) = \sum_{n=1}^{\infty} T_n(t)\sin\frac{n\pi}{l}x. \tag{11.37}$$

Notice that the above method works even when A, B, C are time-dependent.

[162] With this delicate choice of the space-time positions to impose the auxiliary conditions, we need not worry about the compatibility among A, B, C.

Exercise.
(1) Find the solution of the 1d diffusion equation for $x \in [0, \pi]$ and $t \geq 0$ with a homogeneous Neumann condition and the initial condition $u(x, 0) = \sin^2 x$.
(2) Find the solution of the 1d diffusion equation for $x \in [0, \pi]$ and $t \geq 0$ with the initial condition $u(x.0) = x$, and a homogeneous Dirichlet boundary condition.
(3) Solve the diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{11.38}$$

on $[0, 1]$ with the initial condition $u(x, 0) = \sin(\pi x/2)$ and the boundary conditions $u(0, t) = 0$ and

$$\left.\frac{\partial u}{\partial x}\right|_{x=1} = -\frac{1}{\nu} u(1, t), \tag{11.39}$$

where ν is a constant (i.e., a homogeneous Robin condition).
[Hint: Let μ_n be the n-th zero of $\tan x + \nu x = 0$ arranged in the increasing order. Then,

$$\int_0^1 \sin(\mu_n x) \sin(\mu_m x) dx = \delta_{m,n} \frac{1 + \nu \cos^2 \mu_n}{2}. \tag{11.40}$$

]
(4) There is a thermally isolated ring of radius ℓ whose thermal diffusivity is D. The initial temperature distribution is given by

$$T(0, x) = T_0 \cos \frac{2x}{\ell}, \tag{11.41}$$

where x is the coordinate along the ring. Find $T(t, x)$.
(5)There is a thin rod of length ℓ occupying between $x = 0$ and $x = \ell$ whose thermal diffusivity is D. The temperature at one end, say, at $x = 0$ is given as a function of time as $T(x = 0, t) = T_0 e^{-\alpha t}$ ($\alpha > 0$, constant), and the other end is maintained at T_0 for all $t > 0$. Initially the temperature is given by $T(x, 0) = T_0 \sin(3\pi x/\ell)$. Find the temperature field for $t > 0$.

11.6 Obtaining Poisson's formula. Consider the Laplace equation on a disk of radius a centered at the origin (cf. **3.31**):

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \theta^2} = 0 \tag{11.42}$$

The boundary condition is a Dirichlet condition: $u(a, \theta) = f(\theta)$ which is a smooth periodic function with period 2π.

We can of course follow the honest separation strategy, but we may assume that u can be Fourier expanded (as the reader can guess (→**??**), harmonic functions are very smooth (→**??**), so we can do this with confidence) as

$$u(r, \theta) = \frac{A_0(r)}{2} + \sum_{n=1}^{\infty} [A_n(r) \cos n\theta + B_n(r) \sin n\theta]. \tag{11.43}$$

Putting this into the equation, we obtain the following ODE for the coefficients:

$$\frac{d^2A_n}{dr^2}+\frac{1}{r}\frac{dA_n(r)}{dr}-\frac{n^2}{r^2}A_n(r) = 0\ (n=0,1,2,\cdots), \quad (11.44)$$

$$\frac{d^2B_n}{dr^2}+\frac{1}{r}\frac{dB_n(r)}{dr}-\frac{n^2}{r^2}B_n(r) = 0\ (n=1,2,\cdots). \quad (11.45)$$

From this we get the following solutions that are finite at the origin (→**??**):

$$A_n(r)=A_nr^n,\ B_n(r)=B_nr^n, \quad (11.46)$$

where A_n and B_n are constants. With the aid of the boundary condition at $r=a$, these coefficients are uniquely fixed as (→**10.1**)

$$A_n=\frac{1}{\pi}\int_0^{2\pi}f(\phi)\cos n\phi\,d\phi,\ B_n=\frac{1}{\pi}\int_0^{2\pi}f(\phi)\sin n\phi\,d\phi. \quad (11.47)$$

Hnece, our solution (11.43) reads:

$$u(r,\theta)=\frac{1}{2\pi}\int_0^{2\pi}f(\phi)\left(1+2\sum_{n=1}^{\infty}\left(\frac{r}{a}\right)^n\cos n(\phi-\theta)\right)d\phi \quad (11.48)$$

or summing the series, we finally obtain *Poisson's formula* (for $r<a$) (→**9.38**):

$$u(r,\theta)=\frac{1}{2}\int_0^{2\pi}f(\phi)\frac{a^2-r^2}{a^2-2ar\cos(\phi-\theta)+r^2}d\phi. \quad (11.49)$$

11.7 1-space wave equation. Let us consider, as an example, the following 1-wave equation

$$\frac{\partial^2u}{\partial t^2}=c^2\frac{\partial^2u}{\partial x} \quad (11.50)$$

for $x\in[0,a]$ and $t\geq 0$, where c is a positive constant. The auxiliary conditions are:
the initial condition: $u(x,0)=f(x)$, $\partial_t u(x,0)=0$ for $x\in[0,a]$,
the boundary conditions: $u(0,t)=u(a,t)=0$ for $t\geq 0$.
We know that the solution, if exists, is unique for smooth initial conditions (→**1.22**).
Again, we can immediately proceed as in **11.6** to assume the solution in the following form (cf. **10.18**(1), **3.4**):

$$u(x,t)=\sum_{n=1}^{\infty}a_n(t)\sin\left(\frac{n\pi x}{a}\right). \quad (11.51)$$

Now the boundary conditions have been taken into account. The initial condition requires that

$$a_n(0) = \frac{2}{a}\int_0^a f(x)\sin\left(\frac{n\pi x}{a}\right)dx, \tag{11.52}$$

and $a_n'(0) = 0$. The wave equation is translated into a set of infinite ODEs:

$$\frac{d^2a_n(t)}{dt^2} = -c^2\frac{n^2\pi^2}{a^2}a_n(t). \tag{11.53}$$

Thus, we get

$$a_n(t) = a_n(0)\cos\left(\frac{cn\pi t}{a}\right). \tag{11.54}$$

Exercise.
(1) Find the solution for

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2} + 2\frac{\partial u}{\partial t} + u \tag{11.55}$$

for $x \in [0, \pi]$ with a homogeneous Dirichlet boundary condition and the initial condition $u(x, 0) = \sin x$ and $\partial_t u(x, 0) = 0$.
(2) Solve 1-d wave equation with the wave speed c under the initial condition

$$u(0, x) = \sin\frac{3\pi}{2\ell}x,\ \partial_t u(0, x) = 0 \tag{11.56}$$

with the boundary condition $u(t, 0) = 0$ and $\partial_x u(t, 0) = 0$ for $t > 0$ (i.e., $x = 0$ is fixed and $x = \ell$ is open).
(3) There is a string of length l whose both ends are fixed. A concentrated force $A\sin\omega t$ is applied at $x = c$ on the string. Let the density of the string be ρ and its tension T. Then, the speed is given by $c^2 = T/\rho$ (→**??**).
(4) A uniform flexible chain is hanging along the z-axis. Let u be the displacement of the chain in the xz-plane, hanging from the origin. Then

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(x\frac{\partial u}{\partial x}\right). \tag{11.57}$$

Solve this with the aid of the separation of variables. The equation for the spatial function becomes Bessel's equation (→**??**) in this case.
Discussion.
The shape of the string of a violin at time t takes the form in the figure; it looks like a ^ . The breaking pont moves with a constant velocity and its trajectory is on a parabola (see the photos). The formula for the shape is

$$\phi(x, t) = C\sum_{n=1}^{\infty}\frac{1}{n^2}\sin k_n x\sin\omega_n t, \tag{11.58}$$

where $k_n = \pi n/L$ and $\omega_n = ck_n$ with the wave speed c. C is a constant dependent on the loudness of the sound. Demonstrate the statement about the shape (esp.

the motion of the breaking point) from this formula

12 Fourier Transformation

Basics of Fourier transform including the principle of FFT, major qualitative features like the uncertainty principle, sampling theorem, Wiener-Khinchine theorem are discussed in the first two subsections. Then, Fourier analysis of generalized functions and related topics such as Poisson's sum formula, the Plemelj formula are treated in the third subsection. As a related topic, Radon transform is discussed in the last subsection, which underlies many tomographic techniques.

12.A Basics

Fourier analysis is reviewed. The relation between smoothness of the function and the decay rate of its Fourier transform is important. As theoretical applications, uncertainty principle, sampling theorem and the Wiener-Khinchin theorem about spectral analysis are discussed.

Key words: Fourier transform, deconvolution, inverse Fourier transform, sine (cosine) transform, bra-ket notation, Plancherel's theorem, Riemann-Lebesgue lemma

Summary:
(1) Fix your convention of Fourier transform (**12.2**, **12.14**). Deconvolution is often the place where Fourier transformation is effective (**12.3**). Linear differential operators become multiplicative operators (**12.4**).
(2) The decay rate of the Fourier transform and the smoothness of its original function are closely related just as in the Fourier expansion cases (**12.12**).

12.1 Formal limit of Fourier expansion. T229

12.2 Fourier transform. Let f be an integrable function (→**??**) on $\boldsymbol{R}$. If the following integral exists

$$\hat{f}(k) = \mathcal{F}(f)(k) \equiv \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \tag{12.1}$$

it is called the *Fourier transform* of f. Multidimensional cases can be treated similarly.

Exercise.
(A) Consider the Fourier transform of a wave train of finite duration. Or, more concretely, compute the Fourier transform of

$$f(t) = [\Theta(t+T) - \Theta(t-T)] \cos at, \tag{12.2}$$

Sketch the Fourier transform.
(B)
(1) Demonstrate the Fourier transform of the following triangular function

is given by

$$X(\omega) = \frac{4 \sin^2(\omega T/2)}{T\omega^2}. \tag{12.3}$$

(2) Demonstrate

$$\int_{-\infty}^{\infty} \frac{\sin^2 ax}{\pi a x^2} dx = 1. \tag{12.4}$$

for any $a \neq 0$ with the aid of (1).

12.3 Deconvolution. As can be demonstrated with the aid of Fubini's theorem (→**??**).

$$\mathcal{F}(f * g) = \mathcal{F}(f)\mathcal{F}(g), \tag{12.5}$$

This is a very useful relation.

Exercise.
In the following a and b are positive real numbers.
(i) Fourier transform

$$\chi(x) = \Theta(b - |x|). \tag{12.6}$$

(ii) Fourier transform $e^{-a|x|}$.
(iii) Fourier transform

$$f(x) = e^{-a|x|} \frac{\sin bx}{x}. \tag{12.7}$$

12.4 Differentiation becomes multiplication. We have an important relation

$$\hat{f}' = +ik\hat{f}. \tag{12.8}$$

The sign in front of the formula depends on our choice of the definition **12.2**. We have the following formulas (→**3.7**, **3.9**, **3.11**):

$$\begin{aligned} \mathcal{F}(div\,\boldsymbol{v}) &= +i\boldsymbol{k}\cdot\boldsymbol{v}_{\boldsymbol{k}} && (12.9)\\ \mathcal{F}(curl\,\boldsymbol{v}) &= +i\boldsymbol{k}\times\boldsymbol{v}_{\boldsymbol{k}} && (12.10)\\ \mathcal{F}(-\Delta f) &= k^2 f_{\boldsymbol{k}}. && (12.11) \end{aligned}$$

The last formula explains why $-\Delta$ is a natural combination – it is a positive definite operator.
A fundamental reason why differentiation becomes multiplication is this; spatial translation becomes phase change.

12.5 Theorem [Inverse Fourier transformation]. If $f : \boldsymbol{R} \to \boldsymbol{C}$ is continuous (and bounded), and both f and $\hat{f}$ are absolutely integrable, then the inversion formula holds

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \hat{f}(k)e^{+ikx}dk \equiv \mathcal{F}^{-1}(\hat{f}). \tag{12.12}$$

□
The formula could be guessed from the Fourier expansion formula **10.1**; actually Fourier reached this result in this way. (12.12) appears so often that we have fairly a standard abbreviation

$$\int_k \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty}, \quad \int_{\boldsymbol{k}} \equiv \left(\frac{1}{2\pi}\right)^d \int d\boldsymbol{k}. \tag{12.13}$$

12.6 Theorem [Inversion formula for piecewise C^1-function]. Let f be piecewise C^1-function on $\boldsymbol{R}$. Then (cf. **??**)

$$\frac{1}{2}[f(x_0-0)+f(x_0+0)] = \frac{1}{2\pi}P\int_{-\infty}^{\infty} dke^{ikx_0}\hat{f}(k). \tag{12.14}$$

P denotes the Cauchy principal value (→**??**). □
We can write the formula as

$$\frac{1}{2}[f(x_0-0)+f(x_0+0)] = \lim_{\lambda\to\infty}\int_{-\infty}^{\infty} d\xi \frac{\sin[\lambda(x_0-\xi)]}{x_0-\xi}\hat{f}(\xi). \tag{12.15}$$

□

12.7 More general convergence conditions. As can easily be imagined from **10.10** for a pointwise convergence of the Fourier transform, we need some conditions. For example, if f is of bounded variation[163] near x, then (12.12) holds with $f(x)$ being replaced by $[f(x+0)+f(x-0)]/2$. If f is continuous and of bounded variation in (a,b), then (12.12) holds uniformly there.

12.8 Remark
(1) Mathematicians often multiply $1/\sqrt{2\pi}$ to the definition of Fourier transform as

$$\tilde{f} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \tag{12.16}$$

to symmetrize the formulas (as we will see in **12.10** or **12.13** sometimes this is very convenient), because

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk. \tag{12.17}$$

However, this makes the convolution formula (12.5) awkward. For physicists and practitioners, the definition in **12.2** (the sign choice may be different) is the most convenient, because we wish to compute actual numbers.
This notation makes explict the unitary property of Fourier transformation on the space of rapidly decaying functions. T236.
(2) The integral over k may be interpreted as a sum over n such that $k = 2\pi n/L$, where L is the size of the space. The following approximation is very useful in solid-state physics

$$\frac{1}{V} \sum_{\boldsymbol{k}} f_{\boldsymbol{k}} \simeq \frac{1}{2\pi^d} \int f_{\boldsymbol{k}} d\boldsymbol{k} \equiv \int_{\boldsymbol{k}} f_{\boldsymbol{k}}. \tag{12.18}$$

12.9 Sine and cosine transforms. If the space is limited to $x \geq 0$, then *Fourier sine* and *Fourier cosine transformations* may be useful (cf. **10.18**). If $f(0) = f(0+)$, then

$$g(k) = \int_0^{\infty} f(x) \cos kx dx, \quad f(x) = \frac{2}{\pi} \int_0^{\infty} g(k) \cos kx dk. \tag{12.19}$$

If $f(0) = 0$, then

$$g(k) = \int_0^{\infty} f(x) \sin kx dx, \quad f(x) = \frac{2}{\pi} \int_0^{\infty} g(k) \sin kx dk. \tag{12.20}$$

[163] If a function can be written as a difference of two monotonically increasing functions, we say the function is of *bounded variation*.

These can also be written concisely as

$$\frac{2}{\pi}\int_0^\infty \cos kx \cos k'x dx = \delta(k-k'), \tag{12.21}$$

$$\frac{2}{\pi}\int_0^\infty \sin kx \sin k'x dx = \delta(k-k'). \tag{12.22}$$

They can be shown easily with the aid of the Fourier transform of 1 (→**12.36**); Put $\cos kx = (e^{ikx}+e^{-ikx})/2$, etc. into (12.21) or (12.22).

Exercise.
There is an infinite medium whose thermal diffusivity is D. Its initial temperature distribution is given by $T|_{t=0} = T_0(\boldsymbol{x}$. Find the physically meaningful solution (→**1.19** Warning). There are many ways to solve this. For example, we can use the free space Green's function (→**??** and the initial condition trick **9.23**. We can also use the Fourier transformation as follows.
(1) Show that for any[164] function g on $\boldsymbol{R}^3$

$$g(x,y,z) = \frac{1}{\pi^3}\int_0\infty\int_0^\infty\int_0^\infty d\alpha d\beta d\gamma \int_{-\infty}^\infty\int_{-\infty}^\infty\int_{-\infty}^\infty dadbdc \\ g(a,b,c)\cos\alpha(x-a)\cos\beta(y-\beta 0\cos\gamma(z-c). \tag{12.23}$$

(2) The integrands are linearly independent (no mode coupling, or super position principle), so that each term must satisfy the diffusion equation. Introducing $A(t)\cos\alpha(x-a)\cos\beta(y-\beta 0\cos\gamma(z-c)$ into the diffusion equation, show that

$$A(t) = f(a,b,c)e^{-D(\alpha^2+\beta^2+\gamma^2)t}. \tag{12.24}$$

(3) Combining (1) and (2), obtain the following formula, which can be obtained directly with the use of the free space Greeen's function.

$$T(x,y,x,t) = \pi^{-3/2}\int\_{-\infty}^\infty\int\_{-\infty}^\infty\int\_{-\infty}^\infty d\eta d\xi d\zeta e^{-(\eta^2+\xi^2+\zeta^2)} f(x+2\sqrt{DT}\eta, y+2\sqrt{DT}\xi, z+2\sqrt{DT}\zeta). \tag{12.25}$$

[Perform the integration over Greek letters.]

12.10 Bra-ket notation of Fourier transform or momentum (wave-vector) kets. **12.14** has the following symbolic representation (→**??**-**??** for notations).

$$f(x) = \langle x|f\rangle = \int_{-\infty}^\infty \langle x|k\rangle dk\langle k|f\rangle, \tag{12.26}$$

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx}, \tag{12.27}$$

$$\tilde{f}(k) = \langle k|f\rangle = \int_{-\infty}^\infty \langle x|k\rangle dk\langle k|f\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^\infty e^{ikx}f(x). \tag{12.28}$$

[164] If you wish to be within the ordinary calculus, it must be integrable, but we may proceed formally.

$\langle k|f\rangle$ is the Fourier transform of f in this bra-ket symmetrized version (**12.14**), and the normalization is different from that given in **12.2**. Notice that

$$\langle x|y\rangle = \delta(x-y) = \int \langle x|k\rangle dk \langle k|y\rangle = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ik(x-y)}dk. \tag{12.29}$$

To rationalize this, we need the theory of Fourier transform of generalized functions (→**12.36**).

12.11 Plancherel's theorem.

$$\langle f|f\rangle = \int \langle f|k\rangle dk \langle k|f\rangle \tag{12.30}$$

is called *Plancherel's formula*. In our normalization (for physicists) in **12.2** this reads

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} |\hat{f}(k)|^2 dk. \tag{12.31}$$

The theorem tells us that if f is square integrable (that is, the total energy of the wave is finite), then the total energy is equal to the energy carried by individual harmonic modes. This is of course the counterpart of Parseval's equality (→**??**).

12.12 Theorem [**Riemann-Lebesgue Lemma**]. For an integrable function f

$$\lim_{|\boldsymbol{k}|\to\infty} \hat{f}(\boldsymbol{k}) = 0. \tag{12.32}$$

If all the n-th derivatives are integrable, then $\hat{f}(\boldsymbol{k}) = o[|\boldsymbol{k}|^{-n}]$.□
There is an analogue of **10.13**. There we have already discussed its physical meaning.[165]

12.B Applications of Fourier Transform

Fundamental applications of Fourier transformation important in practice are summarized: uncertainty principle, sampling theorem, the Wiener-Khinchine theorem (the relation between power spectrum and correlation function). Also

[165] see Katznelson p123.

the principle of FFT is outlined.

Key words: uncertainty principle, coherent state, band-limited function, sampling theorem, sampling function, aliasing, time-correlation function, power spectrum, Wiener-Khinchine theorem, fast Fourier transform

Summary:
(1) The uncertainty principle is a basic property of Fourier transformation. Its essence is the elementary Cauchy-Schwarz inequality (**12.13**).
(2) If the band width of a signal (function) is finite, then discrete sampling with sufficiently frequent sampling points perfectly captures the signal. This is the essence of the sampling theorem (**12.18**).
(3) Spectral analysis is a fundamental tool of experimental physics. Its theoretical basis is the Wiener-Khinchine theorem – Fourier transform of the time-correlation function is the power spectrum (**12.23**).
(4) Spectral analysis becomes practical after the popularization of fast Fourier transform (FFT) (**12.25-12.26**).

12.13 Theorem [Uncertainty principle]. Let f be in $L_2(\boldsymbol{R})$ ($\rightarrow$**16.19**). Define the following averages

$$\langle x\rangle \equiv \int x|f(x)|^2dx/\int |f(x)|^2dx, \tag{12.33}$$

$$\langle k\rangle \equiv \int k|\hat{f}(k)|^2dk/\int |\hat{f}(k)|^2dk, \tag{12.34}$$

$$\Delta x^2 \equiv \int (x-\langle x\rangle)^2|f(x)|^2dx/\int |f(x)|^2dx, \tag{12.35}$$

$$\Delta k^2 \equiv \int (k-\langle k\rangle)^2|\hat{f}(k)|^2dk/\int |\hat{f}(k)|^2dk. \tag{12.36}$$

Then,

$$\Delta x\Delta k \geq 1/2. \tag{12.37}$$

[Demo] Without loss of generality, we may assume $\langle x\rangle = 0$, and also assume that f is already normalized. Define

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}}\int dxe^{ikx}f(x). \tag{12.38}$$

Using Plancherel's theorem ($\rightarrow$**12.11**), we get (cf. **12.4**)

$$\int dx|f'(x)|^2 = \int |k\tilde{f}(k)|^2dk,\ \int dx|f(x)|^2 = \int |\tilde{f}(k)|^2dk, \tag{12.39}$$

so that

$$\Delta k^2 = \int |f'(x)-\langle k\rangle f(x)|^2dx. \tag{12.40}$$

The Cauchy-Schwarz inequality (→**16.7**) implies

$$\Delta k^2 \Delta x^2 = \int |f'(x) - \langle k \rangle f(x)|^2 dx \int x^2 |f(x)|^2 dx \geq \left| \int [f'(x) - \langle k \rangle f(x)] x \overline{f(x)} dx \right|^2, \tag{12.41}$$

but since $\langle x \rangle = 0$, the last formula reads

$$|f'(x) x \overline{f(x)} dx|^2 \geq |Re \int f'(x) x \overline{f(x)} dx|^2 = 1/4. \tag{12.42}$$

The last number comes from the following integration by parts

$$\int f'(x) x \overline{f(x)} dx = -\int \overline{f'(x)} x f(x) dx - \int |f(x)|^2 dx. \tag{12.43}$$

12.14 Remark. As can be seen from the proof of **12.13**, the uncertainty principle is a disguised Cauchy-Schwarz inequality (→**??**) which says that the modulus of cosine cannot be larger than 1. Note that obvious mathematical theorems can have profound implication in real life.

12.15 Coherent state. The equality in the uncertainty principle is realized if the wave function f is Gaussian

$$f(x) = \frac{1}{\pi^{1/4} \sigma^{1/2}} e^{-x^2/2\sigma^2}. \tag{12.44}$$

Check indeed $\Delta x \Delta k = 1/2$. A state with this equality is called a *coherent state*.

12.16 Hardy's theorem. T289 (on coherence)

12.17 Band-limited function. If a function has a Fourier transform which has a compact support (i.e., $\hat{f}(k)$ is zero if $|k| > k_0$ for some $k_0 > 0$), then f is called a *band-limited function*.

12.18 Theorem [**Sampling theorem**]. Let f be a band-limited function such that $\hat{f}(k)$ be zero if $|k| > k_0 > 0$. Then,

$$f(x) = \sum_{n=-\infty}^{\infty} f(n\pi/k_0) \frac{\sin(k_0 x - n\pi)}{k_0 x - n\pi}. \tag{12.45}$$

That is, f can be reconstructed from the discrete sample values $\{f(n\pi/k_0)\}_{n\in\boldsymbol{Z}}$.□
The sampling theorem is extremely important in communication (multichannel communication, bandwidth compression, etc.), and information storage (digitization as in CD).
[Demo] Since $\hat{f}(k)$ is non-zero only on $[-k_0, k_0]$, we can Fourier expand this as a function of period $2k_0$ (→**10.2**)

$$\hat{f}(k) = \sum_{n\in\boldsymbol{Z}} c_n e^{ikn\pi/k_0} \tag{12.46}$$

with

$$\frac{1}{2k_0}\int_{-k_0}^{k_0} \hat{f}(k)e^{-in\pi k/k_0}dk = c_n. \tag{12.47}$$

On the other hand due to the band-limitedness

$$f(x) = \frac{1}{2\pi}\int_{-k_0}^{k_0} \hat{f}(k)e^{-ikx}dk. \tag{12.48}$$

Comparing (12.47) and (12.48), we get

$$c_n = \frac{\pi}{k_0} f(n\pi/k_0). \tag{12.49}$$

(12.46), (12.48) and (12.49) give the desired result.

Exercise.
Determine the minimum sampling rate (or frequency) for the signal $10\cos\omega t + 2\cos 3\omega t$. This is a trivial question, so do not think too much.

12.19 Sampling function. The function

$$\varphi_n(x) = \frac{\sin(k_0x - n\pi)}{k_0x - n\pi} \tag{12.50}$$

appearing in (12.45) is called the *sampling function*. $\{\varphi_n\}_{n\in\boldsymbol{Z}}$ is an orthogonal system. There is an orthogonality relation:

$$\int_{-\infty}^{\infty} \varphi_n(x)\varphi_m(x)dx = \frac{\pi}{k_0}\delta_{nm}.[\tag{12.51}$$

Exercise.
Demonstrate that the sampling functions $\{\varphi_n\}$ make an orthogonal system. That is, demonstrate (12.51).

12.20 Band-limited periodic function. The sampling theorem would naturally tell us the following. A band-limited periodic function with no harmonics of order higher than N can be uniquely specified by its values sampled at appropriate $2N+1$ points in a single period.

12.21 Aliasing. If the function we sample is strictly band-limited, then the above theorem of course works perfectly. However, often the function has higher frequency components beyond the sample frequency. Then, just as we watch fast rotating wheel in the movie, what we sample is the actual frequency modulo the sample frequency (that is, the beat between these frequencies). This phenomenon is called *aliasing*. To avoid unwanted aliasing, often we filter the original signal (through a low-pass filter) and remove excessively high frequency components.

12.22 Time-correlation function. Let $x(t)$ be a stochastic process or time-dependent data which is statistically stationary. Here 'stochastic' means that we have an ensemble of such signals (more precisely, we have a set of signals $\{x(t;\omega)\}$, where ω is the probability parameter specifying each sample signal. That is, if the reader wishes to start an observation, one ω is given (by God) and she will observe $x(t;\omega)$. The word 'stationary' implies that the ensemble average of $x(t,\omega)$ does not depend on t.[166] Let us denote the ensemble average by $\langle\ \rangle_\omega$. The *time correlation function* is defined by

$$C(t) = \langle x(t)x(0)\rangle_\omega \tag{12.52}$$

and is a fundamental observable in many practical cases.
The ensemble average of

$$\sigma(\nu) = \langle |x_\nu|^2\rangle_\omega \tag{12.53}$$

is called the *power spectrum* of the signal $x(t)$, where x_ν is the Fourier transform of $x(t)$. Thanks to the advent of FFT (→**12.26**), it is easy to obtain the power spectrum experimentally (easier than the correlation function).

12.23 Theorem [Wiener-Khinchin]. The Fourier transform of the power spectrum of a stationary stochastic process is its power spectrum. That is,[167]

$$C(t) \propto \int_{-\infty}^{\infty} e^{-i\nu t}\sigma(\nu)d\nu. \tag{12.54}$$

[166] Actually, in this case we only need the absolute time independence of the correlation function. A process with this property is called a *weak stationary process*.
[167] Actually, if we normalize $C(t)$ so that $C(0) = 1$ (simply regard $C(t)/C(0)$ as $C(t)$), then we have probability measure σ such that

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\nu t}d\sigma(\nu).$$

However, in practice, the numerical constant and normalization are not crucial.

Its demonstration is a straightforward calculation. We compute (→**12.36**)

$$\begin{aligned}\langle x_\nu x_{-\mu}\rangle &= \left\langle \int_{-\infty}^{\infty} dt x(t) e^{i\nu t} \int_{-\infty}^{\infty} ds x(s) e^{-i\mu s} \right\rangle \\ &= \int_{-\infty}^{\infty} dt \int_{-\infty}^{\infty} ds e^{i\nu t} e^{-i\mu s} \langle x(t-s)x(0)\rangle \\ &= 2\pi\delta(\nu-\mu)\int_{-\infty}^{\infty} dt e^{i\nu t} C(t). \end{aligned} \tag{12.55}$$

That is, $\langle x_\nu x_{-\mu}\rangle = \delta(\nu-\mu)\sigma(\nu)$ so that

$$\sigma(\nu) = 2\pi \int_{-\infty}^{\infty} dt e^{i\nu t} C(t). \tag{12.56}$$

12.24 Bochner's theorem. T275

12.25 Discrete Fourier transformation. Let $\boldsymbol{X} \equiv \{X_n\}_{n=0}^{N-1}$ be a sequence of complex numbers, and

$$e(x) \equiv \exp(-2\pi i x). \tag{12.57}$$

The following sequence $\hat{\boldsymbol{X}} \equiv \{X^n\}$ is called the *discrete Fourier transform* of $\boldsymbol{X}$:

$$X^k = \sum_{n=0}^{N-1} e\left(\frac{kn}{N}\right) X_n. \tag{12.58}$$

Its inverse transform is given by

$$X_n = \frac{1}{N}\sum_{k=0}^{N-1} e\left(\frac{-kn}{N}\right) X^k. \tag{12.59}$$

Notice that a straightforward calculation of these sums (N of them) costs $O[N^2]$ operations and is costly.

Exercise.
Demonstrate the above inverse transform formula by showing

$$\frac{1}{N} \sim_{k=0}^{N-1} e^{k(m-n)/N} = \delta_{mn}. \tag{12.60}$$

12.26 Principle of fast Fourier transform.[168] Let $N = N_1 N_2$. $n, k \in \{0, 1, \cdots, N-1\}$ can be uniquely written as[169]

$$n = n_1 + n_2 N_1, \quad k = k_1 N_2 + k_2, \tag{12.61}$$

where $n_i, k_i \in \{0, 1, \cdots, N_i - 1\}$ ($i = 1$ or 2). Notice that

$$e(kn/N) = e(k_1 n_1/N_1) e(k_2 n_2/N_2) e(k_2 n_1/N). \tag{12.62}$$

n_i and k_i are uniquely determined, so we may write, e.g., $(n_1 n_2)$ instead of n. Then, (12.58) can be calculated as

$$\begin{aligned} X^{(k_1 k_2)} &= \sum_{n=0}^{N_1 N_2 - 1} e(k_1 n_1/N_1) e(k_2 n_2/N_2) e(k_2 n_1/N) X_{(n_1 n_2)}, \\ &= \sum_{n_1=0}^{N_1-1} e(k_1 n_1/N_1) \left\{ e(k_2 n_1/N) \left[\sum_{n_2=0}^{N_2-1} e(k_2 n_2/N_2) X_{n_1 n_2} \right] \right\}. \end{aligned} \tag{12.63}$$

Consequently, the calculation of discrete Fourier transfrom can be decomposed into the following three steps:
(1) Compute for any k_2

$${X_{n_1}}^{k_2} = \sum_{n_2=0}^{N_2-1} e(k_2 n_2/N_2) X_{n_1 n_2}. \tag{12.64}$$

(2) Then, rotate the phase:

$$\tilde{X}_{n_1}{}^{k_2} = e(k_2 n_1/N) {X_{n_1}}^{k_2}. \tag{12.65}$$

(3) Finally compute for any k_1

$$\hat{X}^{k_1 k_2} = \sum_{n_1=0}^{N_1-1} e(k_1 n_1/N_1) \tilde{X}_{n_1}{}^{k_2}. \tag{12.66}$$

Now the number of necessary operations is $O[N_1 \times N_2^2] + O[N_1^2 \times N_2]$; if $N_1 = N_2 = \sqrt{N}$, then $O[2N^{3/2}]$. If we can decompose N into m factors of similar order, then the number of necessary operations is roughly $N^{1-1/m} N^{2/m} = N \times N^{1/m}$. Hence, asymptotically, we can guess $N \ln N$ is the best possibility for the discrete Fourier transform of N numbers.

Exercise.
Find the autocorrelation function of the signal

$$f(t) = \Theta(t + T) - \Theta(t - T). \tag{12.67}$$

Then illustrate the Wiener-Khinchine theorem with the example.

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[168] The algorithm, known sometimes as the Cooley-Tukey algorithm (J W Cooley and J W Tukey, Math. Comp. **19**, 297 (1965)), was actually known to Gauss, but the importance was widely recognized after this paper.
[169] This is an example of the so-called *Chinese remainder theorem*.

12.C Fourier Analysis of Generalized Function

Generalized functions can be Fourier transformed and physicists' favorite formulas like $\int e^{ikx}dk = 2\pi\delta(x)$ or the Plemelj formula $1/(x+i0) = P(1/x) - i\pi\delta(x)$ can be demonstrated. Fourier expansion of δ-function gives us the Poisson sum formula which may be used to accelerate the convergence of series.

Key words: Fourier expansion of unity, Poisson sum formula, Euler-MacLaurin sum formula, Plemelj formula

Summary:
(1) Not convergent Fourier series may be interpreted as a generalized function. A typical example is Poisson's sum formula (**12.28**).
(2) Formal calculation of Fourier transform of generalized functions often works, but whenever there is some doubt, return to the definition (**12.34**, **12.36**).

12.27 Delta function.

$$\delta(x) = \sum_{n=-\infty}^{\infty} e^{i2n\pi x} \tag{12.68}$$

for $x \in (-1, 1)$.
[Demo] We know as an ordinary Fourier series

$$\frac{1-2x}{2} = \sum_{n=1}^{\infty} \sin(2n\pi x)/n\pi \tag{12.69}$$

for $x \in (0, 1)$. We may use the RHS to extend the LHS periodically for all $\boldsymbol{R}$. Differentiate this termwisely, interpreting this as a formula for generalized functions (→**7.14**). We get

$$-1 + \delta(x) = 2\sum_{n=1}^{\infty} \cos 2n\pi x \tag{12.70}$$

for $x \in (-1/2, 1/2)$.
The decomposition of unity (→**??**) can also be used to obtain (12.68).

12.28 Poisson's sum formula.

$$\sum_{k=-\infty}^{\infty} \delta(x-k) = \sum_{n=-\infty}^{\infty} e^{i2n\pi x} \tag{12.71}$$

for $x \in \boldsymbol{R}$.

This can be obtained easily from (12.68) by 'tessellating' the formula for $(-1/2, 1/2)$ over the whole range of $\boldsymbol{R}$. From (12.71) we get

$$|\lambda| \sum_{k=-\infty}^{\infty} \delta(x - \lambda k) = \sum_{n=-\infty}^{\infty} e^{i2\pi nx/\lambda} \tag{12.72}$$

(cf. **7.11**). Applying a test function φ to this, we get the following *Poisson sum formula*:

$$|\lambda| \sum_{k=-\infty}^{\infty} \varphi(\lambda k) = \sum_{n=-\infty}^{\infty} \hat{\varphi}(2n\pi/\lambda). \tag{12.73}$$

(Be careful with the normalization constant.) Also we can make a cosine version of the Poisson sum formula

$$\sum_{k=-\infty}^{\infty} \delta(x - k) = 1 + 2\sum_{n=1}^{\infty} \cos(2n\pi x). \tag{12.74}$$

If $f(x)$ is a gently decaying function, then its Fourier transform decays rapidly, and vice versa. The Poisson sum formula is useful because it may help accelerating the convergence of the series.

Exercise.
(1) Demonstrate

$$\sum_{n=1}^{\infty} \frac{\cos na}{1+n^2} = \frac{\pi}{2}\frac{\cosh(\pi - a)}{\sinh \pi} - \frac{1}{2}.$$

(2) Similarly, show

$$\sum \frac{1}{n^2 + t^2} = \frac{\pi}{t}\frac{1 - e^{-2\pi t}}{1 - e^{-2\pi t}}.$$

Then, take the limit $t \to 0$ to obtain

$$\sum \frac{1}{t^2} = \frac{\pi^2}{6}.$$

12.29 Applications of Poisson sum formula.

(1)

$$\sum_{n \in \boldsymbol{Z}} \frac{1}{1 + a^2 n^2} = \frac{\pi}{a} \coth \frac{\pi}{a}. \tag{12.75}$$

The key formulas are

$$\hat{\varphi}(k) = \frac{1}{1 + a^2 k^2/4\pi^2}, \quad \varphi(x) = \frac{\pi}{a} e^{-2\pi|x|/a}. \tag{12.76}$$

(2)

$$\sum_{n=1}^{\infty} \frac{\cos na}{1+n^2} = \frac{\pi}{2}\frac{\cosh(\pi - a)}{\sinh \pi} - \frac{1}{2}. \tag{12.77}$$

12.30 Euler-MacLaurin sum formula.

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} f(x)dx + \frac{1}{2}f(0) - \frac{1}{12}f'(0) + \frac{1}{720}f^{(3)}(0) - \frac{1}{30240}f^{(5)}(0) + \cdots. \tag{12.78}$$

[Demo] Let f be a function defined on the positive real axis. Extend it to the whole $\boldsymbol{R}$ as an even function ($f(x) = f(-x)$). Apply the cosine version of the Poisson sum formula (12.74) and integrate from 0 to ∞. Using the evenness of the function, we get

$$-\frac{1}{2}f(0) + \sum_{k=0}^{\infty} f(k) = \int_0^{\infty} f(x)dx + 2\sum_{n=1}^{\infty}\int_0^{\infty} f(x)\cos(2n\pi x)dx. \tag{12.79}$$

Integrating by parts the last integrals containing cosines, we get

$$\sum_{k=0}^{\infty} f(k) = \frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - \sum_{n=1}^{\infty}\int_0^{\infty} f'(x)\frac{\sin 2n\pi x}{2n\pi}dx. \tag{12.80}$$

Keep applying integration by parts to get

$$\sum_{n=1}^{\infty}\int_0^{\infty} f'(x)\frac{\sin 2n\pi x}{2n\pi}dx = -\sum_{n=1}^{\infty}\left[f'(x)\frac{\cos 2n\pi x}{2(n\pi)^2}\right]_0^{\infty} + \sum_{n=1}^{\infty}\int_0^{\infty} f''(x)\frac{\cos 2n\pi x}{2(n\pi)^2}dx. \tag{12.81}$$

Thus

$$\sum_{k=0}^{\infty} f(k) = \frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - f'(0)\sum_{n=1}^{\infty}\frac{1}{2n^2\pi^2} + \cdots. \tag{12.82}$$

This gives the $f'(0)$ term of the formula.

12.31 Mulholland's formula for canonical partition function for the rotational motion of a heteronuclear diatomic molecule. The rotational partition function $r(T)$ at temperature T is given by

$$r(T) = \sum_{\ell=0}^{\infty}(2\ell+1)\exp\left[-\frac{\hbar^2\ell(\ell+1)}{2Ik_BT}\right], \tag{12.83}$$

where I is the moment of inertia of the molecule, and k_B is the Boltzmann constant. Introduce $\sigma \equiv \hbar^2/2Ik_BT$, and let

$$f(x) = (2x+1)\exp[-x(x+1)\sigma]. \tag{12.84}$$

Apply (12.78) to this function, we get the following Mulholland's formula

$$r(T) = \frac{1}{\sigma} + \frac{1}{3} + \frac{\sigma}{15} + \frac{4\sigma^2}{315} + O[\sigma^3]. \tag{12.85}$$

The first term on the RHS is the classical value.
Apply this to ... T282. Although the convergence is fast, if successful, but do not forget that this is an asymptotic expansion, so conv ergence does not guarantee the accuracy.

12.32 Central limit theorem. T282

12.33 Multidimensional Poisson formula.

12.34 Fourier transform of generalized functions. The crucial observation is (for ˆ see **12.2**): if f and φ both have well-defined Fourier transforms,

$$\langle \hat{f}, \varphi \rangle = \int dk \left[\int dx f(x) e^{-ikx} \right] \varphi(k) = \langle f, \hat{\varphi} \rangle \tag{12.86}$$

The Fourier transform $\hat{\tau} \equiv \mathcal{F}[\tau]$ of a generalized function τ is defined by

$$(\hat{\tau}, \varphi) = (\tau, \hat{\varphi}), \text{ or } (\mathcal{F}[\tau], \varphi) = (\tau, \mathcal{F}[\varphi]), \tag{12.87}$$

where $\varphi \in \mathcal{D}$, a test function.

Exercise.
Demonstrate

$$\lim_{\lambda \to \infty} \frac{\sin \lambda x}{x} = \pi \delta(x). \tag{12.88}$$

$$\lim_{\lambda \to \infty} \int_a^b \sin \lambda x = 0. \tag{12.89}$$

12.35 Convenient test function space. For this definition it is desirable that the set of test functions $\mathcal{D}$ (→**7.8**) and the set of their Fourier transforms $\hat{\mathcal{D}}$ are identical. For the set of Schwartz class functions (→**7.8** footnote) this holds (→**12.12**). [If we choose $\mathcal{D}$ to be the set of all the functions with compact supports, then $\hat{\mathcal{D}}$ becomes very large, so that the class of generalized functions (for which $(\tau, \hat{\varphi})$ must be meaningful) must be severely restricted, and is not very convenient.]

12.36 Fourier transform of unity = delta function.

$$\hat{1} = 2\pi\delta(k). \tag{12.90}$$

This is the *true* meaning of the physicists' favorite

$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} e^{ikx}dk = \delta(x). \tag{12.91}$$

Obviously, $\hat{\delta} = 1$ (direct calculation). That is, $\mathcal{F}^2$ implies multiplication of 2π as we know in **12.11**.
[Demo] $(\hat{1}, \varphi) = (1, \hat{\varphi}) = \int \hat{\varphi}(k)dk = \mathcal{F}^2[\varphi](0)$. Here $\mathcal{F}[\varphi]$ is a function on the configuration space (that is, a function of x) and is equal to $2\pi\varphi(x)$. Therefore we have obtained

$$(\hat{1}, \varphi) = 2\pi\varphi(0) = \int 2\pi\delta(x)\varphi(x)dx = (2\pi\delta, \varphi). \tag{12.92}$$

Exercise.
Show

$$\delta(t) = \frac{1}{\pi}\int_0^{\infty} \cos\omega t d\omega. \tag{12.93}$$

Cf. **12.9**.

12.37 Translation of delta function. The following formulas should be obvious

$$\mathcal{F}[\delta(x-a)] = e^{-iak}, \quad \mathcal{F}[e^{iax}] = 2\pi\delta(a-k). \tag{12.94}$$

12.38 Fourier transform of x, $d/dx \leftrightarrow +ik$. (→**12.4**)

$$\hat{x} = +2\pi i\delta'(k). \tag{12.95}$$

In other words, since $\mathcal{F}^2 \equiv 2\pi$,

$$\hat{\delta}' = +ik. \tag{12.96}$$

[Demo] Start with the definition $(\hat{x}, \varphi) = (x, \hat{\varphi})$ (→**12.34**) which is equal to

$$\int dx x\hat{\varphi}(x) = \int dx x\left[\int e^{-ikx}\varphi(k)dk\right] = \int dx \int dk \left(-\frac{d}{dik}e^{-ikx}\right)\varphi(k). \tag{12.97}$$

Integrating this by parts, taking into account that the test function φ decays sufficiently quickly, we get

$$-\int dx \int dk ie^{-ikx}\varphi'(k) = -i\int dk\hat{1}(k)\varphi'(k) = -2\pi i\int dk\delta(k)\varphi'(k) = 2\pi i\int dk\delta'(k)\varphi(k), \tag{12.98}$$

where we have used (12.90) in **12.36**, and the definition of δ' ($\rightarrow$**7.14**).

A more formal and direct 'demonstration' is

$$\hat{x} = \int xe^{-ikx}dx = \int \left(i\frac{d}{dk}\right)e^{-ikx}dx = 2\pi i\frac{d}{dk}\delta(k). \tag{12.99}$$

Convolution of the derivative of delta function is differentiation ($\rightarrow$**7.24**(2)), and the Fourier transform of a convolution is the product of the Fourier transforms, i.e., $\mathcal{F}(f*g) = \mathcal{F}(f)\mathcal{F}(g)$ ($\rightarrow$**12.3**), so that we easily get)cf. **12.4**)

$$\hat{f}' = +ik\hat{f}. \tag{12.100}$$

12.39 Fourier transform of x^n.

$$\hat{x^n} = 2\pi\left(+i\frac{d}{dk}\right)^n\delta(k). \tag{12.101}$$

In other words,

$$\hat{\delta^{(n)}} = (+ik)^n. \tag{12.102}$$

Since $\delta'*f = f'$, $\delta^{(n)} = \delta'*\delta^{(n-1)} = \delta'*\delta'*\cdots\delta'*\delta$ (n δ' are convoluted) (this is well defined $\rightarrow$**7.24**(2)). This and (12.96) immediately imply (12.102).

12.40 Fourier transform of sign function.

$$\hat{sgn}(k) = \frac{2}{i}P\frac{1}{k}, \tag{12.103}$$

where P denotes the Cauchy principal value ($\rightarrow$**??**).

[Demo] We have demonstrated ($\rightarrow$**??**)

$$\frac{d}{dx}sgn(x) = 2\delta(x). \tag{12.104}$$

Fourier-transforming this, we get ($\rightarrow$(12.100) and $\hat{\delta} = 1$)

$$+ik\mathcal{F}(sgn)(k) = 2. \tag{12.105}$$

With the aid of (2) in **??**, we can solve this equation for $\hat{sgn}$ as

$$\hat{sgn}(k) = 2iP\frac{1}{k} + c\delta(k), \tag{12.106}$$

where c is a constant not yet determined. To fix this constant we apply this equality to an even test function, say e^{-k^2}. Since sgn is an odd generalized function, and since the Fourier transform of a Gaussian function is again Gaussian,

$$(s\hat{g}n, e^{-k^2}) \propto (sgn, e^{-x^2}) = 0. \tag{12.107}$$

$P(1/k)$ is also an odd function, so that this implies $c = 0$.

12.41 Plemelj formula.

$$w\text{-}\lim_{\epsilon\to+0} \frac{1}{x \pm \epsilon i} = P\frac{1}{x} \mp i\pi\delta(x), \tag{12.108}$$

where $w\text{-}\lim_{\epsilon\to+0}$ is the weak limit, that is, the limit is taken *after* integration in which the function appears is completed.
[Demo] Obviously,

$$\lim_{\epsilon\to0+} e^{-\epsilon x}\Theta(x) = \Theta(x), \tag{12.109}$$

If we interpret this equation as an equation for generalized functions, then integration and the limit can be freely exchanged. Therefore, we get

$$\hat{\Theta}(k) = w\text{-}\lim_{\epsilon\to0+} \int_0^\infty e^{-(ik-\epsilon)x} = \lim_{\epsilon\to0+} \frac{1}{ik+\epsilon}. \tag{12.110}$$

Since $sgn(x) = 2\Theta(x) - 1$, (12.103), (12.90) and (12.110) imply

$$2iP\frac{1}{k} = \lim_{\epsilon\to0+} \frac{-2}{ik-\epsilon} - 2\pi\delta(k). \tag{12.111}$$

12.D Radon Transformation

Radon transformation is a theoretical basis of various tomographies. Its inverse transformation is constructed with the aid of Fourier transformation. Radon transformation allows us to solve the Cauchy problem of the wave equation in any dimensional space. The explicit formula clearly demonstrates the marked difference of even and odd dimensional spaces.

Key words: Radon's problem, Radon transform, modified Radon transform, tomography, wave equation, afterglow.

Summary:
(1) The mathematical principle of tomography is Radon transformation (**12.44**) whose inverse transformation is essentially calculable by Fourier transformation (**12.45-12.46**).
(2) Radon transform gives a general method to solve d-wave equation (**12.50**). The resultant solution clearly exhibits the afterglow effect in even dimensional spaces (**12.51**).

NOTATION $f^{\#}$ may be good.

12.42 Radon's problem. Radon (1917) considered the following problem: Reconstruct a function $f(x, y)$ on the plane from its integral along all lines in the plane. That is, the problem is to reconstruct the shape of a hill from the areas of all its vertical cross-sections.

12.43 Radon transform. Let f be a function defined on a region in $\boldsymbol{R}^2$.[170]

$$\mathcal{R}f(s, \boldsymbol{\omega}) \rightleftharpoons \int_{\boldsymbol{R}^2} d\boldsymbol{x}\delta(\boldsymbol{x} \cdot \boldsymbol{\omega} - s)f(\boldsymbol{x}) \tag{12.112}$$

is called the *Radon transform* of f, where $\boldsymbol{\omega}$ is the directional vector $|\boldsymbol{\omega}| = 1$ specifying a line normal to it, and $s \in \boldsymbol{R}$ is the (signed) distance between the line and the origin. The Radon problem **12.42** is to find f from $\mathcal{R}f$.

That (12.112) is the integral of f along the line specified by $\boldsymbol{\omega}\cdot\boldsymbol{x} = s$ can easily be seen if we introduce the rotated Cartesian coordinate system O-x_1x_2 such that the x_2 axis is parallel to the line and x_1 perpendicular to it. The integral now reads $\int \delta(x_1 - s)f(x_1, x_2)dx_1dx_2 = \int f(s, x_2)dx_2$.

12.44 Some properties of Radon transform. Note that
(1) $\mathcal{R}f(s, \boldsymbol{\omega})$ is an even homogeneous function (→**6.8**) of s and $\boldsymbol{\omega}$ of degree -1:

$$\mathcal{R}f(\lambda s, \lambda\boldsymbol{\omega}) = |\lambda|^{-1}\mathcal{R}f(s, \boldsymbol{\omega}). \tag{12.113}$$

(2) The Radon transform of a convolution (→**7.23**) is a convolution of Radon transforms:

$$\left(\mathcal{R}\left[\int_{\boldsymbol{R}^2} f_1(\boldsymbol{y})f_2(\boldsymbol{x} - \boldsymbol{y})d\boldsymbol{y}\right]\right)(s, \boldsymbol{\omega}) = \int_{-\infty}^{\infty} dt\,[\mathcal{R}f_1(t, \boldsymbol{\omega})]\,[\mathcal{R}f_2(s - t, \boldsymbol{\omega})]\,. \tag{12.114}$$

[170] The definition given here can easily be extended to general d-space. See **12.48-12.49**. A good introduction to the topic may be found in I. M. Gel'fand, M. I. Graev and N. Ya. Vilenkin, *Generalized Functions*, vol.5 *Integral Geometry and Representation Theory* (Academic Press, 1966). See also R. S. Strichartz, Am. Math. Month. 1982 June-July.

12.45 Fourier transform of Radon transform.

$$\hat{f}(\rho\boldsymbol{\omega}) = \mathcal{F}(\mathcal{R}f)(\rho,\boldsymbol{\omega}) \rightleftharpoons \int_{-\infty}^{\infty} \mathcal{R}f(s,\boldsymbol{\omega})e^{-i\rho s}ds. \tag{12.115}$$

That is, the Fourier transform of $Rf(s,\boldsymbol{\omega})$ with respect to s is the Fourier transform of the function f itself with the '$\boldsymbol{k}$-vector' parallel to $\boldsymbol{\omega}$.

[Demo] Using the definition (12.112), we have only to perform a straightforward calculation:

$$\int_{-\infty}^{\infty} \mathcal{R}f(s\boldsymbol{\omega})e^{-i\rho s}ds = \int_{-\infty}^{\infty} ds \int d\boldsymbol{x} f(\boldsymbol{x})\delta(s-\boldsymbol{x}\cdot\boldsymbol{\omega})e^{-i\rho s} = \int d\boldsymbol{x} f(\boldsymbol{x})e^{-i\rho\boldsymbol{\omega}\cdot\boldsymbol{x}}. \tag{12.116}$$

Thus f can be reconstructed by

$$f(\boldsymbol{r}) = \frac{1}{(2\pi)^d}\int \hat{f}(\rho\boldsymbol{\omega})e^{i\rho\boldsymbol{\omega}\cdot\boldsymbol{r}}d\rho d\boldsymbol{\omega}. \tag{12.117}$$

12.46 Theorem [Radon inversion formula]. Let f be a piecewise C^1-function defined on a region in $\boldsymbol{R}^2$. Then

$$f(\boldsymbol{x}) = \int \tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega},\boldsymbol{\omega})d\sigma(\boldsymbol{\omega}), \tag{12.118}$$

where $d\sigma$ is the arc length element of the unit circle, and $\tilde{\mathcal{R}}f$ is the *modified Radon transform* defined by

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) \rightleftharpoons \frac{1}{8\pi^2}\int_{-\infty}^{\infty} d\rho e^{-i\rho s}\rho\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega}). \tag{12.119}$$

12.47 X-ray tomography. The Radon transformation is the theoretical underpinning of the particle beam tomographies. These are applied not only medically, but also, e.g., to the anatomical study of fossils such as trilobites.

12.48 *d*-space version. In d-space the Radon transform is defined as

$$\mathcal{R}f(s,\boldsymbol{\omega}) = \int_{\boldsymbol{R}^d} f(\boldsymbol{x})\delta(s-\boldsymbol{\omega}\cdot\boldsymbol{x})d\boldsymbol{x}, \tag{12.120}$$

where $\boldsymbol{\omega}$ is the position vector on the unit $d-1$-sphere S^{d-1} (the skin of the d-unit ball). The d-dimensional version of **12.46** reads:

12.49 Theorem [Recovering f from Radon trasnfrom].

$$f(\boldsymbol{x}) = \int_{S^{d-1}} d\sigma(\boldsymbol{\omega}) \tilde{R}f(\boldsymbol{x}\cdot\boldsymbol{\omega}, \boldsymbol{\omega}), \tag{12.121}$$

where

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) \;\rightleftharpoons\; \frac{1}{2(2\pi)^d}\int_{-\infty}^{\infty} e^{-i\rho s}|\rho|^{d-1}\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega})d\rho, \tag{12.122}$$

$$\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega}) \;\rightleftharpoons\; \int_{-\infty}^{\infty} \mathcal{R}f(s,\boldsymbol{\omega})e^{i\rho s}ds\,(=\hat{f}(\rho\boldsymbol{\omega})\,) \tag{12.123}$$

with σ being the area element of S^{d-1}.

12.50 Solving d-wave equation using Radon transform. Consider a wave equation in the whole d-space

$$(\partial_t^2 - \Delta)u = 0 \tag{12.124}$$

with the initial condition $u = f$ and $\partial_t u = g$ at $t = 0$. If the initial data are constant on all the hyperplanes perpendicular to the direction $\boldsymbol{\omega}$, i.e., $f(\boldsymbol{x}) = F(\boldsymbol{x}\cdot\boldsymbol{\omega})$ and $g(\boldsymbol{x}) = G(\boldsymbol{x}\cdot\boldsymbol{\omega})$, where F and G are functions defined on $\boldsymbol{R}$, then we can apply the method to solve the 1-space problem (→**1.12**) to get the solution as

$$u(\boldsymbol{x},t) = \frac{1}{2}[F(\boldsymbol{x}\cdot\boldsymbol{\omega}+t) + F(\boldsymbol{x}\cdot\boldsymbol{\omega}-t)] + \frac{1}{2}\int_{\boldsymbol{x}\cdot\boldsymbol{\omega}-t}^{\boldsymbol{x}\cdot\boldsymbol{\omega}+t} G(s)ds. \tag{12.125}$$

Therefore, if we can decompose the initial data into a superposition of data depending only on $\boldsymbol{x}\cdot\boldsymbol{\omega}$, the superposition principle (→**3.2**) allows us to reconstruct the solution from the pieces like (12.125). As can be seen from (12.121), d-dimensional Radon transformation is the very tool to accomplish the desired decomposition.
The strategy is as follows:
(1) Calculate the modified Radon transform (12.123) for f and g,
(2) Solve the wave equation for $\tilde{\mathcal{R}}u$.
(3) Use (12.121) to reconstruct u:

$$u(\boldsymbol{x},t) = \int_{S^{d-1}} d\sigma(\boldsymbol{\omega})\left\{\frac{1}{2}[\tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega}+t,\boldsymbol{\omega}) + \tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega}-t,\boldsymbol{\omega})] + \frac{1}{2}\int_{\boldsymbol{x}\cdot\boldsymbol{\omega}-t}^{\boldsymbol{x}\cdot\boldsymbol{\omega}+t}\tilde{\mathcal{R}}g(s,\boldsymbol{\omega})ds\right\}. \tag{12.126}$$

12.51 Waves in odd and even dimensional spaces behave very differently. Let us calculate the modified Radon transform (12.123) explicitly. If d is odd, then $|\rho|^{d-1} = \rho^{d-1}$, so that multiplying ρ can be interpreted as differentiation with respect to s as

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) = \frac{1}{2}(-1)^{(q-1)/2}\left(\frac{1}{2\pi}\right)^{d-1}\frac{\partial^{d-1}}{\partial s^{d-1}}\mathcal{R}f(s,\boldsymbol{\omega}). \tag{12.127}$$

In contrast, if d is even then the non-analyticity of $|\rho|$ must be dealt with as $|\rho|^{d-1} = sgn(\rho)\rho^{d-1}$, so that

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) = \frac{1}{2}(-1)^{(q-1)/2}\left(\frac{1}{2\pi}\right)^{d-1} H\left[\frac{\partial^{d-1}}{\partial s^{d-1}}\mathcal{R}f(s,\boldsymbol{\omega})\right], \tag{12.128}$$

where H is the *Hilbert transform* defined by

$$Hf(x) = P\int \frac{f(s)}{x-s}ds, \tag{12.129}$$

where P denotes the Cauchy principal value (→**??**). This can be obtained from the convolution formula and the Fourier transform of *sgn* (→**??**).

Look at the use of the modified Radon transform in the solution (12.126) when the initial velocity is everywhere zero. This applies to the case of an instantaneous flash of light emitted from a point (that is, $f = \delta(x)$). If $\tilde{\mathcal{R}}f(s\boldsymbol{\omega})$ is determined by $\mathcal{R}f(s,\boldsymbol{\omega})$ only, then the observer at distance sees only a flash of light. That is, the wave is localized in time in odd-dimensional (≥ 3) spaces. On the other hand, if the spatial dimensionality is even, then the Hilbert transform implies that the wave is not localized in time. Thus, after watching a flash, the observer must feel that the world becomes brighter (the *afterglow effect* in even dimensional spaces) (→**9.33**).

APPENDIX XXA Bessel Transform

12.52 Theorem [Hankel]. Let $f \in L_1([0,\infty), r)$ and be piecewise continuous. Then

$$\frac{1}{2}[f(r+0)+f(r-0)] = \int_0^\infty J_\nu(\sigma r)\sigma d\sigma \int_0^\infty f(\rho)J_\nu(\sigma\rho)\rho d\rho \quad (12.130)$$

for $\nu \geq 1/2$. This may also be expressed as

$$\int_0^\infty J_\nu(\sigma r)J_\nu(\sigma r')\sigma d\sigma = \delta(r-r')/r. \quad (12.131)$$

Notice that the RHS is the delta function adapted to the weight r (i.e., $\delta_r(r-r') \to$**??**).[171] □

[Demo] Here (12.130) is proved for continuous L_1 (→**??**) functions and integer $\nu = n$. Let

$$F(x,y) = f(r)e^{in\varphi}, \quad (12.132)$$

where $x = r\cos\varphi$ and $y = r\sin\varphi$. With the aid of the Fourier expression of the delta function (→**12.36**), we can write

$$F(x,y) = \frac{1}{(2\pi)^2}\int dk_x \int dk_y \int d\xi \int d\eta F(\xi,\eta)e^{ik_x(x-\xi)+ik_y(y-\eta)}. \quad (12.133)$$

Introduce polar coordinates as

$$\xi = r'\cos\psi, \quad \eta = r'\sin\psi, \quad (12.134)$$

$$k_x = k\cos\theta, \quad k_y = k\sin\theta. \quad (12.135)$$

(12.133) is rewritten as ($F(\xi,\eta) = f(r')e^{in\psi}$)

$$f(r)e^{in\varphi} = \int_0^\infty dkk \int_0^\infty dr'r'f(r')\left\{\frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{ikr\cos(\theta-\varphi)}\frac{1}{2\pi}\int_{-\pi}^{\pi} d\psi e^{in\psi}e^{-ikr'\cos(\psi-\theta)}\right\}. \quad (12.136)$$

Setting $\psi - \theta = t$, we get

$$\frac{1}{2\pi}\int_{\pi}^{\pi} e^{in\psi}e^{-ikr'\cos(\psi-\theta)}d\psi = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikr'\cos t}e^{in(t+\theta)}dt \quad (12.137)$$

$$= e^{in\pi/2}e^{in\theta}J_n(-kr') = e^{in\pi/2+in\theta}(-1)^n J_n(kr'). \quad (12.138)$$

Here the generating function of Bessels functions (→**??**) has been used. Analogously, we have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikr\cos(\theta-\varphi)}e^{in\theta}d\theta = e^{in\pi/2+in\varphi}J_n(kr). \quad (12.139)$$

Hence, (12.136)–(12.139) implies (12.130) for $\nu = n$.

A more convenient formulas may be

[171] More generally, f may be of bounded variation. See G. N. Watson, *A Treatise on the Theory of Bessel Function* (Cambridge UP, 1962) p456–.

12.53 Bessel transform and its inverse.

$$g(r) = \int_0^\infty h(r')J_\nu(r'r)r'dr', \tag{12.140}$$

$$h(r) = \int_0^\infty g(r')J_\nu(r'r)r'dr'. \tag{12.141}$$

Note that these are the formulas for the Fourier sine (or cosine) transform (→**12.9**) for $\nu = \pm 1/2$ (→**??**).

12.54 Examples. See **??**.

$$\int_0^\infty e^{-ax}J_0(xy)dx = \frac{1}{\sqrt{a^2+y^2}} \leftrightarrow \int_0^\infty \frac{y}{\sqrt{a^2+y^2}}J_0(xy)dy = \frac{e^{-ax}}{x}. \tag{12.142}$$

$$\int_0^\infty \cos ax J_0(xy)dx = \frac{1}{\sqrt{y^2-a^2}} \leftrightarrow \int_0^\infty \frac{y}{\sqrt{y^2-a^2}}J_0(xy)dy = \frac{\cos ax}{x}. \tag{12.143}$$

$$\int_0^\infty e^{-a^2x^2}x^{\nu+1}J_\nu(xy)dx = \frac{y^\nu}{(2a^2)^{\nu+1}}e^{-y^2/4a^2} \leftrightarrow \int_0^\infty \frac{y^{\nu+1}}{(2a^2)^{\nu+1}}e^{-y^2/4a^2}J_\nu(xy)dy = e^{a^2x^2}x^\nu. \tag{12.144}$$

13 Laplace Transformation

Laplace transformation is a disguised Fourier transformation for causal functions (the functions that are zero in the past), and is a very useful tool to study transient phenomena. The inverse transformation is often not easy, but clever numerical tricks may be used to invert the transforms. Appendix **a33** discusses a disguised Laplace transformation, Mellin transformation, which is useful when we wish to solve problems on fan shaped domains.

Key words: Laplace transform, fundamental theorem, convolution, time-delay, fast inverse Laplace transform.

Summary:
(1) Laplace transformation **13.2** allows one to solve many ODE algebraically with the aid of tables (**13.14**).
(2) Basic formulas like the convolution theorem, delay theorem, etc should be known to this end (**13.7-13.10**).

13.1 Motivation. Due to causality, we often encounter functions of time t that are zero for $t < 0$ (or often so for $t \leq 0$ due to continuity). Then, the so-called one-sided Fourier transform

$$F[\omega] = \int_0^\infty f(t)e^{i\omega t}dt \tag{13.1}$$

appears naturally. However, if $f(t)$ grows as e^{at} $(a > 0)$, then this does not make sense even in the sense of generalized functions (→**7.4**). Even in this case, if we choose sufficiently large $c > 0$, the one-sided Fourier transform of $e^{-ct}f(t)$ exists in the ordinary sense. If $f(t)e^{-ct}\Theta(t)$ ($\Theta(t)$ is the Heaviside step function →**??**(3)) is absolutely integrable, and f' is piecewise continuous for $t > 0$, then from the Fourier transform of this function, $f(t)$ for $t > 0$ can be recovered.

13.2 Definition of Laplace transform. The following transformation $\mathcal{L}_s$ is called the *Laplace transformation*:

$$\mathcal{L}_s[u(t)] = \int_0^\infty e^{-st}u(t)dt, \tag{13.2}$$

where $s = c - i\omega$ and c is chosen sufficiently large so that the integral exists. $\mathcal{L}_s[u]$ is called the *Laplace transform* of u.[172]

[172] For a history, see M. F. Gardner and J. L. Barnes, *Transients in Linear Systems* vol.I (Wiley, 1942) Appendix C.

Discussion.
(A) A discrete counterpart is the so-called *z-transformation*: The z-transform $A(z)$ of $\{a_n\}$ is defined by

$$A(z) = \sum_{n=0}^{\infty} a_n z^n. \tag{13.3}$$

This is also called the *generating function* of the sequence $\{a_n\}$. The inverse transform is given by

$$a_n = \frac{1}{2\pi i} \int_{\partial D} dz \frac{A(z)}{z^{n+1}}, \tag{13.4}$$

where D is a disc containing the origin but excluding all the singularities of $A(z)$.
(B) z-transform is a convenient way to solve linear difference equation:

$$a_0 x_{n+r} + a_1 x_{n+r-1} + \cdots + a_{r-1} x_{n+1} + a_r x_n = 0. \tag{13.5}$$

For example, let us solve

$$x_{n+2} - 2x_{n+1} + x_n = 0 \tag{13.6}$$

with the 'initial conditions' $x_0 = 1$, and $x_1 = 0$. The z-transform $X(z)$ obeys

$$X(z) - 1 + 2z(X(z) - 1) + z^2 X(z) = 0. \tag{13.7}$$

From this we can solve $X(z)$. The inverse transform gives $x_n = 1 - n$.
(C) An inhomogeneous linear difference equation is given by

$$a_0 x_{n+r} + a_1 x_{n+r-1} + \cdots + a_{r-1} x_{n+1} + a_r x_n = f_n \tag{13.8}$$

The general solution to this equation is given by the sum of the general solution of (13.5) and a special solution to (13.8) just as the linear differential equation. If we can compute the z-transform of $\{f_n\}$, then at least $X(z)$ can be obtained. However, to obtain x_n from X may not be very easy.

13.3 Who was Laplace (1749-1827) ? The 'Newton of France' was born into a cultivated provincial bourgeois family in Normandy (Beaumont-en-Auge) in 1749. After his secondary school education he attended University of Caen n 1766 to study the liberal arts, but two of his professors (Gadbled and LeCanu) urged this gifted student to pursue mathematics. With LeCanu's letter to d'Alembert (→**1.13**) he left for Paris at age 18 in 1768. He impressed d'Alembert, who secured a position for him at the Ecole Militaire. In 1773 he demonstrated that the acceleration observed in Jupiter and Saturn was not cumulative but periodic. This was the principal advance in dynamical astronomy since Newton toward establishing the stability of the solar system. This work won him election to the Paris Academy in 1773.

Between 1778 and 1789 he was at his scientific prime. Laplace introduced his transformation in 1779, which was related to Euler's work.

In 1780 he worked together with Lavoisier to make a calorimeter to establish that respiration is a form of combustion. Although he played a decisive role to design the metric system in 1790, he wisely avoided Paris when the Jacobins dominated until 1794. In the late 1790s with three well received books (one of which, *Systéme du Monde*, was not only a fine science popularizer but also a model of French prose), he became a European celebrity.

Laplace advanced applied mathematics and theory of probability substantially. He based his theory on generating functions, and extended Jakobi Bernoulli's work on the law of large numbers. He was amply honored by Napoleon and by Louis XVIII. During his final years he lived at his country home in Arceuil, next to his friend chemist Berthollet, surrounded by the adopted children of his thoughts, Arago, Poisson, Biot, Gay-Lussac, von Humboldt and others.

13.4 Fundamental theorem of Laplace transform.

(1) The Laplace transform of f (13.2) exists for s such that $e^{-(Re\, s)t}f(t) \in L_1([0,\infty))$.
(2) There is a one-to-one correspondence between $f(t)$ and its Laplace transform $\mathcal{L}_s[f]$. More explicitly, we have

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} e^{st}\mathcal{L}_s[f]ds, \tag{13.9}$$

where c is a real number larger than the convergence coordinate c^* such that all the singularities of $\mathcal{L}_s[f]$ lie on the left side of $z = c^*$ in $\boldsymbol{C}$.[173]
[Demo] (1) is obvious. At least formally, (2) follows from the motivation **13.1**. Fourier inverse transform of $\mathcal{L}_s[f]$ gives

$$f(t) = e^{ct}\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega t}\mathcal{L}_{c-i\omega}[u(t)]d\omega. \tag{13.10}$$

Since $d\omega = ids$, (13.10) becomes

$$f(t) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} \mathcal{L}_s[f(t)]e^{st}ds. \tag{13.11}$$

For this integral to be meaningful, we need the following theorem:

Discussion.
(1) $f(t) = \exp(t^\sigma)$ with $\sigma > 1$ does not have Laplace transforms.

[173] This was formally shown by Riemann by 1859. Mellin proved this in Acta Soc. Sci. Fenn. **21**, 115 (1896). Hence, there is absolutely no justification to call this integral the 'Bromwitch integral.' History must not be distorted due to national interests.

(2) The minimum real number r making $f(t)e^{-rt} \in L_2([0,+\infty))$ is called the *convergence coordinate.*

Exercise.

Although practically, there is almost no need (→**13.14**) of calculating the integral (13.9), still it is a good exercise of complex integration. Demonstrate the following inverse transform relations with the aid of the residue theorem.

(1)

$$\mathcal{L}_s^{-1}\frac{1}{(s+\alpha)^n} = \frac{t^{n-1}}{(n-1)!}e^{-\alpha t}, \tag{13.12}$$

where $\alpha > 0$ and n is a positive integer.

(2) How can we do a similar thing, if n is not an integer? In this case, $s = 0$ is a branch point. If $n \in (0,1)$, then a straightforward contour integration along the contour in the figure works. The contribution from the small circle vanishes in the small radius limit, and the contribution from the large circle is zero thanks to the Jordan lemma. We need to streamline the formula. If n is larger, then probaly the cleverest way is to use **13.7**(5) and reduce the problem to the case of $n \in (0,1)$.

13.5 Theorem [Holomorphy of Laplace transform]. $\mathcal{L}_s[f]$ is holomorphic where $\mathcal{L}_s[f]$ exists. □[174]

Therefore, if $\mathcal{L}_s[f]$ exists for $c > c^*$, then $\mathcal{L}_s[f]$ has no singularity on the half plane $Re\, z \geq c$.

This implies that

(1) $\mathcal{L}_s[f]$ is differentiable with respect to s,

(2) $\mathcal{L}_s[f]$ is determined by its behavior on the portion of the real axis $x > c^*$ through analytic continuation.

13.6 Theorem [Limits for Laplace transform]. If s goes to s_0 along a curve lying inside the convergence domain, then

$$\lim_{s\to s_0} \mathcal{L}_s[f] = \mathcal{L}_{s_0}[f]. \tag{13.13}$$

Especially,

$$\lim_{s\to\infty} \mathcal{L}_s[f] = 0. \tag{13.14}$$

[Demo] (13.14) follows from (13.13), which follows trivially from an elementary property of the Lebesgue integral.

[174] To prove this we need the following elementary theorem about Lebesgue integration

Theorem. Suppose

(1) $f(x,s)$ is integrable (→**??**) for each s as a function of x,

(2) $f(x,s)$ is holomorphic for almost all x as a function of s,

(3) There is an integrable function Φ such that $|f(x,s)| \leq \Phi(x)$.

Then, $\int dx f(x,s)$ is holomorphic as a function of s. □

13.7 Some properties of Laplace transform.
(1) $a\mathcal{L}_s[f(at)] = \mathcal{L}_{s/a}[f(t)]$, where a is a positive constant. This can be shown by a straightforward calculation.
(2) $\mathcal{L}_s[e^{-bt}f(t)] = \mathcal{L}_{s+b}[f(t)]$. This is straightforward, too.
(3) $\mathcal{L}_s[t^n f(t)] = (-1)^n(d/ds)^n\mathcal{L}_s[f(t)]$. In particular, $\mathcal{L}_s[tf(t)] = -d/ds\mathcal{L}_s[f(t)]$.
(4) $\mathcal{L}_s[f^{(n)}(t)] = s^n\mathcal{L}_s[f(t)] - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - s^{n-k}f^{(k-1)}(0) - \cdots - sf^{(n-2)}(0) - f^{(n-1)}(0)$. In particular,

$$\mathcal{L}_s[f'(t)] = s\mathcal{L}_s[f(t)] - f(0). \tag{13.15}$$

This is due to integration by parts.
(5) $\mathcal{L}_s\left[\int_0^t f(t')dt'\right] = s^{-1}\mathcal{L}_s[f(t)]$.
(6) $\mathcal{L}_s[t^{-1}f(t)] = \int_s^\infty ds\mathcal{L}_s[f(t)]$.
(3) - (6) imply that calculus becomes algebra through the Laplace transformation. This is the most important and useful property facilitating the solution of linear ODE.

Discussion
The following equation is called the *Airy equation* (→**??** Exercise (3))

$$\frac{d^2y}{dt^2} - ty = 0. \tag{13.16}$$

Since the coefficient is only a linear function of t, Laplace transformation is advantageous. Let z be a function of s that is the Laplace transform of y with respect to t. Then,

$$\frac{dz}{ds} - s^2 z = 0, \tag{13.17}$$

which can be solved easily as

$$z = e^{s^3/3}. \tag{13.18}$$

Hence, a solution to can be written as

$$Ai(t) = \frac{1}{2\pi i}\int_C \exp\left(st - \frac{1}{3}t^3\right)ds. \tag{13.19}$$

Here C can be a path as shown in the figure. The integral is called the *Airy integral* .
Show that

$$Ai(0) = 3^{-1/6}\Gamma(1/3)/2\pi. \tag{13.20}$$

13.8 Convolution. If we adapt the ordinary definition of convolution **7.23** to functions that are zero for $t < 0$, we get

$$(f_1 * f_2)(t) = \int_0^t f_1(t-u)f_2(u)du. \tag{13.21}$$

A straightforward calculation gives

$$\mathcal{L}_s[f_1 * f_2] = \mathcal{L}_s[f_1]\mathcal{L}_s[f_2]. \tag{13.22}$$

Exercise.

$$\int_0^x \sin(x-y)u(y)dy + u(x) = \cos x. \tag{13.23}$$

13.9 Time-delay.

$$\mathcal{L}_s[f(at-b)\Theta(at-b)] = \frac{1}{a}e^{-bs/a}\mathcal{L}_{s/a}[f(t)] \tag{13.24}$$

This is also demonstrated by a simple calculation. $e^{-\tau s}$ is often called a delay factor.

13.10 Periodic functions. If f is a function with period T, then

$$\mathcal{L}_s[f(t)] = (1-e^{-sT})^{-1}\int_0^T e^{-st}f(t)dt. \tag{13.25}$$

[Demo] Thanks to the periodicity, we get

$$\int_0^\infty e^{-st}f(t)dt = \int_0^\infty e^{-st}f(t+T)dt = \int_T^\infty e^{-s\tau}f(\tau)d\tau e^{sT}, \tag{13.26}$$

where $t = \tau - T$. This implies that

$$\mathcal{L}_s[f(t)] = \left\{\mathcal{L}_s[f(t)] - \int_0^T e^{-st}f(t)dt\right\}e^{sT}. \tag{13.27}$$

Solving this equation for $\mathcal{L}_s[f]$, we get the desired formula.

13.11 Examples.
(1) $\mathcal{L}_s[1] = 1/s$ is obvious by definition.
(2) This with (2) of **13.7** implies $\mathcal{L}_s[e^{-bt}] = 1/(s+b)$.
(3) Linearity of the Laplace transformation and (2) give, for example,

$$\mathcal{L}_s[\cos\omega t] = \frac{1}{2}(\mathcal{L}_s[e^{i\omega t}] + \mathcal{L}_s[e^{-i\omega t}]) = \frac{s}{s^2+\omega^2}. \tag{13.28}$$

Analogously, we get $\mathcal{L}_s[\cosh at] = s/(s^2 - a^2)$, $\mathcal{L}_s[\sin \omega t] = \omega/(s^2 + \omega^2)$, etc.
(4) (3) with (2) of **13.7** gives for example

$$\mathcal{L}_s[e^{-bt} \cos \omega t] = \frac{s+b}{(s+b)^2 + \omega^2}. \tag{13.29}$$

(5) (1) and (3) of **13.7** imply

$$\mathcal{L}_s \left[\frac{t^n}{n!}\right] = \frac{1}{s^{n+1}}. \tag{13.30}$$

More generally, for $\nu > -1$

$$\mathcal{L}_s \left[\frac{t^\nu}{\Gamma(\nu+1)}\right] = \frac{1}{s^{\nu+1}}. \tag{13.31}$$

This can be shown immediately by the definition of the Gamma function ($\rightarrow$**X**).
(6) Combining (13.30) and (2) of **13.7** gives

$$\mathcal{L}_s[e^{-bt} t^n] = \frac{n!}{(s+b)^{n+1}}. \tag{13.32}$$

(7) An application of **13.10** is

$$\mathcal{L}_s[|\sin t|] = \frac{1}{s^2+1} \coth \frac{\pi s}{2}. \tag{13.33}$$

(8) Applying the convolution theorem **13.8** we can demonstrate

$$\int_0^t J_0(\tau) J_0(t-\tau) d\tau = \sin t \tag{13.34}$$

This follows from ($\rightarrow$**??**)

$$\mathcal{L}_s[J_0(t)] = \frac{1}{\sqrt{s^2+1}}. \tag{13.35}$$

Exercise.
(A) Show

$$\mathcal{L}_s \frac{1}{\sqrt{t}} = \frac{\sqrt{\pi}}{\sqrt{s}}. \tag{13.36}$$

(B) Find
(1) $\mathcal{L}_s \cos^2 \omega t$.
(2) For $\tau > 0$ and $a > 0$ $\mathcal{L}_s (t - t_1) E^{-a(t-t_2}} \Theta(t - \tau)$.

13.12 Laplace transform of delta function. We can define Laplace transforms of generalized functions. We will not discuss this, since the relation between Fourier and Laplace transformations **13.1** explains virtually everything we need practically. A subtlety may remain in the definition of the Laplace transformation of $\delta(x)$, since the definition **13.2** requires an integration from 0. That is, we must consider the product of $\delta(x)$ and $\Theta(x)$, which is meaningless (→**7.6**) as generalized functions. Without any ambiguity for $a > 0$

$$\mathcal{L}_s[\delta(t-a)] = e^{-as}. \tag{13.37}$$

This means the Laplace transform of the weak limit $\lim_{\epsilon\to 0+}\delta(t-\epsilon)$ is 1. Hence, as a generalized function it is sensible to define (→**7.19**)

$$\mathcal{L}_s[\delta(t)] = 1. \tag{13.38}$$

From this (13.37) is obtained with the aid of the time delay formula **13.9**.

13.13 Short time limit.

$$\lim_{t\to 0+} f(t) = \lim_{s\to\infty} s\mathcal{L}_s[f(t)]. \tag{13.39}$$

[Demo] **13.7**(4) with $n = 1$ reads $\mathcal{L}_s[f'(t)] = s\mathcal{L}_s[f(t)] - f(0)$. Apply **13.6** to f', and we get $\lim_{s\to\infty}\mathcal{L}_s[f'(t)] = 0$.

13.14 Practical calculation of Laplace inverse transformation: Use of tables. Although the fundamental theorem **13.4**(2) gives a method to compute the inverse transforms, practically, an easier method is to use a table of Laplace transforms of representative functions. The uniqueness of the transforms (→**13.4**(2)) guarantees that once we can find an inverse transform, that is the inverse transform of a given function of s. Also numerical fast Laplace inverse transform is available.

Exercise.

(1) Solve the following differential equation with the aid of Laplace transformation

$$\frac{d^2y}{dt^2} + 2a\frac{dy}{dt} + (a^2+b^2)y = e^{-at}\sin bt.$$

Here a and b are positive constants, and the initial condition is $y(0) = y'(0) = 0$.

(2) Using Laplace transformation, solve the following integrodifferential equation

$$y(t) = y'(t) + t + 2\int_0^t (t-u)y(u)du$$

with the initial condition $y(0) = 0$.

13.15 Heaviside's expansion formula.[175] Let $F(s)$ be a rational function[176] $F(s) = P(s)/Q(s)$, where P and Q are mutually prime polynomials, and the order of Q is higher than that of P. If $Q(s) = A(s-a_1)\cdots(s-a_n)$ and $a_1, \cdots, a_n$ are all distinct, then

$$\frac{P(s)}{Q(s)} = \sum_{s=1}^{n} \frac{c_k}{s-a_k} \tag{13.40}$$

with $c_k = P(a_k)/Q'(a_k)$. □
This is obvious, and implies that

$$\mathcal{L}_s^{-1}[P(s)/Q(s)] = \sum_{k=1}^{n} P(a_k)e^{a_k t}/Q'(a_k). \tag{13.41}$$

13.16 Examples.

$$\mathcal{L}_s^{-1}\left[\frac{s^2+s+1}{(s^2+1)^3}\right] = \frac{1}{8}(4+t)\sin t - \frac{1}{8}(4t+t^2)\cos t. \tag{13.42}$$

$$\mathcal{L}_s^{-1}\left[\frac{2s+3}{2s^3+3s^2-2s}\right] = -\frac{3}{2} - \frac{1}{10}e^{-2t} + \frac{8}{5}e^{t/2}. \tag{13.43}$$

$$\mathcal{L}_s^{-1}\left[\frac{s^2+1}{2(s^4+s^2+1)}\right] = 1 - \frac{\sqrt{3}}{3}\left[e^{t/2}\cos\left(\frac{\sqrt{3}}{2}t + \frac{\pi}{6}\right) + e^{-t/2}\cos\left(\frac{\sqrt{3}}{2}t - \frac{\pi}{6}\right)\right]. \tag{13.44}$$

Exercise.
(1) Find the inverse transform of

$$g(s) = \frac{s^2 - \omega s + \omega^2}{s(s^2+\omega^2)}. \tag{13.45}$$

(Answer: $\Theta(t) - \sin\omega t$).

$$g(s) = \frac{1+e^{\pi s}}{s(s^2+1)}. \tag{13.46}$$

[175] Heaviside (1850-1925) introduced an algebraic method to solve ODEs, which can be understood as the Laplace transform method explained below. The method, which requires generalized functions like the Heaviside step function, and even the delta function, was never accepted by mathematicians of his day. According to an anecdote, he said that we could eat even though we did not know the mechanism of digestion. This story is often told as a story of a triumph of a self-educated genius. **However**, the method was actually invented by Cauchy long ago. Therefore the story must be quoted as a failure of premature ossification of mathematics due to mediocre mathematicians.
[176] A rational function is a ratio of two polynomials.

13.17 Fast inverse Laplace transform. T. Hosono, "Numerical inversion of Laplace transform and some applications to wave optics," Radio Science **16**, 1015 (1981); *Fast Laplace transform in Basic*, (Kyoritsu Publ., 1984)

Table Mention Mathematica

Appendix XA Mellin Transformation

13.18 Mellin transformation. The *Mellin transform* $\breve{f}$ of $f(r)$ is defined as

$$\breve{f}(p) = \int_0^\infty f(r) r^{p-1} dr. \tag{13.47}$$

This is well-defined for p satisfying $\sigma_1 < Re\, p < \sigma_2$, where

$$\int_0^1 r^{\sigma_1 - 1} |f(r)| dr < +\infty, \quad \int_1^\infty r^{\sigma_2 - 1} |f(r)| dr < +\infty. \tag{13.48}$$

13.19 Theorem [Fundamental theorem of Mellin transformation].
(1)

$$\breve{f}(p) = \int_0^\infty f(r) r^{p-1} dr \tag{13.49}$$

is analytic in the strip $\sigma_1 < Re\, p < \sigma_2$.
(2) Inverse transformation:

$$f(r) = \frac{1}{2\pi i} \int_\Gamma \breve{f}(p) r^{-p} dp, \tag{13.50}$$

where Γ is a straight line in the above strip.□
[Demo] (1) is shown just as the counterpart for the Laplace transformation (→). (2) is also a disguised version of the inversion formula for the Laplace transformation (→**13.2**). Introduce t as $r = e^{-t}$. Then (13.47) reads

$$\breve{f}(p) = \int_0^\infty e^{-pt} f(e^{-t}) dt \tag{13.51}$$

This is the Laplace transformation (→**13.2**). Therefore, we can apply the inverse transformation formula to obtain

$$f(e^{-t}) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \breve{f}(p) e^{pt} dp. \tag{13.52}$$

In terms of r, this is just what we wanted.

13.20 Applications to PDE. If the region of the problem is fan-shaped, then the Mellin transformation is particularly useful. 2-Laplace problem in the cylindrical coordinates is

$$r^2 \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) u + \frac{\partial^2}{\partial \varphi^2} u = 0. \tag{13.53}$$

Melling transforming this, we get

$$p^2 \breve{u} + \frac{d^2}{d\varphi^2} \breve{u} = 0, \tag{13.54}$$

which can be solved easily. The rest is to compute the inverse transform. To calculate it as the Laplace transform (13.52) may be advantageous, since there is the so-called fast Laplace transform algorithm (→**13.17**).

14 Γ-functions

The gamma function was introduced by Euler through his integral; its analytic completion defines an analytic function called the Gamma function. $\Gamma(m+1) = m!$ for $m \in \boldsymbol{N}$ makes this function very useful in theoretical physics. Elementary results are collected here.

Key words Gamma function, Euler's integral, beta function, Schwinger-Feynman's parameter formula, Stirling's formula,

Summary
(1) Remember the definition of Gamma function in terms of Euler's integral (**14.1**). This is practically important in calculating definite integrals (**14.9**).
(2) $N!$ is roughly equal to $(N/e)^N$ for large N (Stirling's formula **14.10**).
(3) Half integer values of Γ can be evaluated exactly (**14.5**).

14.1 Euler's integral. For $\mathbb{R}z > 0$,

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt. \tag{14.1}$$

This is called *Euler's integral*. This integral is defined only for $\mathbb{R}z > 0$, but the *Gamma function* is defined by the analytic completion (→**??**) of (14.1). A rough idea is as follows. Note that

$$\int_0^m \left(1 - \frac{t}{m}\right)^m t^{z-1} dt = \frac{m! m^z}{z(z+1)\cdots(z+m)}. \tag{14.2}$$

This can be shown by repeated integration by parts. Hence, (14.1) can be written as

$$\Gamma(z) = \lim_{m\to\infty} \frac{m! m^z}{z(z+1)\cdots(z+m)}. \tag{14.3}$$

The RHS is well defined for all $z \notin -\boldsymbol{N}$.[177]

Exercise.
Show that

$$H(z) = \int_C (-\zeta)^{z-1} e^{-\zeta} d\zeta = -2i \sin \pi z \Gamma(z). \tag{14.4}$$

[177] A rigorous version may be found in J. W. Dettman, *Applied Complex Analysis*, p194 (Dover, 1965), or E.T. Whittaker and G.N. Watson, *A Course of Modern Analysis*, Chapter XII, which is a convenient reference source of the Γ-function.

From this we obtain the following Hankel's formula

$$\frac{1}{\Gamma(z)} = \frac{i}{2\pi}\int_C (-\zeta)^z e^{-\zeta} d\zeta. \tag{14.5}$$

(2) Draw the graph of $1/\Gamma$ for the interval $[-2, 4]$.

14.2 $\boldsymbol{\Gamma(z+1) = z\Gamma(z)}$. This is for $z \neq 0, -1, -2, \cdots$.
[Demo] From (14.3)

$$z\Gamma(z) = \lim_{m\to\infty} \frac{m! m^{z+1}}{(z+1)(z+2)\cdots(z+1+m)} \frac{z+1+m}{m} = \Gamma(z+1). \tag{14.6}$$

We can compute the Laurent expansion (→**??**) of the Gamma function around negative integers s

$$\Gamma(z) = \frac{(-1)^n}{n!}\frac{1}{z+n} + \cdots. \tag{14.7}$$

The formula can be seen from

$$\Gamma(\zeta - n) = \frac{\Gamma(\zeta)}{(\zeta-n)(\zeta-n+1)\cdots}. \tag{14.8}$$

Exercise.
Laurent-expand $\Gamma(-2+\epsilon)$ around $\epsilon = 0$ and find its principal part. You may use the Taylor expansion formula (→**14.8**), if needed.

14.3 Factorial. Obviously from **14.2**, we have

$$\Gamma(m+1) = m! \tag{14.9}$$

for $m \in \boldsymbol{N}$. $0! = 1$ as usual.

9.4 9.2 directly from Euler's integral. From (14.1) we get with the aid of integration by parts

$$\Gamma(z+1) = -\int_0^\infty (e^{-t})' t^z dt = z\int_0^\infty (e^{-t})' t^{z-1} dt. \tag{14.10}$$

This is **14.2**, which is demonstrated here for $\mathbb{R}z > 0$, but the principle of invariance of functional relations **??** can be invoked to demonstrate **14.2** for all $z \notin -\boldsymbol{N}$.

However, notice that the functional relation **14.2** combined with

$\Gamma(1) = 1$ is not enough to characterize the Γ-function.[178]

Discussion.
Thus

$$\Gamma(z) = \frac{\Gamma(z+1)}{z} \tag{14.11}$$

is true for z on the right half plane. However, the RHS is meaningful for $Re\, z > -1$ except $z = 0$. Continue this argument to show that $\Gamma(z)$ is analytic except negative integer values of z.

14.4 Formula of complementary arguments: For $z \notin \boldsymbol{Z}$

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z}. \tag{14.12}$$

[Demo] We note $\Gamma(1-z) = -z\Gamma(-z)$ from **14.1**.

$$\frac{1}{\Gamma(z)\Gamma(1-z)} = z \prod_{k=1}^{\infty} \left(1 - \frac{z^2}{k^2}\right). \tag{14.13}$$

($\rightarrow$**??**). The RHS is an entire function (let us call it $\phi(z)$) with simple zeros at all $\boldsymbol{Z}$, and $\phi(z)/z$ at $z = 0$ is 1. Actually, the product is $\sin \pi z/\pi z$. An easier demonstration will be given in **14.7** below. $\square$
Analogously, we have

$$\Gamma(z + 1/2)\Gamma(z - 1/2) = \pi/\cos \pi z. \tag{14.14}$$

Exercise.
Show that

$$\Gamma(z)\Gamma(-z) = \frac{\pi}{z \sin \pi z}. \tag{14.15}$$

Using this, demonstrate

$$|\Gamma(iy)|^2 = \frac{\pi}{y \sinh \pi y}. \tag{14.16}$$

14.5 Γ for half integers: The formula of complementary arguments allows us to compute $\Gamma(1/2)$.[179] Since this is positive as seen from the definition (14.3),

$$\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}. \tag{14.17}$$

[178] However, there is a
Theorem [Wielandt] Let $F(z)$ be a holomorphic function in the right half plane having the following two properties:
(i) $F(z+1) = zF(z)$ on the right half plane.
(ii) $F(z)$ is bounded in the strip $\{1 \leq \mathbb{R}z < 2\}$.
Then, $F(z)$ is proportional to $\Gamma(z)$.
See R. Remmert, "Wielandt's theorem about the Γ-function," Am. Math. Month. p214-220, March 1996.
[179] This can be computed directly with the aid of the Gaussian integral as (1) In Exercise.

With **14.1** we get

$$\Gamma\left(n+\frac{1}{2}\right)=\frac{(2n-1)!!}{2^n}\sqrt{\pi}=\frac{(2n)!}{2^{2n}n!}\sqrt{\pi}, \tag{14.18}$$

and

$$\Gamma\left(-n+\frac{1}{2}\right)=\frac{(-1)^n 2^n}{(2n-1)!!}\sqrt{\pi}=\frac{(-4)^n n!}{(2n)!}\sqrt{\pi}. \tag{14.19}$$

Exercise.
(1) $\Gamma(1/2)$ can be computed directly as follows:

$$\Gamma(1/2)=\int_0^\infty e^{-t}\frac{1}{\sqrt{t}}dt=\int_{-\infty}^\infty e^{-x^2}dx. \tag{14.20}$$

Hence, we have only to compute the Gaussian integral. The best method to compute this integral is the following trick:

$$\left\{\int_{-\infty}^\infty e^{-x^2}dx\right\}^2=\int_{\boldsymbol{R}^2}dxdye^{-(x^2+y^2)}=2\pi\int_0^\infty e^{-r^2}rdr. \tag{14.21}$$

Complete the calculation.
(2) Compute $\Gamma(7.5)$ and $\Gamma(-1.5)$.
(3) How fast does $\Gamma(-n+1/2)$ converge to 0 in the $n\to\infty$ limit?
(4) Show

$$\lim_{n\to\infty}\frac{(2n-1)!!}{(2n)!!}n^{1/2}=\pi^{-1/2}. \tag{14.22}$$

14.6 Beta function. The *beta function* $B(p,q)$ is an analytic function of two variables obtained by the analytic completion ($\to$**??**) of the following integral

$$\begin{aligned} B(p,q) &= \int_0^1 t^{p-1}(1-t)^{q-1}dt, && (14.23)\\ &= 2\int_0^{\pi/2}d\theta\cos^{2p-1}\theta\sin^{2q-1}\theta, && (14.24)\\ &= \int_0^\infty dx\,x^{p-1}(1+x)^{-(p+q)}, && (14.25)\end{aligned}$$

where $\Re p$ and $\Re q$ must be positive. The second line can be obtained by setting $t=\sin^2\theta$, and the third line by $t=x/(1+x)$. Assume $p,q\in\boldsymbol{R}$ and positive. We get ($t=x^2$ or y^2 in (14.1))

$$\begin{aligned}\Gamma(p)\Gamma(q) &= 4\int_0^\infty dx\,e^{-x^2}x^{2u-1}\int_0^\infty dy\,e^{-y^2}y^{2u-1} && (14.26)\\ &= 4\int_0^\infty rdr\,e^{-r^2}r^{2(p+q-1)}\int_0^{\pi/2}d\theta\cos^{2p-1}\theta\sin^{2q-1}\theta,\\ &= \Gamma(p+q)B(p,q). && (14.27)\end{aligned}$$

Hence, we have

$$B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{14.28}$$

The RHS is meaningful for all p, q except for negative integers, so that we may define the beta function by this formula.

Exercise.
(1) Because

$$B(p,q) = B(q,p) = \int_0^\infty \frac{x^{q-1}}{(1+x)^{p+q}} dx, \tag{14.29}$$

we obtain

$$B(p,q) = \frac{1}{2}\int_0^\infty \frac{x^{p-1}+x^{q-1}}{(1+x)^{p+q}} dx \tag{14.30}$$

and

$$\int_0^\infty \frac{x^{p-1}-x^{q-1}}{(1+x)^{p+q}} dx = 0. \tag{14.31}$$

(2)

$$I = \int_0^{\pi/2} \sin^p\theta \cos^q\theta d\theta = \frac{1}{2}\int_0^1 x^{(p+1)/2-1}(1-x)^{(q+1)/2-1} dx = \frac{1}{2}B\left(\frac{p+1}{2}, \frac{q+1}{2}\right). \tag{14.32}$$

For example,

$$\int_0^{\pi/2} \sin^p\theta d\theta = \frac{\sqrt{\pi}}{2}\Gamma((p+1)/2)/\Gamma(p/2+1). \tag{14.33}$$

This is called *Wallis' formula*, if p is a positive integer.
(3) Computing

$$\int_{-1}^1 (1-x^2)^{z-1} dx \tag{14.34}$$

with two different change of variables ($t = x^2$ and $t = (x+1)/2$), show

$$\Gamma(2z) = \frac{2^{2z-1}}{\sqrt{\pi}}\Gamma(z)\Gamma\left(z+\frac{1}{2}\right). \tag{14.35}$$

More generally, it is known that

$$\Gamma(nz) = (2\pi)^{(1-n)/2} n^{nz-1/2}\Gamma(z)\Gamma\left(z+\frac{1}{n}\right)\cdots\Gamma\left(z+\frac{n_1}{n}\right). \tag{14.36}$$

14.7 Proof of 9.5: From (14.28) and (14.25) we get for $0 < \Re z < 1$

$$\Gamma(z)\Gamma(1-z) = \Gamma(1)B(z,1-z) = \int_0^\infty dx \frac{x^{z-1}}{1+x} = \frac{\pi}{\sin\pi z}. \tag{14.37}$$

We can apply the principle of invariance of functional relation **??** to complete the proof of **14.4**.

Exercise.
To compute the integral in (14.37) we can also use the transformation $x = e^y$ to convert the integral to

$$\int_{-\infty}^{\infty} \frac{e^{zy}}{1+e^y} dy. \tag{14.38}$$

This is the same problem in **??**.

14.8 Taylor expansion:

$$\Gamma(1+z) = 1 - \gamma z + \frac{1}{2}\left(\gamma^2 + \frac{\pi^2}{6}\right) z^2 + \cdots. \tag{14.39}$$

Here γ is called *Euler's constant* defined by

$$\gamma \equiv \lim_{n\to\infty} \left(1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} - \ln n\right) \tag{14.40}$$

and $\gamma = 0.577215664\cdots$.[180] □
[Demo] Calculate the logarithmic derivative of (14.3) (Uniform convergence allows termwise operations)

$$\frac{\Gamma'(z)}{\Gamma(z)} = -\gamma - \frac{1}{z} + \sum_{k=1}^{\infty}\left(\frac{1}{k} - \frac{1}{k+z}\right), \tag{14.41}$$

so that

$$\Gamma'(1) = -\gamma - 1 + \sum_{k=1}^{\infty}\left(\frac{1}{k} - \frac{1}{k+1}\right) = -\gamma. \tag{14.42}$$

Differentiating (14.41) once more, we get

$$\frac{d^2}{dz^2}\log\Gamma(z) = \sum_{k=0}^{\infty} \frac{1}{(z+k)^2}. \tag{14.43}$$

Hence,

$$\Gamma''(1) - \Gamma'(1)^2 = \sum_{k=1}^{\infty} \frac{1}{k^2} = \frac{\pi^2}{6}.\ ^{181} \tag{14.46}$$

[180] Whether γ is irrational or not is not known; it is known that if it is rational, both the denominator and the numerator must have at least 30,000 digits.
[181] To compute this sum or the *zeta function* (→**??**)

$$\zeta(z) \equiv \sum_{k=1}^{\infty} \frac{1}{k^z}, \tag{14.45}$$

we use

$$\zeta(z)\Gamma(z) = \int_0^{\infty} \frac{t^{z-1}}{e^t - 1} dt. \tag{14.46}$$

See T. M. Apostol, *Math. Intelligencer*, **5**(3), 59-60 (1983) "A proof the Euler missed: evaluation of $\zeta(2)$ the easy way." See **??** Discussion (1).

This gives the desired second derivative. □

Exercise.
(1) Demonstrate that the Γ-function is a convex function (→**??** Discussion) for $x > 0$.
(2) Using the fact

$$\frac{\Gamma'(1)}{\Gamma(1)} = -\gamma, \tag{14.47}$$

demonstrate

$$\gamma = -\int_0^\infty e^{-t} \log t \, dt. \tag{14.48}$$

14.9 Use in perturbative field theories:[182]

(1) When we compute (bare) perturbation series, we have to compute integrals of the following type:

$$I \equiv \int d\boldsymbol{q} \frac{1}{(q^2 + 2\boldsymbol{k}\cdot\boldsymbol{q} + m^2)^\alpha} = \pi^{d/2} \frac{\Gamma(\alpha - d/2)}{\Gamma(\alpha)} (m^2 - k^2)^{d/2-\alpha}. \tag{14.49}$$

Here the integral may not exist even when the RHS exists. In such cases the integral is <u>defined</u> by the RHS (analytic continuation). This formula can be demonstrated as follows: First we exponentiate the denominator with the aid of Euler's integral (14.1)

$$\frac{1}{a^\alpha} = \frac{1}{\Gamma(\alpha)} \int_0^\infty dt \, t^{\alpha-1} e^{-at} \tag{14.50}$$

as

$$I = \int d\boldsymbol{q} \int_0^\infty dt \, t^{\alpha-1} \exp[-t(q^2 + 2\boldsymbol{k}\cdot\boldsymbol{q} + m^2)]. \tag{14.51}$$

This is a standard trick. We can legitimately exchange the order of the two integrations (Fubini's theorem→**15.15**), and perform the d-dimensional Gaussian integral[183] (→**15.20**) to get

$$I = \frac{1}{\Gamma(\alpha)} \int_0^\infty dt \, t^{\alpha-1} \left(\frac{\pi}{t}\right)^{d/2} e^{-(m^2-k^2)t}. \tag{14.52}$$

This gives the desired result. See also (D) below.
(2) We often need the integral of the product of the factors $1/(q^2+m^2)$.

[182] J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, (Oxford, 1989); D. J. Amit, *Field Theory, the Renormalization Group, and Critical Phenomena* (World Scientific, original from McGraw-Hill 1978).

[183]
$$\int_{-\infty}^\infty dq^d e^{-a^2 q^2} = \left(\frac{\sqrt{\pi}}{a}\right)^d.$$

In this case the q-integral (momentum integral) can be reduced to (1) by the so-called *Schwinger-Feynman parameter formula*:

$$\begin{aligned} & \frac{1}{a_1^{\alpha_1} a_2^{\alpha_2} \cdots a_n^{\alpha_n}} \\ = \; & \frac{\Gamma(\alpha_1 + \cdots + \alpha_n)}{\Gamma(\alpha_1)\Gamma(\alpha_2)\cdots\Gamma(a_n)} \int_V dt_1 dt_2 \cdots dt_{n-1} \frac{t_1^{\alpha_1 - 1} \cdots t_n^{\alpha_n - 1}}{(t_1 a_1 + \cdots + t_n a_n)^{\alpha_1 + \cdots + \alpha_n}}, \end{aligned} \tag{14.53}$$

where

$$V = \{(t_1, \cdots, t_{n-1}) : t_i \in [0,1], t_1 + t_2 + \cdots + t_{n-1} \leq 1\}. \tag{14.54}$$

To demonstrate this we start with (14.50). We have, using Fubini's theorem

$$\prod_{i=1}^n a_i^{-\alpha_i} = \int_0^\infty dx_1 dx_2 \cdots dx_n \frac{\prod_{i=1}^n x_i^{\alpha_i - 1} e^{-\sum a_i x_i}}{\prod_{i=1}^n \Gamma(\alpha_i)}. \tag{14.55}$$

Now, introduce new variables $(t_1, t_2, \cdots, t_{n-1}, y)$ as

$$x_i = t_i y, \quad (i = 1, 2, \cdots, n-1), \tag{14.56}$$

$$x_n = (1 - t_1 - t_2 - \cdots - t_{n-1}) y. \tag{14.57}$$

The Jacobian for this transformation is y^{n-1}, so that

$$\prod_{i=1}^n a_i^{-\alpha_i} = \int_0^\infty dy \int_V dt_1 \cdots dt_{n-1} y^{n-1} y^{\sum \alpha_i - n} \frac{e^{-y \sum a_i t_i}}{\prod_{i=1}^n \Gamma(\alpha_i)}. \tag{14.58}$$

This leads to the desired result. □

Exercise.
(A) Demonstrate

$$I = \int \int f(t_1 + t_2) t_1^{a_1 - 1} t_2^{a_2 - 1} dt_1 dt_2 = \frac{\Gamma(a_1)\Gamma(a_2)}{\Gamma(a_1 + a_2)} \int_0^1 f(t) t^{a_1 + a_2 - 1} dt, \tag{14.59}$$

where the integration range is $t_1 + t_2 \leq 1$ and $t_1 > 0$, $t_2 > 0$.

(B) From a similar calculation as (A), we get the following formula:

$$\begin{aligned} & \int \int \cdots \int f(t_1 + t_2 + \cdots + t_n) t_1^{a_1 - 1} t_2^{a_2 - 1} \cdots t_n^{a_n - 1} dt_1 dt_2 \cdots dt_n \\ & \qquad = \frac{\Gamma(a_1)\Gamma(a_2)\cdots\Gamma(a_n)}{\Gamma(a_1 + a_2 + \cdots + a_n)} \int_0^1 f(t) t^{a_1 + a_2 + \cdots + a_n - 1} dt \end{aligned} \tag{14.60}$$

where the integration range is $t_i > 0$ and $t_1 + \cdots + t_n < 1$ as in (A). You need not demonstrate this formula (if you feel it is correct). Using this formula, demonstrate that the volume V of the n-ball of radius r is given by

$$V = \frac{2r^n \pi^{n/2}}{n\Gamma(n/2)}. \tag{14.61}$$

Compute the surface area of the n-ball (i.e., the volume of the $(n-1)$-sphere).

Estimate the ratio of the volume of d-ball and that of its thin skin of thickness $\epsilon \ll 1$ for very large d.[184] [Hint. Actually, dimensional analysis is enough. Look at the ratio of the volume of n-sphere of radius r and that of radius $r - \epsilon$.]

(C) This formula can be generalized to the following. Let D be a domain in n-space defined by

$$\left(\frac{x_1}{a_1}\right)^{b_1} + \cdots + \left(\frac{x_n}{a_n}\right)^{b_n} \le 1 \tag{14.62}$$

and $x_1 \ge 0, \cdots, x_n \ge 0$.

$$\int \cdots \int_D dx_1 dx_2 \cdots dx_n x_1^{l_1 - 1} \cdots x_n^{l_n - 1} = \frac{a_1^{l_1} \cdots a_n^{l_n}}{b_1 \cdots b_n} \frac{\Gamma\left(\frac{l_1}{b_1}\right) \cdots \Gamma\left(\frac{l_n}{b_n}\right)}{\Gamma\left(\frac{l_1}{b_1} + \cdots + \frac{l_n}{b_n} + 1\right)}. \tag{14.63}$$

(D) Demonstrate (14.49). That is,

$$\int dq \frac{1}{(q^2 + 2kq + m^2)^\alpha} = \frac{1}{2} S_{d-1} \frac{\Gamma(d/2)\Gamma(\alpha - d/2)}{\Gamma(\alpha)} (m^2 - k^2)^{d/2 - \alpha}. \tag{14.64}$$

14.10 Stirling's formula.[185] Uniformly in $|\arg z| \le \pi - \delta$ for any small positive δ,

$$\Gamma(z) \sim \sqrt{2\pi} e^{-z} z^{z - 1/2} \left[1 + \frac{1}{12z} + \frac{1}{288z^2} - \frac{139}{51849z^3} + \cdots\right]. \tag{14.65}$$

Here $\sim$ implies that the expansion is asymptotic ($\rightarrow$**21.3**, **21.14**).□

A practical way to remember the salient feature is

$$n! \sim (n/e)^n. \tag{14.66}$$

[Demo][186] We only demonstrate

$$\frac{\Gamma(n) e^n \sqrt{n}}{n^n} \to \sqrt{2\pi} \quad \text{as} \quad n \to \infty. \tag{14.67}$$

In Euler's integral (14.1) set $x = \sqrt{t} - \sqrt{n}$ to find

$$\frac{\Gamma(n) e^n \sqrt{n}}{n^n} = 2 \int_{-\sqrt{n}}^{\infty} \left(1 + \frac{x}{\sqrt{n}}\right)^{2n+1} e^{-2\sqrt{n}x} e^{-x^2} dx \tag{14.68}$$

[184] In very high dimensional spaces, almost all the volume is always very close to the skin. This is a very important fact for statistical mechanics, and coding theory.

[185] James Stirling, 1692-1770.

[186] J. M. Patin, *Am. Math. Month.* **96**, 41-42 (1989).

Now, the integrand is uniformly bounded in n by the integrable function e^{-x^2-1}, because

$$\left(1+\frac{x}{\sqrt{n}}\right)^{2n-1} e^{-2\sqrt{n}x} \le \exp\left\{\frac{x}{\sqrt{n}}(2n-1)\right\}\exp(-2\sqrt{n}x) = e^{-x/\sqrt{n}} \le e. \tag{14.69}$$

Since for each x

$$\lim_{n\to\infty} \log\left\{\left(1+\frac{x}{\sqrt{n}}\right)^{2n-1} e^{-2\sqrt{n}x}\right\} = -x^2, \tag{14.70}$$

the dominated convergence theorem[187] tells us

$$\frac{\Gamma(n)e^n\sqrt{n}}{n^n} \to 2\int_{-\infty}^{\infty} e^{-2x^2}dx = \sqrt{2\pi}. \tag{14.71}$$

□

Discussion.[188] The above proof does not tell us why the ratio (14.67) must be considered. Let us give a more 'constructive' proof.
(1) Notice that for $\mathbb{R}z > 0$

$$\Gamma'(z) = \int_0^{\infty} e^{-t}t^{z-1}\ln t\, dt. \tag{14.72}$$

(2) To rewrite $\ln t$ let us show that integration of

$$\frac{1}{t} = \int_0^{\infty} e^{-xt}dx \tag{14.73}$$

implies for $\mathbb{R}t > 0$

$$\ln t = \int_0^{\infty} \frac{e^{-x}-e^{-xt}}{x}dx. \tag{14.74}$$

This integral is called Frullani's integral.[189]
(3) Combining the above results, we obtain

$$\Gamma'(z) = \int_0^{\infty} \frac{dx}{x}\left[e^{-x}\Gamma(z) - \int_0^{\infty} e^{-t(x+1)}t^{z-1}dt\right]. \tag{14.75}$$

(4) From this we obtain

$$\frac{d}{dz}\ln\Gamma(z+1) = \int_0^{\infty}\left(\frac{e^{-t}}{t} - \frac{e^{-zt}}{e^t-1}\right)dt, \tag{14.76}$$

$$= \int_0^{\infty}\frac{e^{-t}-e^{-tz}}{t}dt + \frac{1}{2}\int_0^{\infty} e^{-tz}dt - \int_0^{\infty}\left(\frac{1}{2}-\frac{1}{t}+\frac{1}{e^t-1}\right)e^{-tz}dt, \tag{14.77}$$

$$= \ln z + \frac{1}{2z} - \int_0^{\infty}\left(\frac{1}{2}-\frac{1}{t}+\frac{1}{e^t-1}\right)e^{-tz}dt. \tag{14.78}$$

[187] Again, this is a rudimentary theorem of Lebesgue integral (→**15.12**).
[188] This is adapted from Lebedev.
[189] To justify the changing the order of integrations, we may rely on Fubini's theorem (→**15.15**). The same is true for the exchange in (3).

(5) Integrating this with z from 0 to z, we obtain

$$\begin{aligned}\ln\Gamma(z) &= \left(z-\frac{1}{2}\right)\ln z - z + 1 \\ &\quad + \int_0^\infty \left(\frac{1}{2} - \frac{1}{t} + \frac{1}{e^t-1}\right)\frac{e^{-t}-e^{-tz}}{t}dt. \end{aligned} \tag{14.79}$$

(6) This can be rewritten as

$$\ln\Gamma(z) = \left(z-\frac{1}{2}\right)\ln z - z + \omega(z) - \omega(1), \tag{14.80}$$

where

$$\omega(z) = \int_0^\infty f(t)e^{-tz}dt \tag{14.81}$$

with

$$f(t) = \left(\frac{1}{2} - \frac{1}{t} + \frac{1}{e^t-1}\right)\frac{1}{t}. \tag{14.82}$$

To compute $\omega(1)$, notice that

$$\omega(1/2) - \omega(1) = \int_0^\infty \left(\frac{e^{-t/2}}{t} - \frac{1}{e^t-1}\right)dt \tag{14.83}$$

but this can be obtained from the result of (5) with $z = 1/2$ (→**9.6**) as

$$\omega(1/2) - \omega(1) = \frac{1}{2}\ln\pi - \frac{1}{2}. \tag{14.84}$$

On the other hand, we can compute $\omega(1/2)$ directly as

$$\omega(1/2) = \frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}. \tag{14.85}$$

Hence, $\omega(1) = -(1/2)\ln 2\pi$
(7) For large $\mathbb{R}z > 0$ we can expect that ω is small. Actually it is of order $1/z$.

15 Integration Revisited

Riemann can integrate piecewise continuous functions. However, there are many functions which cannot be integrated by the Riemann integration, although the values of their integrals are more or less obvious. In this section, the basic idea of the Lebesgue integral is given with a practical summary. The theory is a natural prerequisite for understanding Hilbert space. The most natural integral concept for Fourier expansion is the Lebesgue integral. In the Appendix, rudiments of measure theory is outlined.

Key words: measure zero, almost everywhere, Lebesgue integral, dominated convergence theorem, Beppo-Levi's theorem, Fubini's theorem, Gaussian integral, Wick's theorem.

Remember:
(1) Lebesgue integral is defined by the integral of simple functions (= functions taking only countably many values) (**15.8**-**15.9**).
(2) There are several very powerful theorems for Lebesgue integration (**15.12**-**15.18**). Basically, they justify what looks formally OK to physicists.
(3) Lebesgue integral is the most natural framework to consider Fourier analysis (**15.19**).
(4) Gaussian integrals should be very familiar (**15.20**-**15.21**).

15.1 Practical Check

Exercise. Before going into the discussion of the Lebesgue integration theory, let us check our practical ability to compute Riemann integrals. (1) Compute the following indefinite integrals:

$$\int dx \frac{ax+b}{cx+d}. \tag{15.1}$$

Here we assume that $a, b, c(\neq 0), d$ are constants.
(2) Let $n \in \boldsymbol{N}$. For

$$I_n \equiv \int_0^{\pi/2} \sin^n x dx \tag{15.2}$$

demonstrate that

$$I_n = \left(1 - \frac{1}{n}\right) I_{n-2}. \tag{15.3}$$

Then, compute I_n.
(3) Find the range of α where

$$\int_0^{\infty} \frac{\sin^2 x}{x^{\alpha}} dx \tag{15.4}$$

exists.
(4) [Fresnel integral]. Show that

$$\int_0^\infty \sin(x^2)dx \tag{15.5}$$

exists (as a Riemann integral). cf **??**(1).
(5) Does

$$\int_0^\infty \sin(\cosh x)dx \tag{15.6}$$

exist (as a Riemann integral)?
(6) Show

$$\int_0^\infty \left(\frac{\sin x}{x}\right)^2 dx = \frac{\pi}{2}. \tag{15.7}$$

Use (→**??**)

$$\int_0^\infty e^{-\alpha x}\frac{\sin \lambda x}{x}dx = \frac{\alpha}{\alpha^2+\lambda^2}. \tag{15.8}$$

(7) Show that

$$\int_0^\infty \frac{\sin ax \cos bx}{x} = \frac{\pi}{2}, \tag{15.9}$$

if $a > b > 0$. What happens otherwise?
(8) Show that

$$\int_0^{\pi/2} \log \sin\theta d\theta = -\frac{\pi}{2}\log 2. \tag{15.10}$$

(9) Compute

$$\lim_{n\to\infty}\frac{1}{n}[1+\cos\frac{x}{n}+\cos\frac{2x}{n}+\cdots\cos\frac{(n-1)x}{n}+\cos x] \tag{15.11}$$

(10) Compute

$$\frac{d^n}{dx^n}\int_0^x \frac{(x-y)^{n-1}}{(n-1)!}f(y)dy. \tag{15.12}$$

Discussion.
(1) Let

$$I(a,b) \equiv \int_0^\infty \frac{dx}{\sqrt{(a^2+x^2)(b^2+x^2)}} \tag{15.13}$$

for positive a and b. Show that

$$I(a_n, b_n) = I(a,b) \tag{15.14}$$

for any $n = 1, 2, \cdots$, where $a_{n+1} = (a_n + b_n)/2$ and $b_{n+1} = \sqrt{a_n b_n}$, where $a_1 = a$ and $b_1 = b$. a_n and b_n converge to a common limit μ determined by a and b. Gauss (→**??**) used the bove observation to compute $\mu = \pi/2I$. Show this conclusion.
(2) Let f be integrable on $[0,1]$. Then

$$\int_0^1 \exp(f(t))dt \geq \exp\left(\int_0^1 f(t)dt\right). \tag{15.15}$$

Note that $\int_0^1 f(t)dt$ may be understood as the average of f on $[0,1]$ (→**??**, Discussion (A)).

15.2 Dirichlet function. The Dirichlet function is defined as[190]

$$D(x) = \begin{cases} 0 \text{ for } x \notin \boldsymbol{Q}, \\ 1 \text{ for } x \in \boldsymbol{Q}. \end{cases} \tag{15.16}$$

$\int_0^1 dxD(x)$ must be zero, but obviously this function is not Riemann integrable.

15.3 The area below $D(x)$ must be zero. We know (→**??**(4), **??**) all the rational numbers can be counted, so we may write the totality of rational numbers in $[0,1]$ as $Q \equiv \{y_n\}_{n=1}^{\infty} = \boldsymbol{Q} \cap [0,1]$. Let us cover y_n with an interval E_n of length $\epsilon/2^n$ centered at y_n. Obviously, $\cup E_n \supset Q$ for any positive ϵ, but the total length of $\cup E_n$ is not larger than ϵ, because length$(\cup E_n) \leq \sum($ length $E_n) = \epsilon$. This number is any positive number, so it can be indefinitely small. Hence, the total area occupied by Q must be zero. This must be the area below $D(x)$ on $[0,1]$. Hence, '$\int_0^1 dxD(x)$' $= 0$ (→**15.8**).

15.4 Measure zero. We have demonstrated that $\boldsymbol{Q}$ is *measure zero*. A set $U \subset \boldsymbol{R}$ is called a *measure zero* set, if it can be covered by countably many open intervals the totality of the length of which is less than ϵ for any $\epsilon(> 0)$. **15.3** tells us that any countable set is measure zero. See Appendix a19 for a general discussion about measure (→**15.26**).

15.5 Lebesgue's characterization of Riemann integrability. In his thesis, Lebesgue showed the following theorem.
Theorem. A bounded function f is integrable in the sense of Riemann on $[a,b]$ if and only if the set of discontinuous points of f is measure zero. □
Obviously, $D(x)$ is <u>not</u> integrable in the sense of Riemann.

15.6 "Almost everywhere". Lebesgue also introduced the concept of *almost everywhere*: if a property 'A' is true for a function f except on the measure zero set, we say f has the property 'A' almost everywhere. Thus the theorem above can be restated as: A bounded function f is Riemann integrable if f is almost everywhere continuous.

15.7 Simple function. A function which takes at most countably many (→**??**(4), **??**) values is called a *simple function*. The Dirichlet function (→**15.2**) is a simple function, because it assumes only two values, 0 and 1.

[190] This is the characteristic function of the set of all the rational numbers.

15.8 Lebesgue integral of simple functions. Let f be a real-valued simple function defined on an interval I. If the right-hand-side of the following formula converges absolutely, we say f is *Lebesgue integrable* and the limit is denoted by just the same symbol as the Riemann integral:

$$\int_I f(x)dx \rightleftharpoons \sum_n y_n |I_n|, \tag{15.17}$$

where $|*|$ is the total length of the set $*$, and $I_n \rightleftharpoons \{x | x \in I, f(x) = y_n\}$. Cantor showed $|\boldsymbol{Q}| = 0$ ($\rightarrow$**15.3**). Hence, the Dirichlet function is Lebesgue integrable and the value of the integral is zero.[191]

Note that the values of a function on measure zero sets are irrelevant to the value of the integral.

15.9 Lebesgue integral of general function: $\boldsymbol{L_1([a,b])}$. The Lebesgue integral of a function f on an interval $[a,b]$ is defined as follows. Make a uniform approximation sequence of Lebesgue integrable simple functions f_i for f:

$$\sup_{x\in[a,b]} |f_i(x) - f(x)| \to 0 \text{ as } i \to \infty. \tag{15.18}$$

Then

$$\int_a^b f(x)dx \rightleftharpoons \lim_{i\to\infty} \int_a^b f_i(x)dx. \tag{15.19}$$

[Of course, if we cannot find such a sequence, f is not Lebesgue integrable.]

The totality of functions Lebesgue integrable on the interval $[a,b]$ is denoted by $L_1([a,b])$.

Discussion [Fundamental properties of integrals].
(I) **Double Linearity**. We know that the integral is linear with respect to the integrand. There is one more linearity with respect to the domain as we already noticed in **??**:

$$\int_a^c f(t)dt = \int_a^b f(t)dt + \int_b^c f(t)dt \tag{15.20}$$

or

$$\int_{[a,b]+[b,c]} f(t)dt = \int_{[a,b]} f(t)dt + \int_{[b,c]} f(t)dt. \tag{15.21}$$

[191] In this definition, it is very crucial that all I_n have lengths. Or more generally, if we wish to define an integral of functions on a multidimensional space, then I_n must have a definite volume. Therefore, Lebesgue had to contemplate on the concept 'volume.' This led him to his measurable CHECK if all I_n have well-defined volumes ($\rightarrow$**15.26**). A function f is said to be *measurable* (more precisely, Borel measurable), if the set $\{x \,|\, a < f(x) < b\}$ has a definite length (measure) for any a and $b(> a)$.

If we define

$$\int_{\alpha[a,b]} f(t)dt = \alpha \int_{[a,b]} f(t)dt, \tag{15.22}$$

then $\int$ becomes a linear map on geometrical objects (in this case we discussed only 1D objects, but this can be generalized to general dimensional spaces). Notice that the convention is meaningful if we interpret the integral over $-[a,b]$ to be the integral on $[a,b]$ from b to a instead of a to b ($-$ is the reversing of orientation).
(II) **Non-negativity** and **monotonicity**. If the integrand is nonnegative, its integral is nonnegative. Consequently, if $f \geq g$, then $\int_a^b dt f(t) \geq \int_a^b g(t)dt$.
(III) **Boundedness**. If the integrand is bounded, then its integral over a bounded set is bounded.

15.10 Remark. We must demonstrate that the limit in **15.9** does not depend on the choice of the approximation sequences, but it is a technical detail. An important difference between the Riemann and the Lebesgue integrations is that the latter requires absolute convergence. A. N. Kolmogorov and S. V. Fomin, *Introductory Real Analysis* (Revised English edition, Englewood Cliffs, 1970)[192] is an excellent self-study textbook for the measure theory and Lebesgue integration (and standard functional analysis (say, spectral analysis)).

15.11 Relation between Riemann and Lebesgue integrals.
(1) If f is integrable in both the senses, their values are the same.
(2) If f is bounded and Riemann integrable, then it is Lebesgue integrable. But
(3) There are Riemann integrable but not Lebesgue integrable functions, and vice versa.

The practical merit of the Lebesgue integral is that the conditions for exchanging the order of operations (say, limit and integral) can be simpler than those for Riemann integrals (→**15.12**, **15.15**, **15.18**). This simplicity is due to the absolute convergence in the definition (→**15.8**).

15.12 Theorem [Lebesgue's dominated convergence theorem]. Let I be an interval. If $\lim_{n\to\infty} f_n(x) = f(x)$ for almost all $x \in I$ (i.e., except on a measure zero set (→**15.4**), f_n converges to f), and if there is a Lebesgue integrable function (→**15.9**) $\varphi(x)$ such that $|f_n(x)| < \varphi(x)$ on I, then

$$\lim_{n\to\infty} \int_I f_n(x)dx = \int_I f(x)dx. \tag{15.23}$$

□

[192] Its original Russian version is an undergraduate textbook for Analysis III (designed by Kolmogorov) of Dept of Engineering Mathematics of Moscow State University.

15.13 Theorem [Beppo-Levi]. Let f_n be Lebesgue integrable on an interval I, $\int_I f_n(x)dx < K$ for some number K for all n, and $f_1 \leq f_2 \leq \cdots \leq f_n \leq \cdots$. Then

$$\lim_{n\to\infty} \int_I f_n(x)dx = \int_I \lim_{n\to\infty} f_n(x)dx. \tag{15.24}$$

□

15.14 Example. Termwise integration of $\sum x^n = (1-x)^{-1}$. For $t \in [0,1)$, we may apply Beppo-Levi's theorem to the partial sums to integrate this termwisely:

$$\int_0^t \sum_{n=0}^{\infty} x^n dx = \sum_{n=0}^{\infty} \int_0^t x^n dx = \sum_{n=1}^{\infty} \frac{t^n}{n} = -\ln(1-t). \tag{15.25}$$

Exercise.
Compute the following integrals in the $n \to \infty$ limit:
(1)

$$\int_0^1 \frac{x}{1+nx} dx. \tag{15.26}$$

(2)

$$\int_0^1 \frac{1}{1+nx^2} dx \tag{15.27}$$

Notice that the exchange of the order of limit and integration does not work for

$$\int_0^1 \frac{n}{1+n^2x^2} dx. \tag{15.28}$$

See **??**.

15.15 Theorem [Fubini]. If $\int dx \, (\int dy |f(x,y)|)$ or $\int dy \, (\int dx |f(x,y)|)$ is finite, then we may exchange the order of two integrations in $\int dx \int dy f(x,y)$.
□

Discussion.
(1) Using the integral of $f(x,y) = x^y$ on $[0,1] \times [a,b]$ for $0 < a < b$, demonstrate

$$\int_0^1 \frac{x^b - x^a}{\log x} dx = \log \frac{1+b}{1+a}. \tag{15.29}$$

(2) Demonstrate that

$$\int\int_{x\geq 0, y\geq 0} dxdy f(a^2x^2 + b^2y^2) = \frac{\pi}{4ab} \int_0^{\infty} x f(x) dx. \tag{15.30}$$

(3) Compute

$$\int_1^2 dx \int_1^x dy \frac{x^2}{y^2}, \tag{15.31}$$

$$\int_0^1 dx \int_0^{\sqrt{1-x^2}} dy (1-y^2)^{3/2}, \tag{15.32}$$

$$\int_0^1 dx \int_{\sqrt{x}}^1 dy \sqrt{1+y^2}. \tag{15.33}$$

15.16 Pathological example. Do not think the order of integrations can be freely changed:

$$\int_0^1 dx \int_0^1 dy \frac{x^2-y^2}{(x^2+y^2)^2} = \frac{\pi}{4}, \quad \int_0^1 dy \int_0^1 dx \frac{x^2-y^2}{(x^2+y^2)^2} = -\frac{\pi}{4}. \tag{15.34}$$

Demonstrate that the condition for **15.15** is violated.

Discussion
The reason for the pathology is explained by Legendre with the aid of the following formula:

$$\int_\alpha^1 dx \int_\beta^1 dy \frac{x^2-y^2}{(x^2+y^2)^2} = \frac{\pi}{2} - \arctan \frac{\beta}{\alpha}. \tag{15.35}$$

Demonstrate the formula and complete the argument.

15.17 Good function principle. In short, if a relation is correct for a simple function (→**15.7**), then it is correct for integrable functions. This is sometimes called the *good function principle*.

15.18 Exchanging differentiation and integration. Suppose $f(x,\alpha)$ is integrable for any α in its range, and $\partial_\alpha f$ is integrable, then

$$\frac{d}{d\alpha} \int f(x,\alpha) dx = \int \frac{\partial}{\partial \alpha} f(x,\alpha) dx. \tag{15.36}$$

Very crudely peaking, for Lebesgue integration, if the formal result is mathematically meaningful, then the result is (eventually) justifiable.

Discusiion.
(1) Let f be continuous. Demonstrate that g defined by

$$g(x) = \int_0^x \frac{(x-y)^{n-1}}{(n-1)!} f(y) dy \tag{15.37}$$

is C^n and $g^{(n)}(x) = f(x)$.
(2) **Hadamard representation**. Let $f(x,y)$ be C^1 in the ball of radius r centered at (x_0, y_0). Then

$$f(x,y) = f(x_0,y_0) + f_1(x,y)(x-x_0) + f_2(x,y)(y-y_0), \tag{15.38}$$

where

$$f_1(x,y) = \int_0^1 \frac{\partial f}{\partial x}(x_t, y_t)dt, \quad f_2(x,y) = \int_0^1 \frac{\partial f}{\partial y}(x_t, y_t)dt \tag{15.39}$$

with $x_t = tx + (1-t)x_0$ and $y_t = ty + (1-t)y_0$.

Exercise.

(1) Show that

$$F(x) = \int_0^\infty e^{-y^2} \sin 2xy \, dy \tag{15.40}$$

satisfies

$$F'(x) + 2xF(x) = 1. \tag{15.41}$$

(2) A similar question is: Let

$$I(a) = \int_0^\infty e^{-x^2} \cos 2ax dx. \tag{15.42}$$

Show that

$$\frac{dI}{da} = -2aI. \tag{15.43}$$

Use this to demonstrate that

$$I = \frac{\sqrt{\pi}}{2} e^{-a^2}. \tag{15.44}$$

[Hint. The change of variables $z = x + a/x$ works.]

(3) Let

$$I(a) = \int_0^\infty \exp\left\{-b^2\left(x^2 + \frac{a^2}{x^2}\right)\right\} dx. \tag{15.45}$$

Demonstrate that

$$\frac{dI}{da} = -2b^2 I. \tag{15.46}$$

Then, show

$$I(a) = \frac{\sqrt{\pi}}{2|b|} e^{-2ab^2}. \tag{15.47}$$

15.19 Why is the Lebesgue integral most natural for Fourier analysis? As we have already mentioned in **??**(3) if f is square Lebesgue integrable, then its Fourier series is almost everywhere convergent to f. See also Carlson's theorem (→**??**). Physicists know that Fourier transform is a powerful tool to disentangle convolution (→**28.2**). This can be done freely only when we integrate all integrals as Lebesgue integrals. We can make a continuous and absolute integrable function f such that its convolution to itself $\int dx f(t-x)f(x)$ is Lebesgue integrable, but diverges for all rational t (so that it is not Riemann integrable).[193] That is, if we use the Riemann integral, then we cannot freely use Fourier transformation to disentangle the convolution. The Lebesgue integration theory is much more elegant and fundamental in Fourier analysis than the Riemann integration.

[193] See Körner, Example C.6 on p570.

15.20 Gaussian integral, 'Wick's theorem'. The following integral (the generator of multidimensional Gaussian distribution) is of vital importance in theoretical physics:

$$I(A,\boldsymbol{b}) \equiv \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dx_1\cdots dx_n \exp\left(-\frac{1}{2}\sum_{i,j=1}^{n} A_{ij}x_i x_j + \sum_{i=1}^{n} x_i b_i\right), \tag{15.48}$$

where $A = Matr(A_{ij})$ is an $n\times n$ symmetric non-singular matrix, and $\boldsymbol{b}$ is an n-vector. We get

$$I(A,\boldsymbol{b}) = (2\pi)^{n/2}(detA)^{-1/2}\exp\left(\frac{1}{2}\sum_{i,j} A_{ij}b_i b_j\right). \tag{15.49}$$

$I(A,\boldsymbol{b})/I(A,0)$ is called the generator (generating function) of the Gaussian distribution with mean zero and covariance matrix given by A^{-1}. The standard method to compute this is to shift the origin to the minimum point of the function in the parentheses as

$$y_i = x_i - \sum_j (A^{-1})_{ij}b_j. \tag{15.50}$$

This leads to

$$I(A,\boldsymbol{b}) = \exp\left(\frac{1}{2}\sum_{i,j}(A^{-1})_{ij}b_i b_j\right)\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} dy_1\cdots dy_n \exp\left(-\sum_{i,j=1}^{n} A_{ij}y_i y_j\right) \tag{15.51}$$

The integral can be computed by diagonalizing the matrix.

According to **15.18** we can freely change the order of differentiation with respect to $\boldsymbol{b}$ and integration in (15.48). In this way we arrive at the so-called *Wick's theorem*: For $\boldsymbol{b}=0$

$$\langle x_a x_b\cdots x_z\rangle = \sum (A^{-1})_{k_1k_2}(A^{-1})_{k_3k_4}\cdots(A^{-1})_{k_{n-1}k_n}, \tag{15.52}$$

where $\{k_1,\cdots,k_n\} = \{a,\cdots,z\}$ and the sum is over all the possible pairings of $a,b,\cdots,z$. For example,

$$\langle x_1x_2x_3x_4\rangle = \langle x_1x_2\rangle\langle x_3x_4\rangle + \langle x_1x_3\rangle\langle x_2x_4\rangle + \langle x_1x_4\rangle\langle x_2x_3\rangle. \tag{15.53}$$

Exercise.
(A) Compute the following integrals:
(1)

$$\int\int_{x\geq 0, y\geq 0} dxdy\, e^{-(x^2+2xy\cos\theta+y^2)}. \tag{15.54}$$

(2)

$$\int\int_{\boldsymbol{R}^2} dxdy\, e^{-(x^2+2xy\cos\theta+y^2)}. \tag{15.55}$$

(B) Using the spherical symmetry of the Gaussian integral, find the following integrals in terms of

$$U \equiv \int d^d\boldsymbol{k} e^{-ak^2/2}. \tag{15.56}$$

(1)

$$I = \int d^d\boldsymbol{k} \frac{k_x^2}{k^2} e^{-ak^2/2}. \tag{15.57}$$

(2)

$$J = \int d^d\boldsymbol{k} \frac{k_x^2 k_y^2}{k^4} e^{-ak^2/2}. \tag{15.58}$$

[Hint. (15.53) and $\langle k^4 \rangle = d\langle k_x^4 \rangle + d(d-1)\langle k_x^2 k_y^2 \rangle$. Also differentiation and integration with respect to a (or $-a/2$) is useful.]

15.21 Gaussian integral: complex case. We have the following analogous formula

$$I(A, \boldsymbol{b}) \equiv \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dz_1 d\overline{z}_1 \cdots dz_n d\overline{z}_n \exp\left(- \sum_{i,j=1}^{n} A_{ij} \overline{z}_i z_j + \sum_{i=1}^{n} (\overline{z}_i b_i + z_i \overline{b}_i) \right), \tag{15.59}$$

where A is any nonsingular $n \times n$ matrix, $\boldsymbol{b}$ is a complex n-vector. In terms of real variables x_i and y_i as

$$z_i = (x_i + iy_i)/\sqrt{2}, \tag{15.60}$$

we get $dz_i d\overline{z}_i = dx_i dy_i$.[194] Integration is understood as the integration with respect to these real variables. The result is

$$I(A, \boldsymbol{b}) = (2\pi)^n (detA)^{-1} \exp\left(\sum_{i,j} (A^{-1})_{ij} \overline{b}_i b_j \right). \tag{15.61}$$

The cleverest proof of this relation is: (i) (if necessary) to slightly perturb A so that all the eigenvalues of $A + \delta A$ are distinct (so that $A + \delta A$ is diagonalizable); (ii) compute the integral analogous to **15.20**; then (iii) use the continuity of the integral as a function of the components of A to obtain the result for the unperturbed case.

[194] although formally, the calculation here seems to justify the equality, it is better to undersdand that $dzd\overline{z}$ is a shorthand notation of $dxdy$.

APPENDIX a19 Measure

In this appendix the general theory of the Lebesgue measure is outlined. Without measure theory proper understanding of statistical mechanics and dynamical systems is impossible. However, just as all the important topics, the essence of measure theory is not at all hard to understand. The theory could be read as a very nice example of the analysis of a concept that we seem to know intuitively. For a more formal introduction Kolmogorov-Fomin is strongly recommended.

15.22 Reader's guide to this appendix. (1) + (3) is the minimum of this appendix:
(1) The ordinary Lebesgue measure = volume is explained up to **a19.6**. These entries should be very easy to digest. Remember that Archimedes reached this level of sophistication more than 2000 years ago.
(2) General Lebesgue measure is outlined in **15.31-15.33**. This is an abstract repetition of (1), so the essence should be already obvious.
(3) Lebesgue integral is redefined in terms of the Lebesgue measure in **15.37** with a preparation in **15.36**. This leads us naturally to the concept of functional and path integrals (**a19.16**).
(4) Probability is a measure with total mass 1 (i.e., normalized) (**15.41**).
(5) If we read any probability book, we encounter the triplet $(P, X, \mathcal{B})$. The reason why we need such a nonintuitive device is explained in **15.42-15.43**.

15.23 What is volume? For simplicity, we confine our discussion to 2-space, but our discussion can easily be extended to higher dimensional spaces. The question is: what is 'area' ? It is not easy to answer this question for an arbitrary shape.[195] Therefore, we should start with a seemingly obvious example. The area of a rectangle $[0, a] \times [0, b]$ in $\boldsymbol{R}^2$ is ab. Do we actually know this? Why can we say the area of the rectangle is ab without knowing what area is? To be logically conscientious we must accept:
Definition. The area of a rectangle which is congruent[196] to $\langle 0, a\rangle \times \langle 0, b\rangle$ (Here $\langle$ is [or (and $\rangle$ is] or)) is <u>defined</u> to be ab. Notice that area is defined so that it is not affected by whether the boundary is included or not.

[195] As we will see soon in **15.43**, if we stick to our usual axiomatic system of mathematics ZF+C (→**??** for references), then there are figures without area.
[196] This word is defined by the superposability. That is, if we move (translate, rotate) a figure A and can exactly superpose it on B, we say A and B are congruent. As Hilbert (→**16.4**) realized we must guarantee that the figure does not deform, etc., while being moved, so that we need an axiom, which was never stated in Euclid, although freely used by him (just as the Axiom of Choice in the early 20th century).

15.24 Area of fundamental set. A set which is a direct sum (disjoint union) of finite number of rectangles is called a *fundamental set*. The area of a fundamental set is defined by the sum of the areas of constitutive rectangles.

It should be intuitively obvious that the join and the common set of fundamental sets are again fundamental.

15.25 Heuristic consideration. For an arbitrary shape, the strategy for defining its area should be to approximate the figure with a sequence of fundamental sets. We should use the idea going back to Archimedes; we must approximate the figure from the inside and from the outside. If both sequences converge to the same area, we should define the area to be the are of the figure.

15.26 Outer measure. Let A be a set. We consider a cover of A with finite number of rectangles P_k (inclusion or exclusion of their boundaries can be chosen conveniently →**15.23**), and call it a rectangular cover $P = \{P_k\}$ of A. Let us denote the area of a rectangle P_k by $m(P_k)$. The *outer measure* $m^*(A)$ of A is defined by

$$m^*(A) \equiv \inf \sum_k m(P_k), \tag{15.62}$$

where the infimum is taken over all the finite or countable rectangular covers of A.
$m^*(A) = 0$ is equivalent to A being measure zero (→**15.4** or a *null set*).

15.27 Inner measure. For simplicity, let us assume that $A \in E \equiv [0,1] \times [0,1]$. Then, the inner measure $m_*(A)$ of A is defined by

$$m_*(A) = 1 - m^*(E \setminus A). \tag{15.63}$$

Obviously,

$$m^*(A) \geq m_*(A) \tag{15.64}$$

for any figure A.

15.28 Measurable set, area = Lebesgue measure. Let A be a bounded subset of E.[197] If $m^*(A) = m_*(A)$, then we say A is *measurable* (in the sense of Lebesgue), and $m^*(A)$ written as $\mu(A)$ is called its area (= *Lebesgue measure*).

[197] It should be obvious how to generalize our argument to a more general bounded set in $\boldsymbol{R}^2$.

15.29 Additivity. Assume that all the sets here are in a bounded rectangle, say, E above. The join and the common set of finitely many measurable sets are again measurable. This is true even for countably many measurable sets. The second statement follows from the preceding statement thanks to the finiteness of the outer measure of the join or the common set.

15.30 σ-additivity. Let $\{A_n\}$ be a family of measurable sets satisfying $A_n \cap A_m = \emptyset$ for $n \neq m$. Let $A = \cup_n A_n$. Then,

$$\mu(A) = \sum_n \mu(A_n). \tag{15.65}$$

This is called the *σ-additivity* of the Lebesgue measure. □
[Demo] A is measurable due to **15.29**. Since $\{A_n\}$ covers A, $\mu(A) \leq \sum \mu(A_n)$. On the other hand $A \supset \cup_{n=1}^N A_n$, so that for any N $\mu(A) \geq \sum_{n=1}^N \mu(A_n)$.

15.31 Measure, general case. A map from a family of sets to $\boldsymbol{R}$ is called a *set function*. A set function m satisfying the following three conditions is called a *measure*.
(1) m is defined on a semiring[198] $\mathcal{S}$. [Note that the set of all the rectangles is a semiring.]
(2) $m(A) \geq 0$.
(3) m is an additive function: If A is direct-sum-decomposed in terms of the elements of $\mathcal{S}$ as $A = \cup_{k=1}^n A_k$, then $m(A) = \sum_{k=1}^n m(A_k)$.

Therefroe, the area μ defined in **15.28** is a measure on the set of all the rectangles. In the case of area, the definition of area is extended from rectangles to fundamental sets (→**15.24**). This is the next step:

15.32 Minimum algebra on $\mathcal{S}$, extension of measure. The totality of sets A which is a finite join of the elements in $\mathcal{S}$ is called the *minimum algebra* generated by $\mathcal{S}$. Notice that the totality of fundamental sets in **15.24** is the minimum algebra of sets generated by the totality of rectangles. Just as the concept of area could be generalized to the area of a fundamental set, we can uniquely extend m defined on $\mathcal{S}$ to the measure defined on the algebra generated by $\mathcal{S}$.

15.33 Lebesgue extension. We can repeat the procedure to define μ from m^* and m_* in **??** for any measure m on $\mathcal{S}$ (in an abstract fashion). We define m^* and m_* with the aid of the covers made of the elements in $\mathcal{S}$. If $m^*(A) = m_*(A)$, we define the *Lebesgue extension* μ of m with $\mu(A) = m^*(A)$, and we say A is *μ-measurable*.

[198] If a family of sets $\mathcal{S}$ satisfies the following conditions, it is called a *semiring* of sets:
(i) $\mathcal{S}$ contains $\emptyset$,
(ii) If $A, B \in \mathcal{S}$, then $A \cap B$ and $A \cup B$ are in $\mathcal{S}$,
(iii) if A_1 and A are in $\mathcal{S}$ and $A_1 \subset A$, then $A \setminus A_1$ can be written as a direct sum (the join of disjoint sets) of elements in $\mathcal{S}$.

15.34 Remark. When we simply say the Lebesgue measure, we usually mean the volume (or area) defined as in **??**. However, there is a different usage of the word. μ constructed in **15.33** is also called a Lebesgue measure. That is, a measure constructed by the Lebesgue extension is generally called a Lebesgue measure. This concept includes the much narrower usage common to physicists.

15.35 σ-additivity. (3) in **15.31** is often replaced by the following *σ-additivity* condition: Let A be a sum of countably many disjoint μ-measurable sets $A = \cup_{n=1}^{\infty} A_n$. If

$$\mu(A) = \sum_{n=1}^{\infty} \mu(A_n), \tag{15.66}$$

we say μ is a σ-additive measure.

The Lebesgue measure defined in **15.28** is σ-additive. Actually, if m is σ-additive on a semiring of sets, then its Lebesgue extension is also σ-additive.

15.36 Measurable function. A real function defined on a set D is called a *μ-measurable function* for a Lebesgue measure μ on the set, if any 'level set' $\{x \mid f(x) \in [a, b]\} \cap D$ is μ-measurable. When we simply say a function is measurable, then it means that any level set has a well defined volume in the ordinary sense.

15.37 Lebesgue integral with measure μ. Let μ be Lebesgue measure on $\boldsymbol{R}^n$. Then the Lebesgue integral of a μ-measurable function on $U \subset \boldsymbol{R}^n$ is defined as

$$\int_U f(x) d\mu(x) = \lim_{\epsilon \to 0} \sum a\, \mu(\{x \mid f(x) \in [a - \epsilon/2, a + \epsilon/2)\} \cap U), \tag{15.67}$$

where the sum is over all the disjoint level sets of 'thickness' ϵ (> 0).[199]

15.38 Functional integral. As the reader has seen in **a19.15**, if we can define a measure on a set, we can define an integral over the set. The set need not be an ordinary finite-dimensional set, but can be a function space. In this case the integral is called a *functional integral*. If the set is the totality of paths from time $t = 0$ to T, that is, if the set is the totality of continuous functions: $[0, T] \to \boldsymbol{R}^d$, we call the integral over the set a *path integral*. The Feynman-Kac path integral (→**26.12**) is an example.[200]

[199] There are measures m satisfying $\mu(A) = 0 \Rightarrow m(A) = 0$, where μ is the Lebesgue measure (volume), is said to be *absolutely continuous* with respect to μ. If m is absolutely continuous w.r.t. μ, then Lebesgue extension, Lebesgue integral, etc are easy without any technical difficutly just as the volume. However, careful consideration is needed because there are 'singular' measures.

[200] However, the definition of the Feynman path integral is too delicate to be discussed in the proper integration theory.

15.39 Uniform measure. The Lebesgue measure defined in **15.28** is uniform in the sense that the volume of a set does not depend on its absolute location in the space. That is, the measure is translationally invariant (see **15.42** below for a further comment). However, there is no useful uniform measure in infinite dimensional spaces (→**16.2** Discussion (1)). Thus every measure on a function space or path space must be non-uniform.

15.40 Borel measure. Usually, we mean by a *Borel measure* a measure which makes measurable all the elements of the smallest algebra (→**15.32**) of sets containing all the rectangles.

15.41 Probability. A (Lebesgue) measure P with the total mass 1 is called a *probability measure*. To compute the expectation value with respect to P is to compute the Lebesgue integral w.r.t. the measure P.

When we read mathematical probability books, we always encounter the 'triplet' $(P, X, \mathcal{B})$, where P is a probability measure, X is the totality of elementary events (the event space; $P(X) = 1$) and $\mathcal{B}$ is the algebra of measurable events. This specification is needed, because if we assume that every composite event has a probability, we have paradoxes.[201] This question arose from the characterization of 'uniform measure' in a finite dimensional Euclidean space:

15.42 Lebesgue's measure problem. Consider d-Euclidean space $\boldsymbol{R}^d$. Is it possible to define a set function (→**15.31**) m defined on every bounded set $A \in \boldsymbol{R}^d$ such that
(1) The d-unit cube has value 1.
(2) Congruent sets have the same value,
(3) $m(A \cup B) = m(A) + m(B)$ if $A \cap B = \emptyset$, and
(4) σ-additive
?
This is called *Lebesgue's measure problem*.

15.43 Hausdorff and non-measurable set. Hausdorff demonstrated in 1914 for any d there is no such m satisfying (1)-(4) of **15.42**. Then, Hausdorff asked in 1914 what if we drop the condition (4). He showed that m does not exist for $d \geq 3$.[202] He showed this by constructing a partition of 2-sphere into sets A, B, C, D such that A, B,

[201] There is at least one problem in which the choice of $\mathcal{B}$ is crucial. This is the *first digit problem*. The first significant digits of a table of natural phenomenon such as the height of mountains do not distribute uniformly: 1 appears much more often than 9. Why is this so? A conclusive mathematical explanation was given recently: T P Hill, The Significant-digit Phenomenon, Am. Math. Month. April 1995, p322. If we apparently need a uniform probability on an infinite space (in this case $[0, \infty)$), the choice of $\mathcal{B}$ seems to be the key (→**15.39**).

[202] Banach demonstrated in 1923 that there is a solution for $d = 1$ and for $d = 2$.

C and $B \cup C$ are all congruent and D is countable ($\rightarrow$**??**). Thus if m existed, then we had to conclude $3 = 2$. Therefore, we must admit non-measurable sets.[203]

[203] under the current popular axiomatic system ZF + C.

16 Hilbert Space

Fourier expansion is quite parallel to the expansion of a vector into a linear combination of basis vectors in a finite dimensional vector space. However, function spaces are generally very different from finite dimensional vector spaces. To understand Fourier expansion more intuitively, it is convenient to introduce an infinite dimensional vector space in which our knowledge of finite dimensional vector spaces can be used almost 'freely.' This is the Hilbert space.

Key words: Hilbert space, scalar product, completeness, l_2, L_2, H^2, Cauchy-Schwartz inequality, bra-ket, dual space, K-vector space, orthonormal basis, Gram-Schmidt orthonormalization, generalized Fourier expansion, orthogonal projection, Bessel's inequality, Parseval's equality

Remember:
(1) Hilbert space is an infinite dimensional vector space in which we can define an angle between vectors (**16.3**).
(2) Understand Gram-Schmidt orthonormalization geometrically (**16.16**).
(3) Fourier expansion is a orthogonal decomposition in a Hilbert space (**16.14**).
(4) Be familiar with the bra-ket notation (**16.21-16.24**).
(5) Understand the formal expression of Green's functions (**20.28**).

16.1 Vector space. Let V be a set such that any (finite) linear combination of its elements with coefficients taken from a field K is again in V. V is called a *K-vector space*. K may be $\boldsymbol{R}$ or $\boldsymbol{C}$. A $\boldsymbol{R}$-vector space is called a *real vector space* and a $\boldsymbol{C}$-vector space is called a *complex vector space*. For example, the set $C^0([0,1])$ of continuous real functions on the interval $[0,1]$ is a real vector space. The set of analytic functions on the unit disc is a complex vector space.

Examples.
(1) The set of all the real polynomials of degree n forms a real vector space.
(2) The totality of continuous functions on $[a,b]$ is a vector space (with respect to the ordinary $+$ and $\times$).
(3) The totality of sequences $\{x_i\}$ converging to zero is a vector space, if we introduce $+$ as $\{x_i\}+\{y_i\}=\{x_i+y_i\}$ and scalar multiplication by $c\{x_i\}=\{cx_i\}$.

16.2 Infinite dimensional space. Consider the set $C^0([0,1])$ of all the continuous functions on $[0,1]$. x^n cannot be written as a linear

combination of $1, x, x^2, \cdots, x^{n-1}$ for any n. Thus this function space is obviously infinite dimensional, if we wish to define the 'dimension' of the space as in the ordinary vector space by counting the necessary number of components to specify a vector uniquely. Another approach may be to refer to the interpretation of $f(x)$ as the x-component of a vector f as in functional differentiation (→**??**, **16.21**).[204]

Infinite dimensionality causes special difficulties in convergence. For example, the boundedness of a sequence does not guarantee the existence of a convergent subsequence. For example, consider,

$$(1, 0, \cdots,), (0, 1, 0, \cdots), (0, 0, 1, 0, \cdots), \cdots. \tag{16.1}$$

Discussion.
Infinite dimensional spaces have important peculiar features.
(1) We cannot define a 'uniform volume.' More precisely, there is no uniform measure (=volume) μ (→**19a**) such that for the unit cube C (of infinite dimension) $\mu(C) = 1$ with the translational symmetry (i.e., even if we translate an object, its volume does not change), and the additivity ($\mu(A \cup B) = \mu(A) + \mu(B)$, if $A \cap B = \emptyset$). If such a μ were to exists, then the volumes of most bounded sets are 0 or ∞.[205] Therefore, we cannot define the concept of 'almost everywhere' (→**19.5**).[206]
(2) Compactness and boundedness are distinct. Compactness means (→**??**): if a set A is covered by a family of open sets, then A can already be covered by a finite subset of the family. If the space dimension is finite, this is equivalent to the open boundedness (the Heine-Borel theorem). However, this is obviously untrue for infinite dimensional space: to cover a unit open ball we need infinitely many open balls of radius 1/2. This distinction of compactness and boundedness in infinite dimensional space makes functional analysis much more difficult. A bounded operator and a compact operator are distinct (→**30.20**).

16.3 Hilbert space. An infinite dimensional vector space V, which is complete (see below) with respect to the norm (→**??** footnote) defined by the scalar product (see below) is called a *Hilbert space*.[207]

[204] In this case one might feel that the dimension is uncountable (→**??**(3)). However, usually we do not pay the minute details of the functions, but pay attention to the equivalence classes of functions as individual elements (for example, we ignore the difference on measure zero sets (→**15.4**), so that often the dimension is countable. See Weierstrass' theorem **??**.
[205] Here, we are not discussing 'non-measurable' sets. We confine ourselves to the Borel sets. That is, we discuss the sets which can be constructed as joins and intersections of countable finite cubes. See **19a**.
[206] See B R Hunt, T Sauer, and J A Yorke, "Prevalence: a translational-invariant "almost-every" on infinite dimensional spaces," Bull. Amer. Math. Soc. **27**, 217 (1992). Addendum **28**, 306 (1993).
[207] The definition of 'Hilbert space' can change slightly from book to book. Many authors include finite dimensional vector spaces. Here, following Kolmogorov and

A *scalar product* is a bilinear functional of two vectors $f, g \in V$ denoted by the bracket product $\langle f|g\rangle$ satisfying

$$\begin{aligned}
\langle f|f\rangle &\geq 0, \ \langle f|f\rangle = 0 \iff f = 0, && (16.2)\\
\langle f_1 + f_2|g\rangle &= \langle f_1|g\rangle + \langle f_2|g\rangle, && (16.3)\\
\langle f|g_1 + g_2\rangle &= \langle f|g_1\rangle + \langle f|g_2\rangle, && (16.4)\\
\overline{\langle f|g\rangle} &= \langle g|f\rangle, && (16.5)\\
\langle af|g\rangle &= \overline{a}\langle f|g\rangle, \ \langle f|ag\rangle = a\langle f|g\rangle. && (16.6)
\end{aligned}$$

Here a is a constant scalr (i.e., an element in K). The *norm* in a Hilbert space is defined by $\|f\| = \sqrt{\langle f|f\rangle}$. '*Complete*' means that all the Cauchy sequences[208] do converge: in particular, if $\|f_n - g\| \to 0$, then actually $f_n \to g$.

Introduction of scalar product allows us to introduce the concept of angle between two vectors. We may say that an infinite dimensional space in which we can talk about not only lengths but also angles is a Hilbert space. In other words, in any vector spaces we can define magnitudes by a norm, but the concept of direction is not easy to visualize. To this end, we need a scalar product to introduce the angle between vectors.

Discussion.

(A) **Banach space**. A complete normed space is called a Banach space. It is more important in the study of PDE than the Hilbert space. L_1 (→**15.9**) is a typical Banach space.

(B) **Euclidean space**. In these notes, Hilbert spaces are defined as infinite dimensional spaces. Hilbert spaces and finite dimensional vector spaces (with the ordinary scalar product) are sometimes called Euclidean spaces (written as E^d).

16.4 Who was Hilbert? David Hilbert was born in 1862. He studied mainly at Königsberg, where he befriended Minkowski (who was already famous when he was a high school student. He died relatively young due to appendicitis). From 1895 until his retirement in 1930 he was a named professor at Göttingen. At the Second International Congress of Mathematicians in Paris in 1900, he presented the famous 23 problems for the mathematics of twentieth century. He had a characteristic optimism that new discoveries would continuously be made and that these discoveries were necessary for the vitality of mathematics.

Fomin, we understand that a Hilbert space is always infinite dimensional (need not be countably so).

[208] A Cauchy sequence for a given norm $\|\ \|$ is a sequence $\{y_n\}$ such that $\|y_n - y_m\| \to 0$ as n and m go to infinity. If the sequence is a complex number sequence, then the norm is the usual modulus. We know that $\boldsymbol{C}$ is complete.

His scientific study covers vast area of mathematics, algebra, number theory, functional analysis (as one of the founders; the term 'spectrum' (→**34B**, **34C**) is due to him). His *Grundlagen der Geometrie* (based first on the lectures delivered in 1898-9; there are many versions, because he continued to improve the work) made an epoch.[209] He endeavored to make axiomatic systems more general; he believed that fundamental terms should not have a single privileged interpretation.

Hilbert's last two main scientific interests were theoretical physics and foundation of mathematics. His study of the Boltzmann equation was an important contribution.

He was the major proponent of Formalism, trying hard to prove the consistency of the axiomatic systems on which the modern mathematics is based on (→**??**(5)). This was shown to be untenable by Gödel. However, we must remember that Gödel's sharp result was possible because the problem was posed (formulated) unambiguously by the Hilbert school.

Hilbert died during the World War II (1943). The motto on his grave in Göttingen reads, "Wir müssen wissen, wir werden wissen."[210]

16.5 Examples.

(1) $\boldsymbol{l_2}$-space. Let V be the totality of infinite sequences $\{c_n\} = \{c_1, \cdots, c_n, \cdots\}$ such that $\sum_n c_n^2 < +\infty$. If we introduce the natural linear structure $a\{c_n\} = \{ac_n\}$ and $\{a_n\} + \{b_n\} = \{a_n + b_n\}$ and the scalar product $\{a_n\} \cdot \{b_n\} = \sum a_n b_n$, then V is a Hilbert space, which is called the l_2-*space*.

(2) $\boldsymbol{L}_2([a,b])$. Let V be the totality of square Lebesgue integrable (→**15.9**) functions (complex valued) on the interval $[a,b]$. Then, with the definition of the scalar product

$$\langle f|g\rangle \equiv \int_a^b dx\overline{f(x)}g(x) \tag{16.7}$$

V becomes a Hilbert space called the $L_2([a,b])$-space (→**16.19**).[211]

(3) $\boldsymbol{H}^1([a,b])$. Let V be the totality of Lebesgue square integrable functions defined on $[a,b]$ whose first derivatives are also square integrable. If we introduce the following scalar product

$$\langle f|g\rangle \equiv \int_a^b dx\{\overline{f(x)}g(x) + \overline{f'(x)}g'(x)\}, \tag{16.8}$$

then V becomes a Hilbert space called the H^1-space.[212] The norm based on this scalar product is called in the context of wave equations

[209] Hilbert's axiomatization of Euclidean geometry is summarized in the book of Mac Lane quoted in Book Guide (p63 and on of the book).

[210] We must know; we will know.

[211] Some authors use L^2 and l^2 for L_2 and l_2.

[212] This is an example of the *Sobolev space* (Sergei L'vovich Sobolev, 1908-?).

the energy norm (→**??**).

Discussion.
(A) **Theorem[Riesz-Fischer]**. Let $\{|n\rangle\}$ be an orthonormal set (not necessarily a basis →**??**) of a Hilbert space H. Then for any element $c = \{c_n\}$ of l_2 (→**??**(1)), there is $|a\rangle \in H$ such that $\langle n|a\rangle = c_n$. □
In this sense, any separable (→**??**) Hilbert space is isomorphic.
(B) $\{(2\pi(n^2+1))^{-1/2}e^{inx}\}$ is a complete orthonormal basis of $\boldsymbol{H}^1([-\pi,\pi])$.
(C) Let $u \in L_2[(-\pi,\pi)]$. A condition for $u \in H^1([-\pi,\pi])$ is that $\sum_{n\in\boldsymbol{Z}} n^2|c_n|^2 < \infty$, where c_n is the complex Fourier expansion coefficient (→**??**.

Exercise.
Set up the Gram-Schmidt orthonormalization scheme (→**16.16**) for the $H^1([-1,1])$-space. Apply it to $\{1, x, x^2, \cdots\}$ and obtain the first three polynomials. Compare them with the Legendre polynomials (→**17.5**, **16.16**).

16.6 Parallelogram law and Pythagoras theorem. Let V be a Hilbert space and $x, y \in V$.
(1) **Parallelogram law**. $\|x+y\| + \|x-y\| = 2(\|x\|^2 + \|y\|^2)$.
(2) **Pythagoras' theorem**. If $\langle x|y\rangle = 0$, then $\|x+y\|^2 = \|x\|^2 + \|y\|^2$.

Discussion.
The parallelogram law is a necessary and sufficient condition that the vector space is an Euclidean space (→**16.3**). To demonstrate this we have only to show that

$$\langle x, y\rangle \equiv \frac{1}{4}(\|x+y\| - \|x-y\|)\mathbf{208} \tag{16.9}$$

is a respectable scalar product (→**16.3**). Demonstrating the linearity (**??**) is not very easy. See Kolmogorov-Fomin.

From this we can show that ℓ_p-space defined by $\sum |c_n|^p < \infty$ is a Euclidean space only when $p = 2$. Also the vector space $C_{[a,b]}$ can never be an Euclidean space.

16.7 Cauchy-Schwartz inequality. Let V be a Hilbert space and $f, g \in V$. Then

$$|\langle f|g\rangle| \leq \|f\|\,\|g\|. \tag{16.10}$$

To prove this assume $g \neq 0$, and g is normalized (without loss of generality). Make $h \rightleftharpoons f - g\langle g|f\rangle$. $\langle h|h\rangle \geq 0$ implies the desired inequality.

This inequality tells us a very obvious fact that the modulus of cosine cannot be larger than 1. As is often the case, very obvious things tell us deep things. Heisenberg's uncertainty principle is a disguised version of $|\cos\theta| \leq 1$ (→**28.12**).

From this it is easy to derive the
Triangle inequality: $\|f+g\| \leq \|f\| + \|g\|$.

Discussion.
This inequality allows us to show that + and scalar product are continuous for a Hilbert space. For example, $\langle x_n, y_n\rangle \to \langle x, y\rangle$).

16.8 Bracket notation.
(1) **Ket**. In elementary algebra, we regard an element of a vector space a column vector $\boldsymbol{a}$. Dirac introduced a symbol $|f\rangle$ to denote an element f of a vector space, and called it a *ket*.
(2) **Dual space**. A map from a K-vector space (→**16.1**) V to a field K is called a linear map, if it satisfies the superposition principle (→**??**): $f(\alpha|a\rangle+\beta|b\rangle) = \alpha f(|a\rangle)+\beta f(|b\rangle)$. The totality V^* of these linear maps is again a K-vector space.
Exercise.
Demonstrate this statement.
This space V^* is called the *dual space* of V.
(3) **Scalar product**. In a finite dimensional vector space V, a scalar product is introduced as $\langle \boldsymbol{a}, \boldsymbol{b}\rangle = \boldsymbol{a}^*\boldsymbol{b}$.[213] Any linear map $f(\boldsymbol{a})$ from a K-vector space to K can be uniquely described as a scalar product $f(\boldsymbol{a}) = \langle \boldsymbol{b}, \boldsymbol{a}\rangle$ by choosing an appropriate vector $\boldsymbol{b}$.
Exercise.
Demonstrate the above statement. [It is convenient to use a basis vector set of V.]
This implies that if $\boldsymbol{a} \in V$, then $\boldsymbol{a}^* \in V^*$. That is, (at least for a finite dimensional vector space) we may identify the dual space as the vector space spanned by all the row vectors. We write the hermitian conjugate of a ket $|a\rangle$ as $\langle a|$, which is called a *bra*. We regard V^* the totality of bras.
Notation. The scalar product of $|a\rangle$ and $|b\rangle$ is written as $\langle a|b\rangle$.

16.9 How Dirac introduced brackets. The bra-ket notation was introduced by Dirac. See P. A. M. Dirac, *Principles of Quantum Mechanics* (Oxford UP, 1958). The book is a good example to demonstrate that mathematical depth and mathematical rigor can be different. In this book he introduces kets to describe the states of a quantum mechanical system after explaining superposition of states is required to understand the double slit interference experiment. What he claims is that the state space of a quantum mechanical system is a vector space. Then, he says that for a given vector space, there is always another space, and introduces the space of bras as the dual vectors of kets.

16.10 Orthonormal basis, separability. A subset $\{e_j\}$ of a Hilbert space V is said to be an *orthonormal basis*, if $\langle e_i|e_j\rangle = \delta_{ij}$ and the subspace spanned by $\{e_j\}$ is dense[214] in V. If a Hilbert space has a

[213] * implies the hermitian conjugate. That is, $\boldsymbol{a}^*$ is the complex conjugate of the transposition of $\boldsymbol{a}$.
[214] i.e., for any $f \in V$ there is a sequence $\{a_i\}$ such that $b_N = \sum_{i=1}^N a_i e_i$ converges to f in the norm as $N \to \infty$. That is, $\{e_i\}$ is complete (→**16.3**).

countable dense set, then we say the Hilbert space is *separable*. Separable Hilbert spaces have countable orthonormal basis.

Discussion.
(A) $L_2(\boldsymbol{R}^3)$ is separable.
(B) An example of a non-separable Hilbert space is the totality of functions on $[0,1]$ such that they are nonzero only on a countably many points, and the square sum of these values is finite. The scalar product is defined by $\langle x, y\rangle = \sum x(t)y(t)$, where the sum is over all the countable points on which $x(t)y(t) \neq 0$. (from Kolmogorov-Fomin)
(C) Let $e_n = \{\delta_{nk}\}_{k\in\boldsymbol{N}}$. Then, $\{e_n\}_{n=0}^{\infty}$ is a complete orthonormal system of ℓ_2.

16.11 Bessel's inequality. Let $\{|e_n\rangle\}$ be an orthonormal set of a separable Hilbert space V. Then for $\forall|f\rangle \in V$

$$\sum_{n=1}^{\infty} |\langle e_n|f\rangle|^2 \leq \langle f|f\rangle. \tag{16.11}$$

[Demo]

$$\|f - \sum_{n=1}^{N} |e_n\rangle\langle e_n|f\rangle\|^2 = \langle f|f\rangle - \sum_{n=1}^{N} |\langle e_n|f\rangle|^2 \geq 0 \tag{16.12}$$

for any positive integer N. Hence, (16.11).□

16.12 Parseval's equality. Let $\{|e_n\rangle\}$ be an orthonormal basis of a separable Hilbert space V. Then, for $\forall|f\rangle \in V$

$$\sum_{n=1}^{\infty} |\langle e_n|f\rangle|^2 = \langle f|f\rangle. \tag{16.13}$$

Conversely, if (16.13) holds for $\forall|f\rangle \in V$, then $\{|e_n\rangle\}$ is an orthonormal basis of V. (This follows easily from $|S[f]\rangle = |f\rangle$ (see below **16.14**). This is a natural extension of Pythagoras' theorem **16.6**.)

Discussion.
(A) Let $Q = \{|n\rangle\}$ be an orthonormal set of a Hilbert space. Q is an orthonormal basis, iff[215] $|a\rangle$ satisfying $\langle n|a\rangle = 0$ for all n is actually zero.
[Demo] If Q is an orthonormal basis, vanishing of all the Fourier coefficients implies that $|a\rangle = 0$. Suppose Q is not a basis. Then due to Bessel's inequality **??** and Parseval's equality **??** there is a nonzero vector $|b\rangle$ such that

$$\langle b|b\rangle > \sum_{n} |\langle n|b\rangle|^2. \tag{16.14}$$

[215] i.e., if and only if.

Thanks to the Riesz-Fischer theorem (→**??**), there is a ket $|a\rangle$ such that

$$|a\rangle = \sum_n |n\rangle\langle n|b\rangle. \tag{16.15}$$

Since $\langle b|b\rangle > \langle a|a\rangle$, $|b\rangle - |a\rangle \neq 0$. However, $\langle n|b-a\rangle = 0$ for any n. That is, there is a ket $|c\rangle$ satisfying $\langle n|c\rangle = 0$ for all n but not zero. Hence, if there is no such ket $|c\rangle$, then Q must be a basis.

(B) **Rademacher functions**. Define $r_n(x)$ as $r_0(x) = 1$ and

$$r_n(x) \equiv 1 - 2x_n \tag{16.16}$$

where x_n is the number of the n-th binary place of x. $R' = \{r_n(x)\}_{n\in\boldsymbol{N}}$ is called the *Rademacher orthogonal function system.*

(1) Show that it is an orthonormal system for $L_2([0,1])$.

(2) Show, however, the system is not complete.

(3) Let R be the totality of functions made by multiplying finite number of functions in R'. Then, R is a complete orthonormal system for $L_2([0,1])$.

16.13 Generalized Fourier expansion. Let $\{|e_n\rangle\}$ be an orthonormal basis (→**16.10**) of a Hilbert space V. The following sum for $|f\rangle \in V$

$$|S[f]\rangle = \sum_{n=1}^{\infty} |e_n\rangle\langle e_n|f\rangle \tag{16.17}$$

is called the *generalized Fourier expansion* of f (cf. **16.24**). Due to the definition of the orthonormal basis, actually $|S[f]\rangle = |f\rangle$.[216] The expansion allows us to make a one to one map between any separable Hilbert space (→**16.8**) and the ℓ_2-space (→**16.3**). Hence, all the separable Hilbert spaces are isomorphic.[217]

16.14 Least square approximation and Fourier expansion. **16.11** tells us that the Fourier coefficients can be determined by the following minimization problem:

$$\min \|f - \sum_{n=0}^{N} c_n e_n\|. \tag{16.18}$$

That is, the generalized Fourier series gives the best approximation in the L_2-sense. This gives another reason why L_2 is a natural space to consider Fourier series (Fourier analysis in general) (→**15.19**).

[216] This equality is in the L_2 sense (→**16.5**). When this equality is in the ordinary sense is a non-trivial question as we have seen in **17**.

[217] In these notes, we use the terminology 'Hilbert space' for infinite dimensional cases only.

16.15 Decomposition of unity. The main result of **16.12** can be abstracted as

$$1 \equiv \sum_n |e_n\rangle\langle e_n| \tag{16.19}$$

for an orthonormal basis $\{|e_n\rangle\}$ of a Hilbert space V. This formula is called a *decomposition of unity*.

16.16 Gram-Schmidt orthonormalization. Let V be a Hilbert space, and $\{|1'\rangle, |2'\rangle, \cdots\}$ be a set of linearly independent kets in V whose linear hull is dense in V (i.e., complete →**16.3**). Then, we can construct an orthonormal basis $\{|1\rangle, |2\rangle, \cdots\}$ of V out of these kets as follows. The procedure is called the *Gram-Schmidt orthonormalization*.
(1) $|1\rangle = |1'\rangle/|1'|$, where $|a|$ will denote $\sqrt{\langle a|a\rangle}$ in this entry.
(2) $|2\rangle = |2''\rangle/|2''|$, where $|2''\rangle = (1 - |1\rangle\langle 1|)|2'\rangle$.
(3) $|3\rangle = |3''\rangle/|3''|$, where $|3''\rangle = (1 - |1\rangle\langle 1| - |2\rangle\langle 2|)|3'\rangle$, etc.
This is a method to construct orthogonal polynomials from $1, x, x^2, x^3, \cdots$ (→**17.2**).

16.17 Respect the order in the basis. Hilbert spaces may almost be treated as finite dimensional vector space. However, we must respect the ordering of the basis set. The (generalized) Fourier expansion is not absolutely convergent usually, so this is a very natural thing to respect.

16.18 Orthogonal projection. Let the k-th summand in (16.19) be $P_k \overset{\text{def}}{=} |e_k\rangle\langle e_k|$. Then we have $P_iP_j = P_jP_i = \delta_{ij}P_i$. Especially, $P_iP_i = P_i$. These operators are hermitian, $P_k^* = P_k$.

If a linear operator P satisfies the *idempotency*, i.e., $P^2 = P$, then P is called a *projection* (or a projection operator).
If it is hermitian, then it is called an *orthogonal projection*: For a non-zero ket $|a\rangle$, let $|p\rangle \overset{\text{def}}{=} P|a\rangle$ and $|q\rangle \overset{\text{def}}{=} (1 - P)|a\rangle$. $\langle p|q\rangle = \langle a|P^*(1 - P)|a\rangle = \langle a|(P^* - P^*P)|a\rangle$. If P is hermitian, this vanishes. That is, $|p\rangle$ and $|q\rangle$ are orthogonal.

Discussion.
(A) [**What is P_1P_2?**] Let P_1 and P_2 be orthogonal projection operators. A necessary and sufficient condition for P_1P_2 to be a projection operator is that P_1 and P_2 commute. Let $P_iV = V_i$, where V is a vector space on which these projection operators are defined. What is P_1P_2V?
(B) [**System reduction**]. We wish to study a nonlinear equation

$$\frac{du}{dt} = \mathcal{N}(u). \tag{16.20}$$

Here $\mathcal{N}$ is a nonliner functional (a map). Formally, orthogonal projections are used to reduce a complicated system. Suppose P is a projection to a space spanned by

'important variables' (say, slow variables). Let us write $Q = 1 - P$. We can formally rewrite

$$\frac{dPu}{dt} = P\mathcal{N}(Pu + Qu), \tag{16.21}$$

$$\frac{\partial Qu}{\partial t} = Q\mathcal{N}(Pu + Qu). \tag{16.22}$$

If we could solve the second equation for Qu for any Pu as $Qu = F(Pu)$, then the first member becomes

$$\frac{dPu}{dt} = P\mathcal{N}(Pu + F(Pu)). \tag{16.23}$$

In this way we can get rid of unwanted variables, and reduce the number of variables or the dimension of the space we work. The procedure is only formal, and the crucial point is how to choose P, and how to obtain F. This is a very active field of research now.

16.19 Space $L_2([a,b],w)$. Let $L_2([a,b],w)$ be the totality of the functions which are square integrable[218] with the weight w on the interval $[a,b]$:

$$L_2([a,b],w) \rightleftharpoons \{f \mid \int_a^b |f(x)|^2 w(x)dx < \infty\}. \tag{16.24}$$

This set is a Hilbert space with the following definition of the scalar product

$$\langle f|g\rangle \rightleftharpoons \int_a^b \overline{f(x)} g(x)\, w(x)dx. \tag{16.25}$$

When $w(x) \equiv 1$ we omit w and write $L_2([a,b])$ as in **16.5**. $L_2((-\infty,+\infty))$ is often written as L_2 or $L_2(\boldsymbol{R})$. The convergence with respect to the norm (called the *L_2-norm*) defined by $\|f\| = \sqrt{\langle f|f\rangle}$ is called the *L_2-convergence*. As we know from the theory of Lebesgue integrals (→**15.9**), we may freely change the values of the function on a measure zero set (→**15.4**), so that the convergence in this sense could be quite different from the ordinary sense of convergence (w.r.t the sup norm).

Discussion.
(A) **measure** (→**19a**). Mathematicians usually avoid to discuss the weight functions w, because w need not be an ordinary function (i.e., the density need not be well-behaved). Hence, instead of writing wdx we usually write $d\mu$, introducing a measure μ. Hence, more officially, it is better to call $L_2([a,b],w)$ as $L_2([a,b],\mu)$:

$$L_2([a,b],\mu) \rightleftharpoons \{f \mid \int_a^b |f(x)|^2 d\mu(x) < \infty\}. \tag{16.26}$$

[218] Usually, 'integrable' means 'Lebesgue integrable' (→**15.9**).

(B) $\boldsymbol{L_p}$**-space**. The L_p-space ($p \geq 1$) is defined by the completion[219] of the following function set

$$\{\varphi \,|\, \|\varphi\|_p < +\infty\}, \tag{16.27}$$

where $\| \ \|_p$ is the L_p-norm defined a

$$\|f\|_p \equiv \left(\int |f|^p dx \right)^{1/p}. \tag{16.28}$$

L_p-space is a Banach space (→**16.3** Discussion), but not a Hilbert space except for $p = 2$, because the parallelogram law (→**16.6**) does not hold.

16.20 Dirac's "abuse" of symbols. As we have seen, in a Hilbert space[220] Dirac's bra-ket notation causes no mathematical problem and is quite useful. However, Dirac wished to unify not only the linear space spanned by normalizable states (physically, localized states →**30.19**(4); this part is a Hilbert space) but also the space containing 'plane wave states' which cannot be normalized in the usual way.[221] The starting point of his formal approach is the following interpretation of an ordinary function as a vector with uncountably many components.

16.21 $\boldsymbol{f(x)}$ **as an** $\boldsymbol{x}$**-component of a vector**. It is not an unnatural idea to regard the i-th component of a vector $|v\rangle$ as a 'value' $v(i)$ of a function v defined on $\{1, 2, \cdots, n\}$, where n is the dimension of the vector space. Then, as we have already used the idea (→**??**), it is not outrageous to regard $f(x)$ as the 'x-component' of a vector $|f\rangle$. We know the i-th component of a vector v may be written as $v_i = \langle i|v\rangle$ using the basis vecor $|i\rangle$. Analogously, we write

$$f(x) = \langle x|f\rangle, \quad \overline{f(x)} = \langle f|x\rangle. \tag{16.29}$$

[We Thus we may regard a function as a vector in an infinite dimensional vector space spanned by position kets $\{|x\rangle : x \in [a, b]\}$. These position kets may be regarded as orthonormal vectors (→**20.10**).

16.22 Inner product of functions. It is natural to interpret summations over the coordinate indices as integrations (weighted with a function w as in **16.19**) over the independent variable x. Thus, it is natural to define the scalar product or *inner product* of two functions f and g defined on the same domain as

$$\langle f|g\rangle \equiv \int dx w(x) \langle f|x\rangle\langle x|g\rangle \equiv \int dx w(x) \overline{f(x)} g(x). \tag{16.30}$$

[219] Completion means to add elements to make all the Cauchy sequences have unique limits.

[220] assuming separability (→**16.10**)

[221] Dirac wished to use the Hilbert space notation in a much wider class of spaces now called rigged Hilbert space.

16.23 Decomposition of unity. The formula (16.30) suggests that we can decompose unity (cf. **16.15**) as

$$\int |x\rangle w(x) dx \langle x| \equiv 1. \tag{16.31}$$

This suggests that we may interpret $\{|x\rangle\}$ as an "orthonormal basis." Often unity is written as the following operator:

$$1 = |x\rangle \int dx\, w(x) \langle x|. \tag{16.32}$$

16.24 Trigonometric expansion revisited. Let $V = L_2([-\pi, \pi])$ ($\rightarrow$**16.5**). Let us introduce the kets $|0\rangle, |n, c\rangle, |n, s\rangle$ such that

$$\langle x|0\rangle = \frac{1}{\sqrt{2\pi}}, \quad \langle x|n, c\rangle = \frac{1}{\sqrt{\pi}} \cos nx, \quad \langle x|n, s\rangle = \frac{1}{\sqrt{\pi}} \sin nx. \tag{16.33}$$

Then $\{|0\rangle, |1, c\rangle, |1, s\rangle, |2, c\rangle, |2, s\rangle, \cdots\}$ is an orthonormal basis, because it is a complete set for C^0-functions on $[-\pi, \pi]$, ($\rightarrow$**??**). The standard Fourier expansion **17.1** is

$$|f\rangle = |0\rangle\langle 0|f\rangle + \sum_{n=1}^{\infty} \left\{ |n, c\rangle\langle n, c|f\rangle + |n, s\rangle\langle n, s|f\rangle \right\}. \tag{16.34}$$

[Here, the equality is in the L_2-sense.] Notice, again, that the equality in this formula is in the L_2-sense. Bessel's inequality ($\rightarrow$**16.11**) and Parseval's equality ($\rightarrow$**20.12**) adapted to the trigonometric function set are their original forms.

16.25 δ-function (with weight). We can formally write ($\rightarrow$**16.23**)

$$f(x) = \langle x|1|f\rangle = \int \langle x|y\rangle w(y) dy \langle y|f\rangle = \int f(y) \langle x|y\rangle w(y) dy. \tag{16.35}$$

Therefore, it is natural to introduce

$$\langle x|y\rangle = \delta_w(x - y) \tag{16.36}$$

such that

$$\begin{array}{l} \int \delta_w(x - y) w(y) dy = 1, \\ \delta_w(x - y) = 0 \quad x \neq y. \end{array} \tag{16.37}$$

Obviously, δ_w is a generalization of δ ($\rightarrow$**??**). We should identify as

$$\delta_w(x - y) = \delta(x - y)/w(x). \tag{16.38}$$

Exercise.
Show (for $r' > 0$)

$$\delta(x - x')\delta(y - y')\delta(z - z') = \delta(r - r')\delta(\theta - \theta')\delta(\varphi - \varphi')/r^2 \sin\theta. \tag{16.39}$$

16.26 δ**-function for curvilinear coordinates**. (16.38) tells us that if we wish to use functions defined in terms of the O-$q^1q^2q^3$ coordinates which are orthogonal curvilinear (→**2D.3**), then it is natural to choose the function space whose scalar product uses the weight function $w = h_1h_2h_3$ (→**??**). Thus it is convenient to define the position bra-ket with the normalization

$$\langle q^1, q^2, q^3 | q'^1, q'^2, q'^3 \rangle = \delta(q^1 - q'^1)\delta(q^2 - q'^2)\delta(q^3 - q'^3)/h^1h^2h^3. \quad (16.40)$$

For example, for the spherical coordinate system (→**??**)

$$\langle r, \theta, \varphi | r', \theta', \varphi' \rangle = \frac{\delta(r - r')\delta(\theta - \theta')\delta(\varphi - \varphi')}{r^2 \sin\theta}. \quad (16.41)$$

Exercise.
Write down the δ-function adapted to the elliptic cylindrical coordinates.

16.27 Delta function in terms of orthonormal basis. Since $\delta(x - y) = \langle x|y\rangle$ may be interpreted as $\langle x|1|y\rangle$, we may introduce the decomposition of unity **16.15** into this formula to obtain

$$\delta(x - y) = \sum_n e_n(x)^* e_n(y), \quad (16.42)$$

where $\{|e_n\rangle\}$ is an orthonormal basis, and $e_n(x) \equiv \langle x|e_n\rangle$.

16.28 Green's operator and Green's function – a formal approach. We have already seen the fundamental idea of Green in **??**, and know several examples of Green's functions (→**15**, **16**). We wish to solve the following linear equation:

$$[Lu](z) = f(z) \quad (16.43)$$

with the homogeneous boundary condition. Let $\{|x\rangle\}$ be the position kets w.r.t. the Cartesian coordinates (→**16.21**). With the aid of the decomposition of unity (→**16.23**), we rewrite (16.43) as

$$\langle z|L|y\rangle \int dy \langle y|u\rangle = \langle z|f\rangle \quad (16.44)$$

or

$$\int dy L(z, y)u(y) = f(z), \quad (16.45)$$

where $L(x, y) \equiv \langle x|L|y\rangle$ (a sort of matrix element). If we can invert the 'matrix' $L(x, y)$, then we can solve this equation. In other words, if we can solve

$$LG = 1 \quad (16.46)$$

for G, then $u = Gf$ tanks to superposition (linearity). (16.46) reads

$$\int dy L(x, y)\langle y|G|z\rangle = \langle x|z\rangle = \delta(x - z). \quad (16.47)$$

G is called a *Green's operator*, and $G(x|y) \equiv \langle x|G|y\rangle$ is called a *Green's function*. Formally, $G = L^{-1}$, so that $G(x|y) = \langle x|L^{-1}|y\rangle$.

16.29 Eigenfunction expansion of Green's function – a formal approach. Suppose we know the eigenkets $\{|n\rangle\}$ of the operator L:

$$L|n\rangle = \lambda_n|n\rangle \tag{16.48}$$

If all the eigenvalues are non-zero, then formally

$$G(x,y) = \langle x|L^{-1}|y\rangle = \sum_n u_n(x)\lambda_n^{-1}\overline{u_n(y)}, \tag{16.49}$$

where $\langle x|n\rangle = u_n(x)$. Here we have assumed that the eigenkets of L make a complete orthonormal set. This is the Fourier decomposition formula for the Green's function. We can immediately see the symmetry of the Green's function: $G(x|y) = G(y|x)$ (→**??**, **31.2**, **32.4**, **33.7**). We will later return to a more careful discussion (→**37**).

17 Orthogonal Polynomials

We can construct a polynomial orthonormal basis of a Hilbert space. They are called orthogonal polynomials, which have a beautiful general theory and many important numerical applications (→**22**).

Key words: generalized Fourier expansion, generalized Rodrigues' formula, generating function, three term recursion relation, zeros, Sturm's theorem, Legendre polynomial, Hermite polynomial, Chebychev polynomial

Summary:
(1) Recognize that there is a set of relations and formulas common to many (all classical) orthogonal polynomials (**17.3-17.11**).
(2) Generating function is a useful tool to derive recursion relations (**17.18**, for example).
(3) Remember where the representative polynomials – Legendre, Hermite, and Chebychev – appear (**21B**).

17.A General Theory

17.1 Existence of general theory. The most important fact about orthonormal polynomials is that there is a general theory shared by all the families of (classical →**17.6** Discussion (A)) orthogonal polynomials. The general theory includes generalized Rodrigues' formula, associating (Sturm-Liouville type) eigenvalue problems, generating functions, three term recursion formulas, etc.

17.2 Orthogonal polynomials for $L_2([a,b],w)$ via Gram-Schmidt. $\{1, x, x^2, \cdots\}$ makes a complete set of functions for $L_2([a,b],w)$ (→**16.19**): notice first that $C^0([a,b])$ (the totality of continuous functions on $[a,b]$) is dense in this space. Weierstrass' theorem (→**??**) tells us that any continuous function on a finite interval can be uniformly approximated by a polynomial. Hence, the totality of polynomials is dense in $L_2([a,b],w)$. Therefore, the set of kets $\{|n\rangle\}$ such that $\langle x|n\rangle = x^n$[222] is a complete

[222] For the notational convention see **16.21**.

set (→**16.3**) of the Hilbert space $L_2([a,b],w)$. In this space the scalar product (→**16.5**) is defined by

$$\langle f|g\rangle \equiv \int_a^b \overline{f(x)}g(x)w(x)dx, \tag{17.1}$$

and the norm $\|f\|_w \equiv \sqrt{\langle f|f\rangle}$. We apply the Gram-Schmidt orthonormalization (→**16.16**) to $\{|n\rangle\}$ as follows:
(1) We define $|p_0\rangle = |0\rangle/\sqrt{\langle 0|0\rangle}$.
(2) Normalizing $|1\rangle - |p_0\rangle\langle p_0|1\rangle$, we construct $|p_1\rangle$.
(3) More generally, normalizing

$$|n\rangle - \sum_{k=0}^{n-1} |p_k\rangle\langle p_k|n\rangle, \tag{17.2}$$

we obtain $|p_n\rangle$.
$\{|p_n\rangle\}$ is an orthonormal basis of $L_2([a,b],w)$.

The family of orthogonal polynomials of $L_2([a,b],w)$ is defined by $\langle x|p_n\rangle$ times appropriate n-dependent numerical multiplicative factor as seen in **17.5**.

Exercise.
Apply the Gram-Schmidt orthonormalization method to $\{x^n\}_{n=0}^{\infty}$ and make an ON basis for $L_2([0,1])$. Compute the basis up to the third member of the set.

17.3 Theorem.
(1) $p_n(x) = \langle x|p_n\rangle$ is orthogonal to any $(n-1)$-order polynomial.
(2) The orthonormal polynomials for $L_2([a,b],w)$ are unique, if the coefficients of the highest order terms are chosen to be positive.[223]
These assertions are obviously true by construction, but practically important.

17.4 Least square approximation and generalized Fourier expansion. Let $\mathcal{P}_n$ be the totality of the polynomials order less than or equal to n. The polynomial $P \in \mathcal{P}_n$ which minimizes

$$\|f - P\|_w \tag{17.3}$$

for $f \in L_2([a,b],w)$ is called the n-th order *least square approximation* of f (→**16.13**). The ket $|P\rangle$ satisfying this condition is given by

$$|P\rangle = \sum_{j=0}^{n} |p_j\rangle\langle p_j|f\rangle, \tag{17.4}$$

[223] Here, it is not meant that the orthonormal basis in terms of polynomials is unique (of course, not). If we demand that there are no two polynomials of the same order in the basis, the choice is unique.

where $|p_i\rangle$ are calculated in **17.2** with respect to w. That is, $|P\rangle$ is the n-th partial sum of the following generalized Fourier expansion (→**16.14**) of $|f\rangle$

$$|f\rangle = \sum_{j=0}^{\infty} |p_j\rangle\langle p_j|f\rangle. \tag{17.5}$$

Notice that all the general properties of the Fourier series **??** apply here as well.

Exercise.
(1) Consider the step function $\langle x|a\rangle = \Theta(x-a)$ on $[-1,1]$ ($a \in (-1,1)$). Expand this in terms of Legendre polynomials (→**17.5**).

$$\langle p_n|a\rangle = \sqrt{\frac{1}{2(2n+1)}}(P_{n-1}(a) - P_{n+1}(a)). \tag{17.6}$$

$\langle p_0|a\rangle = (1-a)/\sqrt{2}$ as easily seen. Hence,

$$\Theta(x-a) = \frac{1}{2}(1-a) + \frac{1}{2}\sum_{n=1}^{\infty}[P_{n-1}(a) - P_{n+1}(a)]P_n(x). \tag{17.7}$$

(2) Expand x^5 into the generalized Fourier series in terms of Legendre polynomials.

17.5 Example: Legendre polynomials. A family of orthogonal polynomials of $L_2([-1,1])$ called the Legendre polynomials is defined as

$$P_n(x) = \sqrt{\frac{2}{2n+1}}\langle x|p_n\rangle \tag{17.8}$$

in terms of orthonormal kets $\{|p_n\rangle\}$ constructed for $a=-1$, $b=1$ and $w=1$ in **17.2**. The coefficient $\sqrt{2/(2n+1)}$ is the multiplicative factor mentioned in **17.2**. $P_n(x)$ is called the n-th order *Legendre polynomial*. According to our notational rule (→**20.22**)

$$\langle p_n|f\rangle = \int_{-1}^{1} dx \sqrt{\frac{2n+1}{2}} P_n(x) f(x). \tag{17.9}$$

Hence, the corresponding generalized Fourier expansion (17.5) in terms of the Legendre polynomials reads

$$f(x) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(x) \left[\int_{-1}^{1} dx P_n(x) f(x)\right]. \tag{17.10}$$

17.6 Generalized Rodrigues' formula. Let $F_n(x)$ be defined on $(a,b) \subset \boldsymbol{R}$ as

$$F_n(x) = w(x)^{-1}\frac{d^n}{dx^n}[w(x)s(x)^n], \tag{17.11}$$

where w and s are chosen as

a	b	$w(x)$	$s(x)$
a	b	$(b-x)^\alpha(x-a)^\beta$ $\alpha,\beta>-1$	$(b-x)(x-a)$
a	$+\infty$	$e^{-x}(x-a)^\beta$ $\beta>-1$	$x-a$
$-\infty$	$+\infty$	e^{-x^2}	1

As can easily be seen F_n is an n-th order polynomial (→**??** Exercise (D)). $\{F_n(x)\}$ is a orthogonal polynomial system for $L_2((a,b),w)$ (→**16.17**),[224] because

$$\int_a^b dx\, w(x)F_n(x)F_m(x) = 0 \quad \text{for } n \neq m. \tag{17.12}$$

(Demonstrate this.) If the interval (a,b) and the weight function w are given, the orthogonal polynomial set[225] is uniquely fixed as seen from the Gram-Schmidt construction (up to multiplicative constants) (→**17.2**).

For example, with $w = 1$ (that is, $\alpha = \beta = 0$), $a = -1$ and $b = 1$, F_n must (→**17.3**) be proportional to the Legendre polynomial P_n. Indeed, from (17.11)

$$P_n(x) = \frac{(-2)^{-n}}{n!}F_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(x^2-1)^n. \tag{17.13}$$

This is called *Rodrigues' formula*.

With a suitable n-dependent numerical coefficient K_n a set of orthogonal polynomials $\{f_n\}$ is defined by

$$f_n(x) = \frac{1}{K_n w(x)}\frac{d^n}{dx^n}[w(x)s(x)^n] \tag{17.14}$$

which is called the *generalized Rodrigues formula* (→**21B.1**).[226]

Discussion.

(A) **Classical polynomials**. The generalized Rodrigues' formula can be introduced in a slightly more abstract fashion as follows:

Consider

$$F_n(x) = w(x)^{-1}\frac{d^n}{dx^n}[w(x)s(x)^n], \tag{17.15}$$

where the following conditions are required:

(1) $F_1(x)$ is a first order polynomial.

[224] If a and b are finite, then $L_2((a,b),w) = L_2([a,b],w)$.

[225] We assume that the polynomials are ordered according to their order (→**16.19**).

[226] Not all the orthogonal polynomials can be obtained from the formula; only the so-called *classical polynomials*.

(2) $s(x)$ is a polynomial in x of degree less than or equal to 2 with real roots.
(3) $w(x)$ is real, positive and integrable on $[a, b]$ and satisfies the boundary conditions $w(a)s(a) = w(b)s(b) = 0$.
It turns out that (i)-(iii) implies that we can only have the cases in the table in **18.6** (apart from trivial linear transformations, and multiplicative constants).[227] These polynomials are called *classical polynomials*.
(B) Demonstrate with the aid of Rolle's theorem that all the zeros of $P_n(x)$ are in $[-1, 1]$.

17.7 Relation to the Sturm-Liouville problem. $f_n(x)$ defined by (17.14) obeys the following equation generally called the Sturm-Liouville equation (→**??**, **31.1**)

$$-\frac{d}{dx}\left(w(x)s(x)\frac{d}{dx}f_n(x)\right) = \lambda w(x)f_n(x), \tag{17.16}$$

where λ is a pure number given by

$$\lambda = -n\left(K_1\frac{df_1(0)}{dx} + \frac{n-1}{2}\frac{d^2s(x)}{dx^2}\right). \tag{17.17}$$

This can be demonstrated by a tedious but straightforward calculation. See **31.3** Discussion.

17.8 Generating functions. In general, the following power series of ζ is called the *generating function* of the orthogonal polynomial set $\{p_n(x)\}$

$$Q(\zeta, x) = \sum_{n=0}^{\infty} A_n p_n(x)\zeta^n, \tag{17.18}$$

where A_n is a numerical constant introduced to streamline the formula. That there is such a function for any orthogonal polynomial family can be seen from the rewriting of generalized Rodrigues' formula (17.11). Using Cauchy's theorem (→**??**), we have

$$f_n(z) = \frac{1}{K_n w(z)}\oint_{\partial D} dt \frac{n!}{2\pi i(t-z)^{n+1}} w(t)s(t)^n, \tag{17.19}$$

where $D \subset \boldsymbol{C}$ is a small disk centered at z. We define a new variable ζ as

$$\frac{1}{\zeta} = a\frac{s(t)}{t-z}, \tag{17.20}$$

[227] See P Dennery and A Krzywicki, *Mathematics for Physicists* (Harper and Row, 1967), Section 10.3.

where a is a numerical factor introduced to streamline the final outcome. In terms of this variable (17.19) can be rewritten generally as

$$f_n(z) = \frac{a^n n!}{2\pi i K_n w(z)} \oint_{\partial D'} d\zeta \frac{1}{\zeta^{n+1}} Q(\zeta, z), \tag{17.21}$$

where Q is an appropriate function resulted from the intergrand in (17.19) through the change of variables. This implies

$$Q(\zeta, z) = \sum_{n=0}^{\infty} f_n(z) \frac{K_n w(z) \zeta^n}{a^n n!}. \tag{17.22}$$

17.9 Generating function for Legendre polynomials. For example, for the Legendre polynomials, $K_n = (-2)^n n!$ and $w(x) = 1$. (17.19) reads (or directly from (17.13))

$$P_n(z) = \frac{1}{2\pi i} \oint_{\partial D} \frac{(t^2-1)^n}{[2(t-z)]^n} \frac{dt}{t-z}, \tag{17.23}$$

which is called *Schläfli's integral*. We choose $a = -1/2$ in (17.21) to get

$$P_n(z) = \frac{1}{2\pi i} \oint_{\partial D'} \frac{1}{\zeta^{n+1}} \frac{d\zeta}{\sqrt{1-2z\zeta+\zeta^2}}, \tag{17.24}$$

so that (→**??**(i))

$$w(z, \zeta) = \frac{1}{\sqrt{1-2z\zeta+\zeta^2}} = \sum_{n=0}^{\infty} P_n(z) \zeta^n. \tag{17.25}$$

This is the generating function for the Legendre polynomials.

Exercise.
Derive (17.24). Use the new variable (following (17.20)) ζ as

$$\frac{1}{\zeta} = \frac{t^2-1}{2(t-z)}. \tag{17.26}$$

[Hint. When the reader solves for t, she must choose the correct branch so that $t \to z$ corresponds to $\zeta \to 0$.]

17.10 Three term recursion formula. Let $\{|p_n\rangle\}$ be a complete set of orthonormal polynomial kets, and k_n be the highest order coefficient of the polynomial $p_n(x) = \langle x|p_n\rangle$. Define

$$\gamma_n = k_{n+1}/k_n, \quad \beta_n = \gamma_n/\gamma_{n-1}, \ \alpha_n = \gamma_n \langle p_n|x|p_n\rangle. \tag{17.27}$$

Then,

$$p_{n+1}(x) = (\gamma_n x - \alpha_n) p_n(x) - \beta_n p_{n-1}(x). \tag{17.28}$$

this follows easily from (1) of **17.3**.

Discussion.
Let us demonstrate the assertion.

$$\langle x| \left(|p_n\rangle - x\frac{k_n}{k_{n-1}}|p_{n-1}\rangle \right) \tag{17.29}$$

is a polynomial of degree at most $n-1$. Therefore, it can be expressed as a sum of $\{p_{n-1}, \cdots, p_0\}$.
(1) Demonstrate, because of **17.3**, that only p_{n-2} and p_{n-1} are needed to express $p_n - xk_np_{n-1}/k_{n_1}$. Already we have the form of (21.24). [Hint. What happens if there are other remaining terms?]
(2) Determine the coefficients.

17.11 Zeros of orthogonal polynomials. Let $\{|p_n\rangle\}$ be the orthogonal polynomial kets of $L_2([a,b],w)$ ($\rightarrow$**16.19**). Then
(1) All the zeros of $p_n(x) = \langle x|p_n\rangle$ are in the interval (a,b). This is practically very important ($\rightarrow$**18.3**). For a proof see **31.3** Discussion.
(2) All the zeros of $p_n(x)$ are single and the zeros of $p_{n+1}(x)$ are separated by those of $p_n(x)$.

Discussion.
The three term recurrence relation can be written as

$$x\boldsymbol{P}(x) = A\boldsymbol{P}(x) + \boldsymbol{q}(x), \tag{17.30}$$

where $\boldsymbol{P} = (p_0, p_1, \cdots, p_{n-1})^T$, A is a symmetric matrix, and $\boldsymbol{q} = (0, \cdots, 0, k_{n-1}p_n/k_n)$. Choose x to be a zero x_i of p_n, then we have

$$x_i\boldsymbol{P}(x_i) = A\boldsymbol{P}(x_i) \tag{17.31}$$

That is, the zeros of p_n must be the eigenvalues of A, so that they must be real.

17.12 Remark: how to locate real zeros of polynomials. Drawing graphs with the aid of Mathematica and zooming into the relevant portion of the graphs may be the most practical method. Analytically, there is a famous
Theorem [Sturm]. Assume that the n-th order polynomial P does not have any multiple zero. Let $p_0 \equiv P$ and $p_1 \equiv P'$. Using the theorem of division algorithm, construct p_n as follows:

$$p_{i+1} = p_iq_i - p_{i-1} \quad (i = 1, 2, \cdots, n-1). \tag{17.32}$$

Let $V(c)$ be the number of changes of sign in the sequence $p_0(c), p_1(c), \cdots, p_n(c)$.[228] The number of zeros in the interval $[a,b]$ is given by $V(a) - V(b)$.□

[228] Remove $p_i(c)$ if it is zero from the sequence.

17.13 Example of Sturm's theorem. Let us study $f(x) = x(x^2 - 1)$. We trivially know that $0, \pm 1$ are the real zeros. First we construct p_i in the theorem as follows:

$$p_0 = x(x^2 - 1);\ p_1 = 3x^2 - 1;\ p_2 = 2x/3;\ p_3 = 1. \tag{17.33}$$

Therefore, we can make, for example, the following table exhibiting the signs and V.

a	p_0	p_1	p_2	p_3	$V(a)$
$+\infty$	$+$	$+$	$+$	$+$	0
2	$+$	$+$	$+$	$+$	0
$1/2$	$-$	$-$	$+$	$+$	1
$-1/2$	$+$	$-$	$-$	$+$	2
$-\infty$	$-$	$+$	$-$	$+$	3

For example, $V(-1/2) - V(2) = 2$, so there must be two zeros in $(-1/2, 2)$.

Discussion.
Find the number of positive real roots of the following polynomials.
(1) $P(x) = 3x^4 + 2x^2 - x - 5$,
(2) $P(x) = 13x^{21} + 3x^3 - 2$,
(3) (Runge's example)
$P(x) = 3.22x^6 + 4.12x^4 + 3.11x^3 - 7.25x^2 + 1.88x - 7.84$.

17.14 Descartes' sign rule. Let

$$P(x) = a_0x^n + a_1x^{n-1} + \cdots + a_n \tag{17.34}$$

be a real coefficient polynomial. Let W be the number of the sign change in the sequence $a_0, a_1, \cdots, a_n$ (remove 0 from this sequence before counting). Then the number of strictly positive roots of $P(x) = 0$ is given by W or W minus some even positive number. (Hence, if $W = 1$, that is the answer.)

17.B Representative Examples

17.15 Table of orthogonal polynomials. (→?? Exercise (D)) **17.6** tells us that various orthogonal polynomial families can be obtained by

choosing w and s appropriately and also by choosing appropriate multiplicative numerical factors K_n. Some common examples are given as follows.

name	symbol	domain	$w(x)$	$s(x)$	K_n^{-1}
Legendre	P_n	$[-1,1]$	1	$1-x^2$	$(-1)^n 2^n n!$
Chebychev	T_n	$[-1,1]$	$1/\sqrt{1-x^2}$	$1-x^2$	$(-1)^n(2n-1)!!$
Jacobi	$P_n^{(\alpha,\beta)}$	$[-1,1]$	$(1-x)^\alpha(x+1)^\beta$	$1-x^2$	$(-1)^n 2^n n!$
Laguerre	L_n	$[0,\infty)$	e^{-x}	x	$n!$
Hermite	H_n	$(-\infty,\infty)$	e^{-x^2}	1	$(-1)^n$

Note that L_n is $L_n^{(0)}$ of **??**.

Exercise. Show $T_n = n!\sqrt{\pi}P_n^{(-1/2,1/2)}/\Gamma(n+1/2)$.

17.16 Legendre polynomials. The Legendre polynomials have been discussed above (→**17.5**). The orthonormal basis of $L_2([-1,1])$ (→**16.19**) in terms of the Legendre polynomials is in **17.5** with the generalized Fourier expansion formula. The decomposition of unity (→**16.15**) reads

$$\delta(x-y) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(x)P_n(y). \tag{17.35}$$

Rodrigues' formula is in **17.6**, and the generating function is given in **17.9**. We can write down the general formula starting from Rodrigues' formula as

$$P_n(x) = \frac{1}{2^n} \sum_{j=0}^{[n/2]} \frac{(-1)^j}{j!} \frac{(2n-2j)!}{(n-j)!(n-2j)!} x^{n-2j}. \tag{17.36}$$

($[\cdot]$ is Gauss' symbol denoting the largest integer not exceeding $\cdot$.)

Discussion.
Let $Q_n(x)$ be the n-th order polynomial with its highest order coefficient normalized to be unity. If its L_2-distance from 0 is the smallest among such polynomials, Q_n is proportional to P_n. That is, minimize

$$\int_{-1}^{1} (x^n + a_{n-1}x^{n-1} + \cdots + a_0)^2 dx \tag{17.37}$$

with respect to the coefficients. The resultant polynomial is proportional to P_n.

17.17 Sturm-Liouville equation for Legendre polynomials. The differential equation corresponding to (17.16) reads (→**20.26**)

$$(1-x^2)P_n''(x) - 2xP_n'(x) + n(n+1)P_n(x) = 0, \tag{17.38}$$

or

$$\frac{d}{dx}\left[(1-x^2)\frac{d}{dx}P_n(x)\right] + n(n+1)P_n = 0. \tag{17.39}$$

17.18 Recursion formulas for Legendre polynomials. The three term recursion relation (→**17.10**) reads

$$(n+1)P_{n+1}(x) - (2n+1)xP_n(x) + nP_{n-1}(x) = 0 \tag{17.40}$$

with $P_0(x) = 1$ and $P_1(x) = x$. This can also be obtained easily from the generating function (17.25): expand

$$(1 - 2x\zeta + \zeta^2)\frac{\partial w}{\partial \zeta} + (-\zeta + x)w = 0. \tag{17.41}$$

Similarly, we obtain

$$(1 - 2x\zeta + \zeta^2)\frac{\partial w}{\partial x} - \zeta w = 0. \tag{17.42}$$

This leads to

$$P_{n+1}' - 2xP_n' + P_{n-1}' - P_n = 0. \tag{17.43}$$

If we eliminate P_{n-1}' from (17.40) and (17.43), we get

$$P_{n+1}' - xP_n' = (n+1)P_n. \tag{17.44}$$

If we eliminate P_{n+1}' from (17.40) and (17.43), we get

$$xP_n' - P_{n-1}' = nP_n. \tag{17.45}$$

Combining above two formulas, we obtain

$$P_{n+1}' - P_{n-1}' = (2n+1)P_n. \tag{17.46}$$

17.19 Legendre polynomials, some properties.
(1) $P_n(x)$ is an odd (resp., even) function, if n is odd (resp., even): $P_n(x) = (-1)^n P_n(-x)$, $P_n(1) = 1$ and $P_n(-1) = (-1)^n$. $P_{2n}(0) = \binom{-1/2}{n}$ (see Exercise below).
(2) $|P_n(x)| \leq 1$.
(3) All the zeros of P_n are simple and in $(-1, 1)$ (→**17.11**).
(4) If Π_n is an n-th order polynomial satisfying

$$\int_{-1}^{1} \Pi_n(x) x^k dx = 0 \tag{17.47}$$

for all $k \in \{0, 1, \cdots, n-1\}$, then $\Pi_n \propto P_n$ (→**21A.3(2)**).
[Demo of (2)] This can be proved with the aid of Schläfli's integral (17.23). We choose for the intergration path to be

$$t = z + \sqrt{z^2 - 1} e^{i\phi} \tag{17.48}$$

for $\phi \in [-\pi, \pi)$. Note that $dt/(t - z) = id\phi$. Changing the integration variable from t to ϕ in (17.23), we get the following *Laplace's first integral*

$$P_n(x) = \frac{1}{\pi} \int_0^{\pi} [x + \sqrt{x^2 - 1} \cos\phi]^n d\phi. \tag{17.49}$$

From this we get

$$|P_n(\cos\theta)| \leq \frac{1}{\pi} \int_0^{\pi} |\cos\theta + i \sin\theta \cos\phi|^n d\phi \leq 1. \tag{17.50}$$

Exercise
$P_{2n}(0)$ can be obtained from Rodrigues' formula (21.11), which reads

$$P_{2n}(0) = (-1)^n \frac{\Gamma(n + 1/2)}{\sqrt{\pi}\Gamma(n+1)}. \tag{17.51}$$

17.20 Hermite polynomials. The orthonormal basis $\{|h_n\rangle\}$ for $L_2((-\infty, \infty), e^{-x^2})$ (→**16.19**) obtained by the Gram-Schmidt method applied to monomials (→**17.2**) is written in terms of the *Hermite polynomials* $H_n(x)$ as

$$\langle x|h_n\rangle = \sqrt{\frac{1}{2^n n! \sqrt{\pi}}} H_n(x), \tag{17.52}$$

where

$$H_n(x) = \sum_{m=0}^{[(n+1)/2]} (-)^n \frac{n!}{m!(n+1-2m)!} (2x)^{n+1-2m}. \tag{17.53}$$

($[\cdot]$ is Gauss' symbol denoting the largest integer not exceeding $\cdot$.) The generalized Rodrigues formula (→**17.6**) for the Hermite polynomials is

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} e^{-x^2}. \tag{17.54}$$

The generating function (→**17.8**) is given by

$$W_H(z,\zeta) = e^{2z\zeta-\zeta^2} = \sum_{n=0}^{\infty} \frac{H_n(z)}{n!}\zeta^n. \tag{17.55}$$

H_n is an even (resp., odd) function, if n is even (resp., odd).

Warning. Many authors use the weight $e^{-x^2/2}$ instead of e^{-x^2}. If we write the Hermite polynomials defined for this weight as $H_n^*(x)$, then the generalized Rodrigues formula (→**17.6**) reads

$$H_n^*(x) = (-)^n e^{x^2/2}\frac{d^n}{dx^n}e^{-x^2/2}, \tag{17.56}$$

and

$$H_n(x) = 2^{n/2}H_n^*(\sqrt{2}x), \quad H_n^*(x) = 2^{-n/2}H_n(x/\sqrt{2}). \tag{17.57}$$

Discussion.
To demonstrate the completeness of the Hermite polynomials, Weierstrass' theorem **17.3** is not enough, because the latter is about a finite interval. To show the completeness with respect to the L_2-norm we have only to show the completeness of polynomials. This can be demonstrated with the aid of Weierstrass' theorem on increasingly large intervals.

Exercise.
(A) From the generating function show

$$e^{x^2/2}H_n(x) = \frac{1}{i^n\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ixy-y^2/2}H_n(y)dy. \tag{17.58}$$

This can be split into real and imaginary part relations (Lebedev).
(B) From the generating function we obtain the following generalized Fourier expansion

$$e^{ax} = e^{a^2/4} \sum_0^\infty \frac{a^n}{2^n n!} H_n(x), \tag{17.59}$$

which is good for all $x \in \boldsymbol{R}$.
(C) Compute the generalized Fourier expansion of e^{-ax^2} in terms of Hermite polynomials. The expansion coefficients can be written as

$$c_{2n} = \frac{1}{2^{2n}(2n)!\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-(a+1)x^2} H_{2n}(x) dx. \tag{17.60}$$

To compute the integral use (17.69) below. The x-integration can be done and we are left with

$$c_{2n} = \frac{(-1)^n a^n}{\sqrt{\pi}(2n)!(1+a)^{n+1/2}} \int_0^\infty e^{-s} s^{n-1/2} ds. \tag{17.61}$$

Use the Gamma function (→**14.5**) to obtain the final result (Lebedev)

$$c_{2n} = \frac{(-1)^n a^n}{2^{2n} n!(1+a)^{n+1/2}}. \tag{17.62}$$

17.21 Sturm-Liouville equation for Hermite polynomials. The formula corresponding to (17.16) reads

$$H_n'' - 2xH_n' + 2nH_n = 0. \tag{17.63}$$

17.22 Recurrence equations for Hermite polynomials. The three term recurrence relation (→**17.10**) reads

$$H_{n+1} + 2xH_n + 2nH_{n-1} = 0, \tag{17.64}$$

which can be obtained from

$$\frac{\partial w_H}{\partial \zeta} = -2(z+\zeta)w. \tag{17.65}$$

From

$$\frac{\partial w_H}{\partial z} = 2\zeta w \tag{17.66}$$

we obtain

$$H_{n+1}' = -2(n+1)H_n. \tag{17.67}$$

Exercise.
An integral formula for Hermite polynomials can be obtained with the aid of

$$e^{-x^2} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-t^2} \cos 2xt \, dt. \tag{17.68}$$

[Hint. Note that the integrand is an even function.] Putting this into the generalized Rodrigues' formula (calculate the odd and even n cases separately, and unify the results), we obtain

$$H_n(x) = \frac{2^n(-i)^n e^{x^2}}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-t^2+2itx} t^n dt. \tag{17.69}$$

17.23 Chebychev polynomials. These polynomials are best introduced as

$$T_n(x) = \cos(n \cos^{-1} x). \tag{17.70}$$

The generalized Rodrigues formula (→**17.6**) is given by

$$T_n(x) = \frac{(-1)^n}{(2n-1)!!}\sqrt{1-x^2}\frac{d^n}{dx^n}(1-x^2)^{n-1/2}. \tag{17.71}$$

This can be transformed into (17.70) with the aid of the binomial theorem: it is easy to demonstrate that this formula yields

$$\frac{1}{2}[(x+i\sqrt{1-x^2})^n + (x-i\sqrt{1-x^2})^n] \tag{17.72}$$

which reduces to $\cos n\theta$ with $x = \cos\theta$.

The orthonormal basis $\{|t_n\rangle\}$ of $L^2([-1,1], 1/\sqrt{1-x^2})$ (→**16.19**) obtained by the Gram-Schmidt orthonormalization of monomials (→**17.6**) can be written as

$$\langle x|t_n\rangle = \sqrt{\frac{\pi}{2}}T_n(x). \tag{17.73}$$

The generating function (→**17.8**) is

$$\frac{1-z^2}{1-2xz+z^2} = T_0(x) + 2\sum_{n=1}^{\infty} T_n(x)z^n. \tag{17.74}$$

The highest order coefficient of T_n is 2^{n-1} for $n \geq 1$. The three term recursion formula (→**17.10**) is[229]

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \tag{17.75}$$

for $n = 1, 2, \cdots$ with $T_0 = 1$, $T_1(x) = x$.

[229] This is nothing but $\cos(n+1)x + \cos(n-1)x = 2\cos x \cos nx$.

Exercise.
(1) Demonstrate that

$$(1-x^2)T_n''(x) - xT_n'(x) + n^2 T_n(x) = 0. \tag{17.76}$$

(2) Demonstrate the generating function for Chebychev polynomials (17.74) as elegantly as possible. [Hint. Use (**??**).]

17.24 Remarkable properties of Chebychev polynomials.

(1) Theorem. Let $p_n(x)$ be a polynomial of order $n(\geq 1)$ whose coefficient of x^n is unity. Then,

$$\max_{x\in[-1,1]} |p_n(x)| \geq 2^{1-n}, \tag{17.77}$$

and the equality holds if and only if $p_n(x) = T_n(x)/2^{n-1}$.□
(2) The best (w.r.t. the sup norm) n-th order polynomial approximant of x^{n+1} on $[-1,1]$ is given by $T_{n+1}(x)/2^n - x^{n+1}$. This property makes the Chebychev polynomial very important in approximation theory of functions.
(3) $x_{k+1} = T_n(x_k)$ defines a sequence $x_0, x_1, x_2, \cdots$ from the initial condition x_0. This is a typical chaotic sequence. Among any continuous functions with n laps, $T_n(x)$ gives the most chaotic sequences on the average.

Discussion.
(A) (1) above implies that if the n-th order polynomial Q_n defined on $[-1,1]$ with its highest order coefficient normalized to be unity and if its maximum deviation from zero is the smallest among such polynomials, then Q_n is proportional to the order n Chebychev polynomial.
(B) Take $T_2(x)$. Demonstrate that there are two intervals I and J in $[-1,1]$ which share at most one point such that $T_2(I) \cap T_2(J) \supset I \cup J$. In general, if the reader can find two positive integers and two intervals I and J sharing at most one point such that $f^n(I) \cap f^m(J) \supset I \cup J$, then f exhibits chaos on the inteval containing both I and J. That is, there is an invariant set Ω of f^N for some positive integer N such that f^N restricted to Ω is isomorphic to the coin-tossing process. See the sample Mid Term Report).

18 Numerical Integration

Most integrals cannot be computed analytically. Some of the most important numerical integration algorithms are inseparably connencted to the theory of orthogonal polynomials. Also discussed are the effectiveness of the simple trapezoidal rule and high-dimensional integrals.

Key words: Gauss schemes, IMT formula, DE formula, quasi-Monte Carlo method, Monte Carlo method

Summary:
(1) Roughly speaking, Gauss formulas are versatile and useful. Probably, up to 4 or 5-tuple integrals, direct use of the scheme may be practical. (→**18.3**, **18.5**, **18.6**).
(2) However, if a very accurate integration is needed, variable transformation schemes should be used, esp., the DE formula (→**22B.2**).
(3) If the integration is over a moderately high (~ 10) dimensional region, then quasi-Monte Carlo method **18.18** should be considered first with the conditioning of the function according to **18.15**. I fhte dimension is higher, then currently no better versatile method than the Monte Carlo method is known**18.19**.

18.A Gauss Formulas

18.1 Numerical integration. Simple numerical integration methods as the trapezoidal rule or Simpson's rule has the following general structure

$$\int_{-1}^{1} f(x)dx \simeq \sum_{v=1}^{N} C_v f(\frac{v}{N}) \quad \text{(the general Newton-Cotes formula).} \tag{18.1}$$

We have N freedom to choose C_v. Hence, it is possible to choose them so that the formula is exact for $f(x) = 1, x, \ldots, x^{N-1}$ ((cf. Weierstrass' theorem ß**??**). Gauss pointed out that there is no necessity to choose equidistant points v/N to sample the function values. See the following example.

18.2 Simple demonstration. We choose $N = 2$:

$$\int_{-1}^{1} f(x)dx \sim C_1 f(x_1) + C_2 f(x_2) \tag{18.2}$$

We choose C_i and x_i so that the formula is exact for $f = 1, x, x^2$ and x^3. We have four formulas

$$\begin{aligned} 1 &: 2 = C_1 + C_2, \\ x &: 0 = C_1 x_1 + C_2 x_2, \\ x^2 &: 2/3 = C_1 x_1^2 + C_2 x_2^2, \\ x^3 &: 0 = C_1 x_1^3 + C_2 x_2^3. \end{aligned}$$

From these equations, we solve as

$$\begin{aligned} C_1 = C_2 = 1, \\ x_1 = -x_2 = 1/\sqrt{3}. \end{aligned}$$

Therefore, the $N = 2$ *Gauss-formula* (G2) is

$$\int_{-1}^{1} f(x)dx \simeq f\left(\frac{1}{\sqrt{3}}\right) + f\left(-\frac{1}{\sqrt{3}}\right). \tag{18.3}$$

If we need the integration

$$I = \int_a^b \phi(u)du, \tag{18.4}$$

introduce the variable x running from -1 to 1 such that

$$u = \frac{1}{2}[(b-a)x + a + b] \tag{18.5}$$

and

$$I = \frac{1}{2}(b-a)\int_{-1}^{1} \phi([(b-a)x + a + b]/2)dx. \tag{18.6}$$

Examples for (18.3) are given as[230]

	$\int_0^{\pi/2} \sin x dx$	$\int_0^1 \sqrt{x} dx$	$\int_0^1 x^{3/2} dx$	$\int_0^1 \frac{x}{e^x - 1} dx$	$\int_0^1 f^*(x) dx$
exact	1	2/3	0.4	0.77751164...	0.306853...
G2	0.99848...	0.6738...	0.3987...	0.77750464...	0.2261...

Here $f^*(x) = 1/(x+2)$ for $x \in [0, e-2]$, $f^*(x) = 0$ for $x \in [e-2, 1]$.

As we see, for smooth functions the method is amazingly powerful. If we choose the 4 point formula for $I = \int_0^{\pi/2} \sin x dx$, $I = 1.000000$, correct to six decimal places. (The Simpson rule (→**18.8**) with 64 points

[230] From P. J. Davis and P. Rabinowitz, *Methods of Numerical Integration* (Academic, 1975); not updated but still useful.

produces 0.99999983).
Exercise.
(1) Compute the following integral analytically:

$$\int_{-1}^{1} dx(x^2-1)e^{-x^2/2}. \tag{18.7}$$

Prescribe a method to compute this numerically with the aid of (only) G2 with the relative error of 10^{-5}.
(2) Construct the $N=2$ Gauss formula for the integral of range $[-1,1]$ with the weight $e^{-|x|}$. Apply it to $\cos x$ and compare the result with the ordinary Gauss-Legendre formula with $N=2$ applied to $e^{-|x|}\cos x$ on $[-1,1]$.
(3) Compute

$$\int_0^{\pi/2} \cos x\, sgn(\pi/4-x)dx \tag{18.8}$$

to the relative accuracy of 10^{-4} using only G2. In this case if G2 is naively used for the whole inteval, the error is about 20%.

18.3 Fundamental theorem of Gauss quadrature. Let $w(x)$ be a weight function for the interval $[a,b]$. Then, there exist real numbers $x_1,\ldots,x_N$ and $C_1,\ldots,C_N$ with the following properties
(i) $a<x_1<x_2<\cdots<x_N<b$,
(ii) $C_k>0$ for $k=1,2,\cdots,N$,
(iii)

$$\int_a^b f(x)w(x)dx=\sum_{k=1}^{N} C_k f(x_k) \tag{18.9}$$

is exact for every polynomial $f(x)$ of degree not more than $2N-1$. □
Actually, $x_1\ldots,x_N$ are the zeros of p_N, the N-th member of the orthogonal polynomial family on $[a,b]$ with the weight $w(x)$ (→**17.2**), and

$$C_k=\int_a^b \frac{p_N(x)w(x)dx}{p_N'(x)(x-x_k)} \quad (k=1,\ldots,N).$$

□
For example, for $\int_{-1}^{1} f(x)dx$, $p_N(x)=\sqrt{\frac{2N+1}{2}}P_N(x)$ (→**17.5**) so that the scheme is called the Gauss-Legendre formula.
[Demo] We demonstrate the theorem for $L_2([-1,1])$, the most important case. Let f be an m-th order polynomial, and the desired integration formula is given by

$$\int_{-1}^{1} f(x)dx=\sum_{k=1}^{N} C_k f(x_k), \tag{18.10}$$

as in (iii). Here the fact (→**17.11**) that the zeros of orthogonal polynomials are all in its domain has been fully utilized. Notice that f can be uniquely decomposed as

$$f=P_nQ+R, \tag{18.11}$$

where P_n is the n-th order Legendre polynomial, and R is a polynomial of order less than n. Since the order of Q is $m-n$, if $m-n \leq n-1$ (i.e., $m \leq 2n-1$), then P_n is orthogonal to Q (→**21A.3(1)**). Hence, for $m \leq 2n-1$, we conclude

$$\int_{-1}^{1} f(x)dx = \int_{-1}^{1} R(x)dx. \tag{18.12}$$

According to our formula (18.10), we have

$$\int_{-1}^{1} f(x)dx = \sum_{k=1}^{N} C_k P_n(x_k)Q(x_k) + \sum_{k=1}^{N} C_k R(x_k). \tag{18.13}$$

Therefore, we immediately see that if we can choose x_k to be the zeros of P_n, then the first term on RHS vanishes. That is, (18.12) is true for our formula under construction. For this to be true, we need to set $n = N$ (→**17.11**) and $m = 2N-1$. We have fixed the sampling point locations. If we can choose C_k so that (18.12) holds exactly for all the $N-1$ order polynomials, then we can integrate all the polynomials up to the order $2N-1$ exactly by our integration formula. Therfore, the remaining task is to determine C_k so that

$$\int_{-1}^{1} R(x)dx = \sum_{k=1}^{N} C_k R(x_k) \tag{18.14}$$

is exact for any choice of $N-1$ order polynomial R. Notice that generally we can write

$$R(x) = \sum_{k=1}^{N} R(x_k) l_k(x), \tag{18.15}$$

where[231]

$$l_k(x) = \prod_{i \neq k}^{n} \left(\frac{x - x_i}{x_k - x_i} \right). \tag{18.16}$$

Hence, the following choice solves our problem:

$$C_k = \int_{-1}^{1} l_k(x)dx. \tag{18.17}$$

Since $l_k(x)(x - x_k)$ is proportional to P_N (all the zeros are common!),

$$C_k = \int_{-1}^{1} \frac{P_N(x)}{(x - x_k)P'_N(x_k)}dx = \frac{2}{NP_{N-1}(x_k)P'_N(x_k)} = \frac{2(1-x_k^2)}{[NP_{N-1}(x_k)]^2}. \tag{18.18}$$

Exercise.
Demonstrate the formula for the weight of the Gauss-Legendre formula:

$$C_k = \frac{2(1-x_k^2)}{[NP_{N-1}(x_k)]^2}. \tag{18.19}$$

[231] This is the standard *Lagrange interpolation formula*.

18.4 Error estimate of Gauss formulas.
(1) If f is at least $2N$ times continuously differentiable (i.e., in C^{2N}), then the integration (on $[-1,1]$) error is bounded by

$$|\text{error}| \leq \frac{2^{2N+1}(N!)^4}{(2N+1)((2N)!)^3} \max_{x\in[-1,1]} |f^{(2N)}(x)|. \tag{18.20}$$

(2) If f is holomorphic ($\rightarrow$**??**) in $\Omega \equiv \{z \,|\, |z+1|+|z-1| = \rho+\rho^{-1}\}$ for $\rho > 1$, then

$$|\text{error}| \leq \frac{\pi(\rho+\rho^{-1})}{\rho^{2N+1}} \max_{z\in\Omega} |f(z)|. \tag{18.21}$$

Exercise.
Calculate the following three integrals:

$$(1)\ \int_{-1}^{1} e^{-x^2} dx,\ (2)\ \int_{-1}^{1} \sin|x| dx,\ (3)\ \int_{-1}^{1} \cos x\, sgn(x^2-1/2) dx \tag{18.22}$$

with the aid of the Gauss-Legendre formulas for $N = 2, 4$, and 8 and discuss the results. (The necessary table is on p916 of Abramowitz and Stegun).

18.5 How to get the weights. Abscissa and weight factors are tabulated in, e.g., Abramowitz-Stegun, *Handbook of Mathematical Functions* (Dover, 1972), but it is recommended to compute them to avoid any transcription mistakes.

18.6 Many dimension. We can of course extend the formula for many dimensional cases. [See Davis & Rabinowitz Chapter 5]. For example, a singular integral like

$$\int_{-1}^{1}\int_{-1}^{1} dxdy \frac{1}{1-xy}$$

can be accurately calculated <u>without</u> any special considerations on the singularities.

18.7 Integral equation solver. The Gauss method may be the best general numerical method to solve integral equations.

18.8 Trapezoidal vs. Simpson rule[232] Let

$$I_e = 2h\left\{\sum_{r=1}^{n-1} f(a+2rh) + \frac{1}{2}[f(a)+f(a+2nh)]\right\}, \tag{18.23}$$

$$I_o = 2h\left\{\sum_{r=1}^{n-1} f(a+(2r+1)h)\right\}. \tag{18.24}$$

[232] This section is based on an essay by H. Takahashi, 'Superposition in numerical integration,' Sugaku Seminar, March 1971.

To compute the following integral

$$I = \int_a^{a+2nh} f(x)dx, \tag{18.25}$$

the trapezoidal rule uses

$$I \simeq \frac{1}{2}(I_e + I_o), \tag{18.26}$$

and the Simpson rule uses

$$I \simeq \frac{1}{3}(I_e + 2I_o). \tag{18.27}$$

Usually, it is believed that the Simpson rule is superior to the trapezoidal rule. However, this is not always the case. If

$$I = \int_a^b f(x)dx = \int_{a+h}^{b+h} f(x)dx, \tag{18.28}$$

where h is the increment of integration, then the trapezoidal rule is superior to the Simpson rule. If f vanishes or becomes very small (like $\exp(-x^2)$) outside the domain sufficiently inside $[a, b]$, or if f is a periodic function and $[a, b]$ is a period, then (18.28) hold. [See **18.9** for the computation of Fourier coefficients.] The purpose of the modification in the Simpson rule is to eliminate the end effect of the integration range. This is why the trapezoidal rule can be better if there is no end effect. Therefore, the Simpson rule is better than the trapezoidal rule, when (18.28) does not hold.

18.9 Discrete Fourier transform I. Let

$$a_n = \frac{1}{N}\sum_{k=0}^{2N} X_k \cos\left(\frac{nk\pi}{N}\right), \tag{18.29}$$

$$b_n = \frac{1}{N}\sum_{k=0}^{2N} X_k \sin\left(\frac{nk\pi}{N}\right). \tag{18.30}$$

Then,

$$X_k = \frac{1}{2}(a_0 + a_N \cos k\pi))\sum_{n=1}^{N-1}\left\{a_n \cos\left(\frac{mnk\pi}{N}\right) + b_n \sin\left(\frac{mnk\pi}{N}\right)\right\}, \tag{18.31}$$

if $X_k = f(k\pi/N)$, then (18.30) is obtained from the standard formulas for Fourier coefficients through 'approximating' the integrals with the aid of the trapezoidal rule. However, notice that the formulas are exact. This is an example of the merit of the trapezoidal rule for periodic functions.

18.10 Discrete Fourier transform II. Let $\boldsymbol{X} \equiv \{X_n\}_{n=0}^{N-1}$ be a sequence of complex numbers, and

$$e(x) \equiv \exp(-2\pi i x). \tag{18.32}$$

The following sequence $\hat{\boldsymbol{X}} \equiv \{X^n\}$ is called the *discrete Fourier transform* of $\boldsymbol{X}$:

$$X^k = \sum_{n=0}^{N-1} e\left(\frac{kn}{N}\right) X_n. \tag{18.33}$$

Its inverse transformation is given by

$$X_n = \frac{1}{N} \sum_{k=0}^{N-1} e\left(\frac{-kn}{N}\right) X^k. \tag{18.34}$$

Cf. **28.23**.

18.B Variable Transformation Schemes

18.11 Functions of double exponential decay. If f is an analytic function, then the trapezoidal rule gives an excellent result for the integral over $\boldsymbol{R}$. This seems to be a well known fact. If the integrand decays double exponentially, i.e., for some positive constants A, B and C

$$|f| \sim A \exp(-B \exp(Cx)) \tag{18.35}$$

The error of the trapezoidal rule truncated at N

$$T_h = h \sum_{k=-N}^{N} f(kh) \tag{18.36}$$

for the integral of f from $-\infty$ to $+\infty$ is given by

$$|T_h - I| \leq const. \|f\| \exp(-\tilde{C} N / \ln N) \tag{18.37}$$

for some positive $\tilde{C}$. This means that if N is doubled, then the number of the significant digits doubles.

18.12 Double exponential (DE) formula. The DE formula was proposed by Takahashi[233] and Mori in 1974, and is regarded the most

[233] This is the same person of the 'Takahashi gas', proving that there is no phase transition in 1-space with short range interactions. He is the most creative statistical physicist Japan has ever produced when he was young, but later became the leader of computer research in Japan, saying physics was his hobby.

effective integration formula currently. The essence is to change the independent variable so that the function decays double-exponentially. For example, for the integral of an analytic function f on $[-1,1]$

$$x = \phi(t) \equiv \tanh\left(\frac{\pi}{2}\sinh t\right) \tag{18.38}$$

and the DE formula reads[234]

$$\int_{-1}^{1} f(x)dx \simeq h \sum_{k=-N}^{N} f(\phi(hk))\phi'(hk). \tag{18.39}$$

However, the DE formula is not effective for the integrals of Fourier transformation type.

Discussion.

The DE formula is powerful even for an integrand with end singularities:

$$I \equiv \int_{-1}^{+1} dx(1-x^2)^{-1/2} = \pi \tag{18.40}$$

If we use the Gauss-Legendre formula to this, the error is never less than 10^{-2} for $n \leq 30$. The DE formula with 5 terms is already with only less then 1% error. With 10 points, the error is about 10^{-6}. With $n = 30$ the error is about 10^{-15}. The improvement is roughly exponential $10^{-n/2}$. [This is in conformity with the theoretical error estimate.]

18.13 Numerical estimate of Fourier transform. For

$$\int_0^\infty f(x)\sin\left(\frac{\pi(x-\alpha)}{\lambda}\right)dx \tag{18.41}$$

the following transformation is effective:[235]

$$\psi(t) = \frac{t}{1-\exp(-2\pi\sinh t)}. \tag{18.42}$$

The formula reads

$$\int_0^\infty f(x)\sin\left(\frac{\pi(x-\alpha)}{\lambda}\right)dx \simeq \lambda \sum_{k=-N}^{N} g\left(\frac{\lambda}{h}\psi\left(\frac{h(k\lambda+\alpha)}{\lambda}\right)\right)\psi'\left(\frac{h(k\lambda+\alpha)}{\lambda}\right), \tag{18.43}$$

where $g(x) = f(x)\sin[\pi(x-\alpha)/\lambda]$.

[234] H Takahashi and M Mori, Publ. RIMS **9**, 721 (1974).

[235] T. Ooura and M. Mori, J. Comp. Appl. Math. **38**, 353-360 (1991).

18.C Multidimensional Integrals

18.14 Overview. An immediate idea is to use the one dimensional formulas repeatedly (direct product scheme). Other interesting methods are the Monte Carlo or quasi-Monte Carlo methods. These latter methods are characterized by the error estimate which is independent of the spatial dimensionality but dependent only on the number of sampling points. Here we discuss only two methods for very large dimensions. The quasi Monte Carlo method is becoming increasingly important, because the error improves as $1/N$ instead of $1/\sqrt{N}$. However, there seems to be no versatile general scheme applicable to all the cases. This is a very active field of research esp., in relation to finance.

18.15 Polynomial variable transformation: recommended preconditioning. Let p be an integer not less than 2. If a function $f(\{x_i\})$ has continuous partial derivatives

$$\frac{\partial^{j_1+\cdots+j_s} f(x_1,\cdots,x_s)}{\partial x_1^{j_1}\cdots\partial x_s^{j_s}} \tag{18.44}$$

for all $j_1,\cdots,j_s \in \{0,1,\cdots,p\}$, then we can use the following transformation

$$x_i = \phi(y_i) \equiv \frac{(2p+1)!}{(p!)^2}\int_0^{y_i} u^p(1-u)^p du \tag{18.45}$$

to convert the integrand f to

$$f(\phi(y_1),\cdots,\phi(y_s))\phi'(y_1)\cdots\phi'(y_s) \tag{18.46}$$

whose multidimensional Fourier coefficients have the following estimate:

$$c_k \le const \times |k|^{-p}. \tag{18.47}$$

With this smoothness condition (→**??**), many integration formulas become more effective than without the transformation. Thus usually, it is recommended to transform the integrand with the aid of this transformation prior to application of integration schemes.

18.16 Weyl's equidistribution theorem. If α is irrational, then for any $0 \le a \le b \le 1$ we have

$$\frac{1}{N}\#\{n \,|\, \{n\alpha\} \in [a,b], n \in \{1,2,\cdots,N\}\} \to |b-a|. \tag{18.48}$$

Here $\{a\} = a - [a]$ is the fractional part of a, and $\#A$ is the number of members (the cardinality) of the set A. We will not give any proof

for this,[236] but this should be intuitively clear, if the reader imagines a particle geodesically moving (i.e., going straight) on the 2-torus, and $[0,1]$ is the coordinate of its section (the so-called Poincarè section in the theory of dynamical systems). A multidimensional version should not be hard to formulate and understand in a similar fashion. Thus we get

18.17 Theorem [Weyl]. Let $1, \alpha_1, \cdots, \alpha_s$ be rationally independent.[237] Then,

$$\lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} f(\{k\alpha_1\}, \cdots \{k\alpha_s\}) = \int_{[0,1]^s} f(\{x\}) d\{x\}. \tag{18.49}$$

18.18 Improved Haselgrove method.[238]

$$\int_{[0,1]^s} f(\{x\}) d\{x\} \simeq \frac{1}{N} \sum_{k=1}^{N} w_q(k/N) f(\{k\alpha_1\}, \cdots \{k\alpha_s\}), \tag{18.50}$$

where

$$w_q(x) = \frac{(2q+1)!}{(q!)^2} x^q (1-x)^q. \tag{18.51}$$

The representative irrational numbers $\alpha_1, \cdots, \alpha_s$ are chosen (semi-empirically) as
(1) If $s+3$ is a prime, then $\alpha_j = 2\cos(2j\pi/(2s+3))$,
(2) Otherwise, $\alpha_j = 2^{j/(s+1)}$.
w_q is introduced to reduce the error further. A detailed error estimate is available, but the main features of the error is that it is bounded by the number proportional to N^{-q}.

18.19 Monte Carlo method. To compute

$$I \equiv \int_{[0,1]^s} f(x_1, \cdots, x_s) dx_1 \cdots dx_s \tag{18.52}$$

the Monte Carlo method randomly and uniformly samples points in the cube $[0,1]^s$ as $y_1, y_2, \cdots$ and claim

$$S_N = \frac{1}{N} \sum_{k=1}^{N} f(y_k) \to I. \tag{18.53}$$

[236] See Section 3 of Körner.
[237] That is, there are no integers $p_0, p_1, \cdots, p_s$ (not all of them are simultaneously equal to 0) such that $p_0 + \sum p_k \alpha_k = 0$
[238] M. Sugihara and K. Murota, Math. Computation **39**, 549-554 (1982).

The principle should be understandable from the random analogue of **22C.3**.
Its error can be estimated with the aid of Chebychev's inequality[239] as

$$\text{Probability}(|I - S_N| \geq 2/\sqrt{\epsilon N}) \leq \epsilon \tag{18.54}$$

for f such that $|f| \leq 1$.
For example, if $N = 10^6$, then with probability 99% we can get the answer with 2% relative error independent of the dimension of the space! However, the accuracy improves only as $N^{-1/2}$.
Exercise.
(1) We wish to compute

$$\int_{-1}^{1} \cdots \int_{-1}^{1} e^{-(x_1+x_2+\cdots+x_N)^2/N} dx_1 \cdots dx_N \tag{18.55}$$

with the aid of the Monte Carlo method. Now many samples do we need conservatively to obtain the integral with 5% relative error with probability 99.9%?
(2) We wish to compute the following integral by the Monte Carlo method:

$$I = \int_D dx_1 \cdots dx_{100} r(1-r), \tag{18.56}$$

where $r = \sqrt{\sum_{i=1}^{100} x_i^4}/5$, and the domain D is the 100 dimensional hypercube $[0,1] \times \cdots \times [0,1]$. How many sample points are (conservatively) needed, if we wish to get I with the error less than 2% with the probability more than 99.5%?
(3) **Generalization of the Chebychev inequality**. Let f be a positive function,[240] and $\varphi_A \equiv \inf_{x \in A} \varphi(x)$. Then,

$$\varphi_A \text{Probability}(X \in A) \leq \langle \varphi \rangle. \tag{18.57}$$

The inequality we have used is a special case with $\varphi = x^2$.

[239] $a^2\text{Probability}(|x| \geq a) \leq \langle x^2 \rangle$, which can be derived easily from the obvious inequality $x^2 \geq a^2 \Theta(|x| \leq a)$.
[240] Measurable w.r.t. the probability measure under consideration (→**19a**).

19 Separation of Variables – General Consideration –

Separation of variables is probably the only systematic way to solve linear PDEs. Its essence is the construction of the problem-adapted orthogonal function system. We have already studied the method in **18** when the ordinary Fourier expansion is applicable. The principles have been exhausted there. Here the general features of the method are outlined with a summary of prerequisites and limitations. Practically, if the reader wishes to solve a PDE boundary value problem, consult a collection of worked-out problems. We should not forget that if we need an exact method, it is a sure sign of our ignorance about the problem.

Key words: special function, eigenvalue problem.

Summary:
(1) Practically, the method works only when the domain has a special shape. Possible shapes are best seen in 'style books,' that is, books collecting worked-out problems. If the reader cannot find any good example in them, it may be wise to give up exact solutions (→**23.2**).
(2) The essence of separation is the problem-adapted Fourier-type expansion; consequently, in order to justify the method we need almost all the machinery of functional analysis (→**19.3**).

19.1 Separation of variables: general idea. All our time-dependent linear problems (→**1**) have the following form:

$$L_t\psi(\boldsymbol{x},t) = Q\psi(\boldsymbol{x},t), \tag{19.1}$$

where the operator L_t acts only on the functions of time, and Q on the functions of space coordinates. The time and space coordinates can be separated trivially as

$$L_t\psi_1(t) = \mu\psi_1(t), \tag{19.2}$$
$$Q\psi_2(\boldsymbol{x}) = \mu\psi_2(\boldsymbol{x}). \tag{19.3}$$

Since the first equation is an ODE, it is easy to obtain its general solution. If Q has a 'good' property, we can generalize the eigenvalue expansion method for a finite dimensional vector space. Formally (19.1) can be transformed into

$$L_t\langle\varphi_\mu(\boldsymbol{x})|\psi(\boldsymbol{x},t)\rangle = \mu\langle\varphi_\mu(\boldsymbol{x})|\psi(\boldsymbol{x},t)\rangle, \tag{19.4}$$

where $\varphi_\mu(\boldsymbol{x})$ is the eigenfunction of the operator Q ($Q\varphi_\mu(\boldsymbol{x}) = \mu\varphi_\mu(\boldsymbol{x})$) and (consistently with the notation in **16.21**)

$$\langle\varphi_\mu(\boldsymbol{x})|\psi(\boldsymbol{x},t)\rangle \equiv \int_D dx\overline{\varphi_\mu(\boldsymbol{x})}\psi(\boldsymbol{x},t). \tag{19.5}$$

This is an analogue of the integral to compute the Fourier coefficients (→**16.14**, **16.24**). The final solution is formally given by

$$\psi(\boldsymbol{x},t) = \sum_\mu \langle\varphi_\mu(\boldsymbol{x})|\psi(\boldsymbol{x},t)\rangle\varphi_\mu(\boldsymbol{x}), \tag{19.6}$$

where the summation is over all the eigenvalues. Hence, the key problem of the separation of variables is to find a problem-adapted generalized Fourier expansion.

19.2 Practical procedure via separation of variables. As we have seen in **18** boundary conditions make the separation procedure more complicated than stated above (→**26B**, **27B**). We will see an illustration in **23.9**. A practical procedure to solve a PDE with inhomogeneous boundary conditions by separation of variables can be summarized as follows:
(A) If the domain shape is not regular (roughly speaking, if the boundary does not consist of part of planes and conic surfaces), forget about exact analytic methods (→**19.4**).
(B) If the domain is'well-shaped,' then consult a typical problem source book of the boundary-value problem. For example, the lecturer find N. N. Lebedev, I. P. Skalskaya and Y. S. Ufliand, *Worked Problems in Applied Mathematics* (Dover 1965) very useful.[241] If the reader cannot find any similar problem, unless she wishes to be an expert of special functions, it is wise for her to give up analytical methods to obtain exact solutions.
(C) If the reader insists on analytical solutions:
(1) Decompose the problem into the problems with inhomogeneous boundary conditions only in one coordinate direction with the aid of superposition principle exactly as we did in **??**. The remaining coordinate directions become (generalized) eigenvalue problems.
(2) The (generalized) eigenfunctions of the separated homogeneous problems dictate the form of the solution. (This is the step of constructing the problem-adapted generalized Fourier expansion scheme.)
(3) Fix the expansion coefficients with the aid of the inhomogeneous boundary conditions and the orthogonality of the eigenfunctions as in **18**. See **19.9** for an illustration

[241] This is an accompanying workbook of N. N. Lebedev, *Special Functions & Their Applications* (Dover, 1965), which is an excellent book.

19.3 What do we need to justify and implement our procedure? Here, we summarize the requirements.
(1) When can we justify the expansion (19.6)? To answer this question, we need a rudimentary knowledge of Hilbert space (→**20**) and the operators on it (→**34**). After a suitable preparation we can generalize Fourier expansion and integral transformations (→**30.11**).
(2) We must be able to find explicitly the eigenfunctions of Q defined on a linear space satisfying the auxiliary conditions. We use the method of separation of variables to reduce the problems to lower dimensional (hopefully 1-space) problems. Therefore, we need methods to solve linear ODEs (→**24**) and associated eigenvalue problems (the Sturm-Liouville problems **35**).

Discussion: Fourier expansion of multivariable functions: addendum to separation of variables.
We have claimed that the key element of the justification of the separation of variables is the (generalized) Fourier expansion of the function in terms of the 'equation adapted' orthonormal basis.[242] Generally, we have several variables and we need multiple Fourier expansion. Then a natural question is whether the totality of the tensor products constructed from ON bases for individual coordinates is indeed an ON basis. The answer is in a certain sense affirmative, but somewhat delicate.
(1) The (generalized) Fourier expansion of $f(x_1, \cdots, x_n)$ is well defined if f is integrable thanks to Fubini's theorem (→**16.15**). That is, the value of the Fourier coefficients do not depend on the order of expansion.
(2) To reconstruct the original function from the Fourier coefficients, we can apply the individual inverse transforms successively. This is allowed, but the Fourier coefficients may not be integrable, so to interpret the inverse transform as an n-tuple integral (not as n successive one dimensional integrals) is delicate[243] and some extra condition on f is generally required.[244]

19.4 What problems can we solve by hand?. To have an analytic solutions, we must be able to solve the eigenvalue problem by hand. To this end almost always separation of variables is mandatory. As is mentioned in **19.2**(A), this requires not only a special form of the operator, but also a special shape of the domain.[245] Therefore, problems we can

[242] The reader might say any ON basis will do for our purpose. If we need not worry about the (termwise) differentiability of the Fourier sum, then this is indeed the case. However, we are solving differential equations, so that we must be sensitive about the uniformity of the convergence of the resultant Fourier series (→**??-??**).
[243] That is, we must in general inverse transform in the reverse order of the operation used in the calculation of the coefficients.
[244] See Kolmogorov and Fomin, second ed. Chapter 8, Section 4. Perhaps not available in English.
[245] We must be able to employ the standard orthogonal curvilinear coordinates. For example, for 3d Schrödinger equation, complete separation of variables is possible

solve analytically are very limited even for the Laplace equation. For situations frequently encountered in practice (e.g., the Laplacian in a ball) eigenfunctions of separated operators are well known and called *special functions*. In short, we can solve by hand only very standard PDE under very standard auxiliary conditions. That is why the advice in (B) of **19.2** "see a style book" is practical.

Eercise.
(A) Specify appropriate curvilinear coordinates to solve the following problems (if the problems are separable at all):
(1) From a solid ball of radius a, another ball of radius $b(< a)$ which is completely inside the first ball is removed. Temperatures of inside and outside surfaces are given. Find the steady temperature distribution in the solid.
(2) There are two osculating identical conducting balls. Compute the electric field when the balls are maintained at V with respect to the infinity.
(3) A cylindrical hole of radius r is made through a solid conducting ball of radius $R(> r)$ slightly off the center. Find the electric field when the solid has the total charge Q.
(4) A lens-shaped conductor is maintained at voltage V relative to infinity. Assume that the surfaces are with the same radius of curvature R and the thickness of the lens is $2d$, where $d < R$.
(5) A conducting plane has a semicylindrical boss of radius a. The plane is maintained with the electric potential V. Find the electric field in the space.
(B) Two identical conducting spheres of radius a are placed with the separation of $2l$ between the centers. Both the spheres are maintained at voltage V relative to infinity. Find the electrostatic potential due to these spheres.

Discussion: Lamè's problem.
The most general case we can solve with the aid of separation of variables is the *confocal rectangular parallelepiped* whose surfaces are made of confocal quadratic surfaces given by

$$\frac{x^2}{s-e_1}+\frac{y^2}{s-e_2}+\frac{z^2}{s-e_3}=1. \tag{19.7}$$

The necessary special functions are called Lamè functions which are not studied very well.

19.5 What is a special function? The word 'special function' is used to denote collectively (1) Γ-function (→**9**) and related functions like polygamma functions,[246] (2) functions described by indefinite in-

only when the potential function V has the following form:

$$V = h_1V(q^1) + h_2V(q^2) + h_3V(q^3),$$

where h's are the ones given in **??** (H. P. Robertson, Math. Ann. **98**, 749 (1928); L. P. Eisenstein, Ann. Math. **35**, 284 (1934)).

[246] Polygamma functions: the nth-derivative of $\log\Gamma(z)$ is called the (n+1)-Gamma function. In particular, $n = 1$ is called digamma function, $n = 2$ is called trigamma function, etc.

tegrals of elementary functions like the probability integral (→**21.11**), (3) elliptic functions, (4) solutions of second order ODE obtained by separating variables, and (5) solutions to special ODE like Painlevè equations.[247] Solutions to the second order linear ODE with 3 regular singular points (special functions of hypergeometric type) or with 1 irregular singular point resulting from the merging of two regular singular points (→**20.15**) in the former (special functions of confluent type) are called *classical special functions*.

19.6 Are the analytic solutions useful? It is not easy to say yes. Often the obtained solutions are series solutions in terms of special functions. Since special functions are mere symbols, one must look up tables or use, e.g., Mathematica or Maple (even trigonometric functions are no exceptions; we need a table or a pocket calculator). Hence, if she wants a detailed behavior of the solution, a lot of numerical work is needed anyway. One might say that in order to know qualitative or asymptotic behaviors of a solution, analytic forms are useful. This is true. However, to require a complete solution in order to get qualitative or asymptotic behaviors does not sound elegant.

It should be clearly recognized that necessity of full analytic solution is a clear sign of the sad fact that we do not understand the problem.

19.7 Importance of qualitative understanding. It is important to know how to solve the problems by hand: what special functions are suitable, how they behave qualitatively, etc. To teach these has been the main objective of the conventional math-phys courses.[248] However, for most scientists (esp. pure scientists) to juggle tons of special functions is not important at all.[249] It is much more important to acquire the sense or feeling of correct physics and mathematics so that we will not be outsmarted by computers, or not to be drowned in the flood of numbers. The reader must be able to walk, but in order to go to the Pacific coast she need not retrace the Oregon Trail on foot!

19.8 Use of symbol manipulation programs. Many standard analytic methods, e.g., the series expansion method (→**24B**), are best implemented with the aid of mathematics softwares like Mathematica or Maple. Special functions are available in the standard mathematics softwares. For example, with Mathematica, if the reader types in

[247] For Painlevè equations, see Ince.

[248] See, e.g., H. W. Wyld, *Mathematical Methods for Physics* (Benjamin, 1976).

[249] Perhaps more than 50 years ago there were one-year courses solely devoted to trigonometrics in universities (remember that the universities in those days were not remedial schools of the high school education). This sounds absurd now. To realize that some topics are unimportant is an important progress.

`BesselJ[n,z]`, then she gets $J_n(z)$ (→**23.1**). Hence, we need not be extremely familiar with special functions, although we should know their general features. Most analytical calculations can be mechanized, so it is probably wiser to practice the use of these programs than to experience lengthy practice sessions of analytical methods.

19.9 Case study of separation of variables: Laplace equation with Dirichlet condition. The purpose of this entry is to provide a show case with the aid of a fairly difficult problem. The region is fan-shaped: $z \in [0, h]$, $\varphi \in [0, \phi]$ and $r \in [a, b]$:

$$\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}\right]\psi = 0 \tag{19.8}$$

(→**??**) with the boundary condition

$$\begin{aligned}
\psi(r,\varphi,0) &= f_0(r,\varphi), \quad \psi(a,\varphi,h) = f_h(r,\varphi), && (19.9)\\
\psi(r,0,z) &= g_0(r,z), \quad \psi(r,\phi,z) = g_\phi(r,z), && (19.10)\\
\psi(a,\varphi,z) &= h_a(\varphi,z), \quad \psi(b,\varphi,z) = h_b(\varphi,z). && (19.11)
\end{aligned}$$

First we perform the step (C)(1) of **19.2**. The separation procedure $\psi = R(r)\Phi(\varphi)Z(z)$ gives three distinct eigenvalue problems. The full solution is the superposition of the solutions to all the following three problems (1)-(3).
(1) With the boundary condition (r, φ homogeneous; z inhomogeneous):

$$\begin{aligned}
\psi(r,\varphi,0) &= f_0(r,\varphi), \quad \psi(r,\varphi,h) = f_h(r,\varphi), && (19.12)\\
\psi(r,0,z) &= 0, \quad \psi(r,\varphi,z) = 0, && (19.13)\\
\psi(a,\varphi,z) &= 0, \quad \psi(b,\varphi,z) = 0. && (19.14)
\end{aligned}$$

The separated equations are

$$\begin{aligned}
\frac{d^2\Phi}{d\varphi^2} &= -m^2\Phi, && (19.15)\\
\frac{d^2Z}{dz^2} &= \alpha^2 Z, && (19.16)\\
\frac{1}{R}\left[\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr}\right] - \frac{m^2}{r^2} + \alpha^2 &= 0. && (19.17)
\end{aligned}$$

The eigenvalue problems are (19.15) and (19.17) with homogeneous Dirichlet boundary conditions ($\Phi(0) = \Phi(\phi) = 0$ and $R(a) = R(b) = 0$).

The positivity of α^2 and m^2 follows from the negative definiteness of the operators.[250] The solution must have the following form:

$$\psi = \sum_{m,\alpha}(A_{m,\alpha}J_m(\alpha r)+B_{m,\alpha}N_m(\alpha r))(C_m \sin m\varphi+D_m \cos m\varphi)(E_{m,\alpha}\sinh \alpha z+F_{m,\alpha}\cosh \alpha z). \tag{19.18}$$

Here J_m is the Bessel function (→**??-23.3**), and N_m is the Neumann function (→**23.16**). m, C_m and D_m are fixed by the Dirichlet condition:

$$D_m = 0;\ C_m \sin m\phi + D_m \cos m\phi = 0. \tag{19.19}$$

We may choose $C_m = 1$ without any loss of generality. α, $A_{m,\alpha}$ and $B_{m,\alpha}$ are fixed by the Dirichlet condition

$$A_{m,\alpha}J_m(\alpha a) + B_{m,\alpha}N_m(\alpha a) = 0, \tag{19.20}$$
$$A_{m,\alpha}J_m(\alpha b) + B_{m,\alpha}N_m(\alpha b) = 0. \tag{19.21}$$

That is, $J_m(\alpha a)N_m(\alpha b) = J_m(\alpha b)N_m(\alpha a)$ fixes α. E and F are determined from the inhomogeneous boundary condition (19.14) with the aid of complete orthogonality (→**30.10**) of the eigenfunctions constructed above (not easy or almost impossible bu hand for general a and b).
(2) With the boundary condition (r, z homogeneous; φ inhomogeneous)

$$\psi(r,\varphi,0) = 0;\ \psi(a,\varphi,h) = 0, \tag{19.22}$$
$$\psi(r,0,z) = g_0(r,z);\ \psi(r,\phi,z) = g_\phi(r,z), \tag{19.23}$$
$$\psi(a,\varphi,z) = 0;\ \psi(b,\varphi,z) = 0. \tag{19.24}$$

The separated equations are

$$\frac{d^2\Phi}{d\varphi} = m^2\Phi, \tag{19.25}$$
$$\frac{d^2Z}{dz^2} = -\alpha^2 Z, \tag{19.26}$$
$$\frac{1}{R}\left[\frac{d^2R}{dr^2}+\frac{1}{r}\frac{dR}{dr}\right]+\frac{m^2}{r^2}-\alpha^2 = 0. \tag{19.27}$$

Here the positivity of α^2 is obvious from the condition that (19.26) becomes an eigenvalue problem (it is is not elementary to see this →**30.11** Discussion (B)). m^2 also must be positive so that (19.27) becomes an eigenvalue problem. Hence, we may assume

$$\psi = \sum_{m,\alpha}(A_{m,\alpha}I_{im}(\alpha r)+B_{m,\alpha}K_{im}(\alpha r))(C_m \sinh m\varphi+D_m \cosh m\varphi)(E_\alpha \sin \alpha z+F_\alpha \cos \alpha z), \tag{19.28}$$

[250] Intuitively speaking, the eigenfunctions must be oscillatory functions to satisfy the orthogonality condition. "Negative definiteness" of an operator L means $\langle f|L|f\rangle \le 0$ for any ket $|f\rangle$. The Laplacian Δ is a typical example.

where I and K are modified Bessel functions (→**23.23**). Here α, E_α and F_α are fixed by the Dirichlet condition

$$F_\alpha = 0;\ E_\alpha \sin \alpha h + F_\alpha \cos \alpha h = 0. \tag{19.29}$$

$E_\alpha = 1$ is admissible. m, $A_{m,\alpha}$ and $B_{m,\alpha}$ are determined by the boundary conditions

$$\begin{aligned} A_{m,\alpha} I_{im}(\alpha a) + B_{m,\alpha} K_{im}(\alpha a) &= 0, & (19.30)\\ A_{m,\alpha} I_{im}(\alpha b) + B_{m,\alpha} K_{im}(\alpha b) &= 0. & (19.31) \end{aligned}$$

That is, $I_{im}(\alpha a)K_{im}(\alpha b) = I_{im}(\alpha b)K_{im}(\alpha a)$ determines m. C and D are determined from the inhomogeneous boundary condition (19.23) with the aid of complete orthogonality of the eigenfunctions constructed above.[251]
(3) With the boundary condition (φ, z homogeneous; r inhomogeneous)

$$\begin{aligned} \psi(r,\varphi,0) &= 0,\ \ \psi(r,\varphi,h) = 0, & (19.32)\\ \psi(r,0,z) &= 0,\ \ ,\psi(r,\phi,z) = 0, & (19.33)\\ \psi(a,\varphi,z) &= h_a(\varphi,z),\ \ \psi(b,\varphi,z) = h_b(\varphi,z). & (19.34) \end{aligned}$$

The separated equations are[252]

$$\begin{aligned} \frac{d^2\Phi}{d\varphi} &= -m^2\Phi, & (19.35)\\ \frac{d^2Z}{dz^2} &= -\alpha^2 Z, & (19.36)\\ \frac{1}{R}\left[\frac{d^2R}{dr^2} + \frac{1}{r}\frac{dR}{dr}\right] - \frac{m^2}{r^2} - \alpha^2 &= 0. & (19.37) \end{aligned}$$

The eigenvalue problems are easy ones: (19.35) and (19.36) with homogeneous Dirichlet conditions. We may thus assume

$$\psi = \sum_{m,\alpha} (A_{m,\alpha} I_m(\alpha r) + B_{m,\alpha} K_m(\alpha r))(C_m \sin m\theta + D_m \cos m\theta)(E_\alpha \sin \alpha z + F_\alpha \cos \alpha z). \tag{19.38}$$

Here, I_m and K_m are modified Bessel functions (→**23.23**). A and B must be fixed from the boundary condition (19.34).

[251] This problem is nontrivial, since we need modified Bessel functions of imaginary order. See N. N. Lebedev, *Special Functions & Their Applications* (Dover 1972) Section 6.5.
[252] In this case obviously m^2 and α^2 must be non-negative.

19.10 Remarks to 19.9.
(1) If the region in the z-direction is not bounded, we need Fourier transformations; if the region is not bounded in the r-direction, we need the Fourier-Bessel(-Dini) transformation (→**23.22**).
(2) The boundary condition in the φ direction may be periodic.
(3) The Neumann condition case is analogous.

20 General Linear ODE

The theory of general linear ODE is summarized, and then a constructive solution method (Frobenius' method) is outlined. This series method is best implemented with the aid of symbol manipulation programs. The reader should practice the method for one or two representative examples by hand or a step by step application of mathematics softwares.

Key words: analyticity of solution, fundamental system of solutions, fundamental matrix, Wronskian, separation theorem, Frobenius' theory, (regular and irregular) singular point, indicial equation, index.

Summary:
(1) First-order n-vector continuous ODE preserves the linear independence of the initial condition vectors (the existence of fundamental systems **20.4**, **20.11**).
(2) If the coefficient functions are holomorphic around x, then the solution around x is Taylor-expandable, so a series form fundamental system can be constructed (**20.14**). Even if the coefficients are not holomorphic, if their singularities are not very bad (regular **24B.2**), then still a series form fundamental system can be constructed (Frobenius' theory) (**20.16-20.20**).
(3) The Frobenius method is best implemented by a computer. See **24B.8** for a 'practical Frobenius.'
(4) Separation of variables of the Laplace equation in the spherical coordinates requires Legendre polynomials (**20.26-20.27**) and associate Legendre functions (**20.30**, examples in **26B**).

20.A General Theory

20.1 The problem. We must be able to solve separated equations (→**23**) which are usually ODE. They are linear but with nonconstant coefficients. We know we have only to consider (→**11A.5**)

$$\frac{d\boldsymbol{u}(x)}{dx} = A(x)\boldsymbol{u}(x), \tag{20.1}$$

where $A(x)$ is a $n \times n$ matrix which is continuous[253] on an interval $I \subset \boldsymbol{R}$.

20.2 Theorem [Unique existence of solution]. If $A(x)$ is continuous[254] in an open interval $I \subset \boldsymbol{R}$, then for any $\boldsymbol{u}_0 \in \boldsymbol{R}^n$ and $x_0 \in I$, there is a unique solution $\boldsymbol{u}(x)$ passing through $(\boldsymbol{u}_0, x_0)$ whose domain is I. □
This follows directly from the Cauchy-Peano and Cauchy-Lipschitz theorems (→**??**, **??**).

20.3 Analyticity of solution. $A(x)$ may be considered to be a matrix consisting of functions on $\boldsymbol{C}$ as $A(z)$.
Theorem. Assume $A(z)$ to be analytic (i.e., all the components are analytic functions →**??**, **??**) in $D \subset \boldsymbol{C}$. Then, a solution analytic around $a \in D$ can be analytically continued (→**7**) to any point in D along any curve in D. □

This implies that the singular points of a solution, if any, appear where there are singularities (→**??**-**??**) of $A(z)$.

Discussion.
For 1D Schrödinger equation, the wave function is finite at a point which is not a singularity of the potential. For example, the wave function of the harmonic oscillator is finite for finite x. For the Coulomb potential, the singularity can exist only at the origin.

20.4 Theorem [Fundamental system of solutions]. The totality of solutions of (20.1) makes a n-vector space. Any basis set of this space is called the *fundamental system of solutions*. □
[Demo] Let $\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_n$ be linearly independent vectors and $x_0 \in I$. Write the solution passing through $(\boldsymbol{v}_j, x_0)$ as $\boldsymbol{\phi}_j(x)$ $(j = 1, \cdots, n)$. Let $\boldsymbol{u}_0 = c_1\boldsymbol{v}_1 + c_2\boldsymbol{v}_2 + \cdots + c_n\boldsymbol{v}_n$, and

$$\boldsymbol{u}(x) = c_1\boldsymbol{\phi}_1(x) + c_2\boldsymbol{\phi}_2(x) + \cdots + c_n\boldsymbol{\phi}_n(x). \tag{20.2}$$

It is obvious that the space cannot have a dimension larger than n. If there is x such that $\boldsymbol{u}(x) = 0$, then due to the uniqueness of the solution (→**20.2**) it must agree with the solution starting from 0, which is obviously identically zero, so that $\boldsymbol{u}(x)$ can never be 0. Hence, the dimension of the solution space cannot be less than n. □
Notice that this theorem implies that $\boldsymbol{\phi}_1(x), \boldsymbol{\phi}_2(x), \cdots, \boldsymbol{\phi}_n(x)$ are functionally independent: the identity for $x \in I$

$$c_1\boldsymbol{\phi}_1(x) + c_2\boldsymbol{\phi}_2(x) + \cdots + c_n\boldsymbol{\phi}_n(x) \equiv 0 \tag{20.3}$$

implies $c_j = 0$ for all j[255].

[253] We say that $\boldsymbol{u}(x)$ is continuous, analytic, etc., if all its components are, as functions, continuous, analytic, etc.
[254] Our problem is a linear problem, so this is enough. A related discussion is in **??** Discussion (B).
[255] This is of course a stronger condition that $\boldsymbol{u} \neq 0$.

20.5 Fundamental matrix. The matrix $\Phi(x) = (\boldsymbol{\phi}_1(x), \boldsymbol{\phi}_2(x), \cdots, \boldsymbol{\phi}_n(x))$ is called a *fundamental matrix* of (20.1), if $\{\boldsymbol{\phi}_1(x), \boldsymbol{\phi}_2(x), \cdots, \boldsymbol{\phi}_n(x)\}$ is a fundamental system of solutions ($\rightarrow$**20.4**).[256]

20.6 Wronskian. Let $\boldsymbol{u}_1(x), \boldsymbol{u}_2(x), \cdots, \boldsymbol{u}_n(x)$ be n solutions to (20.1). The determinant of the matrix $(\boldsymbol{u}_1(x), \boldsymbol{u}_2(x), \cdots, \boldsymbol{u}_n(x))$ is called the *Wronskian* of the set of solutions $\{\boldsymbol{u}_1(x), \boldsymbol{u}_2(x), \cdots, \boldsymbol{u}_n(x)\}$.

If the Wronskian of the set $\{\boldsymbol{u}_1(x), \boldsymbol{u}_2(x), \cdots, \boldsymbol{u}_n(x)\}$ is nonzero, then this set is a fundamental system of solutions.

The converse is also true according to **20.4**. In other words:

20.7 Theorem. A regular matrix $X(x)$ satisfying

$$\frac{dX(x)}{dx} = A(x)X(x) \tag{20.4}$$

is a fundamental matrix of (20.1).

20.8 Theorem. Let $W(x)$ be the Wronskian of the set of (any) n solutions to (20.1). Then,

$$\frac{dW(x)}{dx} = [Tr\, A(x)]W(x). \tag{20.5}$$

This should be obvious from

$$det[(1 + At)X] = detX + t\, Tr A\, detX + O[t^2]. \tag{20.6}$$

This formula follows from

$$detX = \exp[Tr \ln X], \tag{20.7}$$

which is a very important formula and essentially follows from $detX = \prod \lambda_i$, where λ_i are eigenvalues of X.

20.9 . Let $\Phi(x)$ be a fundamental matrix ($\rightarrow$**20.5**) of (20.1). Then, for any non-singular matrix P, $\Phi(x)P$ is again a fundamental matrix of (20.1). Conversely, if $\Phi(x)$ and $\Psi(x)$ are two fundamental matrices of (20.1), then there is a constant non-singular matrix P such that $\Psi(x) = \Phi(x)P$. $\square$

[Demo] Obviously, $\Phi(x)P$ satisfies (20.4) and non-singular, so it is a fundamental matrix. Next, let $P = \Phi(x)^{-1}\Psi(x)$, then a straightforward calculation shows $dP/dx = 0$. Hence, P must be a constant matrix, and non-singular by definition.

[256] The evolution operator $T(x, y)$ such that $\boldsymbol{u}(x) = T(x, y)\boldsymbol{u}(y)$ is given by $T(x, y) = \Phi(x)\Phi(y)^{-1}$.

20.10 Second order linear ODE. Separation of variables (→**23**) of linear second order PDE often gives second order linear ODE of the following type:

$$\frac{d^2u}{dx^2} + P(x)\frac{du}{dx} + Q(x)u = 0, \tag{20.8}$$

where P and Q are functions of $x \in \boldsymbol{R}$. This can be transformed into the first order ODE of the form discussed in **20.1**:

$$\frac{d\boldsymbol{u}}{dx} = A(x)\boldsymbol{u} \tag{20.9}$$

with $\boldsymbol{u}(x) = (u, du/dx)^T$ and

$$A(x) = \begin{pmatrix} 0 & 1 \\ -Q & -P \end{pmatrix}. \tag{20.10}$$

20.11 Fundamental system of solutions. Let u_1 and u_2 be two solutions for (20.8). The Wronskian $W(x)$ (→**20.6**) for these solutions is defined as

$$W(x) = \begin{vmatrix} u_1 & u_2 \\ u_1'(x) & u_2'(x) \end{vmatrix}. \tag{20.11}$$

Tha is, W is the Wronskian of (20.9). If we can find u_1 and u_2 with $W(x) \neq 0$, then the set $\{u_1, u_2\}$ is called a *fundamental system of solutions*. The general solution to (20.8) is $c_1u_1 + c_2u_2$ for arbitrary constants c_1 and c_2 (cf. **20.4**).

20.12 Theorem [Separation theorem]. Let u and v make a fundamental system of solutions of (20.8). Then
(1) The zeros of u and v are all of multiplicity one.
(2) The zeros of u and v separate each other.□
[Demo] Suppose u has a zero of multiplicity larger than one. Then u and u' can vanish simultaneously, so that the Wronskian W (→**20.6**) of u and v can vanish. This contradicts the assumption. Thus (1) must be true. To prove (2) note that u and v cannot have a common zero, since $W \neq 0$. Let a_1 and a_2 $(> a_1)$ be two adjacent zeros of u, and assume that v does not vanish in the interval $J = (a_1, a_2)$. Then u/v is well defined in J, and is differentiable:

$$\frac{d(u/v)}{dx} = \frac{W(x)}{v^2}. \tag{20.12}$$

This cannot vanish. However, $u/v = 0$ at the both ends of J, so Rolle's theorem asserts that (20.12) must vanish in J, a contradiction. We can exchange u and v to complete the proof.

Exercise.
Consider the following 1-Schrödinger problem

$$(-\Delta + V)\psi = E\psi, \tag{20.13}$$

where V vanishes at infinity. If this equation has a bound state, it cannot be degenerate. In particular, the lowest energy bound state (ground state) cannot be degenerate. Prove this showing or answering the following:
(1) Degeneracy implies that there are two independent solutions for a given energy. What must be their Wronskian?
(2) The Wronskian for localized state is zero.

20.13 Making a partner. Suppose we have found one solution v to (20.8). We wish to make u (a partner of v) so that $\{u, v\}$ becomes a fundamental system of solutions (→**20.11**). We use (20.12). To compute the Wronskian W we can use (20.5) (→**20.8**) with $Tr\, A = -P$ for (20.8). W can be solved as

$$W = W_0 \exp\left(-\int^x P(y)dy\right). \tag{20.14}$$

From (20.12) we obtain

$$u = v\left[\int^z d\xi v^{-2} e^{-\int^\xi P(\xi')d\xi'} + c\right], \tag{20.15}$$

where c is a constant.

Exercise.
One solution of

$$\frac{d^2y}{dx^2} - \left(\frac{1}{x} + 1\right)\frac{dy}{dx} + \frac{1}{x}y = 0 \tag{20.16}$$

is e^x. Find its partner.

20.B Frobenius' theory

20.14 Analiticity of solutions. **20.3** implies that if P and Q are analytic in a region D, then the solution to (20.8) is unique and analytic in D. Hence, a local solution can be assumed to be in the power series form around a point where P and Q are holomorphic.

20.15 Singular points. If P or Q becomes singular (→**8A.2**) at a point a, a is called a *singular point* of the ODE (20.8).
(1) At a singular point a, if the singularity of P is at worst a pole of order one, and that of Q is at worst a pole of order two (→**??**(4)(ii)), then a is called a *regular singular point* of the ODE.
(2) Otherwise, a is called an *irregular singular point* of the ODE.

Discussion.[257]

[257] Yosida p86

In general (in more standard pure math literatures) the definition of a regular singular point is as follows. Let u be any solution of (20.8).

Definition. z_0 is a regular singular point of (20.8), if there is a positive number ρ such that for any of its solution u satisfies

$$\lim_{z\to z_0}(z-z_0)^\rho u(zz)=0 \tag{20.17}$$

That is, if the singularity of the solution (remember **20.3**, **24B.1**) is at worst algebraic at z_0, we say z_0 is a regular singular point.

Theorem [Fuchs].A necessary and sufficient condition for z_0 to be a regular singular point of (20.8) is that z_0 is a regular singular point in the sense of **20.15**. □

Its proof is not very simple (elementary but lengthy). An intuitive understanding is the 'balance condition' of the singularities (divergences) around z_0 in (20.8). Consider only the most singular terms in (20.8) near z_0. If the 'magnification' of singularities by differentiation balances the singularities in the coefficients, then we say the singularity is regular.

20.16 Expansion around regular singular point. Frobenius showed that power series expansion can give a local solution around a regular singular point as well. Around a regular singular point a, which we may set to be 0 without any loss of generality, we expect the following form

$$u(z)=z^\mu\sum_{k=0}^{\infty}a_k z^k, \tag{20.18}$$

where μ is an appropriate complex constant. We may expand P and Q as (Laurent expansion →**??**)

$$zP(z)=\sum_{k=0}^{\infty}p_k z^k, \tag{20.19}$$

$$z^2Q(z)=\sum_{k=0}^{\infty}q_k z^k. \tag{20.20}$$

Formally substituting these expansions into the differential equation (20.8), we get conditions for the equation to be satisfied identically:

$$a_0\phi(\mu) = 0, \tag{20.21}$$

$$a_1\phi(\mu+1)+a_0\theta_1(\mu) = 0 \tag{20.22}$$

and generally for $n=1,2,\cdots$

$$\phi(\mu+n)a_n+\sum_{k=1}^{n}a_{n-k}\theta_k(\mu+n-k)=0, \tag{20.23}$$

where

$$\phi(\mu) = \mu^2+(p_0-1)\mu+q_0, \tag{20.24}$$

$$\theta_i(\mu) = \mu p_i+q_i. \tag{20.25}$$

20.17 Indicial equation. We may assume $a_0 = 1$ without any loss of generality. However, if (20.23) couples only even coefficients $\{a_{2n}$ with each other (or only odd coefficients), then even and odd coefficients are decoupled. Therefore, the choice $a_0 = 1$, $a_1 = 0$ and that $a_0 = 0$, $a_1 = 1$ both give different solutions (cf. **20.27**). (20.21) or $\phi(\mu) = 0$ is called the *indicial equation*. It determines two (possibly identical) values of μ, μ_1 and μ_2 (Henceforth, we assume $Re\mu_1 \geq Re\mu_2$).

Exercise.
Find the indicial equation for

$$\frac{d}{dz}\left\{(1-z^2)\frac{d}{dz}u\right\} + \left\{l(l+1) - \frac{m^2}{1-z^2}\right\}u = 0. \tag{20.26}$$

20.18 Use of symbol manipulation programs. Expanding and regrouping expanded terms is performed by symbol manipulating programs very efficiently. In practice, Frobenius' method will not be used often, but if needed, the best way is to use computers to compute the series.

20.19 Theorem. Assume that $z = 0$ is a regular singular point ($\rightarrow$**20.15**(1)) of (20.8) and μ_1, μ_2 are the roots of the indicial equation $\phi(\mu) = 0$ (cf.(20.24)). Then
[1] If $\mu_1 - \mu_2 \notin \boldsymbol{N}$, there is a fundamental system of solutions ($\rightarrow$**20.11**) in the form of (20.18) converging in some neighborhood of 0.
[2] If $\mu_1 - \mu_2 \in \boldsymbol{N}$, generally only one solution in the form of (20.18) is uniquely determined by the expansion method. See **20.20** for further classification. □

[Demo] Choose $\mu = \mu_1$. Then, $\phi(\mu + n)$ cannot be zero for any $n = 1, 2, \cdots$, so that a_n can be uniquely determined from (20.23). The resultant series is convergent in some small neighborhood of $z = 0$. This can be demonstrated by constructing a majorizing series.[258] If $\mu_1 - \mu_2$ is not in $\boldsymbol{N}$, then $\mu = \mu_2$ also allows us to determine a_n uniquely, and the resultant solution is distinct from the one obtained for μ_1. However, if $\mu_1 - \mu_2 \in \boldsymbol{N}$, then there is $m \in \boldsymbol{N}$ such that $\mu_2 + m = \mu_1$ or $\phi(\mu_2 + m) = 0$. Therefore, we may not generally determine a_m for this μ_2.

20.20 Theorem [For $\boldsymbol{\mu_1 - \mu_2 \in N}$]. In case **[2]** of Theorem **20.19**.
[21] If $\mu_1 = \mu_2$, then any partner u (to make a fundamental system) of the solution v constructed for μ_1 in the form (20.18) must contain a logarithmic term and has the following general form

$$u(z) = Av(z)\ln z + z^{\mu_1}\psi(z), \tag{20.27}$$

[258] See, for example, H. S. Wilf, *Mathematics for the Physical Sciences* (Dover, 1962), or E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge UP, 1927), Sect. 10.31 for an explicit demonstration.

where A is a nonzero constant, and ψ is analytic around $z = 0$. This function can be determined by substituting the series expansion form of (20.27) into (20.8).
[22] If $\mu_1 - \mu_2 \in \boldsymbol{N} \setminus \{0\}$, then a partner u of the solution v constructed for μ_1 in the form (20.18) has the following general form

$$u(z) = Av(z) \ln z + z^{\mu_2} \psi(z), \tag{20.28}$$

where v is again the solution constructed for μ_1 in the form (20.18), A is a constant (can be zero), and ψ is analytic around $z = 0$. This function can be determined by substituting the series expansion form of (20.28) into (20.8).
□
[Demo] According to (20.15) (→**20.13**) the ratio $q(z) = u/v$ of v and its partner u is given by (c_1 and c_0 are integration constants)

$$\begin{aligned} q(z) &= c_1 + c_0 \int^z d\zeta v(\zeta)^{-2} \exp\left[-\int^\zeta P(\zeta') d\zeta' \right] \\ &= c_1 + c_0 \int^z d\zeta \frac{1}{[\zeta^{\mu_1}(1 + a_1\zeta + \cdots)]^2} \exp\left[-\int^\zeta \left(\frac{p_0}{\zeta'} + p_1 + \cdots \right) d\zeta' \right] \\ &= c_1 + c_0 \int^z \zeta^{-(p_0 + 2\mu_1)} h(\zeta) d\zeta, \end{aligned} \tag{20.29}$$

where $h(z)$ is analytic around $z = 0$ as can be seen from

$$h(z) = \exp\left[-\int^z d\zeta (p_1 - p_2\zeta + \cdots) \right] / (1 + a_1\zeta + \cdots)^2. \tag{20.30}$$

Since from the indicial equation (→**20.17**) or $\phi(\mu) = 0$ (cf.(20.24)) $-p_0 + 1 = \mu_1 + \mu_2$, we know $p_0 + 2\mu_1 = 1 + \mu_1 - \mu_2 \in \boldsymbol{N} \setminus \{0\}$. Therefore, (20.29) has the following form

$$q(z) = A \ln z + z^{\mu_2 - \mu_1} \varphi(z), \tag{20.31}$$

where A is a constant and φ is a function analytic around $z = 0$. Hence, u must have the form (20.28). For $\mu_1 = \mu_2$ A cannot be zero to make u functionally independent of v.□.

20.21 Practical Frobenius.

(0) Check the expansion center is at worst regularly singular (→**20.15**).
(1) Compute the indices μ_1 and μ_2 according to **20.17**.
(2) Choose the index with the larger real part μ_1 and construct the series solution following Frobenius (**20.16**).
(3) If μ_2 is not equal to μ_1, try to construct the second solution just as before. If the obtained solution is different (functionally independent[259]

[259] That is, their Wronskian (→**24A.6**) is not identically zero. Often, without checking the Wronskian, we can recognize the independence by inspection.

from the first one, we are done.
(4) If we obtain the same solution or $\mu_1 = \mu_2$, assume the form with logarithm as in **20.20**, and determine v in a power series form.

Exercise.[260]
(1) Show that two solutions of the equation

$$\frac{d^2u}{dx^2} + xu = 0 \tag{20.32}$$

are given by

$$u_1 = x - \frac{1}{12}x^4 + \cdots, \tag{20.33}$$

$$u_2 = 1 - \frac{1}{6}x^3 + \cdots. \tag{20.34}$$

(2) Show that two solutions of the equation

$$\frac{d^2u}{dx^2} + \frac{1}{4x^2}(1 - x^2)u = 0 \tag{20.35}$$

are given by

$$u_1 = x^{1/2}\left\{1 + \frac{1}{16}x^2 + \frac{1}{1024}x^4 + \cdots\right\}, \tag{20.36}$$

$$u_2 = u_1(x)\log x - \frac{1}{16}x^{3/2} + \cdots. \tag{20.37}$$

20.22 Construction of the second solution by differentiation. Let us write the solution obtained by Frobenius' method with the index λ as $u(x;\lambda)$. If $u(x,\lambda_1)$ and $u(x,\lambda_2)$ are functionally independent, then we can use $u(x,\lambda_1)$ and a linear combination of the two as a fundamental system of solutions. Consider

$$\frac{(\lambda_1 - \lambda_2)u(x,\lambda_1) - m\,u(x,\lambda_2)}{\lambda_1 - \lambda_2 - m}. \tag{20.38}$$

For the case (**21**), we choose $m = 0$ and compute the limit of $\lambda_1 \to \lambda_2$ with the aid of l'Hospital's rule. That is, we compute

$$\frac{\partial}{\partial\lambda}u(x;\lambda)\bigg|_{\lambda=\lambda_1}. \tag{20.39}$$

Computing this explicitly, we obtain the general form given in **24B.7**[**21**]. When $\lambda_1 - \lambda_2 = m \in \boldsymbol{N}$, we perform a similar calculation:

$$\frac{\partial}{\partial\lambda}[(\lambda - \lambda_2)u(x;\lambda)]\bigg|_{\lambda=\lambda_1}. \tag{20.40}$$

[260] We have obtained the form asserted in **20.20**.

20.23 Examples.[261]
(1) Case [**1**]: $\mu_1 - \mu_2 \neq \boldsymbol{N}$.

$$x^2 y'' + \left(x^2 + \frac{5}{36}\right) y = 0 \tag{20.41}$$

with

$$v = x^{5/6}\left(1 - \frac{3}{16}x^2 + \frac{9}{896}x^4 + \cdots\right), \tag{20.42}$$

$$u = x^{1/6}\left(1 - \frac{3}{8}x^2 + \cdots\right). \tag{20.43}$$

(2) Case [**21**]: $\mu_1 = \mu_2$

$$x(x-1)y'' + (3x-1)y' + y = 0 \tag{20.44}$$

with

$$v = 1/(1-x),\ u = \ln x/(1-x). \tag{20.45}$$

(3) Case [**22**]: $\mu_1 - \mu_2 \in \boldsymbol{N} \setminus \{0\}$ with a logarithmic term.

$$(x^2-1)x^2 y'' - (x^2+1)xy' + (x^2+1)y = 0 \tag{20.46}$$

with

$$v = x,\ \ u = x\ln x + 1/2x. \tag{20.47}$$

(4) Case [**22**] $\mu_1 - \mu_2 \in \boldsymbol{N} \setminus \{0\}$ without any logarithmic term (cf. **23.19**, **23.25**).

$$x^2 y'' + xy' + \left(x^2 - \frac{1}{4}\right) y = 0 \tag{20.48}$$

with

$$v = \sin x/\sqrt{x},\ \ u = \cos x/\sqrt{x}. \tag{20.49}$$

See **??** also, for example.

20.24 Singularity at infinity. To study the singularity of the equation (20.8) at infinity, we introduce $\zeta = z^{-1}$ as usual in complex function theory. The equation reads in terms of ζ

$$\frac{d^2u}{d\zeta^2} + \left[\frac{2}{\zeta} - \frac{1}{\zeta^2}P(\zeta^{-1})\right]\frac{du}{d\zeta} + \frac{1}{\zeta^4}Q(\zeta^{-1})u = 0. \tag{20.50}$$

Therefore (→**20.15**),
(1) If $2z - z^2P(z)$ and $z^4Q(z)$ is regular at ∞, $z = \infty$ is a non-singular point.
(2) If $zP(z)$ and $z^2Q(z)$ are regular at ∞, then $z = \infty$ is a regular singular point.
(3) Otherwise, $z = \infty$ is an irregular singular point.

[261] Taken from E. Kreyszig, *Advanced Engineering Mathematics* (Wiley, 1983 Fifth edition) p163.

20.25 How to solve inhomogeneous problem. To solve the inhomogeneous version of (20.8)

$$\frac{d^2u}{dx^2} + P(x)\frac{du}{dx} + Q(x)u = f(x), \tag{20.51}$$

where f is a piecewise continuous function, we have only to find one special solution to this inhomogeneous equation; the general solution is the sum of that for (20.8) and this special solution. If one cannot get it by inspection, then perhaps the most systematic way is to use Lagrange's method of variation of constants described in **??**.

20.C Representative Examples

20.26 Legendre equation. If the method of separation of variables is used in the spherical coordinates for the Laplace equation (→**??**), the angular part can further be split into the parts $\Theta(\theta)$ and $\Phi(\varphi)$ as (cf. **22.2**)

$$\frac{d^2\Phi}{d\varphi^2} + m^2\Phi = 0, \tag{20.52}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left(\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right)\Theta = 0. \tag{20.53}$$

If there is no φ dependence, then $m = 0$, and (20.53) simplifies to (→**22.21**)

$$\frac{d^2P}{dz^2} - \frac{2z}{1-z^2}\frac{dP}{dz} + \frac{\ell(\ell+1)}{1-z^2}P = 0, \tag{20.54}$$

where $z = \cos\theta$ and $P(z) = \Theta(\theta)$. Or, we get

$$\frac{d}{dz}(1-z^2)\frac{d}{dz}P + \ell(\ell+1)P = 0, \tag{20.55}$$

which is called the *Legendre equation*. $z = \pm 1$ are regular singular points (→**20.15**) of (20.54). ($z = \infty$ is also a regular singular point. See **20.24**.)

20.27 Series expansion method applied to Legendre's equation; around $z = 0$. Since $z = 0$ is a regular point, solutions can be obtained in the series form $P(z) = \sum_{k=0}^{\infty} a_k z^k$ with the radius of convergence at least unity (→**20.14**, **??**).
(1) Introducing this into (20.55), we get

$$(n+1)(n+2)a_{n+2} + (\ell - n)(\ell + n + 1)a_n = 0. \tag{20.56}$$

(2) This implies that a_n can be expressed in terms of a_0 and a_1. The choice $a_0 = 1$, $a_1 = 0$ gives an even power series

$$P_{even} = 1 - \frac{\ell(\ell+1)}{2!}z^2 + \frac{\ell(\ell+1)(\ell-2)(\ell+3)}{4!} - \cdots, \tag{20.57}$$

and $a_0 = 0$, $a_1 = 1$ gives an odd power series

$$P_{odd} = z - \frac{(\ell-1)(\ell+2)}{3!}z^3 + \frac{(\ell-1)(\ell+2)(\ell-3)(\ell+4)}{5!}z^5 - \cdots. \tag{20.58}$$

(3) Notice that these two solutions make a fundamental system of solutions (→**20.11**). If $\ell = n \in \boldsymbol{N} \setminus \{0\}$, then they become polynomials called the *Legendre polynomials* $P_n(z)$ (→**17.16**).

20.28 Series expansion method applied to Legendre's equation; around $z = 1$. The indicial equation (20.24) is $\phi(\mu) = \mu^2 = 0$, so this is the case [**21**] of Theorem **20.20**. One solution in the series form is

$$P_\ell(z) = \sum_{k=0}^{\infty} \frac{(\ell+1)(\ell+2)\cdots(\ell+k)(-\ell)(-\ell+1)\cdots(-\ell+k-1)}{k!^2}\left(\frac{1-z}{2}\right)^k. \tag{20.59}$$

This is called the *Legendre function of degree ℓ of the first kind*. Its partner in the fundamental system is obtained in the form of (20.28) (→**20.20**). For a positive integer $\ell = n$

$$Q_n(z) = \frac{1}{2}P_n(z)\ln\frac{1+z}{1-z} - \sum_{k=1}^{n}\frac{2n-4k+3}{(2k-1)(n-k+1)}P_{n-2k+1}(z). \tag{20.60}$$

This is called the *Legendre function of degree ℓ of the second kind*. Since P_n and Q_n make a fundamental system of solutions (→**20.11**), their zeros separate each other (→**20.12**(2)).

20.29 Gauss' hypergeometric equation. The following equation is called *Gauss' hypergeometric equation*

$$z(1-z)\frac{d^2u}{dz^2} + [\gamma - (\alpha+\beta+1)z]\frac{du}{dz} - \alpha\beta u = 0, \tag{20.61}$$

where α, β and γ are constants. $z = 0, 1$ and ∞ are the regular singular points (→**20.15**(1)). The indicial equation (→**20.17**) around $z = 0$ is

$$\phi(\mu) = \mu(\mu - 1 + \gamma) = 0. \tag{20.62}$$

For $\mu = 0$ we can get (→**20.19**) for $-\gamma \notin \boldsymbol{N}$

$$F(\alpha, \beta, \gamma; z) \equiv \sum_{k=0}^{\infty} \frac{(\alpha)_k (\beta)_k}{k!(\gamma)_k} z^k, \tag{20.63}$$

where

$$(\lambda)_k = \lambda(\lambda + 1) \cdots (\lambda + k - 1). \tag{20.64}$$

F is called the *hypergeometric function*. For $\mu = 1 - \gamma$, if $\gamma - 2 \notin \boldsymbol{N}$, we get a partner of the above solution as

$$z^{1-\gamma} F(\alpha + 1 - \gamma, \beta + 1 - \gamma, 2 - \gamma; z). \tag{20.65}$$

Notice that from (20.59)

$$P_\nu(z) = F(\nu + 1, -\nu, 1; (1 - z)/2). \tag{20.66}$$

Discussion.
If we scale z as kz in Gauss's equation, we obtain the equation of the following form:

$$z(1 - kz)u'' + (c - bz)u' - au = 0. \tag{20.67}$$

Its regular singular points are at 0, $1/k$ and ∞. There is no other singularities. Take the $k \to 0$ limit to make $1/k$ confluent to ∞. Then, we obtain

$$zu'' + (c - bz)u' - au = 0. \tag{20.68}$$

If we set $b = 0$, the equation is Bessel's equation (→**23.1**). Indeed, replacing az with $-t^2/4$, $c = \nu + 1$, and $v = t^\nu u$, then

$$t^2 v'' + tv' + (t^2 - \nu^2)v = 0. \tag{20.69}$$

It is obvious that ∞ is its irregular singularity (→**20.15**).

20.30 Associate Legendre functions. Consider the case with $m \neq 0$ for (20.53) (→**20.26**). Using the same transformation of the variable $z = \cos\theta$, (20.53) becomes

$$\frac{d}{dz}\left((1 - z^2)\frac{d\Theta}{dz}\right) + \left(\ell(\ell + 1) - \frac{m^2}{1 - z^2}\right)\Theta = 0. \tag{20.70}$$

$z = \pm 1$ are regular singular points (→**20.15**). Instead of solving this with the aid of the series expansion, introduce Z as

$$\Theta = (1 - z^2)^{m/2} Z(z). \tag{20.71}$$

Then, we have

$$(1-z^2)\frac{d^2Z}{dz^2} - 2(m+1)z\frac{dZ}{dz} + (\ell-m)(\ell+m+1)Z = 0. \quad (20.72)$$

Differentiate Legendre's equation (20.55) m times, we get

$$(1-z^2)\frac{d^{2+m}u}{dz^{2+m}} - 2(m+1)z\frac{d^{m+1}u}{dz^{m+1}} + (\ell-m)(\ell+m+1)\frac{d^m u}{dz^m} = 0. \quad (20.73)$$

Therefore, in terms of Legendre functions P_ℓ and Q_ℓ (→**20.28**)

$$P_\ell^m(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}P_\ell(z), \quad Q_\ell^m(z) = (1-z^2)^{m/2}\frac{d^m}{dz^m}Q_\ell(z) \quad (20.74)$$

are the fundamental system of solutions (→**20.11**) of (20.70), and are called *associate Legendre functions* (→**22.5**-**22.6**). Notice that P_ℓ^m is not a polynomial, if m is odd. Also

$$P_\ell^m(\pm 1) = 0 \quad \text{for } m \geq 1. \quad (20.75)$$

20.31 Confluent hypergeometric equation. Replace z in the hypergeometric equation (20.61) with z/β and let $\beta \to \infty$. We get

$$z\frac{d^2u}{dz^2} + (\gamma - z)\frac{du}{dz} - \alpha u = 0 \quad (20.76)$$

This is called the *confluent hypergeometric equation* or *Kummer's equation*. $z = 0$ is a regular singular point (→**20.15**), but $z = \infty$ is an irregular singular point (→**20.15**), which is created by the confluence of two regular singular points 1 (which is scaled to β by the variable change) and ∞ of the hypergeometric equation. The indicial equation (20.24) is $\phi(\mu) = \mu(\mu-1) + \gamma\mu = 0$. The series solution method gives

$$u_1 = F(\alpha, \gamma; z), \quad u_2 = z^{1-\gamma}F(\alpha - \gamma + 1, 2 - \gamma; z), \quad (20.77)$$

where

$$F(\alpha, \gamma; z) \equiv \sum_{k=0}^{\infty} \frac{(\alpha)_k}{k!(\gamma)_k} z^k, \quad \gamma \neq 0, 1, 2, \cdots. \quad (20.78)$$

This function is called the *confluent hypergeometric function*.

Exercise.
Show that
(1) $(1+z)^n = F(-n, \beta, \beta, z)$
(2) $(1/z)\log(1+z) = F(1, 1, 2, -z)$.

APPENDIX a24 Floquet Theory

20.32 We consider (20.1) with periodic $A(x)$, that is, there is $\omega > 0$ such that

$$A(x+\omega) = A(x). \tag{20.79}$$

20.33 Theorem [Floquet]. If A in (20.1) is periodic, then there is a fundamental matrix such that

$$\Phi(x) = F(x)e^{x\Lambda}, \tag{20.80}$$

where F is a $n \times n$ matrix with period ω, and Λ is a constant $n \times n$ matrix. □
[Demo] Let $\Phi(x)$ be a fundamental matrix (→**20.5**) for (20.1). Then $\Phi(x+\omega)$ is also a fundamental matrix. Therefore, Theorem **??** tells us that there is a constant non-singular matrix M such that $\Phi(x+\omega) = \Phi(x)M$. Since M is non-singular, its logarithm $\ln M = N$ is well defined. Define $\Lambda = N/\omega$, and set

$$F(x) = \Phi(x)e^{-x\Lambda}. \tag{20.81}$$

We get with the aid of $\Phi(x+\omega) = \Phi(x)M$

$$\Phi(x+\omega) = F(x+\omega)e^{(x+\omega)\Lambda} = F(x+\omega)e^{x\Lambda}M = F(x)e^{x\Lambda}M. \tag{20.82}$$

Hence,

$$F(x+\omega) = F(x). \tag{20.83}$$

In other words,

20.34 Theorem. A linear ordinary differential equation (20.1) with a periodic matrix A can be converted into a constant coefficient ordinary differential equation

$$\frac{d\boldsymbol{v}(x)}{dx} = \Lambda\boldsymbol{v}(x) \tag{20.84}$$

with $\boldsymbol{u} = F(x)\boldsymbol{v}$, where F is defined by (20.81).□

20.35 Characteristic exponents. The eigenvalues of Λ in (20.81) are called the *characteristic exponents*. There is no systematic way to obtain these exponents.

21 Asymptotic Expansion

A formal expansion of a solution of a linear ODE discussed in the previous section around an irregular singular point gives generally a divergent series, but the series may still be useful as asymptotic series. Almost all the expansion series obtained by perturbation calculations in physics are divergent but asymptotic series. The famous perturbation series of QED are examples. We cannot uniquely reconstruct the function from its asymptotic series expansion in general, but we can with some auxiliary conditions. A famous example is the Borel summability.

Key words: asymptotic sequence, asymptotic series, optimal truncation, Watson's lemma, Laplace's method, Stirring's formula, acceleration of convergence, Borel sum, Borel transformation, Nevanlinna's theorem.

Summary:
(1) If Frobenius' method is blindly applied around an irregular singular point, we usually obtain divergent formal series, but they are often asymptotic (**21.1**). Most perturbation series in physics are only asymptotic (**21.17**).
(2) Divergence does not automatically mean asymptoticity; A series is an asymptotic expansion of a function, if the truncation error at the n-th order is smaller than the n-th order term (**21.3**). Therefore, its optimal truncation (**21.5**) is practically very useful.
(3) Computation involving asymptotic series can be performed termwisely except differentiation (**21.10**).
(4) There are several standard methods to obtain the asymptotic expansion of functions and integrals (**21.11**-**21.13**, **21.15**).
(5) The asymptotic expansion (in terms of a given asymptotic sequence) of a function is unique (**21.6**), but an asymptotic series cannot uniquely determine a function (**21.7**).
(6) However, if the function satisfies certain auxiliary conditions, then it can be recovered from the asymptotic series. The most important condition is the Borel summability (Nevanlinna's theorem **21.20**). In this case the Borel summation allows us to reconstruct the function (**21.18**-**21.20**).

21.1 Irregular singularity and divergence. Try to solve (20.8) following Frobenius (**24B**) blindly, assuming that $x = 0$ is an irregular

singular point (→**20.15**):

$$u(x) = x^\lambda \sum_{k=0}^{\infty} c_k x^k. \tag{21.1}$$

Formally, we get a set of formulas for c_k and λ as in **20.16**. If, fortunately, $c_l = 0$ for all l larger than some N, we can get a regular solution. However, this is an accidental case, and usually we can prove that for some $k > 0$

$$\lim_{n\to\infty} \left|\frac{c_{n-k}}{c_n}\right| = 0, \tag{21.2}$$

that is, the series (21.1) is divergent.[262] However, the resultant divergent series may be used as an *asymptotic series* around $x = 0$.

21.2 Asymptotic sequence. Let $\{\phi_n(x)\}$ be an infinite sequence of continuous functions. If $\phi_{n+1}(x) = o[\phi_n(x)]$ around x_0, i.e.,

$$\lim_{x\to x_0} \phi_{n+1}(x)/\phi_n(x) = 0, \tag{21.3}$$

for all $n > 0$, the sequence is called an *asymptotic sequence* (around x_0).

21.3 Asymptotic series. Let $\{\phi_n\}$ be an asymptotic sequence around x_0. Then, the following formal series

$$a_0\phi_0(x) + a_1\phi_1(x) + \cdots + a_n\phi_n(x) + \cdots \tag{21.4}$$

is called an *asymptotic series* for a function f at x_0, if for each fixed n

$$f(x) = a_0\phi_0(x) + a_1\phi_1(x) + \cdots + a_n\phi_n(x) + o[\phi_n(x)] \tag{21.5}$$

as $x \to x_0$. That is, if

$$\lim_{x\to x_0} \frac{f(x) - \sum_{k=0}^{n} a_n\phi_n(x)}{\phi_n(x)} = 0 \tag{21.6}$$

for all n, we say (21.5) is an *asymptotic expansion* of f around x_0 in terms of asymptotic function sequence $\{\phi_j\}$, and write

$$f(z) \sim a_0\phi_0(z) + a_1\phi_1(z) + \cdots + a_n\phi_n(z) + \cdots. \tag{21.7}$$

[262] See E L Ince, *Ordinary Differential Equations* (Dover, 1956; original 1926), p422. Also see W R Wasow, *Asymptotic Expansions for Ordinary Differential Equations* (Intescience, 1965).

Discussion.
(A) Let $A_a(\alpha,\beta)$ denote the angular region

$$A_a(\alpha,\beta) \equiv \{z \,|\, \alpha < Arg(z-a) < \beta, \tag{21.8}$$

where Arg is the principal argument (→**??**). We say a function f is expanded in the (generalized) asymptotic power series around a in the angular region $A_a(\alpha,\beta)$, if (21.5) hold when $z \to a$ is taken inside the angular region. The boundary of the maximal angular region where a given asymptotic expansion holds is called a Stokes line (→**21.8**).
(B) The Stirling formula **14.10** is admissible in the angular region $A_0(-\pi,\pi)$. This can be shown with the aid of

$$\log\Gamma(z) = \left(z-\frac{1}{2}\right)\log z - z + \log\sqrt{2\pi} - \frac{1}{\pi}\int_0^\infty \frac{z}{z^2+t^2}\log(1-e^{-2\pi t}). \tag{21.9}$$

21.4 Example. A typical example is:

$$F(x) = \int_0^\infty \frac{e^{-t/x}}{1+t}dt \sim \sum_{n=0}^{\infty}(-1)^n n! x^{n+1}. \tag{21.10}$$

This is an asymptotic series around $x=0$. If $x=1/2$, then the series read

$$\frac{1}{2} - \frac{1}{4} + \frac{1}{4} - \frac{3}{8} + \frac{3}{4} + \cdots. \tag{21.11}$$

This is hardly useful. However, if x is small, then the series should be usable as a numerical tool:[263]

$$F(0.1) \sim \frac{1}{10} - \frac{1}{100} + \frac{2}{1000} - \frac{6}{10000} + \cdots. \tag{21.12}$$

21.5 Optimal truncation of asymptotic series. As is clear from the definition **21.3**, to evaluate $f(\epsilon)$, if we truncate the asymptotic sequence at the n-th order, then the error (i.e., the difference between the true value and the estimate obtained from the truncated series) must be smaller than $a_n\phi_n(\epsilon)$. Hence, for a given ϵ we can find an optimal n to truncate the series by looking for n which minimizes $a_n\phi_n(\epsilon)$.

For example, for (21.10), with the aid of Stirling's formula (→**9.11**, also see **21.14**)

$$n! x^{n+1} \sim e^{(n+1)\ lnx + n\ln(n/e)}. \tag{21.13}$$

Hence, $n \sim 1/\epsilon$ gives the optimal truncation position.

[263] Read a conversation between a numerical analyst and an asymptotic analyst on p19 of N. G. de Bruijn, *Asymptotic Methods in Analysis* (Dover, 1958, 1981).

Discussion: How to efficiently compute series.
(1) **Euler transformation**. Let

$$f(x) = \sum_{n=0}^{\infty} a_n x^n \tag{21.14}$$

be a convergent series. Define the difference operator D as

$$\mathrm{D}a_n = a_{n+1} - a_n. \tag{21.15}$$

Then,

$$f(x) = (1-x)^{-1}a_0 + (1-x)^{-1}\sum_{n=0}^{\infty} \mathrm{D}a_n x^{n+1}. \tag{21.16}$$

This transformation is called the *Euler transformation*. Practically it is wise to use this beyond some finite terms.
(2) **Subtraction trick**. The above idea may be understood as subtracting the expansion of $(1-x)^{-1}a_0$ from $f(x)$. If we could find a function g which is close to f and easily expandable analytically, then considering $f-g$ may be a good idea to compute the series for f. For example, to compute

$$f = \sum_{n=0}^{\infty} \frac{1}{(1+n^2)}, \tag{21.17}$$

it is advantageous to use the knowledge

$$\sum_{n=0}^{\infty} \frac{1}{n(n+1)} = 1. \tag{21.18}$$

Hence,

$$f - 1 = \sum_{n=0}^{\infty} \frac{n-1}{n(n+1)(n^2+1)}. \tag{21.19}$$

(3) We wish to compute

$$S = \sum_{n=1}^{\infty} \frac{1}{1+n^2} \tag{21.20}$$

(i) The remainder satisfies the following inequalities

$$\int_N^{\infty} \frac{dx}{1+x^2} < S_N \equiv \sum_{n=N}^{\infty} \frac{1}{1+n^2} < \int_{N-1}^{\infty} \frac{dx}{1+x^2}. \tag{21.21}$$

Using this, find the necessary number of terms to obtain S within a 0.01% error.
(ii) Now we use the subtraction trick (→**??**) with the aid of

$$\sum_{n=1}^{\infty} \frac{1}{n^2} = \frac{\pi^2}{6}, \ \sum_{n=1}^{\infty} \frac{1}{n^4} = \frac{\pi^4}{90}. \tag{21.22}$$

What N do you need to obtain the same accuracy?
(4) The same idea works for integrals as well. Consider

$$I(\epsilon) = \int_0^1 \frac{1}{\sqrt{\epsilon + x}} dx. \tag{21.23}$$

In this case $I(0) = 2$ is easy, so let us subtract $1/\sqrt{x}$:

$$\int_0^1 \left[\frac{1}{\sqrt{\epsilon + x}} - \frac{1}{\sqrt{x}} \right] dx. \tag{21.24}$$

Introducing $u = x/\epsilon$ (*rescaling trick*), we realize that this integral is of order $\epsilon^{1/2}$. The integration range may be replaced by $[0, \infty)$ to the lowest nontrivial order.

21.6 Uniqueness of asymptotic expansion. The asymptotic expansion up to a given number of terms of a given function is unique if an asymptotic sequence is specified. □
This follows from the explicit formula for the coefficients:

$$a_n = \lim_{x \to x_0} \frac{f(x) - \sum_{k=0}^{n-1} a_k \phi_k(x)}{\phi_n(x)}. \tag{21.25}$$

21.7 Warning. However, an asymptotic series cannot uniquely determine a function. $(1+x)^{-1}$, $(1+e^{-x})/(1+x)$ and $(1+e^{-\sqrt{x}}+x)^{-1}$ all have the same asymptotic expansion $\sum(-1)^{n-1}x^{-n}$ $(x \to \infty)$ (Demonstrate this statement). If we try to asymptotically expand $e^{-1/x}$ in terms of the asymptotic sequence $\{x^n\}$ $(x \to 0)$, all the coefficients vanish, but obviously the function is not equal to 0. Hence, we cannot generally recover a function from its asymptotic expansion, because transcendentally small terms are ignored by asymptotic expansion.

21.8 Stokes line. The transcendentally small term $e^{-1/x}$ $(x \to +0)$ cannot be seen through asymptotic expansions as seen in **25.7**. However, obviously this is no more small for $x < 0$. Hence, if we consider the function $f(x)$ as a function $f(z)$ of the complex variable z instead of x, then its 'expandability into asymptotic series' should change drastically according to the sectors or regions on the complex plane. The occurrence of this drastic change is called *Stokes' phenomenon* and the boundary of these regions is called a *Stokes line* (curve). The existence of this phenomenon signifies nonconvergent asymptotic series.

21.9 Convergent power series is asymptotic. If $f(x)$ is Taylor-expandable at $x = a$ (i.e., is analytic (→**7.1**) around a), then the Taylor series is an asymptotic series. Conversely, if $f(x)$ is holomorphic (→**??**) and single valued in $0 < |x - a| < r$ for some positive r, then a is a removable singularity (→**??**(i)), and the asymptotic series is the Taylor series of f around a. [264]

[264] *Encyclopedic Dictionary of Mathematics* vol I p124-6.

21.10 Operations with asymptotic series.
(1) Termwise addition and subtraction of two asymptotic series (with the same asymptotic sequence **21.2**) is again an asymptotic series.
(2) In the case of power series $f \sim \sum a_n x^n$ and $g \sim \sum b_n x^n$, their product fg has the asymptotic power series $\sum c_n x^n$ with $c_n = \sum_{r=0}^{n} a_{n-r} b_r$.
(3) Also for power series the asymptotic series of $f(g)$ is obtained from that of f and g by substitution.
(4) The termwise integration of the power asymptotic series is the asymptotic series of the integral:

$$\int_0^x f(x)dx \sim \sum_{n=0}^{\infty} \frac{a_n}{n+1} x^{n+1}. \tag{21.26}$$

(5) However, termwise differentiation may not be allowed. A famous counter example is $e^{-1/x}\sin(e^{1/x})$, which has 0 as its asymptotic power series as guessed easily from **21.7**, but its derivative cannot be expanded in powers.
(6) Termwise differentiation is allowed if the derivative of the function also has an asymptotic expansion. See the Discussion below.

Discussion.
In this case, if f is holomorphic near a in the angular region and has an asymptotic power series, then termwise differentiation is allowed so long as a is reached within $A_a(\alpha, \beta)$ (→**21.3** Discussion (A)).

21.11 How to obtain expansion I: Integration by parts
(1) Let us estimate the tail of the normal distribution

$$G(x) = \frac{1}{\sqrt{2\pi}} \int_x^{\infty} e^{-y^2/2} dy. \tag{21.27}$$

Integrating by parts, we get

$$\sqrt{2\pi} G(x) = \frac{1}{x} e^{-x^2/2} - \int_x^{\infty} e^{-y^2/2} dy. \tag{21.28}$$

From this we easily get

$$\frac{x}{1+x^2} e^{-x^2/2} \leq \sqrt{2\pi} G(x) \leq \frac{1}{x} e^{-x^2/2}. \tag{21.29}$$

This suggests that $G(x)\exp x^2/2$ can be asymptotically expanded in powers of x^{-1}. See also **21.12**.
(2)

$$-Ei(-t) \equiv \int_t^{\infty} \frac{e^{-s}}{s} ds \sim \frac{e^{-t}}{t} - \int_t^{\infty} \frac{e^{-s}}{s^2} ds \tag{21.30}$$

etc., gives an asymptotic expansion.
(3) The decay rate of the Fourier expansion coefficients of a C^k- function discussed in **??** is an application of this method thanks to the Riemann-Lebesgue lemma (→**??**).
(4) Fourier expansion of piecewise C^k-functions. To compute

$$\int_{-\infty}^{\infty} f(x)e^{i\omega x}dx \tag{21.31}$$

we decompose the integration range into piecewise C^k sections, and then estimate the integral asymptotically by integration by parts (again thanks to the Riemann-Lebesgue lemma) in each section.

Exercise.
(A) Find the asymptotic expansion of Fresnel integrals

$$C(x) \equiv \int_0^x \cos\frac{\pi u^2}{2}du;\ S(x) \equiv \int_0^x \sin\frac{\pi u^2}{2}du; \tag{21.32}$$

[Hint. Use $\int_0^\infty$ →**??**.]
(B) Approximate estimation of integrals[265]
(1)

$$I(x) = \int_0^x e^{t^2}\frac{dt}{\sqrt{x^2-t^2}}. \tag{21.33}$$

For $x \ll 1$, we may replace $e^{t^2} \simeq 1$. For $x \gg 1$, we introduce $\xi = x - t$, and

$$I(x) = e^{x^2}\int_0^x e^{-2\xi x+\xi^2}\frac{d\xi}{\sqrt{2\xi x-\xi^2}}. \tag{21.34}$$

Plotting the exponent in the integrand, we realize that the exponential factor is the largest when $\xi = 0$, so that

$$I(x) \simeq e^{x^2}\int_0^x e^{-2\xi x}\frac{d\xi}{\sqrt{2x\xi}} \simeq \frac{e^{x^2}}{2x}\int_0^\infty e^{-z}\frac{dz}{\sqrt{z}} \sim \frac{e^{x^2}}{2x}. \tag{21.35}$$

(2)

$$I(a,b) = \int_0^\infty e^{-ax^2}\sin^2 bx dx. \tag{21.36}$$

This can be rewritten as

$$I(a,b) = \frac{1}{\sqrt{a}}\int_0^\infty e^{-z^2}\sin^2\left(\frac{b}{\sqrt{a}}z\right)dz. \tag{21.37}$$

If $b \gg \sqrt{a}$, then the sine factor oscillates very rapidly, so we may replace it with its average value 1/2. Therefore, $\simeq 1/\sqrt{a}$. Compare this with the exact value of I.

[265] Migdal

21.12 How to obtain asymptotic series II: Watson's lemma. Consider the following Laplace integral[266]

$$F(s) = \int_0^\infty e^{-st} f(t) dt. \tag{21.38}$$

Assume that $f(t)$ has a power series expansion

$$f(t) = \sum_{n=0}^{\infty} a_n t^n \tag{21.39}$$

with the radius of convergence R. Replace f in the integral (21.38) with its series expansion (21.39), and perform the integration termwisely. Then we get the following formal result:

$$F(s) \text{ ‘} = \text{’ } \sum_{n=0}^{\infty} \frac{a_n}{s^{n+1}}. \tag{21.40}$$

Watson's Lemma. If there is $a > 0$ such that $|f(t)| = O[e^{at}]$ for sufficiently large t, then (21.40) is actually an asymptotic expansion of F around $s = \infty$. □[267]

Example. An asymptotic expansion of the error function may easily be obtained with the help of Watson's lemma:

$$Erfc(x) = \frac{2}{\sqrt{\pi}} \int_x^\infty e^{-t^2} dt = \frac{2}{\sqrt{\pi}} e^{-x^2} \int_0^\infty e^{-2xt - t^2} dt. \tag{21.41}$$

Now introduce $u = xt$ and expand e^{-u^2/x^2} in power series.

$$Erfc(x) = \frac{2e^{-x^2}}{x\sqrt{\pi}} \int_0^\infty e^{-2u} \left(1 - \frac{u^2}{x^2} + \frac{u^4}{2x^4} - \frac{u^6}{6x^6} + \cdots\right) du. \tag{21.42}$$

This lemma can be used to estimate the asymptotic form of Fourier transforms as well.

Exercise.
(1) Show for $x > 0$

$$\int_0^\infty \frac{e^{-xt}}{1+t^2} dt = \frac{1}{x} - \frac{2!}{x^2} + \frac{4!}{x^4} - \cdots. \tag{21.43}$$

[266] F is the Laplace transform of f (→**33**).
[267] For a proof see B. Friedman, *Lectures on Application-Oriented Mathematics* (Wiley, 1969), p78.

[Hint. Use $s = xt$ as a new integration variable.]
(2) Show

$$\int_0^\infty \frac{e^{-xt}}{1+t^3}dt \sim \sum +n = 0^\infty (-1)^n \frac{(3n)!}{x^{3n+1}}. \tag{21.44}$$

(3) The asymptotic expansion of Ci and si:

$$Ci(x) \equiv \int_x^\infty \frac{\cos t}{t}dt,\ si(x) \equiv \int_x^\infty \frac{\sin t}{t}dt. \tag{21.45}$$

This is the real and imaginary parts of

$$J(x) = \int_x^\infty \frac{e^{it}}{t}dt = \int_0^\infty \frac{e^{i(x+u)}}{x+u}du. \tag{21.46}$$

Apply Watson's theorem to obtain the asymptotic expansions of these functions. Of course, repeated integration by parts should also work as can be guessed from the example in **21.11**.
(4) (This problem need not be here.) Find the asymptotic expansion in the $x \to \infty$ limit of

$$E_n(x) = \int_1^\infty t^{-n}e^{-xt}dt \tag{21.47}$$

in powers of $1/x$ For $n = 1$, what is the optimum truncation of the resultant asymptotic series to compute $E_1(N)$?

21.13 How to obtain asymptotic series III: Laplace's method. Consider

$$F(\theta) = \int_{-\infty}^{+\infty} e^{\theta h(x)}dx, \tag{21.48}$$

where h is a real C^2-function with the following properties:
(i) $h(0) = 0$ is an absolute maximum of h, and $h < 0$ for any nonzero x.
(ii) There are positive constant a and b such that $h \le -a$ for $|x| \ge b$.
We must of course assume that the integral converges for sufficiently large θ. Then, in the $\theta \to \infty$ limit, we get

$$F(\theta) \sim \sqrt{2\pi}(-\theta h''(0))^{-1/2}. \tag{21.49}$$

21.14 Gamma function and Stirling's formula. Although we can apply Watson's lemma to get the asymptotic expansion of Gamma function (→**14.1**), it is not very easy, so we use the Laplace method. Substituting $t = z(1+x)$ in (14.3), we get

$$\Gamma(z+1) = e^z z^{z+1} \int_{-1}^\infty \left[e^{-x}(1+x)\right]^z dx. \tag{21.50}$$

h in **21.13** reads $-x+\ln(1+x)$, so it satisfies the condition of Laplace's method, and $h''(0) = -1$. Hence, we get

$$n! \sim \sqrt{2\pi}e^{-n}n^{n+1/2}, \tag{21.51}$$

which is the famous *Stirling's formula* (→**14.10**) obtained by Laplace in this way.

21.15 How to obtain asymptotic series IV: Method of steepest descent. This is perhaps the most famous method to obtain asymptotic expansions of integrals. The principle is explained as follows. We wish to compute the following contour integral on the complex plane

$$I = \int_C G(z) e^{tf(z)} dz, \tag{21.52}$$

where C is a contour from infinity to infinity on the complex plane such that on both ends the holomorphic function (→**??**) f goes to $-\infty$. G is also assumed to be holomorphic and t is a large positive constant. Let us split f into its real and imaginary parts as $f = \phi + i\psi$. Since ϕ is a harmonic function (→**??**), it can have a saddle point (→**25.6**) z^*, which satisfies $f'(z^*) = 0$. Modify the contour C to C^* so that it can pass through z^* and parallel to $grad\, \phi$ near z^*. Along this pass

$$f(z) = f(z^*) + \frac{1}{2}(z - z^*)^2 f''(z^*) + \cdots \tag{21.53}$$

and ψ must be almost constant, because the Cauchy-Riemann equation (→**??**) tells us that gradients of ϕ and ψ are orthogonal. Hence the second term in the above expansion along C^* near z^* must be real non-positive. We may introduce a real coordinate ζ such that $f(z) = f(z^*) - \zeta^2/2 + \cdots$. Let α be the angle between the real axis and the tangent of C^* at z^*. Then

$$\frac{d\zeta}{dz} = e^{i\alpha} \sqrt{|f''(z)|}. \tag{21.54}$$

Changing the integration variable, we get

$$I = e^{tf(z^*)} G(z^*) e^{-i\alpha} \left| \frac{2\pi}{tf''(z^*)} \right|^{1/2}. \tag{21.55}$$

21.16 Acceleration or improvement of asymptotic series. If we could convert the asymptotic series around 0 in powers of x into another asymptotic sequence which is in terms of an asymptotic sequence converging much more quickly to 0 than x^n, then the asymptotic estimate should become much more accurate. An example is given here.[268] Consider (21.10)

$$F(x) = \frac{1}{x} - \frac{1}{x^2} + \frac{2}{x^3} + \cdots. \tag{21.56}$$

[268] See, for example, C. N. Moore, *Summable Series and Convergence Factors* (Dover, 1966).

We wish to convert this into the power series in $y = \phi(x)$. We assume $y/x \to 1$ in the $x \to \infty$ limit, and the Taylor-expandability: $x/y = 1 + a/y + b/y^2 + \cdots$. Substituting this into (21.56), we get

$$\begin{aligned} F(x) &= \frac{1}{y + a + b/y} - \frac{1}{(y+a)^2} + \cdots \\ &= \frac{1}{y}\left(1 - \frac{a}{y} + \frac{a^2}{y^2} - \frac{b}{y^2} + \cdots\right) - \frac{1}{y^2}\left(1 - \frac{2a}{y} + \cdots\right) + \cdots . \end{aligned} \tag{21.57}$$

Hence, choosing $a = -1$, we can kill the $1/y^2$ term. That is, we get

$$F(x) = \frac{1}{x+1} + O\left[\frac{1}{(x+1)^3}\right]. \tag{21.58}$$

This is much better than the original expansion for $x \gg 1$. Of course, one should not believe that the improvement is increasingly better if we continue this procedure indefinitely; the outcome is still an asymptotic expansion.

Discussion.
Consider the summation

$$S = \sum_{r=1}^{\infty} f(r), \tag{21.59}$$

where f is well-behaved. Let $S(n)$ be the partial sum up to the n-th term. Then, often

$$S(n) = S + \frac{B}{n} + \frac{C}{n^2} + o[n^{-2}]. \tag{21.60}$$

This can be used to estimate S from partial sums.

A variant of this idea is the estimation of integral from numerical integration with increment h. Let the integral be I and its approximately computed value with the increment h be $I(h)$. Then, often

$$I(h) = I + Bh + Ch^2 + o[h^2]. \tag{21.61}$$

21.17 Most perturbation series in physics are at best asymptotic. In field theory and statistical mechanics, in many cases we can perform analytical work only with the aid of some sort of perturbation techniques. The resultant perturbation series are usually divergent. Physicists often claim that they are asymptotic, but divergence does not automatically mean that the series is asymptotic. Hence, we have two problems: (1) To show that the series is asymptotic and (2) To recover the desired quantity from the asymptotic series. As we have seen in **21.7**, (2) is impossible without some auxiliary knowledge about the function. Read Fejer's theorem (→**??**) for Fourier series. A certain

summation method may recover the original function from a divergent series under an appropriate auxiliary conditions. (For Fejer's theorem the needed auxiliary condition is the continuity of the function.) Thus, we may expect that a function satisfying certain auxiliary condition could be recovered from its asymptotic series by a particular summation method. A representative method is the Borel summation (→**21.18**). Often the perturbation series in field theory are proved to be *Borel summable* (i.e., the original quantity can be recovered from its asymptotic series as a Borel sum).

21.18 Borel transform. Even if the RHS of

$$f(z) \sim \sum_{n=0}^{\infty} a_n z^n \tag{21.62}$$

diverges, its "Borel sum"

$$B(t) = \sum_{n=0}^{\infty} a_n \frac{t^n}{n!} \tag{21.63}$$

may converge. $B(t)$ is called the *Borel transform* of the series (21.62).

21.19 Heuristics. Consider

$$\frac{1}{z}\int_0^{\infty} \frac{t^n}{n!} e^{-t/z} dt = z^n. \tag{21.64}$$

Inserting this into (21.62), and formally changing the order of intergration and summation, we obtain

$$f(z) = \frac{1}{z}\int_0^{\infty} B(t) e^{-t/z} dt = \int_0^{\infty} B(\lambda z) e^{-\lambda} d\lambda. \tag{21.65}$$

Essentially, the Laplace transform (→**33**) of $B(t)$ is the desired function.

Exercise.
(1) Apply this to $(1+x)^{-1} \sim \sum (-)^n x^n$.
(2) We can asymptotically expand as

$$Erfc(x) = \frac{2}{\sqrt{\pi}} \int_x^{\infty} e^{-t^2} dt \sim \frac{2}{\sqrt{\pi}} \frac{e^{-x^2}}{x} \sum_n = 0^{\infty} \frac{(-1)^n (2n)!}{n!(2x)^{2n}}. \tag{21.66}$$

Apply the Borel summation method to this series and recover the error function.

21.20 Nevanlinna's theorem. Let $f(z)$ be analytic on the open disc D in the figure, and its asymptotic expansion satisfies

$$f(z) = \sum_{k=0}^{n-1} a_k z^k + R_n(z) \tag{21.67}$$

with

$$|R_n(z)| \leq \text{const.}\sigma^n n!|z|^n \tag{21.68}$$

uniformly for all n and all $z \in D$ for some positive σ. Then (21.67) is Borel summable (→**21.17**). That is, the Borel transform $B(t)$ of the series converges for $|t| < \sigma^{-1}$ and can be analytically continued to an analytical function $B(t)$ (→**??**) on the strip containing the entire positive real axis. From this f can be recovered as[269]

$$f(z) = \frac{1}{z}\int_0^\infty B(t)e^{-t/z}dt. \tag{21.69}$$

Exercise.
(1) Apply the Borel summation method to (25.8) (you must check the condition for the possibility).
(2) Demonstrate the following asymptotic expansion for $x \to \infty$

$$e^{x^2/2}\int_x^\infty e^{-y^2/2}dy \sim \frac{1}{x} - \frac{1}{x^3} + \cdots + (-1)^n\frac{(2n-1)!!}{x^{2n+1}} + \cdots. \tag{21.70}$$

Then, recover the integral from the series with the aid of the Borel summation method (if possible).

[269] For an elegant proof see A D Sokal, J. Math. Phys. **21**, 261-3 (1980). However, this is not the general form given by the original author. For applications, see, for example, Itzykson and Zuber, *Quantum Field Theory* (McGraw-Hill, 1980), Section 9.4. J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon Press, 1989) Section 27.

22 Spherical Harmonics

Separation of variables of the Laplace equation in the spherical coordinates requires the spherical harmonic functions which make a complete orthonormal set of functions of spatial directions (i.e., functions on a unit sphere). Derivation of functional forms, the orthonormal relation, addition theorem related to the multipole expansion, and the application to PDE boundary value problems (potential problems) are discussed.

Key words: spherical harmonics, spherical harmonic function, addition theorem, multipole expansion, interior problem, exterior problem, annular problem

??:
(1) The angular part of the Laplacian in the spherical coordinates have the orthonormal eigenfunctions called spherical harmonics Y_n^m (**22.8**-**22.9**). They are simultaneous eigenfunctions of the total and the z-component of the quantum mechanical angular momentum (**22.10**).
(2) The addition theorem is used to decouple two spatial directions (**26A.12**), and applied to the multipole expansion of the electrostatic potential (**22.14**-**22.15**).
(3) Spherical potential problems have different general expansion forms depending on the domain of the problem (**22.17**-**22.20**).

22.A Basic Theory

22.1 Separating variables in spherical coordinates. In the polar coordinate system, the 3-Laplacian reads (→**??**)

$$\Delta = \frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{1}{r^2} L, \tag{22.1}$$

where

$$L = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}. \tag{22.2}$$

Separating the solution as $u(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$, we get

$$\frac{d^2}{dr^2} rR(r) = l(l+1)\frac{R(r)}{r}, \tag{22.3}$$

$$LY(\theta,\varphi) = -l(l+1)Y(\theta,\varphi). \tag{22.4}$$

L is essentially the Laplacian on the unit sphere, and is a negative definite operator.

22.2 Further separation of angular variables. Let us further assume $Y(\theta,\varphi) = \Theta(\theta)\Phi(\varphi)$. The φ-direction must be the periodic direction, so the equation for Φ must be an eigenvalue problem (cf. **19.9** or **??**). Hence,

$$\frac{d^2\Phi}{d\varphi^2} = -m^2\Phi, \tag{22.5}$$

and the rest is

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \left(l(l+1) - \frac{m^2}{\sin^2\theta}\right)\Theta = 0. \tag{22.6}$$

22.3 Legendre's equation. If we introduce $x = \cos\theta$, the (22.6) reads

$$\frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right) + \left(l(l+1) - \frac{m^2}{1-x^2}\right)\Theta = 0, \tag{22.7}$$

which is called (modified) *Legendre's equation.*

22.4 $\boldsymbol{m = 0}$. For $m = 0$ Legendre's equation reads (→**24C.1**)

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right] + l(l+1)\Theta = 0, \tag{22.8}$$

The general solution to this can be written as (→**20.28**)

$$\Theta = AP_l(x) + BQ_l(x), \tag{22.9}$$

where P_l and Q_l are Legendre functions of first and second kind, respectively. Q_l is divergent at $x = \pm 1$, so that for a sphere problem this function should not appear. Furthermore, P_l is not finite at $x = 1$ if l is not an integer. Hence, we need P_n ($n \in \boldsymbol{N}$), the Legendre polynomials (→**17.16**, **20.27**(3)). That is, l must be a nonnegative integer (the eigenvalue problem has been solved).

22.5 $m \neq 0$. For convenience **20.30** is repeated here. If we define $Z(x)$ by

$$\Theta = (1-x^2)^{m/2}Z(x), \tag{22.10}$$

(22.7) becomes

$$(1-x^2)\frac{d^2Z}{dx^2} - 2(m+1)x\frac{dZ}{dx} + (n-m)(n+m+1)Z = 0. \tag{22.11}$$

This equation can be obtained by differentiating (22.7) m times. Therefore, the general solution of (22.7) is given by (→**20.30**)

$$P_n^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x),\ Q_n^m(x) = (1-x^2)^{m/2}\frac{d^m}{dx^m}Q_n(x). \tag{22.12}$$

These functions are called *associate functions* of P_n and Q_n. If we require that the solution is finite at $x = 1$, then P_n^m is the functions appearing in the solution.

22.6 Associate Legendre functions. If m is odd, then P_n^m is not a polynomial:

$$P_1^1(x) = (1-x^2)^{1/2} = \sin\theta, \tag{22.13}$$

$$P_2^1(x) = 3(1-x^2)^{1/2}x = 3\sin\theta\cos\theta = \frac{3}{2}\sin\theta, \tag{22.14}$$

$$P_2^2(x) = 3(1-x^2) = 3\sin^2\theta\frac{3}{2}(1-\cos 2\theta), \tag{22.15}$$

$$P_3^1(x) = \frac{3}{2}(1-x^2)^{1/2}(5x^2-1) = \frac{3}{8}(\sin\theta + 5\sin 3\theta), \tag{22.16}$$

$$P_3^2(x) = 15(1-x^2)x = \frac{15}{4}(\cos\theta - \cos 3\theta), \tag{22.17}$$

$$P_3^3(x) = 15(1-x^2)^{3/2} = 15\sin^3\theta = \frac{15}{4}(3\sin\theta - \sin 3\theta), \tag{22.18}$$

etc., where $x = \cos\theta$.

22.7 Orthonormalization of associate Legendre functions. We have

$$\int_{-1}^{1} P_k^m(x) P_l^m(x) dx = \frac{(l+m)!}{(l-m)!} \frac{2}{2l+1} \delta_{k,l}. \tag{22.19}$$

[Demo]. The LHS is, for $l > m$, $k > m$

$$\begin{aligned} f(m) &\equiv \int_{-1}^{1} (1-x^2)^m \frac{d^m P_k}{dx^m} \frac{d^m P_l}{dx^m} dx & (22.20) \\ &= -\int_{-1}^{1} \frac{d^{m-1} P_k}{dx^{m-1}} \frac{d}{dx} \left((1-x^2)^m \frac{d^m P_l}{dx^m} \right) dx. & (22.21) \end{aligned}$$

On the other hand, replacing m with $m-1$ and n with l in (22.11) and multiplying $(1-x^2)^{m-1}$, we get

$$\frac{d}{dx}(1-x^2)^m \frac{d^m P_l}{dx^m} = -(l+m)(l-m+1)(1-x^2)^{m-1} \frac{d^{m-1} P_l}{dx^{m-1}}. \tag{22.22}$$

Hence, (22.21) implies

$$f(m) = (l+m)(l-m+1) f(m-1) = \cdots = \frac{(l+m)!}{(l-m)!} f(0). \tag{22.23}$$

$f(0) = 2/(2l+1)$ is obtained from **17.5**.

22.8 Spherical harmonics. Now we can construct a complete orthonormal set of $L_2(S_2, \sin\theta)$ (S_2 is the unit 2-sphere) (→**16.19**). Let us define the kets $\{|l,m\rangle\}$ by (→**16.21**-)

$$\begin{aligned} \langle \theta, \varphi | l, m \rangle &= Y_l^m(\theta, \varphi) \\ &= (-)^{\{1+(-1)^m\}/2} \sqrt{\frac{2l+2}{2} \frac{(l-|m|)!}{(l+|m|)!}} P_l^{|m|}(\cos\theta) \frac{1}{\sqrt{2\pi}} e^{im\varphi}, \end{aligned} \tag{22.24}$$

where the ket $|\theta, \varphi\rangle$ satisfies (→**16.23**, **16.25**)

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta |\theta, \varphi\rangle \sin\theta \langle \theta, \varphi| = 1. \tag{22.25}$$

and

$$\langle \theta, \varphi | \theta', \varphi' \rangle = \delta(\theta - \theta') \delta(\varphi - \varphi') / \sin\theta. \tag{22.26}$$

22.9 Orthonormal relation for spherical harmonics. The decomposition of unity (→**16.15**) reads

$$1 = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} |l, m\rangle\langle l, m| \tag{22.27}$$

with the normalization

$$\langle l, m|l', m'\rangle = \delta_{l,l'}\delta_{m,m'}. \tag{22.28}$$

In the ordinary notation these formulas read (→**16.26**-**16.27**)

$$\frac{\delta(\theta - \theta')\delta(\varphi - \varphi')}{\sin\theta} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\theta, \varphi)\overline{Y_l^m(\theta', \varphi')}, \tag{22.29}$$

and

$$\int_0^{\pi} d\theta \int_0^{2\pi} d\varphi \sin\theta \overline{Y_l^m(\theta, \varphi)} Y_{l'}^{m'}(\theta, \varphi) = \delta_{l,l'}\delta_{m,m'}. \tag{22.30}$$

22.10 Angular momentum. Quantum mechanically, $-\hbar^2 L^2$ is the total angular momentum operator. $|l, m\rangle$ is the simultaneous eigenket of the total angular momentum operator and the z-component of the momentum M_z:

$$(i\hbar)^2 L|l, m\rangle = \hbar^2 l(l+1)|l, m\rangle, \tag{22.31}$$

$$M_z|l, m\rangle = m|l, m\rangle. \tag{22.32}$$

22.11 Spherical harmonic function. A function X of angular coordinates θ and φ is called a *spherical harmonic function* of order n, if $r^n X$ becomes a harmonic function (→**??**). X satisfies

$$LX + n(n+1)X = 0, \tag{22.33}$$

where L is in **22.1**. Because of the completeness (→**??**) of the spherical harmonics (essentially, its proof is in **33.1**), any spherical harmonic function of order n can be written as

$$X(\theta, \varphi) = \sum_{m=-n}^{n} A_m Y_m^n(\theta, \varphi). \tag{22.34}$$

22.12 Addition theorem. Let γ be the angle between the directions specified by the angular coordinates (θ, φ) and (θ', φ').[270] Then,

$$P_n(\cos\gamma) = \frac{4\pi}{2n+1} \sum_{m=-n}^{n} \overline{Y_n^m(\theta', \varphi')} Y_n^m(\theta, \varphi). \tag{22.35}$$

This theorem allows us to decouple two directions.
[Demo]. Notice that $P_n(\cos\gamma)$ is a spherical harmonic function of order n (due to spherical symmetry), so that we can expand it as

$$P_n(\cos\gamma) = \sum_{m=-n}^{n} Y_n^m(\theta, \varphi) A_m(\theta', \varphi'). \tag{22.36}$$

The coefficients are fixed immediately from the following formula and the orthogonality of $\{Y_n^m\}$.

22.13 Lemma. Let X be a spherical harmonic function of order n, and γ is the angle in **22.12**. Then,

$$\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta X(\theta, \varphi) P_n(\cos\gamma) = \frac{4\pi}{2n+1} X(\theta', \varphi'). \tag{22.37}$$

[Demo]. The integration is all over the sphere, so we can freely choose the $\theta = 0$ direction. Let us choose it to be the direction of (θ', φ'), and write the new angular coordinates as (γ, ψ). The integral we wish to compute becomes

$$I = \int_0^{2\pi} d\psi \int_0^{\pi} d\gamma \sin\gamma \hat{X}(\gamma, \psi) P_n(\cos\gamma), \tag{22.38}$$

where $\hat{X}$ is X in new variables. $\hat{X}$ is again a spherical harmonic function of order n (look at the spherical symmetry of (22.33)), so that it can be expanded as

$$\hat{X}(\gamma, \psi) = \sum_{m=-n}^{n} B_m Y_n^m(\gamma, \psi). \tag{22.39}$$

Hence,

$$I = \sqrt{\frac{4\pi}{2n+1}} B_0. \tag{22.40}$$

To calculate B_0 note the fact that $Y_n^m(0, \varphi) = 0$ if $m \neq 0$ (see the definition of P_n^m in **22.5**), and $Y_n^0(0, \varphi) = \sqrt{(2n+1)/4\pi}$ ($P_n(1) = 1 \rightarrow$**21B.5**(1)). Hence, from (22.39) we obtain

$$B_0 = \hat{X}_n(0, \psi) \sqrt{\frac{4\pi}{2n+1}} = X(\theta', \varphi') \sqrt{\frac{4\pi}{2n+1}}. \tag{22.41}$$

[270] We have $\cos\gamma = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\varphi - \varphi')$.

22.14 Multipole expansion. Let $\rho(x)$ be the charge distribution. Then the potential due to this charge distribution with respect to the zero potential at infinity is given by

$$V(x) = \int dy \frac{\rho(y)}{4\pi\epsilon_0 |x-y|}. \tag{22.42}$$

If $\rho(x)$ vanishes for $|x| \geq R$, then

$$V(x) = \sum_{n=0}^{\infty} \frac{1}{\epsilon_0 R^{n+1}} \left[\sum_{m=-n}^{n} \frac{1}{2m+1} q_n^m Y_n^m(\theta, \varphi) \right], \tag{22.43}$$

where

$$q_n^m = \int_0^R dr \int_0^\pi d\theta \sin\theta \int_0^{2\pi} d\varphi \, r^n \overline{Y_n^m(\theta,\varphi)} \rho(r,\theta,\varphi). \tag{22.44}$$

The expansion (22.43) is called the *multipole expansion.* □
[Demo]. Let the angle between x and y be γ, $R = |x|$ and $r = |y|$. Then

$$|x-y| = R\sqrt{1 - 2\zeta\cos\gamma + \zeta^2}, \tag{22.45}$$

where $\zeta = r/R$ (< 1). With the aid of the generating function of the Legendre polynomials (→**17.9**), we get

$$\frac{1}{|x-y|} = \frac{1}{R} \sum_{n=0}^{\infty} P_n(\cos\gamma) \zeta^n. \tag{22.46}$$

Now we use the addition theorem **22.12** to separate the x and y directions as

$$\frac{1}{|x-y|} = \frac{1}{R} \sum_{n=0}^{\infty} \left(\frac{r}{R}\right)^n \left[\sum_{m=-n}^{n} \overline{Y_n^m(\theta',\varphi')} Y_n^m(\theta,\varphi) \right]. \tag{22.47}$$

Putting this into (22.42) and exchanging the order of summation and integration (→**15.12**), we get the desired formula.

22.15 Lower order multipole expansion coefficients. For low order expansions, the Cartesian expression is much more popular. It reads

$$V(\boldsymbol{R}) = \frac{q}{R} + \frac{\boldsymbol{p}\cdot\boldsymbol{R}}{r^3} + \frac{1}{2}\frac{\sum_{i,j} Q_{ij} R_i R_j}{R^5} + \cdots, \tag{22.48}$$

where $\boldsymbol{R}$ is the position vector from the center of the charge distribution, q is the total charge, $\boldsymbol{p}$ is the dipole moment

$$\boldsymbol{p} = \int d\boldsymbol{x} \rho(\boldsymbol{x}) \boldsymbol{x}, \tag{22.49}$$

and Q_{ij} is the *quadrupole moment tensor*

$$Q_{ij} = \int d\boldsymbol{x}(3x_i x_j - x^2\delta_{ij})\rho(\boldsymbol{x}). \tag{22.50}$$

In terms of these more familiar moments, we can write

$$\begin{aligned}
q_0^0 &= \frac{1}{\sqrt{4\pi}}q, && (22.51)\\
q_1^1 &= -\sqrt{\frac{3}{8\pi}}(p_x - ip_y), && (22.52)\\
q_1^0 &= \sqrt{\frac{3}{4\pi}}p_z, && (22.53)\\
q_1^{-1} &= \sqrt{\frac{3}{8\pi}}(p_x + ip_y), && (22.54)\\
q_2^2 &= \frac{1}{12}\sqrt{\frac{15}{2\pi}}(Q_{11} - 2iQ_{12} - Q_{22}), && (22.55)\\
q_2^1 &= -\frac{1}{3}\sqrt{\frac{15}{8\pi}}(Q_{13} - iQ_{23}), && (22.56)\\
q_2^0 &= \frac{1}{2}\sqrt{\frac{5}{4\pi}}Q_{33}, && (22.57)\\
q_2^{-1} &= \frac{1}{3}\sqrt{\frac{15}{8\pi}}(Q_{13} + iQ_{23}), && (22.58)\\
q_2^{-2} &= \frac{1}{12}\sqrt{\frac{15}{2\pi}}(Q_{11} + 2iQ_{12} - Q_{22}). && (22.59)
\end{aligned}$$

Note that, generally

$$q_n^m = \overline{q_n^{-m}}. \tag{22.60}$$

22.B Application to PDE

22.16 Formal expansion of harmonic function in 3-space. **22.1**-**22.3** and **22.9** tell us that a harmonic function ψ (→**??**) can have the following (formal)[271] expansion in 3-space in terms of spherical harmonic functions:

$$\psi = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} R_{lm}(r)Y_l^m(\theta,\varphi), \tag{22.61}$$

[271] If we wish, we could say an expansion as a generalized function (→**14**).

where $R_{lm}(r)$ obeys (→**22.1**)

$$\frac{d^2}{dr^2} r R_{lm} = l(l+1)\frac{R}{r}. \tag{22.62}$$

Hence, R_{lm} has the following general solution (→**??**)

$$R_{lm}(r) = A_{lm} r^l + B_{lm} r^{-l-1}. \tag{22.63}$$

That is, we get the following formal expansion:

$$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (A_{lm} r^l + B_{lm} r^{-l-1}) Y_l^m(\theta, \varphi). \tag{22.64}$$

22.17 Interior problem. A harmonic function on 3-ball of radius a centered at the origin must be finite at the origin, so its general form must be

$$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm} r^l Y_l^m(\theta, \varphi). \tag{22.65}$$

for $r \in [0, a]$.
(1) Dirichlet condition on the sphere. The solution to the Lapalce equation on the sphere with the boundary condition at the surface

$$\psi(a, \theta, \varphi) = V(\theta, \varphi) \tag{22.66}$$

must have the form of (22.65). Hence we must have

$$V(\theta, \varphi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} A_{lm} a^l Y_l^m(\theta, \varphi). \tag{22.67}$$

With the aid of the orthonormality in **22.9**, we obtain

$$A_{lm} a^l = \int_0^{\pi} d\theta \, \sin\theta \int_0^{2\pi} d\varphi \overline{Y_m^l(\theta, \varphi)} V(\theta, \varphi). \tag{22.68}$$

(2) Neumann condition on the sphere. The solution to the Lapalce equation on the sphere with the boundary condition at the surface

$$\left. \frac{\partial \psi}{\partial r} \right|_{r=a} = E(\theta, \varphi). \tag{22.69}$$

Differentiating (22.65), we obtain

$$\frac{\partial \psi}{\partial r} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} l r^{l-1} A_{lm} Y_l^m(\theta, \varphi). \tag{22.70}$$

Hence, it is easy to obtain an explicit formula analogous to (1).

22.18 Exterior problem. If the harmonic function outside of a sphere is bounded, then the solution must have the following form

$$\psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} B_{lm} r^{-l-1} Y_l^m(\theta, \varphi). \tag{22.71}$$

B_{lm} are determined with the aid of orthonormality of spherical harmonics just as the interior problem.

22.19 Uniqueness condition for exterior problem. We have discussed that if the domain D is not bounded, then the uniqueness condition is not trivial (→**??**, **25.9**). To study this, first we study the problem in the domain $D \cap V$, where V is a sphere of radius R. Suppose ψ_1 and ψ_2 are solutions to a given Dirichlet problem. Let $\psi = \psi_1 - \psi_2$. Then, it is a solution to a homogeneous Dirichlet problem. Green's formula tells us that

$$\int_{D\cap V} (grad\,\psi)^2 d\tau = \int_{\partial(D\cap V)} \psi\, grad\,\psi \cdot d\boldsymbol{S} = \int_{\partial V \cap D} \psi\, grad\,\psi \cdot d\boldsymbol{S}. \tag{22.72}$$

Hence, for the integral to vanish a sufficient condition is

$$|\psi| < const. R^{-1/2-\epsilon} \tag{22.73}$$

Boundedness of ψ is generally not enough to guarantee the unique solution.

22.20 Annular problem. If the domain is a concentric sphere, the problem is called an annular problem. In this case both terms in R_{lm} in **22.16** are needed. The boundary conditions on two spherical boundary surfaces allow us to determine the coefficients uniquely.

Exercise.
Find the harmonic function on the annular region $r \in [a, 3a]$ with the boundary conditions $u = \cos\phi$ on $r = a$ and $u = \cos 3\phi$ on $r = 3a$.

22.21 Cylindrically symmetric case. If the system under consideration is independent of φ (→**20.26**), then the general solution has the following formal expansion:

$$\psi(r, \theta, \varphi) = \sum_{l=0}^{\infty} (A_l r^l + B_l r^{-l-1}) P_l(\cos\theta). \tag{22.74}$$

This is certainly a solution of the Laplace equation as can be seen from the result in **22.16** (also **??**). The uniqueness of the solution tells us that this is the general solution.

22.22 Examples.
(1) A conducting sphere of radius a is separated into the upper and the lower halves. The upper half is maintained at potential V_1, and the lower at V_0. The electric potential outside the sphere is given by

$$V+\frac{V_1-V_0}{2}\frac{a}{r}-(V_1-V_0)\sum_{\text{odd}\,l}(-1)^{(l-1)/2}\frac{2l+1}{\sqrt{2}}\left(\frac{a}{r}\right)^{l+1}\frac{(l-2)!!}{(l+1)!!}P_l(\cos\theta). \tag{22.75}$$

(2) The electric potential due to uniformly charged disk of radius a. For $r > a$

$$V=\frac{Q}{2\pi\epsilon_0 r}\sum_{n=1}^{\infty}(-1)^{n-1}\frac{(2n-3)!!}{(2n)!!}\left(\frac{a}{r}\right)^{2n}P_{2n-1}(\cos\theta). \tag{22.76}$$

Here Q is the total charge on the disk. For $r < a$ there is an extra complication, because $\theta = \pi/2$ is in the disk. However, for $\theta \in [0, \pi/2)$ there is no problem, and the solution is

$$V=\frac{Q}{2\pi\epsilon_0 r}\left[1-\frac{r}{a}P_1(\cos\theta)+\sum_{n=1}^{\infty}\frac{(-1)^{n-1}(2n-2)!}{2^{2n-1}(n-1)!n!}\left(\frac{r}{a}\right)^{2n}P_{2n-1}(\cos\theta)\right]. \tag{22.77}$$

For $\theta > \pi/2$ we use the symmetry $V(r,\theta,\varphi) = V(r,\pi-\theta,\varphi)$.
(3) The equilibrium temperature distribution of a half ball of radius a with the surface temperature specified as $T = f(\cos\theta)$ and the bottom disk is maintained at $T = 0$. In this case we use the reflection principle (→**??**) to extend the problem to the whole ball. The boundary condition for the extended problems is given by $T_{r=a} = g(\cos\theta)$, where $g(x) = sgn(x)f(x)$. From the symmetry, the boundary condition on the bottom surface is automatically satisfied. The formal expansion of the interior problem with cylindrical symmetry (→**22.21**) is given by **22.18**, so the answer reads

$$T=\sum_{l=0}^{\infty}A_l r^l Y_l^0(\theta,\varphi) \tag{22.78}$$

with

$$A_l a^l=\sqrt{(2l+1)\pi}\{1-(-1)^n\}\int_0^1 dx P_l(x)f(x). \tag{22.79}$$

Exercise.
(1) Find the gravitational potential due to a sphere of radius R with the density distribution given by

$$\rho = r^k X_m(\theta,\varphi), \tag{22.80}$$

where X_m is a spherical harmonics of order m ($\rightarrow$**22.11**).
In this case due to the superposition principle, the potential V is given by

$$V(\boldsymbol{x}) = \int d^3\boldsymbol{y} \frac{\rho(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}. \tag{22.81}$$

Use (22.46) in **22.14** to expand the Green's function. Then, use **22.13** to perform the angular integral. In this way, we arrive at

$$V(\boldsymbol{x}) = \frac{4\pi}{2m+1} \frac{R^{m+k+3}}{m+k+3} X_m(\theta, \varphi). \tag{22.82}$$

(2) Discuss the waves in a thin spherical layer of radius R. The equation of motion is the wave equation written in the spherical coordinates with r suppressed ($r = R$).

23 Cylinder Functions

Separation of variables of the Laplace equation in the cylindrical coordinates requires Bessel and modified Bessel functions, which may perhaps be the most representative special functions. Bessel and Neumann functions make a fundamental system for the radial part of the separated equation called the Bessel equation. Classical results about Bessel and Neumann functions are summarized such as orthonormal relations (Fourier-Bessel-Dini expansion), generating functions, integrals containing Bessel functions. Bessel functions with half odd integer parameter (or their streamlined version: spherical Bessel functions) are required to solve the Helmholtz equation in the spherical coordinates.

Key words: Bessel equation, Bessel function, Bessel's integral, generating function, recurrence relations, cylinder functions, zeros of Bessel functions, Neumann function, Hankel function, Fourier-Bessel-Dini expansion, Modified Bessel function, spherical Bessel function, partial wave expansion.

Summary:
(1) The Laplace equation in the cylindrical coordinates requires Bessel and Neumann functions (**23.1**, **??**, **23.16**). Pay attention to the general shapes of these functions (**??**, **23.16**).
(2) Bessel functions make an orthonormal eigenfunction set for the radial part of the Laplacian (**23.21**-**23.22**).
(3) The Helmholtz equation in the spherical cooridnates requires spherical Bessel functions (**23.25**-**23.26**).
(4) Many second order linear ODE can be solved in terms of cylinder functions (**23.28**).

23.A General Theory

23.1 Bessel's equation. In terms of $z = \alpha r$, the equation (19.17) ($\rightarrow$**19.9**(1)) becomes

$$\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz} + \left(1 - \frac{m^2}{z^2}\right)u = 0. \tag{23.1}$$

$z = 0$ is a regular singular point (→**20.15**(1)), and $z = \infty$ is an irregular singular point (→**20.15**(2)).[272]

23.2 Series solution to Bessel's equation around $z = 0$. The indicial equation (20.24) (→**20.17**) is $\phi(\mu) = \mu^2 - m^2 = 0$. Choose $\mu = m$, $a_1 = 0$, $a_0 = 1/2^m\Gamma(m+1)$ and follow **20.16**. We get

$$J_m(z) = \left(\frac{z}{2}\right)^m \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(m+k+1)} \left(\frac{z}{2}\right)^{2k}. \tag{23.2}$$

This is called the *Bessel function of order m* (of the first kind). If $\mu_1 - \mu_2 = 2m$ is not an integer (→**??**[1]), then J_{-m} is a partner (→**20.13**) of J_m in a fundamental system of solutions (→**20.11**) of (23.1). If m is a half odd integer, then J_m and J_{-m} are still functionally independent (that is, this is the case with no logarithmic term in **??**).

If m is a positive integer, then J_m and J_{-m} are not functionally independent:

$$J_m = (-1)^m J_{-m}. \tag{23.3}$$

This can be demonstrated from (23.2) with the aid of $\Gamma(-m+k+1) = \infty$ for $k < m$ (→**14.1** or **23.7**). In this case we need a different partner: Neumann functions (→**23.15**).

Exercise.
(A)
(1) Show that

$$\frac{(-1)^k}{k!\Gamma(m+k+1)} \left(\frac{z}{2}\right)^{m+2k} = \left(\frac{z}{2}\right)^m \frac{(-1)^k}{\Gamma(m+1/2)\Gamma(1/2)} \frac{z^{2k}}{(2k)!} B\left(m + \frac{1}{2}k + \frac{1}{2}\right). \tag{23.4}$$

(2) With the aid of the integral expression of the Beta function (9.22), show that formally[273]

$$J_m(z) = \frac{1}{\Gamma(1/2)\Gamma(m+1/2)} \left(\frac{z}{2}\right)^m \int_0^1 t^{m-1/2}(1-t)^{-1/2} \cos[z(1-t)^{1/2}]dt \tag{23.5}$$

for $m + 1/2 > 0$.
(3) Now, changing the integration variable as $t = \sin^2\theta$, this formula can be rewritten as

$$J_m(z) = \frac{1}{\Gamma(1/2)\Gamma(m+1/2)} \left(\frac{z}{2}\right)^m \int_0^{\pi} \cos(z\cos\theta) sin^{2m}\theta d\theta. \tag{23.6}$$

Notice that the integration from 0 to $\pi/2$ and from $\pi/2$ to π are identical in this case, so $\int_0^{\pi}$ can be replaced by $2\int_0^{\pi/2}$. This formula is called *Poisson's integral*

[272] Therefore, the Bessel function is a special function of confluent type (→**19.5**).
[273] The exchange of the order of summation and integration can be justified.

representation.
(4) If $1-t=x^2$ is introduced, then (23.5) can be rewritten as

$$J_m(z)=\frac{1}{\Gamma(1/2)\Gamma(m+1/2)}\left(\frac{z}{2}\right)^m\int_{-1}^{1}(1-x^2)^{m-1/2}e^{izx}dx. \tag{23.7}$$

(B) Demonstrate the following *Whittaker's integral representation*

$$J_{n+1/2}(z)=(-i)^n\sqrt{\frac{\pi}{2z}}\int_{-1}^{1}e^{izx}P_n(x)dx. \tag{23.8}$$

Here P_n is the Legendre polynomial.
(C) Show

$$\int_0^{\pi/2}J_0(x\cos\theta)\cos\theta d\theta=\frac{\sin x}{x}. \tag{23.9}$$

[Hint. Use the integral of $\cos^n\theta$.]

23.3 Definition. The *Bessel function* of order ν can also be defined by

$$J_\nu(z)=\frac{1}{2\pi i}\int_C e^{\frac{z}{2}(t-\frac{1}{t})}t^{-(\nu+1)}dt, \tag{23.10}$$

where C can be a unit circle centered at the origin, and ν any real number. Obviously,

$$J_0(0)=1,\quad J_n(0)=0 \text{ for positive integer } n. \tag{23.11}$$

For integer ν this definition and the result in **23.1** are identical as seen in **??**.

Discussion: Where did the Bessel functions appear first?
The position of the earth (x,y) on the rotation plane can be written as

$$x=a(\cos\phi-e),\ y=a\sqrt{1-e^2}\sin\phi, \tag{23.12}$$

where e is eccentricity, a the and ϕ the angle of rotation measured from the peligy, and

$$\phi-e\sin\phi=vt, \tag{23.13}$$

where t is the time since the earth passed the peligy, and v is the average angular velocity. Hence, if we can write down ϕ as a function of t, then we can explicitly obtain $x(t)$ and $y(t)$. Consider

$$\frac{d\phi}{dvt}=\frac{1}{1-e\cos\phi}, \tag{23.14}$$

which is an even periodic function of vt. Hence, we can Fourier-expand it as

$$\frac{d\phi}{dvt}=1+\sum_{n=1^\infty}a_n\cos nvt. \tag{23.15}$$

The coefficient can be computed as

$$a_n = \frac{1}{2\pi}(1 - e\cos\phi)^{-1}\cos nvtd(vt), \tag{23.16}$$

$$= \frac{2}{\pi}\int_0^\pi \cos[n(\phi - e\cos\phi)]d\phi. \tag{23.17}$$

Comparing this with the generating equation in **23.5**, we obtain

$$a_n = 2J_n(ne) \tag{23.18}$$

Exercise.
Demonstrate

$$J_n(z) = \frac{1}{\pi i^n}\int_0^\pi e^{iz\cos\theta}\cos n\theta d\theta. \tag{23.19}$$

23.4 Series expansion. With the change of variables from t to $u = tz/2$, we rewrite the RHS of (23.10) as

$$\frac{1}{2\pi i}\left(\frac{z}{2}\right)^\nu \int_{C'} e^{u-z^2/4u}u^{-(\nu+1)}du = \frac{1}{2\pi i}\left(\frac{z}{2}\right)^\nu \sum_{m=0}^\infty \frac{(-1)^m}{m!}\left(\frac{z}{2}\right)^m \int_{C'} e^u u^{-(\nu+m+1)}du. \tag{23.20}$$

The integral can be computed with the residue theorem (→**??**) as

$$J_\nu(z) = \left(\frac{z}{2}\right)^\nu \sum_{m=0}^\infty \frac{(-1)^m}{m!\Gamma(\nu+m+1)}\left(\frac{z}{2}\right)^{2m}, \tag{23.21}$$

which is in agreement with (23.2). The series is convergent on the whole complex plane. Due to the factor $(-1)^m$ it is clear that J_ν cannot have any pure imaginary zero. From the formula, near the origin

$$J_\nu(z) \sim z^\nu. \tag{23.22}$$

Exercise.
(This problem need not be here.) Demonstrate

$$\int_0^1 t^{n+1} J_n(t) dt = J_{n+1}(1). \tag{23.23}$$

23.5 Generating function.

$$e^{\frac{1}{2}z(t-\frac{1}{t})} = \sum_{n=-\infty}^{+\infty} J_n(z) t^n. \tag{23.24}$$

This is from (23.10). This equation implies that J_n for integer n is the coefficients of the Laurent expansion (→**??**) of $\exp[z(t-t^{-1})/2]$ around $t = 0$.

23.6 Bessel's integral. Replacing t in (23.10) with $e^{i\theta}$, we have *Bessel's integral*

$$J_n(z) = \frac{1}{\pi} \int_0^\pi \cos(n\theta - z \sin\theta) d\theta. \tag{23.25}$$

Exercise.
Show

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix \sin\theta} d\theta. \tag{23.26}$$

23.7 $J_{-n}(z) = (-1)^n J_n(z)$. This can be obtained by replacing θ with $\pi - \theta$ in (23.25). (We have already shown this in **??**.)

23.8 Sine of sine → Bessel functions.

$$\sin(z \sin\theta) = 2J_1(z) \sin\theta + 2J_3(z) \sin 3\theta + 2J_5(z) \sin 5\theta + \cdots. \tag{23.27}$$

To show this rewrite (23.24) with the aid of **23.7** as

$$e^{\frac{1}{2}z(t-\frac{1}{t})} = J_0(z) + \sum_{n=1}^{\infty} J_n(z)[t^n + (-)^n t^{-n}]. \tag{23.28}$$

Now replace t with $e^{i\theta}$, and we get

$$e^{iz \sin\theta} = J_0(z) + 2iJ_1(z) \sin\theta + 2J_2(z) \cos 2\theta + 2iJ_3(z) \sin 3\theta + \cdots. \tag{23.29}$$

Splitting this into real and imaginary part, we get (23.27) and

$$\cos(z \sin\theta) = J_0(z) + 2J_2(z) \cos 2\theta + 2J_4(z) \cos 4\theta + \cdots.. \tag{23.30}$$

Thus, when sine appears inside a trigonometric function, recall J_n.

23.9 Recurrence relations. Differentiating (23.24) with respect to z and comparing the coefficients of the power of t, we get

$$2J'_m(z) = J_{m-1}(z) - J_{m+1}(z). \tag{23.31}$$

In particular, with the aid of **23.7** we have

$$J'_0(z) = -J_1(z) \tag{23.32}$$

If we differentiate (23.24) with respect to t and then compare the coefficients of t^n, we get

$$\frac{2m}{z}J_m(z) = J_{m-1}(z) + J_{m+1}(z). \tag{23.33}$$

23.10 Cylinder function. Any function $f(z,\nu)$ satisfying the following relations is called a *cylinder function*:

$$f(z,\nu-1) + f(z,\nu+1) = 2\frac{\nu}{z}f(z,\nu), \tag{23.34}$$

$$f(z,\nu-1) - f(z,\nu+1) = 2\frac{\partial}{\partial z}f(z,\nu). \tag{23.35}$$

(23.31) and (23.33) thus imply that Bessel functions are cylinder functions.

Exercise.
(1) These relations can be rewritten as

$$\frac{d}{dz}[z^\nu J_\nu(z)] = z^\nu J_{\nu-1}(z), \tag{23.36}$$

$$\frac{d}{dz}[z^{-\nu} J_\nu(z)] = -z^{-\nu} J_{\nu+1}(z). \tag{23.37}$$

(2) Derive

$$z^{-(\nu+m)}J_{\nu+m}(z) = (-1)^m \left(\frac{1}{z}\frac{d}{dz}\right)^m [z^{-\nu}J_\nu]. \tag{23.38}$$

Similarly, we can obtain

$$z^{\nu-m}J_{\nu-m}(z) = \left(\frac{1}{z}\frac{d}{dz}\right)^m [z^{\nu}J_\nu]. \tag{23.39}$$

(3) Integral related to the Fraunhofer diffraction through a circular aperture:

$$J = \int_0^a \int_0^{2\pi} e^{ibr\cos\theta} d\theta r dr = \frac{2\pi a}{b}J_1(ab). \tag{23.40}$$

[Hint. Use **23.6** and **23.10**.]

23.11 Zeros of Bessel functions.
(1) There are infinitely many zeros of $J_n(z)$.
(2) All the zeros of J_n for $n > -1$ are real and of multiplicity one except $z = 0$.
(3) $z^{-n}J_n(z)$ has no zero of multiplicity larger than one.
(4) The zeros of $J_n(z)$ separate the zeros of $J_{n\pm1}(z)$.
[Demo] From the Bessel equation (23.1) by scaling with a constant α we get

$$\frac{d^2J_n(\alpha z)}{dz^2} + \frac{1}{z}\frac{dJ_n(\alpha z)}{dz} + \left(\alpha^2 - \frac{n^2}{z^2}\right)J_n(\alpha z) = 0. \tag{23.41}$$

Hence,

$$\frac{1}{z}\frac{d}{dz}\left\{z\frac{dJ_n(\alpha z)}{dz}J_n(\beta z) - z\frac{dJ_n(\beta z)}{dz}J_n(\alpha z)\right\} = (\beta^2 - \alpha^2)J_n(\alpha z)J_n(\beta z), \tag{23.42}$$

where β is another constant. Multiplying x and integrationg (23.42) gives

$$(\beta^2 - \alpha^2)\int_0^b xJ_n(\alpha x)J_n(\beta x)dx = \left[x\frac{dJ_n(\alpha x)}{dx}J_n(\beta x) - x\frac{dJ_n(\beta x)}{dx}J_n(\alpha x)\right]_0^b. \tag{23.43}$$

Since $J_n(x)$ is of order x^n near $x = 0$ ($\rightarrow$(23.22)), if $n > -1$, the contribution from $x = 0$ of the RHS of (23.43) vanishes. Choose α to satisfy $J_n(\alpha b) = 0$, and set $\beta = \overline{\alpha}$. Then $J_n(\beta b) = 0$ since all the coefficients in (23.21) are real ($\overline{J_n(z)} = J_n(\overline{z})$). For these choices, the RHS of (23.43) is zero, so we have

$$(\beta^2 - \alpha^2)\int_0^b x|J_n(\alpha x)|^2dx = 0. \tag{23.44}$$

This implies $\beta^2 = \alpha^2$, that is $\alpha = \overline{\alpha}$, since there is no pure imaginary zeros ($\rightarrow$**??**). That is, the zeros of J_n are all real if $n > -1$.

The multiplicity of the zeros is known from the general property of the fundamental system ($\rightarrow$**20.12**). At $z = 0$ the coefficient function is not C^1, so this argument is not applicable to $z = 0$. Thus (2) and (3) have been demonstrated. Bessel's equation can be rewritten as

$$\frac{d^2U}{dz^2} + HU = 0 \tag{23.45}$$

with $U(z) = J_n/\sqrt{z}$ and $H(z) = 1 + (1/4 - n^2)/z^2$. Let $x \in \boldsymbol{R}$ be sufficiently large to make $H(x) > 0$. Suppose $U > 0$. Then, irrespective of the sign of dU/dx (23.45) tells $d^2U/dx^2 < 0$. Hence, as long as $U > 0$, dU/dx decreases with the increase of x. This continues until $U = 0$, but there $dU/dx < 0$ so U becomes eventually $U < 0$. This argument can be continued indefinitely. Thus, there must be infinitely many zeros for J_n. This is (1). (4) follows from

$$\frac{d}{dz}(z^{\pm\nu}J_\nu) = \pm z^\nu J_{\nu\mp1}, \tag{23.46}$$

which can be derived from the nature of J_ν as cylinder functions ($\rightarrow$**23.10**).

23.12 Proposition. For $x \in \boldsymbol{R}$

$$\begin{aligned} |J_0(x)| &\leq 1 && (23.47)\\ |J_n(x)| &\leq 1/\sqrt{2} \text{ for } n = 1, 2, \cdots . && (23.48) \end{aligned}$$

The first inequality follows from (23.25). The second inequality follows from the Gegenbauer-Neumann formula (→**23.14**. Expand the LHS and compare it with the RHS. cf. **23.15**(2).).

23.13 Addition theorem.

$$\begin{aligned} J_n(x+y) &= \sum_{s=-\infty}^{\infty} J_{n-s}(x)J_s(y), && (23.49)\\ &= \sum_{s=0}^{n} J_s(x)J_{n-s}(y) + \sum_{s=1}^{\infty}(-)^s[J_s(x)J_{n+s}(y) + J_{n+s}(x)J_s(y)]. && (23.50) \end{aligned}$$

This follows from the generating function (23.24):

$$\sum_{n=-\infty}^{\infty} J_n(x+y)t^n = e^{(x+y)(t-1/t)/2} = \sum_{n=-\infty}^{\infty} J_n(x)t^n \sum_{n=-\infty}^{\infty} J_n(y)t^n. \tag{23.51}$$

23.14 Gegenbauer-Neumann formula.

$$\begin{aligned} J_0(\sqrt{R^2 + 2Rr\cos\gamma + r^2}) &= J_0(R)J_0(r) + 2\sum_{m=1}^{\infty}(-1)^m J_m(R)J_m(r)\cos m\gamma,\\ J_0(\sqrt{R^2 - 2Rr\cos\gamma + r^2}) &= J_0(R)J_0(r) + 2\sum_{m=1}^{\infty} J_m(R)J_m(r)\cos m\gamma. \end{aligned} \tag{23.52}$$

[Demo] The second formula can be obtained from the first by $r \to -r$ and **23.7**. With the aid of the generating function **23.5**, we obtain

$$\sum_{n=-\infty}^{\infty} \lambda^n J_n(x)t^n = \exp\left\{\frac{x}{2t}\left(\lambda - \frac{1}{\lambda}\right)\right\} \sum_{n=-\infty}^{\infty} J_n(\lambda x)t^n. \tag{23.53}$$

Setting $\lambda = e^{i\theta}$, this equation becomes

$$\sum_{n=-\infty}^{\infty} J_n(e^{i\theta}x)t^n = e^{-(ix/t)\sin\theta} \sum_{n=-\infty}^{\infty} e^{in\theta} J_n(x)t^n. \tag{23.54}$$

Following the demonstration of the addition theorem **23.13**, we obtain

$$\sum_{n=-\infty}^{\infty} J_n(e^{i\theta}x+e^{i\varphi}y)t^n = e^{-(i/t)(x\sin\theta+y\sin\varphi)}\left[\sum_{n=-\infty}^{\infty} e^{in\theta}J_n(x)t^n\right]\left[\sum_{n=-\infty}^{\infty} e^{in\varphi}J_n(y)t^n\right]. \tag{23.55}$$

Let x, y, θ and φ be real and $xe^{i\theta}+ye^{i\varphi}$ be real. Then, $x\sin\theta+y\sin\varphi=0$. Compare the coefficients of t^0:

$$J_0(x\cos\theta+y\cos\varphi) = \sum_{m=-\infty}^{\infty} e^{im(\theta-\varphi)}J_m(x)J_{-m}(y) \tag{23.56}$$

Notice that if the imaginary part of $Re^{i\theta}+re^{i\varphi}$ vanishes, we can write

$$\sqrt{R^2+2Rr\cos\gamma+r^2} = Re^{i\theta}+re^{i\varphi} \tag{23.57}$$

with $\gamma=\theta-\varphi$. This concludes the proof. See **??**.

Exercise.
Show

$$J_n(z)J_n(z') = \frac{1}{\pi}\int_0^{\pi} J_0(\sqrt{z^2+z'^2-2zz'\cos\theta})\cos n\theta d\theta \tag{23.58}$$

for $n=0,1,2,\cdots$.

23.15 Integrals containing Bessel functions.

(1) From Bessel's integral **23.6** for $a\geq 0$ and $b>0$

$$\int_0^{\infty} e^{-ax}J_0(bx)dx = \frac{1}{\sqrt{a^2+b^2}}. \tag{23.59}$$

Especially $\int_0^{\infty} J_0(bx)dx = 1/b$. Replacing a in (23.59) with ia we get ($b>a$ assumed)

$$\int_0^{\infty} J_0(bx)\cos axdx = \frac{1}{\sqrt{b^2-a^2}}. \tag{23.60}$$

Differentiating these equations w.r.t. a, we compute similar integrals with insertions of powers of x. With the aid of (23.32) and integration by parts, we obtain

$$\int_0^{\infty} e^{-ax}J_1(bx)xdx = \frac{b}{(b^2+a^2)^{3/2}}. \tag{23.61}$$

(2) From the Gegenbauer-Neumann formula **23.14** with the aid of the orthogonality of $\{\cos n\gamma\}$ we obtain ($\rightarrow$**??** with $l=\pi$)

$$\frac{1}{\pi}\int_0^{\infty} J_0(x\sqrt{R^2-2Rr\cos\gamma+r^2})\cos n\gamma d\gamma = J_n(Rx)J_n(rx). \tag{23.62}$$

From this and (23.59), we get

$$\int_0^{2\pi} J_n(Rx)J_n(rx)dx = \frac{1}{\pi}\int_0^{\pi} \frac{\cos\gamma}{\sqrt{R^2-2Rr\cos\gamma+r^2}}d\gamma. \qquad (23.63)$$

Notice that this formula contains the generating function for the Legendre polynomials (→**17.9**), so that expansion in terms of r/R can be calculated with the aid of $P_n(\cos\gamma)$.
(3) [Weber's integral] Expanding $J_\nu(bx)$ as in **??** and termwise integration (→**15.12**) give for $a>0$, $b>0$ and for $Re\,\nu > -1$

$$\int_0^{\infty} e^{-a^2x^2}J_\nu(bx)x^{\nu+1}dx = \frac{b^\nu}{(2a^2)^{\nu+1}}e^{b^2/4a^2}. \qquad (23.64)$$

(4) [Lommel's integral]

$$\int_0^x J_n(\alpha x)J_n(\beta x)xdx = \frac{x}{\alpha^2-\beta^2}\left\{\alpha J_n(\beta x)J_{n+1}(\alpha x)-\beta J_n(\alpha x)J_{n+1}(\beta x)\right\}, \qquad (23.65)$$

$$= \frac{x}{\alpha^2-\beta^2}\left\{\beta J_n(\alpha x)J_{n-1}(\beta x)-\alpha J_n(\beta x)J_{n+1}(\alpha x)\right\}. \qquad (23.66)$$

This follows from (23.43) and recurrence relations (→**23.9**).

Exercise.
Show

$$J_0(x) = \frac{2}{\pi}\int_0^{\infty} \frac{\cos xt}{\sqrt{1-t^2}}dt. \qquad (23.67)$$

23.16 Neumann function of order m. When $m \in \boldsymbol{N}\setminus\{0\}$, we may use the general theory or the procedure in **20.20**[22], but traditionally, the following partner is chosen:

$$N_m(z) = [J_m(z)\cos m\pi - J_{-m}(z)]/\sin m\pi, \qquad (23.68)$$

which is called the *Neumann function of order* m. For non-integer m (23.68) is well defined and obviously a partner of J_m in **20.14**. If $m \in \boldsymbol{N}$, (23.68) becomes $0/0$, so we interpret the formula with the aid of l'Hospital's rule:[274]

$$N_m(z) = \frac{1}{\pi}\left[\frac{\partial J_m(z)}{\partial m} - (-1)^m\frac{\partial J_{-m}(z)}{\partial m}\right] \quad \text{for } m \notin \boldsymbol{N}\setminus\{0\}. \qquad (23.69)$$

[274] If we explicitly compute (23.69), we get

$$N_m(z) = \frac{2}{\pi}J_m(z)\ln\left(\frac{z}{2}\right) - \frac{1}{\pi}\sum_{k=0}^{m-1}\frac{(m-k-1)!}{k!}\left(\frac{z}{2}\right)^{-m+2k} - \frac{1}{\pi}\sum_{k=0}^{\infty}\frac{\psi(k+1)+\psi(m+k+1)}{k!(m+k)!}(-1)^m\left(\frac{z}{2}\right)^{m+2k},$$

where $\psi(z) = \Gamma'(z)/\Gamma(z)$. Thus this form is in conformity with the general theory **20.20**[22].

The general solution of Bessel's equation (23.1) is given by

$$AJ_m(z) + BN_m(z). \tag{23.70}$$

Notice that Neumann functions are cylinder functions as easily explicitly checked (→**23.10**).

Exercise.
Demonstrate that

$$W(J_\nu(x), N_\nu(x)) = \frac{2}{\pi x}. \tag{23.71}$$

23.17 $N_n(z)$ is singular at $z = 0$. This follows from explicit formulas in the $z \to 0$ limit (see the footnote of the previous entry):

$$N_0(z) \sim (2/\pi)\ ln(z/2), \tag{23.72}$$
$$N_n(z) \sim -(n-1)!(x/2)^{-n}/\pi \text{ for } n = 1, 2, \cdots. \tag{23.73}$$

23.18 Lommels' formula. Since J_ν and N_ν make a fundamental system of Bessel's equation (→**23.16** and **24A.4**), their Wronskian (→**20.6**) W must satisfy **24A.13**, i.e.,

$$W(x) = W_0 e^{-\ln x} = \frac{W_0}{x}. \tag{23.74}$$

To calculate W_0 we may use $\lim_{x\to 0} xW(x) = W_0$. If ν is not an integer, J_ν and $J_{-\nu}$ make a fundamental system (→**??**), so

$$\lim_{x\to 0} xW(J_\nu(x), J_{-\nu}(x)) = \lim_{x\to 0} x[J_\nu(x)J'_{-\nu}(x) - J'_\nu(x)J_{-\nu}(x)] = -\frac{2\sin\nu\pi}{\pi}, \tag{23.75}$$

where we have used the formula of complementary arguments for the Gamma function **14.4**. Thus, we obtain

$$W(J_\nu(x), J_{-\nu}(x)) = -\frac{2\sin\nu\pi}{\pi x}. \tag{23.76}$$

The result is correct even if ν is an integer due to continuity. With the aid of this formula and the definition of N_n in **23.16**, we obtain

$$W(J_n(x), N_n(x)) = \frac{2}{\pi x}. \tag{23.77}$$

This is called *Lommel's formula*.

Exercise.
Show
(1)

$$J_n N_{n+1} - J_{n+1} N_n = -\frac{2}{\pi x}. \tag{23.78}$$

(2)

$$J_n J_{-n+1} + J_{-n} J_{n-1} = \frac{2\sin n\pi}{\pi x}. \tag{23.79}$$

23.19 Bessel function with half odd integer parameters (See spherical Bessel functions in **23.25**). The Bessel and Neumann functions with half odd integer parameters can be written in terms of elementary functions:

$$J_{1/2}(z) = \sqrt{\frac{2}{\pi}}\frac{\sin z}{\sqrt{z}},\ J_{-1/2}(z) = \sqrt{\frac{2}{\pi}}\frac{\cos z}{\sqrt{z}} \tag{23.80}$$

$$J_{3/2} = \sqrt{\frac{2}{z\pi}}\left(\frac{\sin z}{z} - \cos z\right), \tag{23.81}$$

$$N_{1/2}(z) = -\sqrt{\frac{2}{z\pi}}\cos z,\quad N_{-1/2}(z) = \sqrt{\frac{2}{z\pi}}\sin z, \tag{23.82}$$

$$N_{3/2}(z) = 1\sqrt{\frac{1}{z\pi}}\left(\sin z + \frac{\cos z}{z}\right). \tag{23.83}$$

Exercise.
Derive

$$J_{m+1/2} = (-1)^m \frac{z^{m+1/2}\sqrt{2}}{\sqrt{\pi}}\left(\frac{1}{z}\frac{d}{dz}\right)^m\left(\frac{\sin z}{z}\right). \tag{23.84}$$

23.20 Hankel functions. Hankel functions are defined as follows:

$$H_n^{(1)}(z) \rightleftharpoons J_n(z) + iN_n(z), \tag{23.85}$$

$$H_n^{(2)}(z) \rightleftharpoons J_n(z) - iN_n(z). \tag{23.86}$$

$H_n^{(1)}$ and $H_n^{(2)}$ make a fundamental system of solutions (→**20.11**) for the Bessel equation (→**23.1**).

Exercise.
Show

$$H_n^{(2)}(x)H_{n+1}^{(1)}(x) - H_n^{(1)}(x)H_{n+1}^{(2)}(x) = \frac{4}{\pi x}. \tag{23.87}$$

23.21 Orthonormal basis in terms of Bessel functions. The set of kets $|i,\nu\rangle$ defined as follows is an orthonormal basis (→**16.10**) of $L_2([0,a],x)$ (→**16.19**)

$$\langle x|i,\nu\rangle = \frac{\sqrt{2}}{aJ_{\nu+1}(r_i^{(\nu)})} J_\nu(r_i^{(\nu)}x/a), \tag{23.88}$$

where $r_i^{(\nu)}$ is the i-th zero of $J_\nu(x)$ (→**23.11**). That $\{|i,\nu\rangle\}$ is a basis follows from the corresponding eigenvalue problem and the general theory (→**32.3**). That this is normalized (orthogonality follows from the general theory) is seen with the aid of Lommel's integral (→**23.15**(4)). Using l'Hospital's rule, we take the $\alpha \to \beta$ limit to obtain

$$\int_0^\alpha x J_\nu(r_i^{(\nu)}x/a)^2 dx = \frac{a^2}{2}[J'_\nu(r_i^{(\nu)})]^2. \tag{23.89}$$

This can be further transformed into the desired result with the aid of a recurrence relation in **23.9**.

The corresponding decomposition of unit operator $1 = \sum_{i=1}^\infty |i,\nu\rangle\langle i,\nu|$ (**16.15**) implies (cf. **16.26** for the delta function with a weight)

$$\frac{\delta(x-y)}{x} = \sum_{i=1}^\infty \frac{2}{[aJ_{\nu+1}(r_i^{(\nu)})]^2} J_\nu(r_i^{(\nu)}x/a) J_\nu(r_i^{(\nu)}y/a). \tag{23.90}$$

23.22 Fourier-Bessel-Dini expansion. $f \in L^2([0,a],x)$ (→**16.19**) can be expanded as

$$f(x) = \sum_{m=1}^\infty C_m J_\nu(r_m^{(\nu)}x/a), \tag{23.91}$$

where

$$C_m = \frac{2}{[aJ_{\nu+1}(r_i^{(\nu)})]^2} \int_0^a f(x) J_\nu(r_i^{(\nu)}x/a) x dx. \tag{23.92}$$

Notice that this is nothing but a standard generalized Fourier expansion with a special choice of the orthonormal basis. Hence the analogues of three key facts (→**??**) holds.

23.23 Modified Bessel functions. In terms of $z = \alpha r$, the equation (19.37) becomes (→**19.9**(3))

$$\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz} - \left(1 + \frac{m^2}{z^2}\right) u = 0. \tag{23.93}$$

$z = 0$ is a regular singular point (→**20.15**(1)), and $z = \infty$ is an irregular singular point (→**20.15**(2)). If z in (23.1) is replaced with iz, we get this equation. Hence, $J_m(iz)$ and $N_m(iz)$ are solutions. However, with a suitable phase factor the following set is usually chosen as a fundamental system of solutions (→**20.11**)

$$I_m(z) = e^{m\pi i/2} J_m(iz) = \sum_{n=0}^{\infty} \frac{1}{n!\Gamma(n+m+1)} \left(\frac{z}{2}\right)^{2n+m}, \tag{23.94}$$

$$K_m(z) = \frac{\pi}{2}\frac{I_{-m}(z) - I_m(z)}{\sin m\pi} = \frac{\pi}{2}\frac{e^{m\pi i/2} J_{-m}(iz) - e^{-m\pi i/2} J_m(iz)}{\sin m\pi}. \tag{23.95}$$

I and K are called *modified Bessel functions*. They are <u>not</u> cylinder functions.

Exercise.
(1) Show the leading singularities:

$$K_0(x) = -\ln x - \gamma + \ln 2 + \cdots, \tag{23.96}$$

$$K_n(x) = 2^{n-1}(n-1)! x^{-n} + \cdots. \tag{23.97}$$

(2) Demonstrate

$$\cosh x = I_0(x) + 2\sum_{n=1}^{\infty} I_{2n}(x). \tag{23.98}$$

(3) The solution to

$$u'' - zu = 0 \tag{23.99}$$

is called *Airy functions*. They become usful to study asymptotic behaviors of the Bessel functions for large $|z|$ and $|\nu|$. We can easily find a fundamental system for this equation, looking at the table in **23.28**:

$$\begin{aligned} u_1 &= Ai(z) \equiv \frac{1}{\pi}\left(\frac{z}{3}\right)^{1/2} K_{1/3}\left(\frac{2z^{3/2}}{3}\right) = \frac{z^{1/2}}{3}\left[I_{-1/3}\left(\frac{2z^{3/2}}{3}\right) - I_{1/3}\left(\frac{2z^{3/2}}{3}\right)\right] \\ u_2 &= Bi(z) \equiv \frac{z^{1/2}}{3}\left[I_{-1/3}\left(\frac{2z^{3/2}}{3}\right) + I_{1/3}\left(\frac{2z^{3/2}}{3}\right)\right]. \end{aligned} \tag{23.100}$$

Ai (resp., *Bi*) is called the *Airy function of the first (resp., second) kind*.

23.24 Helmholtz equation. For the equation of the type $L_t\psi = \Delta\psi$, where L_t is a differential operator with respect to time, the separation of variables gives us the *Helmholtz equation*

$$\Delta\psi = -\kappa^2\psi, \tag{23.101}$$

where $-$ is explicitly written, because the Laplacian is a non-positive operator. The separation of variables in the spherical coordinates $\psi = R(r)Y(\theta,\varphi)$ gives

$$\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right)Y(\theta,\varphi) = -\ell(\ell+1)Y(\theta,\varphi), \tag{23.102}$$

and

$$\frac{1}{r}\frac{d^2}{dr^2}rR(r) = \left(-\kappa^2 + \frac{\ell(\ell+1)}{r^2}\right)R(r). \tag{23.103}$$

(23.102) with the periodic boundary condition on the sphere gives eigenfunctions $Y_\ell^m(\theta,\varphi)$ ($\rightarrow$**22.8**) ($\ell = 0, 1, 2, \cdots$ and $m = -\ell, -\ell+1, \cdots, -1, 0, 1, \cdots, \ell$ for each ℓ). We may assume

$$\psi = \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} R_{lm}(r)Y_\ell^m(\theta,\varphi). \tag{23.104}$$

Here R_{lm} obeys (23.103).

23.25 Spherical Bessel functions. Introducing $u = \sqrt{\kappa r}R(r)$ and $z = \kappa r$, (23.103) becomes

$$\frac{d^2u}{dz^2} + \frac{1}{z}\frac{du}{dz} + \left(1 - \frac{(\ell + 1/2)^2}{z^2}\right)u = 0. \tag{23.105}$$

This is Bessel's equation (23.1) with $m = \ell + 1/2$. Therefore, the fundamental system of solutions for (23.103) consists of $J_{\ell+1/2}(\kappa r)/\sqrt{\kappa r}$ and $N_{\ell+1/2}\kappa r)/\sqrt{\kappa r}$. Thus the following *spherical Bessel function* j_ℓ and *spherical Neumann function* n_ℓ are defined:

$$j_\ell(z) \rightleftharpoons \sqrt{\frac{\pi}{2z}}J_{\ell+1/2}(z), \quad n_\ell(z) \rightleftharpoons \sqrt{\frac{\pi}{2z}}N_{\ell+1/2}(z). \tag{23.106}$$

The general solution to (23.103) is given by

$$Aj_\ell(z) + Bn_\ell(z). \tag{23.107}$$

The *spherical Hankel function* is also defined analogously

$$h_l^{(1,2)}(x) = \sqrt{\frac{\pi}{2x}}H_{l+1/2}^{(1,2)}(x). \tag{23.108}$$

Exercise.
(1) Demonstrate

$$j_0(x) = \frac{\sin x}{x} \tag{23.109}$$

with the aid of the series expansion of the Bessel function. Also demonstrate

$$n_0(x) = -\frac{\cos x}{x} \tag{23.110}$$

(2) Show

$$j_n(x) = (-1)^n x^n \left(\frac{1}{x}\frac{d}{dx}\right)^n \left(\frac{\sin x}{x}\right). \tag{23.111}$$

(3) Show

$$j_n(x)n_n'(x) - j_n'(x)n_n(x) = \frac{1}{x^2}. \tag{23.112}$$

23.26 Orthonormal basis in terms of spherical Bessel functions. There is nothing new in the present case, since we know the corresponding result for the Bessel function (→**23.17**). Therefore,

$$\left\{\sqrt{\frac{2}{a^3}}\frac{1}{j_{l+1}(\rho_i^{(l)})}j_l(\rho_i^{(l)}r/a)\right\}_{i=1}^{\infty}, \tag{23.113}$$

where $\rho_i^{(l)} = r_i^{(l+1/2)}$ is the zeros of $J_{l+1/2}$ (→**23.11**), is an orthonormal basis of $L_2([0,a], r^2)$ (→**16.19**). For example, the decomposition of unit operator reads (cf. **16.27**)

$$\frac{\delta(x-y)}{x^2} = \sum_{i=1}^{\infty} \frac{2}{a^3} \frac{1}{j_{l+1}(\rho_i^{(l)})^2} j_l\left(\frac{\rho_i^{(l)} x}{a}\right) j_l\left(\frac{\rho_i^{(l)} y}{a}\right). \tag{23.114}$$

23.27 Partial wave expansion of plane wave.

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta). \tag{23.115}$$

[Demo] $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ satisfies the Helmholtz equation $(\Delta + k^2)u(r) = 0$ (→**23.24**). Hence, we may assume

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} c_l j_l(kr) P_l(\cos\theta). \tag{23.116}$$

Therefore, the problem is to determine the coefficients c_l. With the aid of the orthogonality of the Legendre polynomial (→**17.5**), we obtain

$$c_l j_l(kr) = \frac{2l+1}{2} \int_{-1}^{1} dx e^{ikrx} P_l(x). \tag{23.117}$$

To evaluate the integral, integrate it by parts and ignore $o[1/r]$. We have

$$\int_{-1}^{1} dx e^{ikrx} P_l(x) \sim \frac{1}{ikr}[e^{ikr} - (-)^l e^{-ikr}] = \frac{2i^l}{kr} \sin\left(kr - \frac{l\pi}{2}\right). \tag{23.118}$$

Comparing this with the asymptotic formula for $r \to \infty$, we arrive at $c_l = (2l+1)i^l$.

23.28 ODE solvable in terms of Cylinder functions. Many second order linear ODE can be solved in terms of cylinder functions. See the table.

Exercise.
Find the general solution to the following ODE

$$\frac{d^2u}{dz^2} + \left(\frac{1}{2} + \sinh^2 z - \frac{3}{4}(\tanh^2 z + \coth^2 z)\right) u = 0. \tag{23.119}$$

23.B Applications to Solving PDE

(1) A circular membrane of radius a is applied a uniform force $b \sin \omega t$ over the membrane. Find the forced oscillation.[275]
(2)[276] Consider a disc of radius a whose center is located at the origin in the xy-plane. The boundary is maintained at $T = 0$, and the initial temperature is given by

$$T(x, y, 0) = T_0 \left(1 - \frac{x^2 + y^2}{r^2}\right). \tag{23.120}$$

Assume that the thermal diffusivity is κ. Find $T(x, y, t)$. The solution is given in the form of Fourier-Bessel-Dini expansion (→**23.22**). Compute the expansion coefficients explicitly with the aid of the following formula

$$\int_0^{\pi/2} d\phi \sin^{\mu+1} \phi \cos^{2\nu+1} \phi J_\mu(z \sin \phi) = \frac{2^\nu \Gamma(\nu + 1)}{z^{\nu+1}} J_{\mu+\nu+1}(z). \tag{23.121}$$

(3) **Circular wave guide**: The equation for $\phi = B_z$ reads

$$(\Delta_2 + k^2)\psi = 0 \tag{23.122}$$

on $r = a$ with the boundary condition $\phi = 0$. The field can be separated as

$$\phi(r, \varphi) = B(r) e^{im\varphi}, \tag{23.123}$$

where $m \in \boldsymbol{Z}$ due to the univalency of the field. $B(r)$ obeys

$$\frac{d^2B}{dr^2} + \frac{1}{r}\frac{dB}{dr} + \left(k^2 - \frac{m^2}{r^2}\right) B = 0. \tag{23.124}$$

Therefore, $B = J_m(kr)$ is the eigenfunction.

[275] LSU82.
[276] L138.

24 Diffusion Equation: How irreversibility is captured

Our discussion on the diffusion equation in **1** relied very heavily on our physics intuition. We wish to see whether our intuition is correctly captured by the diffusion equation. The maximum principle tells us that the diffusion equation captures well irreversible nature of diffusion processes. This in turn implies that the diffusion problems are well-posed in Hadamard's sense. Diffusion equations allow infinite speed of propagation of signals and matter, but adding second order time derivative terms cure this unphysical nature.

Key words: maximum principle, well-posedness, preservation of order, infinite propagation speed, telegrapher's (Maxwell-Cattaneo) equation.

Summary:
(1) The solution to the diffusion equation evolves in time generally toward the more 'featureless' function. This is guaranteed by the maximum principle (**24.2**).
(2) When the solution of a problem is unique and depends on the auxiliary conditions continuously, the problems is said to be well-posed in the sense of Hadamard (**24.3**). Diffusion problems are well-posed (**28.4**).
(3) Diffusion equations allow infinite speed of propagation (**28.9**). Only the addition of higher order time derivatives can cure this (**24.10**).

24.1 Elementary summary. We have learned where diffusion equations appear (→**??**, **??**, **??**, **??**, **??**). Some Green's functions have been constructed (→**16B**), and we physically argued that if they exist, it is unique in the bounded domain in particular, under the following condition with a given initial field (→**??**):
(1) Dirichlet condition: At the boundary all the values of ψ are specified. For the heat conduction problem, this is the condition with the given wall temperature (i.e., thermostated).
(2) Neumann condition: At the boundary the normal derivative of ψ is given. For the heat conduction problem, this is the condition with the given heat flux through the wall.

We heavily relied on the zeroth law of thermodynamics: there is a unique equilibrium state if we wait long enough. Our argument is, however, in a certain sense circular, because we have shown that if the diffusion equation is physically reasonable, then we can rely on physics

argument. To break this circle, we must demonstrate that indeed diffusion equation reflects thermodynamics correctly. This is equibvalent to demonstrating that our intuition and our mathematics could be in harmony (at least for the diffusion equation).

Exercise.
Solve

$$\frac{\partial u}{\partial t} = \Delta u + \boldsymbol{b} \cdot \nabla u + e^t \sin(x - b_x t), \tag{24.1}$$

with the initial condition $u(\boldsymbol{r}, 0) = |\boldsymbol{r}|$. Here $\boldsymbol{b}$ is a constant vector and b_x is its x-component.

24.2 Maximum principle. Let u be a solution[277] of the diffusion equation

$$u_t = u_{xx} \tag{24.2}$$

on $\Omega \rightleftharpoons I \times [0, T]$, where I is an interval on the x-axis. Then, its maximum value is taken on the *parabolic boundary* $\Gamma = \partial I \times [0, T] \cup I \times \{0\}$. In particular, this means the maximum value of $|u|$ on I is a decreasing function of time.
[Demo] Let μ be the maximum value of u on the parabolic boundary Γ, and define

$$v = e^{-t}(u - \mu). \tag{24.3}$$

v satisfies

$$v_t + v = v_{xx} \tag{24.4}$$

in Ω°.[278] If we can prove that $v \leq 0$ on Γ implies $v \leq 0$ in $I^\circ \times (0, T]$, then we are almost done. Suppose v has a maximum value $v = v_0 > 0$ at $(x_0, t_0) \in \Omega^\circ$. At this point $v_{xx} \leq 0$ and $v_t = 0$, so that (24.4) implies that $v_0 \leq 0$, a contradiction. If there is a maximum at the boundary $t = T$, then $v_t \geq$ and $v_{xx} \leq 0$, so $v < 0$. We are done.
(1) This principle also holds in d-space. An analogous demonstration works in any d-space, replacing I with a bounded region.
(2) As can be seen from the demonstration, if the solution may be assumed to be bounded everywhere, then the principle holds even if the problem is on an unbounded region.

Discussion.
(1) What can you say about the evolution of the number of peaks of a solution to the diffusion equation (under, say, a time-independent Neumann condition)?
(2) A more general theorem can be obtained almost as easily as the maximum

[277] There are actually several kinds of solutions. A solution in the ordinary sense of the calculus (requiring necessary differentiability, etc.) is called a *classical solution*.
[278] A° denotes the open kernel of the set A. That is, A° is the largest open set in A.

principle.
Gevrey's uniqueness theorem. Consider

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} + a(x,t)u = 0. \tag{24.5}$$

Here a is positive and continuous in the closed space time domain in the figure.[279] Let u be a solution to (24.5) that is continuous in the closed domain U considered above, satisfying (24.5) on the region $\hat{U} = U$ subtracted its parabolic boundary, and with continuous $\partial_t u$ and $\partial_x^2 u$ there. Then, u cannot have any positive maximum nor negative minimum in $\hat{U}$.□
[Demo]. Suppose we have a positive maximum inside DABC. Then, at the point

$$u > 0 \;\; \frac{\partial u}{\partial t} = 0, \;\; \frac{\partial^2 u}{\partial x^2} \leq 0, \tag{24.6}$$

so that this contradicts $a > 0$. If there is a positive maximum on the open segment CD, then there,

$$u > 0 \;\; \frac{\partial u}{\partial t} \geq 0, \;\; \frac{\partial^2 u}{\partial x^2} \leq 0, \tag{24.7}$$

This also contradicts $a > 0$. To show the statement about the minimum, consider $-u$ instead.

24.3 Well-posedness (in the sense of Hadamard).[280] Even if the unique solution exists, if the solution is extremely sensitive to the auxiliary conditions such as boundary and initial data, then the PDE may be useless for describing reproducible natural phenomena. A problem is said to be *well-posed (in the sense of Hadamard)*, if
(1) there is a solution which is unique,
and
(2) the solution depends continuously on the data (initial and other auxiliary conditions).

Otherwise, the problem is called *ill-posed*.[281] Physically reasonable problems are often well-posed as we will see later. For example, the Dirichlet problem for the Laplace equation is well-posed (→**25.9**).[282]

The existence of a solution implies that the problem is not *overdetermined*. The uniqueness of the solution implies that the problem is not *underdetermined*.

[279] A and B can be coincident. Furthermore, the side curves can wiggle wildly so long as they do not cross the upper and lower lines.
[280] Jacque Salomon Hadamard, 1865-1963. Read J. Hadamard, *The Psychology of Invention in the Mathematical Field* (Dover, 1945) on creativity.
[281] The condition (2) must be stated more precisely with the aid of some norm (→**??** footnote) to make the concept 'continuous' meaningful.
[282] One might suggests that chaos is an example of the lack of well-posedness, but most examples of chaos are well-posed, because the continuous dependence of the solution on the initial condition is trivially satisfied for any finite time.

24.4 Cauchy problem of diffusion equation with Dirichlet condition is well-posed. That is, the solution is unique and depends continuously on the initial and boundary data. [This theorem is proved for a bounded region here. Also we will not discuss the existence of a solution.]

[Demo] Let u_1 and u_2 be two solutions of the same problem. Then, due to the linearity of the problem, the difference $u = u_1 - u_2$ obeys the same diffusion equation with a homogeneous Dirichlet boundary condition (i.e., $u = 0$ at the boundary of the domain) and $u = 0$ initially as we have discussed (→**??**). From the maximum principle u cannot be larger than 0, and $-u$ cannot be larger than 0. Hence, $u_1 = u_2$. That is, if there is a solution, it is unique. Now, we compare two different problems 1 and 2 with the auxiliary conditions which are different slightly. Let the solutions of 1 and 2 be u_1 and u_2, respectively. Then, the maximum principle tells us that the maximum value of $|u_1 - u_2|$ in the region cannot be larger than the differences in the initial and boundary data. Hence, the solution depends on the auxiliary conditions continuously.[283] That is, the problem is well posed in Hadamard's sense.

Exercise.

Show that $\int u \ln u dx$ is non-increasing, if u obeys a diffusion equation. Assume the initial $u \geq 0$, and consider the problem in $\boldsymbol{R}^2$. (We define $u \ln u = 0$ for $u = 0$.)

24.5 Anti-diffusion: violation of second law. Thermodynamically destabilizing the world can produce ill-posed problems. A typical example is the 'anti'-diffusion equation.

$$\frac{\partial u}{\partial y} + \frac{\partial^2 u}{\partial x^2} = 0 \tag{24.8}$$

Notice that the amplitude of the mode e^{ikx} is amplified as $e^{+k^2 y}$, so unless the initial data decay faster than this factor in k-space, a kind of Hadamard instability occurs for any finite 'time' $y > 0$.[284]

Discussion.

$$\frac{\partial u}{\partial t} + t\frac{\partial^2 u}{\partial x^2} = f(x,t) \tag{24.9}$$

cannot make a well-posed problem. The reason should be obvious.[285]

[283] That is, when the sup norm of the change in the auxiliary condition is made small indefinitely, so does the sup norm of the corresponding change of the solution.
[284] As we have seen, the ill-posedness of a problem is closely related to instability in the ultraviolet limit ($k \to \infty$).
[285] Y. Kannai, Israel J. Math. **9**, 306 (1971).

24.6 Preservation of order, positivity. Let u_1 and u_2 be two solutions of the diffusion equation on the domain Ω as in **24.2**. If $u_1 \leq u_2$ on the parabolic boundary ($\rightarrow$**24.2**), then $u_1 \leq u_2$ in Ω°. Hence, for example, if $u_1 \leq u_2$ at $t = 0$, then this relation holds forever. In particular, if the initial condition is positive and the boundary value is non-negative, then the solution is positive forever. This should be obvious from the maximum principle.

24.7 Spatially inhomogeneous and/or anisotropic diffusion. Physically, the consequences of irreversibility should not be affected by the existence of spatial inhomogeneity and/or anisotropy (with time-dependence). We encounter the following equation in such a case (with the summation convention):

$$\frac{\partial u}{\partial t} = a_{ij}(x,t)\frac{\partial^2 u}{\partial x_i \partial x_j} + b_i(x,t)\frac{\partial u}{\partial x_i} + c(x,t)u \tag{24.10}$$

or its divergence form (with different coefficient functions):

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x_i}a_{ij}(x,t)\frac{\partial u}{\partial x_j} + b_i(x,t)\frac{\partial u}{\partial x_i} + c(x,t)u. \tag{24.11}$$

The second law requires the positive definiteness of the matrix $Matr(a_{ij})$. Under this condition it is known that so long as $c \leq 0$ the maximum principle ($\rightarrow$**24.2**) holds. Thus everything we can conclude intuitively about diffusion based on thermodynamics should also be captured in the spatially inhomogeneous diffusion equation. It is physically very sensible that the existence of the advection ($\rightarrow$**??**) term with b is irrelevant to the maximum principle.

24.8 Unbounded space. So far we have heavily relied on the boundedness of the domain of the problem. Note that the diffusion equation can have a rapidly growing solution even if the initial data is zero $u(x,0) = 0$ as Tikhonov demonstrated.[286] See also the warning in **??**(5). In any case, this episode tells us a danger of mathematical modeling: since diffusion equations are derived as a balance condition of conserved quantities ($\rightarrow$**??**), it is physically unthinkable that initially everywhere 0 solution can grow. (However, if the growth rate of the solution as a function of x is not too rapid, then the initial value problem can be solved uniquely. In particular, a bounded solution is unique.)

[286] F. John, p211-3.

24.9 Infinite propagation speed. For a very short time, the solution of the diffusion equation is almost independent of the (bounded) boundary condition away from the boundary, and is given by (3.6). In particular, if the thermal energy is concentrated at the origin at $t = 0$ (i.e., $T(\boldsymbol{x}, 0) = \delta(\boldsymbol{x}) \rightarrow$**??**):

$$T(\boldsymbol{x}, t) = \frac{1}{\sqrt{4\pi t}^d} e^{-x^2/4t} \tag{24.12}$$

is an accurate solution of $\partial_t T = \Delta T$ for short time in d-space ($\rightarrow$**??**). For any positive t, however small it may be, $T(x, t) > 0$ for any x. Therefore, we must conclude that heat can travel at infinite speed. This is true for the diffusion equation for chemical species as well, and is physically unrealistic. However, for most applications of diffusion equations, this is good enough because the tail part of T is much smaller than exponentially small quantities, and because significant error could occur only for extremely short times (when a collective description like diffusion is not applicable).

24.10 Short-time modification of diffusion equation: the Maxwell-Cattaneo equation.[287] We must modify the diffusion equation, if we wish to describe the short time behavior of the system more realistically. This is only possible by adding higher order time derivatives.[288] Hence, the following modification has been proposed:

$$c\frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = D_T \Delta T, \tag{24.13}$$

where c is a positive constant. This is called, in the context of heat conduction, the *Maxwell-Cattaneo equation*. We have already come across this type of equation in conjunction to the propagation of electromagnetic wave in matter (e.g., the telegrapher's equation $\rightarrow$**??**). Therefore, obviously, infinite speed of propagation is eliminated.[289]

[287] cf. Compt. Rend. **247**, 431 (1958).

[288] In Newton's equation of motion, the inertial effect is described by the second order time derivative, and the dissipative effect by the first order time derivative as in $\ddot{x} = -\eta\dot{x} + f$, where η is the friction constant, and f an external driving force. If we pay our attention only to the very short time behavior of the system, we do not see the dissipation term. The effect of dissipation sets in only later. Such an observation is also important in hydrodynamics. The Euler equation ($\rightarrow$**??**) accurately describes the initial motion of a body in a viscous fluid under impulsive force.

[289] The equation now becomes a hyperbolic equation ($\rightarrow$**??**). One of the important properties of hyperbolic equations is the finiteness of the propagation speed ($\rightarrow$**??**).

25 Laplace Equation: Consequence of spatial moving average

A solution of the Laplace equation is called a harmonic function. This must be a function invariant under spatial moving averaging as we discussed in **??**. This property almost determines the important features of the solutions of the Laplace equation and guarantees its well-posedness, etc.

key words: harmonic function, Green's formula, mean-value theorem, its converse, maximum principle, analyticity of solution, Liouville's theorem

Summary:
(1) Solutions to the Laplace equation must be invariant under spatial moving average; a precise statement is the spherical mean-value theorem and its converse (**25.4**-**25.5**). The resulting smoothness can also be stated precisely (**25.10**).
(2) From this, we immediately know that harmonic functions cannot have any local extremum inside the domain (**25.6**, **25.8**). This denies the existence of any stable electrostatic structure (**25.7**).
(3) Typical potential problems are well-posed (**25.9**).

25.1 Elementary summary. We have learned where the Laplace equation appears (→**??**, **??**, **??**, **??**), and physically argued what auxiliary conditions can ensure the uniqueness of the solution (→**??**). The most important boundary conditions are Dirichlet conditions in which the value of the function ψ on the boundary of the domain is fixed, and Neumann conditions in which the normal derivative of ψ on the boundary is given.

Discussion.
Cauchy problem of the Laplace equation is not well-posed. This was seen in Discussion **??**(7). Physically, this is not surprising. To obtain the Laplace equation instead of the wave equation for electromagnetic wave, we must change the sign of Faraday's law (→**??**). This implies that we replace Lenz's law with 'anti-Lenz's law'. Lenz's law is a manifestation of the stability of the world, so there is no surprise that the Laplace equation does not describe the well-behaved time evolution in our world.

25.2 Laplace equation and harmonic functions. Any classical solution to the Laplace equation is called a *harmonic function*. The

electric potential due to point charges is a harmonic function where there is no charge (→**??**), and charges correspond to the singularities of the functions. The equilibrium drumhead is described by a harmonic function. The real and imaginary parts of an analytic function are harmonic functions (→**??**).

Discussion.
(1) There is no solution to the 3-Laplace equation on the unit ball centered at the origin with the origin removed with the boundary condition $u = 1$ on the $|x| = 1$ and $u(0) = 0$.
(2) Consider the 2D Laplace equation $\Delta u = 0$ on the half plane $x > 0$ with the 'initial condition' $u(0, y) = 0$ and $\partial_x u(0, y) = f(y)$. If f is analytic, then there is a local analytic solution, but if it is not, then there is not even a local solution.

25.3 Green's formula. Let $D \subset \boldsymbol{R}^n$ be a bounded region, and u and v be C^2-functions defined on the closure of D. Here, we record the formulas again for convenience (→**??**).

$$\int_D (v\Delta u + grad\, u \cdot grad\, v) d\tau = \int_{\partial D} v\, grad\, u \cdot d\boldsymbol{S}, \tag{25.1}$$

and

$$\int_D (v\Delta u - u\Delta v) d\tau = \int_{\partial D} (v\, grad\, u - u\, grad\, v) \cdot d\boldsymbol{S}. \tag{25.2}$$

25.4 Spherical mean-value theorem. Let u be harmonic on a region $D \subset \boldsymbol{R}^n$, and $B_r(x)$ be a ball of radius r centered at x such that $B_r(x) \subset D$. Then, we have

$$u(x) = \frac{1}{S_{n-1}(r)} \int_{\partial B_r(x)} u(y) d\sigma(y), \tag{25.3}$$

where $d\sigma(y) = |d\boldsymbol{S}(y)|$, the area of the surface element, and $S_{n-1}(r)$ is the surface area of $(n-1)$-sphere (i.e., the skin of the n-ball) of radius r.[290] □

This should be intuitively expected from the interpretation of the Laplacian (→**??**).
[Demo] Set $v(y) = 1/|x-y|^{n-2}$ $(n > 2)$ or $\ln|x-y|$ $(n = 2)$ in (25.2), and $D = B_r(x) \setminus B_\epsilon(x)$ $(r > \epsilon)$.[291] Since v is harmonic in $\boldsymbol{R}^n \setminus \{x\}$ as a function of y, $v(y)$ is harmonic on D. To calculate the RHS of (25.2) we need the normal derivatives on $\partial B_r(x)$:

$$\frac{\partial v}{\partial n} = (2-n) r^{1-n}. \tag{25.4}$$

[290] $S_{n-1}(r) = 2\pi^{n/2} r^{n-1}/\Gamma(n/2)$.
[291] $A \setminus B$ is the set of all the points in A but not in B: $A \setminus B \equiv \{x | x \in A, x \notin B\}$.

Since both $u(y)$ and $v(y)$ are harmonic on D, (25.2) reads

$$\begin{aligned} 0 &= \int_{\partial D} (v\partial_n u - u\partial_n v) d\sigma(y) \\ &= \int_{\partial B_r(x)} (v\partial_n u - u\partial_n v) d\sigma(y) - \int_{\partial B_\epsilon(x)} (v\partial_n u - u\partial_n v) d\sigma(y). \end{aligned} \quad (25.5)$$

Using (25.4) and (9.19), we can rewrite this as

$$0 = -(2-n)\left[r^{1-n} \int_{\partial B_r(x)} u d\sigma(y) - \epsilon^{1-n} \int_{\partial B_\epsilon(x)} u d\sigma(y) \right], \quad (25.6)$$

which implies

$$\lim_{\epsilon \to 0} \epsilon^{1-n} \int_{\partial B_\epsilon(x)} u d\sigma(y) = S_{n-1}(r) u(x). \quad (25.7)$$

The converse of this theorem is also true:

25.5 Theorem [Converse of mean-value theorem]. Let u be a continuous function on a region D. If the mean value theorem **25.4** holds for any $r > 0$ and x such that $B_r(x) \subset D$, then u is C^∞ and harmonic on D. □[292]

25.6 Maximum principle. Let D be an open region and u be harmonic (→**25.2**) there. Suppose $\sup_{x \in D} u(x) \equiv A < \infty$. If $u \not\equiv A$ for $\forall x \in D$, then $u(x) < A$ for $\forall x \in D$. □
This should be obvious from the mean-value theorem **25.4**. Also, since a harmonic function is a steady solution of a diffusion equation, from the maximum principle for the diffusion equation (→**24.2**), this should be physically sensible. Changing u to $-u$ gives the minimum counterpart. This theorem implies:
Corollary. Let D be a compact set, and u be a harmonic function on the open kernel of D and continuous on D, then the extremum of u on D is achieved on ∂D. □
This implies that static electric potential cannot have its extreme values where there is no charge. A grave consequence is the collapse of classical physics.

Discussion.
Consider

$$\Delta u = u - u^3 \quad (25.8)$$

in 3-space on a bounded region Ω. Assume $u = 0$ on $\partial\Omega$. Show that $-1 \le u \le 1$.

25.7 Classical physics cannot explain atoms: Earnshaw's theorem. It is impossible to have a stable static configuration of charges in any static electric field. □
Unstable stationary configurations are not impossible (give an example). This theorem and electromagnetic radiation inevitable from accelerated charges conclusively killed the possibility of explaining atoms within classical physics.

[292] For a classical proof, see Folland p91 (2.5).

25.8 Strong maximum principle. Let Ω be a bounded region in $\boldsymbol{R}^n$, and u be harmonic there. If u attains its maximum value M at an inner point of Ω, then u is constant on Ω.

This is obvious from the mean value theorem.

25.9 Uniqueness and well-posedness. The solution of the Laplace equation on a bounded domain D, if exists,[293] is unique and depends continuously on the boundary data (→**25.11**).□
The proof is quite parallel to that for the diffusion equation (→**24.4**).
[Demo] Let u_1 and u_2 be two solutions of the same problem. Then, due to the linearity of the problem, the difference $u = u_1 - u_2$ obeys the Laplace equation with the homogeneous Dirichlet boundary condition (i.e., $u = 0$ at the boundary of the domain). From the maximum principle (→**25.6**) u cannot be larger than 0, and $-u$ cannot be larger than 0. Hence, $u_1 = u_2$. That is, if there is a solution, it is unique. Now, we compare two different problems 1 and 2 with the auxiliary conditions different slightly. Let the solutions of 1 and 2 be u_1 and u_2, respectively. Then, the maximum principle tells us that the maximum value of $|u_1 - u_2|$ in the region cannot be larger than the differences in the boundary data.

Discussion.
The existence of a solution in a domain in 3 or higher dimensional space is a very difficult problem, even if the boundary condition is continuous.

25.10 Smoothness of the solution. Since a harmonic function is, roughly speaking, invariant under spatial moving average, it must be smooth. Actually,
Theorem. All the solutions of the Laplace equation are real analytic (→**??** for $d = 2$. Here the assertion is for all $d \geq 2$. Analyticity means the convergence of the Taylor series.). □

Discussion.
(1) A solution to $\Delta u = f$ is analytic if f is analytic (Courant-Hilbert).
(2) Hadamard's example
Let D be a bounded region. There exists a continuous function $F : \partial D \to \boldsymbol{R}$ such that it becomes the boundary value of a harmonic function ϕ on D for which $\int_D |grad\phi|^2 d\sigma$ is not bounded. In this case although ϕ is C^∞, the derivatives of F behave wilder and wilder as the point approaches the boundary of the domain.

If the boundary value is continuous, then the corresponding Dirichlet problem of the Laplace equation on a bounded domain has at most one solution.

25.11 Well-posedness of Poisson's equation. The general Poisson problem has the following form

$$\Delta u = F \text{ in } \Omega,\ u = f \text{ on } \partial\Omega. \tag{25.9}$$

[293] We have not yet constructed the solution!

Here Ω is a bounded region. If we are interested in smooth solution (for example, C^2), then

$$\|u_1 - u_2\|_\Omega \leq c_1\|f_1 - f_2\|_{\partial\Omega} + c_2\|F_1 = F_2\|_\Omega, \tag{25.10}$$

where $\| \ \|_D$ is the L_2-norm on D, and c_1, c_2 are positive constants. This inequality clearly implies the well-posedness of our problem.

It is a good occasion to learn something about the so-called a priori estimate.

The inequality can be demonstrated as follows.

(1) First, the problem is split into v and w: $\Delta v = F$ in Ω, $v = 0$ on $\partial\Omega$ and $\Delta w = 0$ in Ω, $w = f$ on $\partial\Omega$.

(2) From the properties of the algebraic and geometric averages we get

$$2|(v, w)| = 2|(\epsilon^{-1/2}v, \epsilon^{1/2}w)| \leq \epsilon\|v\| + (\epsilon)^{-1}\|w\| \tag{25.11}$$

for any positive ϵ.

(3) Therefore,

$$\|v + w\|^2 \leq (1 + \epsilon)\|v\| + (1 + \epsilon^{-1})\|w\|. \tag{25.12}$$

That is, we have only to find bounds for v and w, respectively.

(4) With the aid of the variational problem (→**30.24**) for the eigenvalue of the Laplacian $-\Delta$:

$$0 < \lambda_1 = \inf_{v|_{\partial\Omega}=0} \frac{\int_\Omega v(-\Delta)v dx}{\int_\Omega v^2 dx}. \tag{25.13}$$

Hence, with the aid of the Schwarz inequality (→**16.7**)

$$\|v\|_\Omega^2 \leq \frac{1}{\lambda}\left(\int_\Omega v(-\Delta)v dx\right) \leq \frac{1}{\lambda}\left(\int_\Omega v^2 dx\right)^{1/2}\left(\int_\Omega (\Delta v)^2 dx\right)^{1/2} \tag{25.14}$$

Hence,

$$\|v\|^2 \leq \frac{1}{\lambda_1^2}\int_\Omega F^2 dx. \tag{25.15}$$

(5) Introduce an auxiliary function φ such that $\Delta\varphi = w$ on Ω and the homogeneous Dirichlet condition on $\partial\Omega$ (the existence of the solutions w and φ is a prerequisite of our argument). With the aid of Green's formula (→**25.3**)

$$\int_{\partial\Omega} w\frac{\partial\varphi}{\partial n}d\sigma - \int_{\partial\Omega}\varphi\frac{\partial w}{\partial n}d\sigma = \int_\Omega w\Delta\varphi dx - \int_\Omega \varphi\Delta w dx. \tag{25.16}$$

Hence,

$$\int_\Omega w^2 dx = \int_{\partial\Omega} w\frac{\partial\varphi}{\partial n}d\sigma \leq \left(\int_{\partial\Omega} w^2 dx\right)^{1/2}\left(\int_{\partial\Omega}\left(\frac{\partial\varphi}{\partial n}\right)^2 d\sigma\right)^{1/2}. \tag{25.17}$$

We have used the Schwarz inequality.

(6) For a function vanishing on the boundary

$$\int_{\partial\Omega}\left(\frac{\partial\varphi}{\partial n}\right)^2 d\sigma \leq C\int_\Omega (\Delta\varphi)^2 dx. \tag{25.18}$$

Hence, $\|w\|^2$ is bounded by $\|F\|^2$. [294]

Discussion.
Partial derivatives of a harmonic function with respect to the Cartesian coordinates are again harmonic. However, the partial derivatives with respect to curvilinear coordinates are not necessarily so.

25.12 Comparison theorem. Let u and v be harmonic functions on a bounded domain Ω, and $u \geq v$ on $\partial\Omega$. Then, $u \geq v$ throughout Ω.

25.13 Liouville's theorem.[295] If u is a bounded harmonic function on the whole space $\boldsymbol{R}^n$, then u is a constant.□[296]

25.14 More general elliptic equation. The essence of the Laplacian is that it is an operator giving the deviation of the value of the function from its local average. The Laplacian is obtained when we assume that the weight for the average is everywhere uniform (→**??**). We should be able to choose a weighted average. Then, a more general equation like

$$a_{ij}\frac{\partial^2 u}{\partial x_i x_j} + b_i \frac{\partial u}{\partial x_i} + c(x)u = 0 \tag{25.20}$$

with the positive definite matrix $Matr(a_{ij})$ appears. We may expect that the key properties of the Laplacian should be true even for $a_{ij}\partial_i\partial_j$, because they are due to the averaging principle. Indeed the maximum principle is true if $c \leq 0$ as intuitively expected. (The most statements above hold if $c \leq 0$[297]).

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[294] The following theorem is also relevant.
Aleksandrov's theorem. The solution to Poisson's equation smoothly depends on the charge distribution. Or, more precisely: Let D be a bounded domain and u be a solution of $\Delta u = f$ in D with a homogeneous Dirichlet condition and is continuous up to the boundary of D. Then,

$$\sup_D u \leq C||f||_d, \tag{25.19}$$

where C is a constant dependent on the spatial dimensionality and the radius of D, and $||\cdot||_d$ is the L^d-norm. [L^p-norm for any positive p is defined by $||f||_p \equiv \left(\int |f|^p dx\right)^{1/p}$, where the integral is the Lebesgue integral (→**19**).] See Egorov-Shubin, p93.
[295] Joseph Liouville, 1809-1882.
[296] Folland p94 (2.11).
[297] See, Yu. V. Egorov and M. A. Shubin (eds) *Partial Differential Equations III*, Chapter 2 (Springer, 1991)

26 Wave Equation: Finiteness of propagation speed

Wave equations are representative hyperbolic equations. With the aid of energy conservation, we discuss the well-posedness of wave equation problems. A general method to solve 3-space wave equation is given (method of spherical means due to Poisson), which clearly shows Huygens' principle. Finally, the characterization of hyperbolic equation with constant coefficients due to Gårding is summarized.

Key words: characteristic curve, domain of dependence (influence), energy conservation, Huygens' principle, method of spherical means, focusing, hyperbolicity in Gårding's sense, finiteness of propagation speed.

Summary:
(1) Wave equations have well-defined domains of dependence and influence: they are called the past and the future in relativity (**30.3**). Huygens' principle is correctly captured by the wave equation (**26.8**).
(2) Wave equations allow propagation of a solution which is not smooth along a special curve (characteristic curve) (**26.2**).
(3) Wave equations preserve energy. This implies well-posedness of wave equation problems (**26.4**, **26.6**).
(4) All the general methods to solve d-space wave equations are based on reducing them to 1D wave equations (**??**. For another, see **28.45**). In $d(\geq 2)$-space, the time evolution due to wave equations may reduce the smoothness in the initial waves (**26.10**).
(5) Gårding conclusively characterized hyperbolicity (**26.12**-**26.14**), which implies finiteness of propagation speed (**26.15**).

26.1 Elementary summary. We have learned where the wave equations appear (→**??**, **??**-**??**, **??**), and physically argued what auxiliary conditions can ensure the uniqueness of the solution (→**??**). We know how to obtain the unique solution to the initial value problem in $\boldsymbol{R}$ as d'Alembert's formula (→**??**) for the 1-space problem

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2}. \tag{26.1}$$

We know from the telegrapher's equation (→**??** or the Maxwell-Cattaneo equation →**24.10**) that the second order time derivative prohibits infinite speed propagation of the signal.

Exercise.
Solve

$$u_{tt} - u_{xx} = e^{-|x-t|} \tag{26.2}$$

on $\boldsymbol{R} \times \boldsymbol{R}$.

26.2 Characteristic curve. The solution method in **??**(1) reduces the 1-wave equation (26.1) to two first order PDEs whose characteristic curves (→**??**) are $x \pm ct = const.$ These curves (actually lines) are called the *characteristic curves* of the wave equation (→(C) below). If u is a solution to (26.1), then we can prove the following general identity:

$$u(A) + u(C) = u(B) + u(D), \tag{26.3}$$

where A-D are the apices of any parallelogram ABCD in space-time whose edges are parallel to the characteristic curves $x \pm ct = const.$ This equality can be shown easily with the aid of d'Alembert's solution (→**??**). We may characterize a 'generalized solution' to (26.1) as any function u satisfying (26.3).

Discussion.
(A) Hyperbolic equations allow propagation of discontinuity without smoothing. Rewrite the wave equation (3.1) in the following form:

$$\frac{\partial v}{\partial t} = c\frac{\partial u}{\partial x}, \ \frac{\partial u}{\partial t} = c\frac{\partial v}{\partial x}. \tag{26.4}$$

Is there any curve $\phi(x,t) = 0$ on which u and v are continuous but their derivatives jump? [We have already discussed this in detail in **??** Discussion.]
(B) Try the same thing as above for the telegrapher's equation.
(C) We have already discussed the meaning of the characteristic curve in (A). Let us continue the discussion for more general cases. Consider

$$\frac{\partial^2 u}{\partial t^2} - c^2(x)\frac{\partial^2 u}{\partial x^2} = 0 \tag{26.5}$$

where $c(x)$ is a positive valued function. Suppose there is a discontinuity of the solution of this equation along a curve $\varphi(x,t) = 0$. We assume the solution is smooth except on this curve. We rewrite the equation with the new coordinate $X = \varphi(x,t)$ and $Y = \psi(x,t)$, where ψ is chosen to make (X,Y) a well-behaved coordinate system.
(1) Show that the result can be written as

$$Q(\varphi,\varphi)\frac{\partial^2 u}{\partial X^2} + 2Q(\varphi,\psi)\frac{\partial^2 u}{\partial X \partial Y} + Q(\psi,\psi)\frac{\partial^2 u}{\partial Y^2} + L(\varphi)\frac{\partial u}{\partial X} + L(\psi)\frac{\partial u}{\partial Y} = 0, \tag{26.6}$$

where

$$Q(\varphi,\psi) = \frac{\partial \varphi}{\partial t}\frac{\partial \psi}{\partial t} - c^2(x)\frac{\partial \varphi}{\partial x}\frac{\partial \psi}{\partial x}, \tag{26.7}$$

$$L(\varphi) = \frac{\partial^2 \varphi}{\partial t^2} - c^2(x)\frac{\partial^2 \varphi}{\partial x^2}. \tag{26.8}$$

(2) Suppose $\partial u/\partial X$ has a discontinuity across $\varphi(x,t)=0$. Then, show that

$$Q(\varphi,\varphi)=0 \tag{26.9}$$

must be satisfied. This equation is called the *characteristic equation*, and $\varphi=$ const. is called a *characteristic curve*.
(3) See that $x=\pm ct=$ const. are characteristic curves for the ordinary wave equation.
(4) There are two characteristic curves passing through a given point. The singularity we are discussing is constrained on them, so its propagating speed should be given by

$$\frac{dx}{dt}=-\frac{\partial\varphi(x,t)}{\partial t}\Big/\frac{\partial\varphi(x,t)}{\partial x}=\pm c(x). \tag{26.10}$$

(5) Notice that to solve the equation $Q=0$ is equivalent to solving (6.9).

26.3 Domain of dependence, finite propagation speed. D'Alembert's solution (→**??**) clearly shows that u at x at time t is completely determined by the initial data in the interval $[x-ct,x+ct]$. This interval is called the *domain of dependence*. Conversely, the initial data at ζ can influence the interval $[\zeta-ct,\zeta+ct]$ of the space at time t. This of course means that the disturbance can propagate at fastest with speed c in contradistinction to parabolic equations (→**24.9**).

Discussion: Characteristic initial value problem.
The light cone is a characteristic surface. If u is given on a characteristic surface as is shown in figure, then the solution is uniquely determined within its domain of influence. Hence, generally no boundary value problem in a closed domain has a solution for wave equations.

26.4 Energy conservation. The *energy integral*

$$E(t)=\frac{1}{2}\int_0^l\left\{\left(\frac{\partial u}{\partial t}\right)^2+c^2\left(\frac{\partial u}{\partial x}\right)^2\right\} \tag{26.11}$$

is time independent for classical solutions (→**??**). A formal calculation exchanging the order of differentiation with respect to time and integration is justifiable (→**15.18**).

Discussion.
Suppose that a vibrating string of length L with a fixed end condition is subjected to a damping force $-a\frac{\partial\psi}{\partial t}$. Discuss how the energy conservation is violated.

26.5 Uniqueness revisited. Although we already know the unique existence of the solution to the initial value problem of (26.1) in $\boldsymbol{R}$, let us reconsider the problem in terms of the energy integral. Since the equation is linear, to prove the uniqueness, we have only to consider that

the homogeneous problem has only the zero solution: if v satisfies (26.1) and the auxiliary conditions $v(x,0)=0$ for $x\in D$, and $v(x,t)=0$ for $x\in\partial D$ for $t\geq 0$, then $v(x,t)=0$ in $D\times[0,t]$. For this initial condition the total energy (26.11) is zero, so that the constancy of energy integral implies that $\partial_t v(x,t)=\partial_x v(x,t)=0$. This implies (with the aid of the mean value theorem) v is a constant. Since v is continuous, this implies that $v\equiv 0$.

Discussion.
(1) **Riemann's method**. Let

$$L\equiv\rho(x)\frac{\partial^2}{\partial t^2}-\frac{\partial^2}{\partial x^2}. \tag{26.12}$$

Find the solution satisfying

$$\begin{aligned} Lv &= 0, && (26.13)\\ v|_{t=t_0,x=x_0} &= 1, && (26.14)\\ 2\sqrt{\rho(x)}\frac{\partial v}{\partial s}+\frac{\partial\sqrt{\rho(x)}}{\partial s}v &= 0 \ \text{ on characteristic curves.} && (26.15)\end{aligned}$$

The solution v is called the *Riemann function* (fundamental solution). In terms of this function, the solution to the initial value problem can be obtained as

$$(\sqrt{\rho(x)}u)(P)=\frac{1}{2}\left[(\sqrt{\rho(x)}uv)(A)+(\sqrt{\rho(x)}uv)(B)\right]+\frac{1}{2}\int_{x_A}^{x_B}\rho(x)\left(\frac{\partial u}{\partial t}v-u\frac{\partial v}{\partial t}\right)dx, \tag{26.16}$$

wher A, B, P are the points in the figure. The formula is called *Riemann's formula*, and d'Alembert's formula is its special case.
(2) How can we determine Riemann's function? The problem is to solve v for which the auxiliary conditions are given on the characteristic curves. Such a problem is called a *Goursa's problem* or *characteristic boundary value problem*. We change the independent variables from x,t to φ_+ and φ_- (characteristic curves $\rightarrow$**26.2**(C)). The problem now reads

$$\frac{\partial^2 v}{\partial\varphi_-\partial\varphi_+}-a\frac{\partial v}{\partial\varphi_-}-b\frac{\partial v}{\partial\varphi_+}=0 \tag{26.17}$$

with the boundary conditions

$$v(\varphi_-,0)=f_-,\ \ v(\varphi_+,0)=f_+. \tag{26.18}$$

Here a, b and$f_\pm$ are given functions. If we define

$$\Psi_\pm=\frac{\partial v}{\partial\varphi_\pm}, \tag{26.19}$$

then, the PDE can be cast in the following simultaneous Volterra integral equation:

$$\Psi_- \ = \ f_-'+\int_0^{\varphi_+}[a(\varphi_-,\eta)\Psi(\varphi_-,\eta)+b(\varphi_-,\eta)\Psi_+(\varphi_-,0)]d\eta,$$

(26.20)

$$\Psi_+ = f'_+ + \int_0^{\varphi_-} [a(\xi,\varphi_+)\Psi_-(\xi,\varphi_+) + b(\xi,,\varphi_+)\Psi_+(\xi,\varphi_+)]d\xi.$$

(26.21)

This can be solved by an interative replacement method with the starting choice of $\Psi_- = f'_-$, $\Psi_+ = f'_+$.

26.6 Well-posedness. We consider two problems (26.1) with $u(x,0) = f_i(x)$ and $\partial_t u(x,0) = g_i(x)$ in $\boldsymbol{R}$ $(i = 1, 2)$. Denoting each solution as u_i, we can easily get

$$|u_1(x,t) - u_2(x,t)| \leq ||f_1 - f_2||_{max} + |t|\,||g_1 - g_2||_{max} \tag{26.22}$$

from d'Alembert's formula (→**??**). Hence, the solution depends on the data continuously. That is, small changes of the data cause a small change in the solution for any finite time.

26.7 Inhomogeneous wave equation. Consider

$$\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial^2 u}{\partial x^2} = F(x,t) \tag{26.23}$$

in $\boldsymbol{R} \times \boldsymbol{R}$ with the initial condition $u(x,0) = f(x)$ and $\partial_t u(x,0) = g(x)$, where f is C^2 and g is C^1. The problem is a superposition of the homogeneous equation with the inhomogeneous initial conditions studied in **??** and the following problem of inhomogeneous equation with homogeneous initial conditions:

$$\frac{\partial^2 v}{\partial t^2} - c^2\frac{\partial^2 v}{\partial x^2} = F(x,t) \tag{26.24}$$

with $v(x,0) = 0$ and $\partial_t v(x,0) = 0$. The problem can be solved easily with the introduction of the new variables (a standard trick →**??**) $x \pm ct$ as in

$$v(x,t) = \frac{1}{2c}\int_0^t d\tau \int_{x-c(t-\tau)}^{x+c(t-\tau)} F(\sigma,\tau)d\sigma. \tag{26.25}$$

Notice that if $F(x,t)$ is an odd function of x, then so is v for all t.

26.8 Wave equation in 3-space, Huygens' principle. The initial value problem

$$\partial_t^2 u = c^2\Delta u \tag{26.26}$$

with the initial condition

$$u = f(x), \partial_t u = g(x) \text{ for } t = 0 \tag{26.27}$$

in 3-space has the following solution:

$$u(x,t) = \frac{1}{4\pi c^2 t}\int_{|y-x|=ct} g(y)d\sigma(y) + \frac{\partial}{\partial t}\left(\frac{1}{4\pi c^2 t}\int_{|y-x|=ct} f(y)d\sigma(y)\right). \tag{26.28}$$

This is an explicit expression of *Huygens' principle*. This equation can be a starting point of a numerical scheme. A demonstration of the equation follows.

Exercise.
Solve the following 3-wave equation:

$$u_{tt} = \Delta u \tag{26.29}$$

with the initial condition $u = x^2 + y^2 + z^2$ and $u_t = z$.

Needless to say, an inhomogeneous problem $\Box u = q$ can be solved by linear decomposition. The inhomogeneous problem with a homogeneous auxiliary conditions can be solved easily in terms of Green's functions (→**40**)

26.9 Method of spherical means [Poisson]. Define

$$M_h(\boldsymbol{x}, r) = \frac{1}{4\pi^2}\int_{|y|=1} h(\boldsymbol{x} + r\boldsymbol{y})d\sigma(\boldsymbol{y}), \tag{26.30}$$

where h is a C^2-function, and σ is the area element of the sphere. M_h is an even function of r. Using Gauss' theorem (→**??**), we get the following *Darboux's equation*

$$\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) M_h(\boldsymbol{x}, r) = \Delta M_h(\boldsymbol{x}, r). \tag{26.31}$$

Here Δ is the Laplacian acting on the function of $\boldsymbol{x}$. (26.26) is converted to

$$\frac{\partial^2}{\partial t^2}(rM_u) = c^2\frac{\partial^2}{\partial r^2}(rM_u), \tag{26.32}$$

where M_u is interpreted as a function of $\boldsymbol{x}$, r and t as $M_u(\boldsymbol{x}, r, t)$, and the initial condition becomes

$$M_u = M_f, \quad \partial_t M_u = M_g \quad \text{for } t = 0. \tag{26.33}$$

Notice that $M_u(\boldsymbol{x}, 0, t) = u(\boldsymbol{x}, t)$. (26.32) can be solved as (→**??**):

$$rM_u(\boldsymbol{x}, r, t) = \frac{1}{2}[(r+ct)M_f(\boldsymbol{x}, r+ct)+(r-ct)M_f(\boldsymbol{x}, r-ct)]+\frac{1}{2c}\int_{r-ct}^{r+ct} yM_g(\boldsymbol{x}, y)dy. \tag{26.34}$$

Using the fact that M_f and M_g are even functions of r, we can rewrite this as

$$M_u(\boldsymbol{x}, r, t) = \frac{(ct+r)M_f(\boldsymbol{x}, ct+r) - (ct-r)M_f(\boldsymbol{x}, ct-r)}{2r} + \frac{1}{2cr}\int_{ct-r}^{ct+r} yM_g(\boldsymbol{x}, y)dy. \tag{26.35}$$

Now, take the $r \to 0$ limit (l'Hospital's rule is used) and we finally arrive at (26.28)

26.10 Focusing effect. (26.28) implies that the smoothness of the solution u can be less than that of the initial data due to the derivative in the formula. This effect is called the *focusing effect*. This can happen when the initial condition is focussed into a small set, making caustics. This does not happen in 1-space.

26.11 What is the mathematical essence of the wave equation? Physically, that the singularity can be propagated without smoothing (propagation of shock waves, for example) is a remarkable distinction from the diffusion equation (parabolic equation). Also the finiteness of the speed of propagation is in striking contrast to the diffusion equation (→**24.9**). Since the wave equation is nothing but Newton's equation of motion of an idealized elastic body (→**??**), the Newton-Laplace determinacy should apply. That is, the Cauchy problem must be well-posed (→**24.3**). Gårding[298] answered the question decisively at least for the constant coefficient linear partial differential equations (of any order).

26.12 Hyperbolicity in Gårding's sense. Let $L \rightleftharpoons L(\partial_t, \nabla)$ be a N-th order linear PDE operator with constant coefficients. If L contains $\partial^N/\partial t^N$[299] and if the real parts of the zeros $\lambda_i(\xi)$ of the characteristic equation $L(\lambda, i\xi) = 0$[300] considered as an equation for λ are bounded as a function of ξ, then we say $Lu = 0$ is a *hyperbolic equation in Gårding's sense*.

26.13 Example.
(1) Wave equation $(\partial_t^2 - c^2\Delta)u = 0$. $L(\lambda, i\xi) = \lambda^2 + c^2\xi^2$. Therefore, $\lambda(\xi) = \pm ic|\xi|$. That is, the characteristic roots are purely imaginary, so obviously the equation is hyperbolic in Gårding's sense.

[298] Gårding wrote a nice book on mathematics: L. Gårding, *Encounter with Mathematics* (Springer, 1977). Those who are interested in mathematics as a part of the modern culture will enjoy the book.
[299] If the highest order derivative is not ∂_t^N, then **26.15** below does not hold. That is, the propagation of front has infinite speed.
[300] Here not only the highest order terms but all the derivatives are taken into account. Furthermore i accompanies with ξ.

(2) Diffusion equation $(\partial_t - D\Delta)u = 0$. $L(\lambda, i\xi) = \lambda + D\xi^2$, so that $\lambda(\xi) = -D\xi^2$ is real and is not bounded as a function of ξ.
(3) However, if we add a second order time derivative term with a small positive coefficient as $(\epsilon\partial_t^2 + \partial_t - D\Delta)u = 0$, which is called the telegrapher's equation or Maxwell-Cattaneo equation (→**??**, **24.10**), the situation is drastically different from the diffusion equation. For this $L(\lambda, i\xi) = \epsilon\lambda^2 + \lambda + D\xi^2$, so that $\lambda(\xi) = (-1 \pm \sqrt{1 - 4\epsilon D\xi^2})/2\epsilon$. Hence its real part is bounded as a function of ξ. That is, the telegrapher's equation is hyperbolic in Gårding's sense.
(4) Certainly, the Laplace equation $\Delta u = 0$ is not hyperbolic.

Discussion.
The equation for transversal oscillations of a beam is given by

$$\frac{\partial^4 u}{\partial x^4} + c^{-4}\frac{\partial^2 u}{\partial t^2} = f(x,t), \tag{26.36}$$

where f is essentially the external load. This equation is hyperbolic.

26.14 Theorem [Gårding]. The Cauchy problem $Lu = 0$ under the Cauchy condition $\partial^k f/\partial t^k(0,x) = u_k(x)$ $(0 \le k \le N-1)$ is well-posed in the sense of Hadamard (→**24.3**) if and only if L is hyperbolic in Gårding's sense. □[301]
Hence, the determinacy (and more) for the wave equation is vindicated.

26.15 Theorem [Finiteness of the propagation speed]. Let Ω be the support of the Cauchy data for $Lu = 0$, where L is a linear partial differential operator with constant coefficients, and is hyperbolic in the sense of Gårding (→**26.12**). Then the support of the solution at time $t > 0$ is included in the set $\{x : \cup_{\xi\in\Omega}|x - \xi| \le ct\}$, where c is a finite number such that

$$c \ge \max_{i-1,\cdots,m;|\xi|=1} \bar{\lambda}_i(\xi). \tag{26.37}$$

Here $\overline{\lambda}_i$ are zeros of the symbol of the principal part of the differential operator (and are real for hyperbolic equations).□[302]

[301] See John, Section 5.2.
[302] S. Mizohata, *Partial Differential Equations* (Iwanami, 1965), Theorem 4.9.

27 Numerical Solution of PDE

Although we have been discussing analytical methods to solve PDE, most problems are intractable by exact methods. In this section elementary numerical methods to solve PDE are outlined. We require a numerical scheme to be stable and consistent (i.e., converging to the original problem in the continuum limit). This is a section for ABC of numerical analysis.

Key words: discretization, consistency, stability, convergence, von Neumann condition, Courant-Friedrichs-Lewy condition

Summary:
(1) There are two major methods to discretize a continuum problem: the Galerkin method and sampling at space-time lattice points (**31.2**). There can be many unconventional discretization schemes (**31.4**).
(2) Any discrete scheme must recover the original problem in the continuum limit (consistency of the scheme). If the solution to a scheme is bounded, then the scheme is said to be stable. For linear problems Consistency and stability imply convergence of the scheme (i.e., the solution to the scheme converges to the true solution in the continuum limit) (**27.7**).
(3) Stability conditions for a scheme may be understood, roughly, by the condition that physical propagation speed of the signal does not outrun the numerical propagation speed (**27.9**, **27.11**).

27.1 Discretization. To use computers to solve a differential equation, unless we use symbolic manipulation, we must discretize everything and express quantities in a finite number of rational numbers. Thus the fundamental question of numerical computations of differential equations is how faithful this map to the discrete world is.
Numerical analysis is a discipline to analyze numerical algorithms and is as old as analysis itself. Already Newton discussed a series expansion method to solve ODE in his first calculus paper (1669). Euler introduced discretization methods in 1743.

Discussion.
Consider[303]

$$\frac{du}{dt} = f(u), \tag{27.1}$$

[303] M. Yamaguti and H. Matano, Euler's finite difference scheme and chaos, Proc. Japan Acad. **55** Ser.A, 78-80 (1979).

where f satisfies $f(0) = f(1) = 0$, $f(u) > 0$ for $u \in (0,1)$ and $f(u) < 0$ for $1 < u < \kappa$ for some positive $\kappa > 1$. Then, its Euler differencing result

$$u_{n+1} = u_n + \Delta t f(u_n) \tag{27.2}$$

exhibits chaos for $\Delta t > c_1$ for some positive c_1. Here 'exhibiting chaos' means that the solution has a 'natural' relation to random numbers (or the outcome of coin-tossing).[304]

(B) Consider the following *logistic equation*

$$\frac{du}{dt} = u(1-u). \tag{27.3}$$

(1) Solve this equation with the initial condition $u = u_0 \in (0,1)$ analytically.

(2) Get the following type of difference equation with the aid of the center differencing scheme:

$$u_{n+1} = v_n + \alpha u_n(1-u_n), \quad v_{n+1} = u_n, \tag{27.4}$$

where $\alpha = 2\Delta t$, $u_n = u(n\Delta t)$ and $v_n = u_{n-1}$.

(3) The equation (27.4) defines a map from $\boldsymbol{R}^2$ into itself. The map exhibits chaos irrespective of the size of Δt.[305] A more careful statement is as follows. Let time T be fixed and $N \equiv T/\Delta t$. If $\Delta t \to 0$, then up to N there is no pathological behavior. However, if Δt is fixed, then for sufficiently large N (consequently for large T), pathological behavior will show up.

(4) The equation (27.4) converges to (more generally, see **27.3** Discussion)

$$\frac{du}{dt} = v(1-v), \quad \frac{dv}{dt} = u(1-u). \tag{27.5}$$

This equation does not exhibit chaos, but is unstable near $u = v = 1$.

27.2 Two major methods of discretization. There are two major methods to map a continuous problem to a discrete problem. One is the sampling method (recall Green's approach →**??**), and the other is the Fourier expansion method.

The sampling method tries to represent a function $f(x)$ by a set of function values sampled at appropriately located sampling points, and is usually called "the discrete variable method." We have already used its primitive version in **1** (**??**, **??**, **??**).

The Fourier expansion method tries to describe a function $f(x)$ as a truncated generalized Fourier expansion $f_N(x)$ (→**16.14**). A typical method is the one called the *Galerkin method*: Put $f_N(x) = \sum_{n=1}^{N} a_n \phi_n(x)$, where ϕ_n denotes orthonormal functions (→**16.10**), into the original equation. Then, multiply $\phi_m(x)$ and integrate over x. This will give a set of equations for the Fourier coefficients. This is a finite set of algebraic equations, so there are many ways to solve it.[306]

[304] S. Y. Oono, Period $\neq 2^n$ implies chaos, Prog. Theor. Phys. **59**, 1029-1030 (1978).

[305] S. Ushiki, Central differencing scheme and chaos, Physica D **4**, 407-424 (1982).

[306] The Galerkin method is often used to solve PDE. In this case the resultant set of equations become a simultaneous set of ODEs. The method is also very important

27.3 Consistency, stability and convergence. If the discretization scheme recovers the original equation in the limit which recovers a function from its discretized version, we say the method is *consistent*. If the discretized solution is bounded in terms of the input data (initial condition, etc), we say the method is *stable*. Consistency and stability imply the convergence of the scheme. That is, if a numerical scheme is consistent and stable, then the scheme gives the solution which converges to the true solution of the original continuous problem in the limit recovering a function from its discretized version. There are consistent but unstable schemes.[307]

Discussion.
Probably the most famous example is the center differencing scheme:[308]
Since $dx/dt \simeq [x(t_{n+1}) - x(t_{n-1})]/2h$, where h is the time increment $t_{n+1} - t_n = h$ for all n, we might be able to rewrite $dx/dt = f(x)$ as

$$\frac{x(t_{n+1}) - x(t_{n-1})}{2h} = f(x(t_n)). \tag{27.6}$$

The scheme is called the *center differencing scheme*. It is known that this equation converges to the following simultaneous equation:

$$\frac{dx}{dt} = f(y), \quad \frac{dy}{dt} = f(x). \tag{27.7}$$

If $x = y$ is stable, then there is no problem, but often this is not the case. The method doubles the dimensionality of the phase space (= the space where the trajectories are). Hence, even a two dimensional ODE could produce chaos as artifact after center differencing discretization.

27.4 Discretization of PDE. The simplest method to discretize a PDE is to use a regular mesh on its domain and use the values of the functions sampled at the mesh points.[309] As explained in **27.2** we can also use the Galerkin method to discretize the PDE with the aid of generalized Fourier expansion (in terms of an appropriate complete set). Always the consistency and stability of the scheme are crucial.

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as a tool to prove the existence of the solutions to PDEs like the Navier-Stokes equation. See Ladyzhenskaya quoted in **??** Discussion.

[307] One might think that if a scheme is not consistent, then the scheme is useless. However, the situation is not this simple, because we do not take the $h \to 0$ limit in practice. Hence, even if the limit may be different from the original equation, still the numerical solution for a finite h may be a good solution.

[308] M. Mizutani, T. Niwa and T. Ohno, Chaos and bifurcation phenomena in limiting central difference scheme, J. Math. Kyoto Univ. **23**, 39-54 (1983).

[309] A. Iserles, *A First Course in the Numerical Analysis of Differential Equations* (Cambridge UP, 1996) is an excellent introdution to the mathematical side of numerical analysis. Although, as the author explicitly says, it is not for practitioners, still the comments in the end of each chapter contain updated information and are useful.

An important point recognized explicitly in recent years is that good modeling of physics on a discrete space can motivate a useful numerical solver for PDE.

Discussion.
A typical example is the numerical schemes for the simple equation

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0, \tag{27.8}$$

where c is a constant. We can solve this equation analytically easily (→**??** Discussion(2), **??**, **??**), e.g., for the initial condition $u(x,0) = 1$ for $x > 0$ and 0, otherwise. Ordinary discretization methods give miserable results (Try to solve this with the simple Euler scheme). However, we know the essence of the equation is the translational symmetry of space:

$$u(x, t+\delta t) = u(x - c\delta t, t) \tag{27.9}$$

for any δt (this is the equation for weak solutions, cf. **2B.3**). The problem is that if we discretize u, then we know only $u(x_i)$ at sampling points $\{x_i\}$. Therefore, it is very hard to describe the translational symmetry. The most natural idea is: (i) first reconstruct the continuous u from the discrete sampled values by interpolation, (ii) then translate the reconstructed continuous function according to (27.9), (iii) Finally sample the values of the shifted function at the grid points (see Figure). Actually, this reconstruction-resampling scheme is used in one of the best schemes for (27.8). Thus, the reader should keep in mind that there is still an ample room to devise unconventional numerical schemes for PDE.

27.5 Discretization of Poisson's equation. Practically useful numerical schemes use simple discretization to solve a Poisson's equation:[310]

$$\Delta u = f \tag{27.10}$$

on a region D with the boundary condition $u = g$ on ∂D. Let us consider this in 2-space. To discretize this, we follow Euler: Let h be the lattice spacing of the sampling regular square lattice; the sampling points are (ih, jh), where i and j are integers. Let us denote the value of a function f at (ih, jh) as $f[i,j]$. The simplest scheme is

$$\Delta_h u[i,j] \equiv \frac{u[i+1,j] + u[i,j+1] + u[i-1,j] + u[i,j-1] - 4u[i,j]}{h^2} = f[i,j] \tag{27.11}$$

with $u[i,j] = g[i,j]$ if (ih, jh) is on the discretized boundary. Let us denote the set of grid points in the domain by D_h and the discretized boundary by Γ_h.

[310] If the domain is regular, say, a square, then, Fourier transform methods are practical.

27.6 CHECK algebraic equation, so that if the matrix defined by Δ_h is non-singular, then we can solve it. The non-singularity of the matrix can be shown with the aid of the maximum principle (→**25.6**) which is still true after discretization, because the mean value theorem is correct as can be seen from the form of Δ_h (→**??**). More precisely, we can show easily that if

$$\Delta_h v \geq 0 \text{ on } D_h \text{ and } v \geq 0 \text{ on } \Gamma_h, \tag{27.12}$$

then $v \geq 0$ on $D_h \cup \Gamma_h$. This implies that if v and $-v$ both satisfy (27.12), then $v = 0$ on $D_h \cup \Gamma_h$. That is, if $\Delta_h v = 0$ on D_h and $v = 0$ on Γ_h, then its unique solution is $v = 0$ everywhere. Hence, the matrix defining the simultaneous linear equation (27.11) is regular, and (27.11) has a unique solution. The matrix is very sparse, so many sparse marix solvers can be used.

27.7 Consistency and stability ⇒ convergence. Is this discretization scheme consistent? That is, in the $h \to 0$ limit can we claim that the discretized version converges to the original equation? If u is C^3 on the domain, we can demonstrate

$$\max_{x \in D_h} |\Delta_h u - \Delta u| \leq \frac{h}{3} \max_{x \in D} \left\{ \left| \frac{\partial^3 u}{\partial x^3} \right|, \left| \frac{\partial^3 u}{\partial y^3} \right| \right\}. \tag{27.13}$$

Since we know the solution to Poisson's equation is very smooth (→**25.10**) this is enough to demonstrate that indeed our scheme is consistent.

Our scheme is also stable: the solution to (27.11) is bounded by the 'magnitudes' of f and g in the problem as

$$\max_{x \in D_h \cup \Gamma_h} |u(x)| \leq c(\max_{x \in D_h} |f| + \max_{x \in \Gamma_h} |g|), \tag{27.14}$$

where c is a positive constant independent of h, f and g.[311]
Now we have
Theorem. The solution u_h to (27.11) converges uniformly to the solution to the original problem. More precisely,

$$\max_{x \in D_h \cup \Gamma_h} |u_h(x) - u(x)| \leq ch \max_{x \in D} \left\{ \left| \frac{\partial^3 u}{\partial x^3} \right|, \left| \frac{\partial^3 u}{\partial y^3} \right|, \left| \frac{\partial u}{\partial x} \right|, \left| \frac{\partial u}{\partial y} \right| \right\}. \tag{27.15}$$

□
We thus know that u_h converges to the true solution, but actually this is shown only on the dense set that are limit points of the lattice points. Since we know from the general theory that the true solution is very smooth, this should be enough.

[311] In this case, we need not restrict the size of h, but usually the stability holds for h up to some upper bound as we will see in the case of diffusion equation (→**27.8**).

27.8 Discretizing diffusion equation: θ-method. Let us consider 1-space diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + f \tag{27.16}$$

on $Q_T = \{(x,t); x \in (0,1), t \in (0,T)\}$. We impose the initial condition $u(x,0) = a(x)$ for $x \in (0,1)$. We must also specify a boundary condition at $x = 0$ and 1, but we will not explicitly write it down. The 1-space version of Δ_h is given by

$$\Delta_h u[i] = \frac{u[i+1] + u[i-1] - 2u[i]}{h^2}. \tag{27.17}$$

We must discretize the time axis with the spacing τ. We introduce the following notation

$$u_n[i] = u(ih, n\tau), \tag{27.18}$$

and

$$u_{n+\theta}[i] = \theta u_{n+1}[i] + (1-\theta)u_n[i]. \tag{27.19}$$

We introduce the following scheme called the *θ-method*:

$$\frac{u_{n+1}[i] - u_n[i]}{\tau} = \Delta_h u_{n+\theta}[i] + f_{n+\theta}[i]. \tag{27.20}$$

For $\theta = 0$ this is the standard Euler method; for $\theta = 1/2$ it is called the *Cranck-Nicholson method*; for $\theta = 1$ it is called the *backward Euler method*. The latter two methods are called implicit methods, because we cannot immediately read off the updated data.

27.9 Stability analysis. A standard method to analyze the stability of a scheme is to compute the so-called *amplification factor* A:

$$u_n[l] = A^n e^{iklh}. \tag{27.21}$$

The basic idea is that we prepare spatially bounded 'initial condition' (that is why e^{ikl}) and study its time evolution. If $|A| > 1$, we are in trouble.

27.10 Von Neumann's stability condition.[312] In our case the scheme is stable if $u_n[i]$ is bounded for all i and n by a number proportional to the 'magnitude' of the initial condition a. Let us measure the 'magnitude' with the following 'normalized ℓ_2-norm':

$$||v||_h \equiv \left\{ \frac{1}{N} \sum_{i=0}^{N-1} v[i]^2 \right\}^{1/2}. \tag{27.22}$$

[312] John von Neumann, 1903-1957.

The stability is defined by the inequality

$$||u_n||_h \leq c||a||_h \tag{27.23}$$

for all n with some positive constant c independent of a, h and $\tau(< 1)$.
Theorem [von Neumann]. A necessary and sufficient condition for the scheme (27.20) to be stable is that there is a nonnegative constant b such that for any k

$$\left| \frac{h^2 - 4(1-\theta)\sin^2 \frac{\pi k}{4N}}{h^2 + 4\theta\tau \sin^2 \frac{\pi k}{4N}} \right| < 1 + b\tau \tag{27.24}$$

for any $k \in \boldsymbol{Z}$. In particular, the scheme is stable for $\theta \in [1/2, 1]$ unconditionally and for $\theta \in [0, 1/2]$ under the condition

$$\frac{\tau}{h^2} \leq \frac{1}{2(1-2\theta)}, \tag{27.25}$$

which is called the stability condition.[313] □
Generally speaking, implicit schemes are more stable as seen here. However, implicit schemes are usually computationally more time consuming. The reader might think that exploiting the stability, we can choose a large τ to compensate the complexity. Sometimes, this indeed works, but stability does not mean that the obtained solution is accurate, so that choosing a large τ is not usually wise.

Discussion.
(A) In (27.20) put $\theta = 0$ and $f = 0$. Assume

$$u_{n,j} = \lambda(k)^n e^{ik\ (jh)}. \tag{27.26}$$

Then, this is a solution to (27.20), if

$$\lambda(k) = 1 - 4\frac{\tau}{h^2}\sin^2(kh/2). \tag{27.27}$$

This $\lambda(k)$ is the amplification factor for the mode k. From this we conclude that

$$\frac{\tau}{h^2} < \frac{1}{2} \tag{27.28}$$

is required for the scheme to be stable. The condition can be rewritten as

$$D < \frac{h^2}{2\tau}. \tag{27.29}$$

This may be interpreted as a condition for the numerical diffusion constant to be larger than the physical diffusion constant.

[313] The stability condition may depend on the norm used. If we use the ℓ_∞-norm, then the RHS of (27.25) reads $1/2(1-\theta)$ for $\theta \in [0, 1]$.

If $\tau/h^2 = 1/2$, the scheme may violate the maximum principle.
(B) In **27.8** try the same and derive the formula for the amplification factor for the θ method:

$$\lambda(k) = \frac{1 - 4(1-\theta)(\tau/h^2)\sin^2(kh/2)}{1 + 4\theta(\tau/h^2)\sin^2(kh/2)}. \tag{27.30}$$

From this the stability condition is given by (the von Neumann stability condition **27.9**)

$$\frac{\tau}{h^2}(1-2\theta) < \frac{1}{2}. \tag{27.31}$$

For $\theta = 1/2$, the method is called the *Cranck-Nicolson scheme*. In this case, if $\tau/h^2 = 1$, the scheme is stable, but does not satisfy the maximum principle (the number of peaks may increase).
(C) Consider the following diffusion-advection equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - b\frac{\partial u}{\partial x}, \tag{27.32}$$

where b is a continuous function of x and t with boundedness: $|b| < B$. Apply a discretization scheme (not complicated one, please) and study its stability.

27.11 Consistency and convergence of θ-method. If u is smooth enough,[314] then we can show that the θ-method is consistent. Under the stability condition discussed in **27.10**, the solution u_h to (27.20) converges to the solution to the original PDE in the $h \to 0$ limit. More precisely,

$$\max_n ||u_{hn} - u_n||_h \le T\left\{\left|\theta - \frac{1}{2}\right| \tau \max\left|\frac{\partial^2 u}{\partial t^2}\right| + \frac{\tau^2}{12}\max\left|\frac{\partial^3 u}{\partial t^3}\right| + \frac{h^2}{12}\max\left|\frac{\partial^4 u}{\partial t^4}\right|\right\}. \tag{27.33}$$

27.12 Courant-Friedrichs-Lewy condition. Let us return to the simple advection problem (27.8). Consider the following simple Euler scheme

$$\frac{u_n[i] - u_{n-1}[i]}{\tau} + c\frac{u_n[i] - u_n[i-1]}{h} = 0. \tag{27.34}$$

This is called the *upstream approximation*, because if c is interpreted as the stream velocity, the scheme uses the upstream information only. The scheme satisfies the stability condition, if

$$\tau \le \frac{h}{c}. \tag{27.35}$$

The condition is called the *Courant-Friedrichs-Lewy condition*[315] (CFL condition). This implies that the numerical propagation speed h/τ

[314] C^4 in space and C^3 in time, for example.
[315] Richard Courant, 1888-1972; Kurt Otto Friedrichs, 1901-1983.

must not be smaller than the physical propagation speed c. In other words, if physics outruns computation, the scheme becomes unstable. A similar interpretation may be possible for **27.10**.

Exercise.
(1) Compute the amplification factor for (13.28) and derive the Courant-Friedrichs-Lewy condition.
(2) Show that the down stream scheme, which replaces $u_n[i] - u_n[i-1]$ in the upstream scheme with $u_n[i+1] - u_n[i]$ is always unstable.

27.13 Wave equation. A standard differencing practice to solve 1-space wave equation $u_{tt} - c^2 u_{xx} = 0$ is the simple Euler scheme:

$$\begin{aligned} u_{n+1}(i) &= 2u_n(i) - u_{n-1}(i) \\ &\quad + \left(\frac{c\Delta t}{\Delta x}\right)^2 \{u_n(i+1) + u_n(i-1) - 2u_n(i)\}. \end{aligned} \tag{27.36}$$

It is easy to generalize this to d-space (The stability limit due to the CFL condition is $c\Delta t/\Delta x \leq 1/\sqrt{d}$). This is a very stable and simple scheme, and is widely used. However, it suffers from the dispersion error (The scheme conserves energy very well, but distorts initial conditions with steep wave fronts.)

Discussion
The following scheme is called the *angled derivative method*:

$$u_{n+2}(i) = \left(1 - 2\frac{\Delta t}{\Delta x}\right)(u_{n+1}(i) - u_{n+1}(i-1)) + h_n(i-1). \tag{27.37}$$

Since the method intertwines space and time discretization, it cannot be derived by the consideration of discretizing time evolution. The method is an excellent one to propagate steep waves.
Exercise.
Study the stability condition of this simple scheme and demonstrate that we indeed need the Courant-Friedrichs-Lewy condition (the numerical propagation speed must be faster than the physical speed).

28 Fourier Transformation

Basics of Fourier transform including the principle of FFT, major qualitative features like the uncertainty principle, sampling theorem, Wiener-Khinchine theorem are discussed in the first two subsections. Then, Fourier analysis of generalized functions and related topics such as Poisson's sum formula, the Plemelj formula are treated in the third subsection. As a related topic, Radon transform is discussed in the last subsection, which underlies many tomographic techniques.

28.A Basics

Fourier analysis is reviewed. The relation between smoothness of the function and the decay rate of its Fourier transform is important. As theoretical applications, uncertainty principle, sampling theorem and the Wiener-Khinchin theorem about spectral analysis are discussed.

Key words: Fourier transform, deconvolution, inverse Fourier transform, sine (cosine) transform, bra-ket notation, Plancherel's theorem, Riemann-Lebesgue lemma

Summary:
(1) Fix your convention of Fourier transform (**28.1**, **28.7**). Deconvolution is often the place where Fourier transformation is effective (**28.2**). Linear differential operators become multiplicative operators (**28.3**).
(2) The decay rate of the Fourier transform and the smoothness of its original function are closely related just as in the Fourier expansion cases (**28.11**).

28.1 Fourier transform. Let f be an integrable function ($\rightarrow$**15.9**) on $\boldsymbol{R}$. If the following integral exists

$$\hat{f}(k) = \mathcal{F}(f)(k) \equiv \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \tag{28.1}$$

it is called the *Fourier transform* of f. Multidimensional cases can be treated similarly.

Exercise.
(A) Consider the Fourier transform of a wave train of finite duration. Or, more concretely, compute the Fourier transform of

$$f(t) = [\Theta(t+T) - \Theta(t-T)] \cos at, \tag{28.2}$$

Sketch the Fourier transform.
(B)
(1) Demonstrate the Fourier transform of the following triangular function

is given by

$$X(\omega) = \frac{4\sin^2(\omega T/2)}{T\omega^2}. \tag{28.3}$$

(2) Demonstrate

$$\int_{-\infty}^{\infty} \frac{\sin^2 ax}{\pi a x^2} dx = 1. \tag{28.4}$$

for any $a \neq 0$ with the aid of (1).

28.2 CHECK aid of Fubini's theorem (→**15.15**).

$$\mathcal{F}(f * g) = \mathcal{F}(f)\mathcal{F}(g), \tag{28.5}$$

This is a very useful relation.

Exercise.
In the following a and b are positive real numbers.
(i) Fourier transform

$$\chi(x) = \Theta(b - |x|). \tag{28.6}$$

(ii) Fourier transform $e^{-a|x|}$.
(iii) Fourier transform

$$f(x) = e^{-a|x|} \frac{\sin bx}{x}. \tag{28.7}$$

28.3 Differentiation becomes multiplication. We have an important relation

$$\hat{f}' = +ik\hat{f}. \tag{28.8}$$

The sign in front of the formula depends on our choice of the definition **28.1**. We have the following formulas (→**??**, **??**, **??**):

$$\mathcal{F}(div\, \boldsymbol{v}) = +i\boldsymbol{k} \cdot \boldsymbol{v}_{\boldsymbol{k}} \tag{28.9}$$

$$\mathcal{F}(curl\, \boldsymbol{v}) = +i\boldsymbol{k} \times \boldsymbol{v}_{\boldsymbol{k}} \tag{28.10}$$

$$\mathcal{F}(-\Delta f) = k^2 f_{\boldsymbol{k}}. \tag{28.11}$$

The last formula explains why $-\Delta$ is a natural combination – it is a positive definite operator.

28.4 Theorem. If $f : \boldsymbol{R} \to \boldsymbol{C}$ is continuous (and bounded), and both f and $\hat{f}$ are absolutely integrable, then the inversion formula holds

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \hat{f}(k) e^{+ikx} dk \equiv \mathcal{F}^{-1}(\hat{f}). \tag{28.12}$$

□
The formula could be guessed from the Fourier expansion formula **??**; actually Fourier reached this result in this way. (12.12) appears so often that we have fairly a standard abbreviation

$$\int_k \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty}, \quad \int_{\boldsymbol{k}} \equiv \left(\frac{1}{2\pi}\right)^d \int d\boldsymbol{k}. \tag{28.13}$$

28.5 Theorem [Inversion formula for piecewise C^1-function]. Let f be piecewise C^1-function on $\boldsymbol{R}$. Then (cf. **??**)

$$\frac{1}{2}[f(x_0 - 0) + f(x_0 + 0)] = \frac{1}{2\pi} P \int_{-\infty}^{\infty} dk e^{ikx_0} \hat{f}(k). \tag{28.14}$$

P denotes the Cauchy principal value (→**??**, **??**). □
We can write the formula as

$$\frac{1}{2}[f(x_0 - 0) + f(x_0 + 0)] = \lim_{\lambda \to \infty} \int_{-\infty}^{\infty} d\xi \frac{\sin[\lambda(x_0 - \xi)]}{x_0 - \xi} \hat{f}(\xi). \tag{28.15}$$

□

28.6 More general convergence conditions. As can easily be imagined from **??** for a pointwise convergence of the Fourier transform, we need some conditions. For example, if f is of bounded variation[316] near x, then (12.12) holds with $f(x)$ being replaced by $[f(x+0)+f(x-0)]/2$. If f is continuous and of bounded variation in (a, b), then (12.12) holds uniformly there.

28.7 Remark
(1) Mathematicians often multiply $1/\sqrt{2\pi}$ to the definition of Fourier transform as

$$\tilde{f} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx f(x) e^{-ikx}, \tag{28.16}$$

to symmetrize the formulas (as we will see in **28.9** or **28.12** sometimes this is very convenient), because

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \tilde{f}(k) e^{ikx} dk. \tag{28.17}$$

[316] If a function can be written as a difference of two monotonically increasing functions, we say the function is of *bounded variation*.

However, this makes the convolution formula (12.5) awkward. For physicists and practitioners, the definition in **??** (the sign choice may be different) is the most convenient, because we wish to compute actual numbers.
(2) The integral over k may be interpreted as a sum over n such that $k = 2\pi n/L$, where L is the size of the space. The following approximation is very useful in solid-state physics

$$\frac{1}{V}\sum_{\boldsymbol{k}} f_{\boldsymbol{k}} \simeq \frac{1}{2\pi^d}\int f_{\boldsymbol{k}} d\boldsymbol{k} \equiv \int_{\boldsymbol{k}} f_{\boldsymbol{k}}. \tag{28.18}$$

28.8 Sine and cosine transforms. If the space is limited to $x \geq 0$, then *Fourier sine* and *Fourier cosine transformations* may be useful (cf. **??**). If $f(0) = f(0+)$, then

$$g(k) = \int_0^\infty f(x)\cos kx dx, \quad f(x) = \frac{2}{\pi}\int_0^\infty g(k)\cos kx dk. \tag{28.19}$$

If $f(0) = 0$, then

$$g(k) = \int_0^\infty f(x)\sin kx dx, \quad f(x) = \frac{2}{\pi}\int_0^\infty g(k)\sin kx dk. \tag{28.20}$$

These can also be written concisely as

$$\frac{2}{\pi}\int_0^\infty \cos kx\cos k'x dx = \delta(k-k'), \tag{28.21}$$

$$\frac{2}{\pi}\int_0^\infty \sin kx\sin k'x dx = \delta(k-k'). \tag{28.22}$$

They can be shown easily with the aid of the Fourier transform of 1 (→**??**); Put $\cos kx = (e^{ikx} + e^{-ikx})/2$, etc. into (12.21) or (12.22).

Exercise.
There is an infinite medium whose thermal diffusivity is D. Its initial temperature distribution is given by $T|_{t=0} = T_0(\boldsymbol{x}$. Find the physically meaningful solution (→**??**(5) Warning). There are many ways to solve this. For example, we can use the free space Green's function (→**??** and the initial condition trick **??**. We can also use the Fourier transformation as follows.
(1) Show that for any[317] function g on $\boldsymbol{R}^3$

$$g(x,y,z) = \frac{1}{\pi^3}\int_0 \infty \int_0^\infty \int_0^\infty d\alpha d\beta d\gamma \int_{-\infty}^\infty \int_{-\infty}^\infty \int_{-\infty}^\infty dadbdc$$
$$g(a,b,c)\cos\alpha(x-a)\cos\beta(y-\beta 0\cos\gamma(z-c). \tag{28.23}$$

[317] If you wish to be within the ordinary calculus, it must be integrable, but we may proceed formally.

(2) The integrands are linearly independent (no mode coupling, or super position principle), so that each term must satisfy the diffusion equation. Introducing $A(t)\cos\alpha(x-a)\cos\beta(y-\beta 0\cos\gamma(z-c)$ into the diffusion equation, show that

$$A(t) = f(a,b,c)e^{-D(\alpha^2+\beta^2+\gamma^2)t}. \tag{28.24}$$

(3) Combining (1) and (2), obtain the following formula, which can be obtained directly with the use of the free space Greeen's function.

$$T(x,y,x,t) = \pi^{-3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\eta d\xi d\zeta e^{-(\eta^2+\xi^2+\zeta^2)} f(x+2\sqrt{DT}\eta, y+2\sqrt{DT}\xi, z+2\sqrt{DT}\zeta) \tag{28.25}$$

[Perform the integration over Greek letters.]

28.9 Bra-ket notation of Fourier transform or momentum (wave-vector) kets. **28.7** has the following symbolic representation (→**16.21-16.23** for notations).

$$f(x) = \langle x|f\rangle = \int_{-\infty}^{\infty}\langle x|k\rangle dk\langle k|f\rangle, \tag{28.26}$$

$$\langle x|k\rangle = \frac{1}{\sqrt{2\pi}}e^{-ikx}, \tag{28.27}$$

$$\tilde{f}(k) = \langle k|f\rangle = \int_{-\infty}^{\infty}\langle x|k\rangle dk\langle k|f\rangle = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ikx}f(x). \tag{28.28}$$

$\langle k|f\rangle$ is the Fourier transform of f in this bra-ket symmetrized version (**28.7**), and the normalization is <u>different</u> from that given in **28.1**. Notice that

$$\langle x|y\rangle = \delta(x-y) = \int\langle x|k\rangle dk\langle k|y\rangle = \frac{1}{2\pi}\int_{\infty}^{\infty} e^{ik(x-y)}dk. \tag{28.29}$$

To rationalize this, we need the theory of Fourier transform of generalized functions (→**??**).

28.10 Plancherel's theorem.

$$\langle f|f\rangle = \int\langle f|k\rangle dk\langle k|f\rangle \tag{28.30}$$

is called *Plancherel's formula*. In our normalization (for physicists) in **28.1** this reads

$$\int_{-\infty}^{\infty}|f(x)|^2dx = \frac{1}{2\pi}\int_{-\infty}^{\infty}|\hat{f}(k)|^2dk. \tag{28.31}$$

The theorem tells us that if f is square integrable (that is, the total energy of the wave is finite), then the total energy is equal to the energy carried by individual harmonic modes. This is of course the counterpart of Parseval's equality (→**16.12**).

28.11 Theorem [Riemann-Lebesgue Lemma]. For an integrable function f

$$\lim_{|\boldsymbol{k}|\to\infty} \hat{f}(\boldsymbol{k}) = 0. \tag{28.32}$$

If all the n-th derivatives are integrable, then $\hat{f}(\boldsymbol{k}) = o[|\boldsymbol{k}|^{-n}]$.□
There is an analogue of **??**. There we have already discussed its physical meaning.[318]

28.B Applications of Fourier Transform

Fundamental applications of Fourier transformation important in practice are summarized: uncertainty principle, sampling theorem, the Wiener-Khinchine theorem (the relation between power spectrum and correlation function). Also the principle of FFT is outlined.

Key words: uncertainty principle, coherent state, band-limited function, sampling theorem, sampling function, aliasing, time-correlation function, power spectrum, Wiener-Khinchine theorem, fast Fourier transform

Summary:
(1) The uncertainty principle is a basic property of Fourier transformation. Its essence is the elementary Cauchy-Schwarz inequality (**28.12**).
(2) If the band width of a signal (function) is finite, then discrete sampling with sufficiently frequent sampling points perfectly captures the signal. This is the essence of the sampling theorem (**28.16**).
(3) Spectral analysis is a fundamental tool of experimental physics. Its theoretical basis is the Wiener-Khinchine theorem – Fourier transform of the time-correlation function is the power spectrum (**28.21**).
(4) Spectral analysis becomes practical after the popularization of fast Fourier transform (FFT) (**28.22**-**??**).

28.12 Theorem [Uncertainty principle]. Let f be in $L_2(\boldsymbol{R})$ (→**16.19**). Define the following averages

$$\langle x \rangle \equiv \int x|f(x)|^2 dx / \int |f(x)|^2 dx, \tag{28.33}$$

[318] see Katznelson p123.

$$\langle k\rangle \equiv \int k|\hat{f}(k)|^2dk/\int |\hat{f}(k)|^2dk, \tag{28.34}$$

$$\Delta x^2 \equiv \int (x-\langle x\rangle)^2|f(x)|^2dx/\int |f(x)|^2dx, \tag{28.35}$$

$$\Delta k^2 \equiv \int (k-\langle k\rangle)^2|\hat{f}(k)|^2dk/\int |\hat{f}(k)|^2dk. \tag{28.36}$$

Then,

$$\Delta x\Delta k \geq 1/2. \tag{28.37}$$

[Demo] Without loss of generality, we may assume $\langle x\rangle = 0$, and also assume that f is already normalized. Define

$$\tilde{f}(k) = \frac{1}{\sqrt{2\pi}}\int dx e^{ikx}f(x). \tag{28.38}$$

Using Plancherel's theorem (→**28.10**), we get (cf. **28.3**)

$$\int dx|f'(x)|^2 = \int |k\tilde{f}(k)|^2dk, \quad \int dx|f(x)|^2 = \int |\tilde{f}(k)|^2dk, \tag{28.39}$$

so that

$$\Delta k^2 = \int |f'(x)-\langle k\rangle f(x)|^2dx. \tag{28.40}$$

The Cauchy-Schwarz inequality (→**16.7**) implies

$$\Delta k^2\Delta x^2 = \int |f'(x)-\langle k\rangle f(x)|^2dx\int x^2|f(x)|^2dx \geq \left|\int [f'(x)-\langle k\rangle f(x)]x\overline{f(x)}dx\right|^2, \tag{28.41}$$

but since $\langle x\rangle = 0$, the last formula reads

$$|f'(x)x\overline{f(x)}dx|^2 \geq |Re\int f'(x)x\overline{f(x)}dx|^2 = 1/4. \tag{28.42}$$

The last number comes from the following integration by parts

$$\int f'(x)x\overline{f(x)}dx = -\int \overline{f'(x)}xf(x)dx - \int |f(x)|^2dx. \tag{28.43}$$

28.13 Remark. As can be seen from the proof of **28.12**, the uncertainty principle is a disguised Cauchy-Schwarz inequality (→**16.7**) which says that the modulus of cosine cannot be larger than 1. Note that obvious mathematical theorems can have profound implication in real life.

28.14 Coherent state. The equality in the uncertainty principle is realized if the wave function f is Gaussian

$$f(x) = \frac{1}{\pi^{1/4}\sigma^{1/2}}e^{-x^2/2\sigma^2}. \tag{28.44}$$

Check indeed $\Delta x\Delta k = 1/2$. A state with this equality is called a *coherent state*.

28.15 Band-limited function. If a function has a Fourier transform which has a compact support (i.e., $\hat{f}(k)$ is zero if $|k| > k_0$ for some $k_0 > 0$), then f is called a *band-limited function.*

28.16 Theorem [Sampling theorem]. Let f be a band-limited function such that $\hat{f}(k)$ be zero if $|k| > k_0 > 0$. Then,

$$f(x) = \sum_{n=-\infty}^{\infty} f(n\pi/k_0) \frac{\sin(k_0 x - n\pi)}{k_0 x - n\pi}. \tag{28.45}$$

That is, f can be reconstructed from the discrete sample values $\{f(n\pi/k_0)\}_{n\in \boldsymbol{Z}}$.□
The sampling theorem is extremely important in communication (multichannel communication, bandwidth compression, etc.), and information storage (digitization as in CD).
[Demo] Since $\hat{f}(k)$ is non-zero only on $[-k_0, k_0]$, we can Fourier expand this as a function of period $2k_0$ (→**??**)

$$\hat{f}(k) = \sum_{n\in \boldsymbol{Z}} c_n e^{ikn\pi/k_0} \tag{28.46}$$

with

$$\frac{1}{2k_0} \int_{-k_0}^{k_0} \hat{f}(k) e^{-in\pi k/k_0} dk = c_n. \tag{28.47}$$

On the other hand due to the band-limitedness

$$f(x) = \frac{1}{2\pi} \int_{-k_0}^{k_0} \hat{f}(k) e^{-ikx} dk. \tag{28.48}$$

Comparing (12.47) and (12.48), we get

$$c_n = \frac{\pi}{k_0} f(n\pi/k_0). \tag{28.49}$$

(12.46), (12.48) and (12.49) give the desired result.

Exercise.
Determine the minimum sampling rate (or frequency) for the signal $10\cos\omega t + 2\cos 3\omega t$. This is a trivial question, so do not think too much.

28.17 Sampling function. The function

$$\varphi_n(x) = \frac{\sin(k_0 x - n\pi)}{k_0 x - n\pi} \tag{28.50}$$

appearing in (12.45) is called the *sampling function.* $\{\varphi_n\}_{n\in \boldsymbol{Z}}$ is an orthogonal system. There is an orthogonality relation:

$$\int_{-\infty}^{\infty} \varphi_n(x)\varphi_m(x) dx = \frac{\pi}{k_0} \delta_{nm}. \tag{28.51}$$

Exercise.
Demonstrate that the sampling functions $\{\varphi_n\}$ make an orthogonal system.

28.18 Band-limited periodic function. The sampling theorem would naturally tell us the following. A band-limited periodic function with no harmonics of order higher than N can be uniquely specified by its values sampled at appropriate $2N + 1$ points in a single period.

28.19 Aliasing. If the function we sample is strictly band-limited, then the above theorem of course works perfectly. However, often the function has higher frequency components beyond the sample frequency. Then, just as we watch fast rotating wheel in the movie, what we sample is the actual frequency modulo the sample frequency (that is, the beat between these frequencies). This phenomenon is called *aliasing*. To avoid unwanted aliasing, often we filter the original signal (through a low-pass filter) and remove excessively high frequency components.

28.20 Time-correlation function. Let $x(t)$ be a stochastic process or time-dependent data which is statistically stationary. Here 'stochastic' means that we have an ensemble of such signals (more precisely, we have a set of signals $\{x(t;\omega)\}$, where ω is the probability parameter specifying each sample signal. That is, if the reader wishes to start an observation, one ω is given (by God) and she will observe $x(t;\omega)$. The word 'stationary' implies that the ensemble average of $x(t,\omega)$ does not depend on t.[319] Let us denote the ensemble average by $\langle\ \rangle_\omega$. The *time correlation function* is defined by

$$C(t) = \langle x(t)x(0)\rangle_\omega \tag{28.52}$$

and is a fundamental observable in many practical cases.
The ensemble average of

$$\sigma(\nu) = \langle |x_\nu|^2\rangle_\omega \tag{28.53}$$

is called the *power spectrum* of the signal $x(t)$, where x_ν is the Fourier transform of $x(t)$. Thanks to the advent of FFT (→**28.23**), it is easy to obtain the power spectrum experimentally (easier than the correlation function).

28.21 Theorem [Wiener-Khinchin]. The Fourier transform of the power spectrum of a stationary stochastic process is its power spectrum.

[319] Actually, in this case we only need the absolute time independence of the correlation function. A process with this property is called a *weak stationary process*.

That is,[320]

$$C(t) \propto \int_{-\infty}^{\infty} e^{-i\nu t}\sigma(\nu)d\nu. \tag{28.54}$$

Its demonstration is a straightforward calculation. We compute (→**??**)

$$\begin{aligned}\langle x_\nu x_{-\mu}\rangle &= \left\langle \int_{-\infty}^{\infty} dt x(t)e^{i\nu t}\int_{-\infty}^{\infty} ds x(s)e^{-i\mu s}\right\rangle \\ &= \int_{-\infty}^{\infty} dt\int_{-\infty}^{\infty} ds e^{i\nu t}e^{-i\mu s}\langle x(t-s)x(0)\rangle \\ &= 2\pi\delta(\nu-\mu)\int_{-\infty}^{\infty} dt e^{i\nu t}C(t). \end{aligned}\tag{28.55}$$

That is, $\langle x_\nu x_{-\mu}\rangle = \delta(\nu-\mu)\sigma(\nu)$ so that

$$\sigma(\nu) = 2\pi\int_{-\infty}^{\infty} dt e^{i\nu t}C(t). \tag{28.56}$$

28.22 Discrete Fourier transformation. Let $\boldsymbol{X} \equiv \{X_n\}_{n=0}^{N-1}$ be a sequence of complex numbers, and

$$e(x) \equiv \exp(-2\pi i x). \tag{28.57}$$

The following sequence $\hat{\boldsymbol{X}} \equiv \{X^n\}$ is called the *discrete Fourier transform* of $\boldsymbol{X}$:

$$X^k = \sum_{n=0}^{N-1} e\left(\frac{kn}{N}\right)X_n. \tag{28.58}$$

Its inverse transform is given by

$$X_n = \frac{1}{N}\sum_{k=0}^{N-1} e\left(\frac{-kn}{N}\right)X^k. \tag{28.59}$$

Notice that a straightforward calculation of these sums (N of them) costs $O[N^2]$ operations and is costly.

Exercise.
Demonstrate the above inverse transform formula by showing

$$\frac{1}{N}\sum_{k=0}^{N-1} e^{k(m-n)/N} = \delta_{mn}. \tag{28.60}$$

[320] Actually, if we normalize $C(t)$ so that $C(0) = 1$ (simply regard $C(t)/C(0)$ as $C(t)$), then we have probability measure σ (→**15.41**) such that

$$C(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\nu t}d\sigma(\nu).$$

However, in practice, the numerical constant and normalization are not crucial.

28.23 Principle of fast Fourier transform.[321] Let $N = N_1 N_2$. $n, k \in \{0, 1, \cdots, N-1\}$ can be uniquely written as[322]

$$n = n_1 + n_2 N_1, \quad k = k_1 N_2 + k_2, \tag{28.61}$$

where $n_i, k_i \in \{0, 1, \cdots, N_i - 1\}$ ($i = 1$ or 2). Notice that

$$e(kn/N) = e(k_1 n_1/N_1) e(k_2 n_2/N_2) e(k_2 n_1/N). \tag{28.62}$$

n_i and k_i are uniquely determined, so we may write, e.g., $(n_1 n_2)$ instead of n. Then, (12.58) can be calculated as

$$\begin{aligned} X^{(k_1 k_2)} &= \sum_{n=0}^{N_1 N_2 - 1} e(k_1 n_1/N_1) e(k_2 n_2/N_2) e(k_2 n_1/N) X_{(n_1 n_2)}, \\ &= \sum_{n_1=0}^{N_1-1} e(k_1 n_1/N_1) \left\{ e(k_2 n_1/N) \left[\sum_{n_2=0}^{N_2-1} e(k_2 n_2/N_2) X_{n_1 n_2} \right] \right\}. \end{aligned} \tag{28.63}$$

Consequently, the calculation of discrete Fourier transfrom can be decomposed into the following three steps:
(1) Compute for any k_2

$$X_{n_1}{}^{k_2} = \sum_{n_2=0}^{N_2-1} e(k_2 n_2/N_2) X_{n_1 n_2}. \tag{28.64}$$

(2) Then, rotate the phase:

$$\tilde{X}_{n_1}{}^{k_2} = e(k_2 n_1/N) X_{n_1}{}^{k_2}. \tag{28.65}$$

(3) Finally compute for any k_1

$$\hat{X}^{k_1 k_2} = \sum_{n_1=0}^{N_1-1} e(k_1 n_1/N_1) \tilde{X}_{n_1}{}^{k_2}. \tag{28.66}$$

Now the number of necessary operations is $O[N_1 \times N_2^2] + O[N_1^2 \times N_2]$; if $N_1 = N_2 = \sqrt{N}$, then $O[2N^{3/2}]$. If we can decompose N into m factors of similar order, then the number of necessary operations is roughly $N^{1-1/m} N^{2/m} = N \times N^{1/m}$. Hence, asymptotically, we can guess $N \ln N$

[321] The algorithm, known sometimes as the Cooley-Tukey algorithm (J W Cooley and J W Tukey, Math. Comp. **19**, 297 (1965)), was actually known to Gauss, but the importance was widely recognized after this paper.
[322] This is an example of the so-called *Chinese remainder theorem*.

is the best possibility for the discrete Fourier transform of N numbers.

Exercise.
Find the autocorrelation function of the signal

$$f(t) = \Theta(t+T) - \Theta(t-T). \tag{28.67}$$

Then illustrate the Wiener-Khinchine theorem with the example.

28.C Fourier Analysis of Generalized Function

Generalized functions can be Fourier transformed and physicists' favorite formulas like $\int e^{ikx}dk = 2\pi\delta(x)$ or the Plemelj formula $1/(x+i0) = P(1/x) - i\pi\delta(x)$ can be demonstrated. Fourier expansion of δ-function gives us the Poisson sum formula which may be used to accelerate the convergence of series.

Key words: Fourier expansion of unity, Poisson sum formula, Euler-MacLaurin sum formula, Plemelj formula

Summary:
(1) Not convergent Fourier series may be interpreted as a generalized function. A typical example is Poisson's sum formula (**28.25**).
(2) Formal calculation of Fourier transform of generalized functions often works, but whenever there is some doubt, return to the definition (**28.29**, **??**).

28.24 Delta function.

$$\delta(x) = \sum_{n=-\infty}^{\infty} e^{i2n\pi x} \tag{28.68}$$

for $x \in (-1, 1)$.
[Demo] We know as an ordinary Fourier series

$$\frac{1-2x}{2} = \sum_{n=1}^{\infty} \sin(2n\pi x)/n\pi \tag{28.69}$$

for $x \in (-1/2, 1/2)$. We may use the RHS to extend the LHS periodically for all $\boldsymbol{R}$. Differentiate this termwisely, interpreting this as a formula for generalized functions ($\rightarrow$**??**). We get

$$-1 + \delta(x) = 2\sum_{n=1}^{\infty} \cos 2n\pi x \tag{28.70}$$

for $x \in (-1/2, 1/2)$.
The decomposition of unity (→**16.27**) can also be used to obtain (12.68).

28.25 Poisson's sum formula.

$$\sum_{k=-\infty}^{\infty} \delta(x-k) = \sum_{n=-\infty}^{\infty} e^{i2n\pi x} \tag{28.71}$$

for $x \in \boldsymbol{R}$.

This can be obtained easily from (12.68) by 'tessellating' the formula for $(-1/2, 1/2)$ over the whole range of $\boldsymbol{R}$. From (12.71) we get

$$|\lambda| \sum_{k=-\infty}^{\infty} \delta(x-\lambda k) = \sum_{n=-\infty}^{\infty} e^{i2\pi nx/\lambda} \tag{28.72}$$

(cf. **??**). Applying a test function φ to this, we get the following *Poisson sum formula*:

$$|\lambda| \sum_{k=-\infty}^{\infty} \varphi(\lambda k) = \sum_{n=-\infty}^{\infty} \hat{\varphi}(2n\pi/\lambda). \tag{28.73}$$

(Be careful with the normalization constant.) Also we can make a cosine version of the Poisson sum formula

$$\sum_{k=-\infty}^{\infty} \delta(x-k) = 1 + 2\sum_{n=1}^{\infty} \cos(2n\pi x). \tag{28.74}$$

If $f(x)$ is a gently decaying function, then its Fourier transform decays rapidly, and vice versa. The Poisson sum formula is useful because it may help accelerating the convergence of the series.

Exercise.
Demonstrate

$$\sum_{n=1}^{\infty} \frac{\cos na}{1+n^2} = \frac{\pi}{2}\frac{\cosh(\pi-a)}{\sinh \pi} - \frac{1}{2}.$$

28.26 Applications of Poisson sum formula.
(1)

$$\sum_{n \in \boldsymbol{Z}} \frac{1}{1+a^2n^2} = \frac{\pi}{a}\coth\frac{\pi}{a}. \tag{28.75}$$

The key formulas are

$$\hat{\varphi}(k) = \frac{1}{1+a^2k^2/4\pi^2}, \quad \varphi(x) = \frac{\pi}{a}e^{-2\pi|x|/a}. \tag{28.76}$$

(2)

$$\sum_{n=1}^{\infty} \frac{\cos na}{1+n^2} = \frac{\pi}{2}\frac{\cosh(\pi-a)}{\sinh \pi} - \frac{1}{2}. \tag{28.77}$$

28.27 Euler-MacLaurin sum formula.

$$\sum_{n=0}^{\infty} f(n) = \int_0^{\infty} f(x)dx + \frac{1}{2}f(0) - \frac{1}{12}f'(0) + \frac{1}{720}f^{(3)}(0) - \frac{1}{30240}f^{(5)}(0) + \cdots. \tag{28.78}$$

[Demo] Let f be a function defined on the positive real axis. Extend it to the whole $\boldsymbol{R}$ as an even function ($f(x) = f(-x)$). Apply the cosine version of the Poisson sum formula (12.74) and integrate from 0 to ∞. Using the evenness of the function, we get

$$-\frac{1}{2}f(0) + \sum_{k=0}^{\infty} f(k) = \int_0^{\infty} f(x)dx + 2\sum_{n=1}^{\infty}\int_0^{\infty} f(x)\cos(2n\pi x)dx. \tag{28.79}$$

Integrating by parts the last integrals containing cosines, we get

$$\sum_{k=0}^{\infty} f(k) = \frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - \sum_{n=1}^{\infty}\int_0^{\infty} f'(x)\frac{\sin 2n\pi x}{2n\pi}dx. \tag{28.80}$$

Keep applying integration by parts to get

$$\sum_{n=1}^{\infty}\int_0^{\infty} f'(x)\frac{\sin 2n\pi x}{2n\pi}dx = -\sum_{n=1}^{\infty}\left[f'(x)\frac{\cos 2n\pi x}{2(n\pi)^2}\right]_0^{\infty} + \sum_{n=1}^{\infty}\int_0^{\infty} f''(x)\frac{\cos 2n\pi x}{2(n\pi)^2}dx. \tag{28.81}$$

Thus

$$\sum_{k=0}^{\infty} f(k) = \frac{1}{2}f(0) + \int_0^{\infty} f(x)dx - f'(0)\sum_{n=1}^{\infty}\frac{1}{2n^2\pi^2} + \cdots. \tag{28.82}$$

This gives the $f'(0)$ term of the formula.

28.28 Mulholland's formula for the canonical partition function for the rotational motion of a heteronuclear diatomic molecule. The rotational partition function $r(T)$ at temperature T is given by

$$r(T) = \sum_{\ell=0}^{\infty}(2\ell+1)\exp\left[-\frac{\hbar^2\ell(\ell+1)}{2Ik_BT}\right], \tag{28.83}$$

where I is the moment of inertia of the molecule, and k_B is the Boltzmann constant. Introduce $\sigma \equiv \hbar^2/2Ik_BT$, and let

$$f(x) = (2x+1)\exp[-x(x+1)\sigma]. \tag{28.84}$$

Apply (12.78) to this function, we get the following Mulholland's formula

$$r(T) = \frac{1}{\sigma} + \frac{1}{3} + \frac{\sigma}{15} + \frac{4\sigma^2}{315} + O[\sigma^3]. \tag{28.85}$$

The first term on the RHS is the classical value.

28.29 Fourier transform of generalized functions. The crucial observation is (for ˆ see **28.1**): if f and φ both have well-defined Fourier transforms,

$$\langle \hat{f}, \varphi \rangle = \int dk \left[\int dx f(x) e^{-ikx} \right] \varphi(k) = \langle f, \hat{\varphi} \rangle \tag{28.86}$$

The Fourier transform $\hat{\tau} \equiv \mathcal{F}[\tau]$ of a generalized function τ is defined by

$$(\hat{\tau}, \varphi) = (\tau, \hat{\varphi}), \text{ or } (\mathcal{F}[\tau], \varphi) = (\tau, \mathcal{F}[\varphi]), \tag{28.87}$$

where $\varphi \in \mathcal{D}$, a test function.

Exercise.
Demonstrate

$$\lim_{\lambda \to \infty} \frac{\sin \lambda x}{x} = \pi \delta(x). \tag{28.88}$$

$$\lim_{\lambda \to \infty} \int_a^b \sin \lambda x = 0. \tag{28.89}$$

28.30 Convenient test function space. For this definition it is desirable that the set of test functions $\mathcal{D}$ (→**??**) and the set of their Fourier transforms $\hat{\mathcal{D}}$ are identical. For the set of Schwartz class functions (→**??** footnote) this holds (→**28.11**). [If we choose $\mathcal{D}$ to be the set of all the functions with compact supports, then $\hat{\mathcal{D}}$ becomes very large, so that the class of generalized functions (for which $(\tau, \hat{\varphi})$ must be meaningful) must be severely restricted, and is not very convenient.]

28.31 Fourier transform of unity = delta function.

$$\hat{1} = 2\pi \delta(k). \tag{28.90}$$

This is the *true* meaning of the physicists' favorite

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk = \delta(x). \tag{28.91}$$

Obviously, $\hat{\delta} = 1$ (direct calculation). That is, $\mathcal{F}^2$ implies multiplication of 2π as we know in **28.10**.
[Demo] $(\hat{1}, \varphi) = (1, \hat{\varphi}) = \int \hat{\varphi}(k) dk = \mathcal{F}^2[\varphi](0)$. Here $\mathcal{F}[\varphi]$ is a function on the configuration space (that is, a function of x) and is equal to $2\pi\varphi(x)$. Therefore we have obtained

$$(\hat{1}, \varphi) = 2\pi\varphi(0) = \int 2\pi \delta(x) \varphi(x) dx = (2\pi\delta, \varphi). \tag{28.92}$$

Exercise.
Show

$$\delta(t) = \frac{1}{\pi} \int_0^\infty \cos \omega t d\omega. \tag{28.93}$$

Cf. **28.8**.

28.32 Translation. The following formulas should be obvious

$$\mathcal{F}[\delta(x-a)] = e^{-iak}, \quad \mathcal{F}[e^{iax}] = 2\pi\delta(a-k). \tag{28.94}$$

28.33 Fourier transform of x, $d/dx \leftrightarrow +ik$. (→**28.3**)

$$\hat{x} = +2\pi i\delta'(k). \tag{28.95}$$

In other words, since $\mathcal{F}^2 \equiv 2\pi$,

$$\hat{\delta'} = +ik. \tag{28.96}$$

[Demo] Start with the definition $(\hat{x}, \varphi) = (x, \hat{\varphi})$ (→**28.29**) which is equal to

$$\int dx x\hat{\varphi}(x) = \int dx x \left[\int e^{-ikx}\varphi(k)dk\right] = \int dx \int dk \left(-\frac{d}{dik}e^{-ikx}\right)\varphi(k). \tag{28.97}$$

Integrating this by parts, taking into account that the test function φ decays sufficiently quickly, we get

$$-\int dx \int dk ie^{-ikx}\varphi'(k) = -i\int dk\hat{1}(k)\varphi'(k) = -2\pi i\int dk\delta(k)\varphi'(k) = 2\pi i\int dk\delta'(k)\varphi(k), \tag{28.98}$$

where we have used (12.90) in **32C.8**, and the definition of δ' (→**??**).

A more formal and direct 'demonstration' is

$$\hat{x} = \int xe^{-ikx}dx = \int \left(i\frac{d}{dk}\right)e^{-ikx}dx = 2\pi i\frac{d}{dk}\delta(k). \tag{28.99}$$

Convolution of the derivative of delta function is differentiation (→**??**(2)), and the Fourier transform of a convolution is the product of the Fourier transforms, i.e., $\mathcal{F}(f*g) = \mathcal{F}(f)\mathcal{F}(g)$ (→**28.2**), so that we easily get)cf. **28.3**)

$$\hat{f'} = +ik\hat{f}. \tag{28.100}$$

28.34 Fourier transform of x^n.

$$\hat{x^n} = 2\pi\left(+i\frac{d}{dk}\right)^n\delta(k). \tag{28.101}$$

In other words,

$$\hat{\delta^{(n)}} = (+ik)^n. \tag{28.102}$$

Since $\delta'*f = f'$, $\delta^{(n)} = \delta'*\delta^{(n-1)} = \delta'*\delta'*\cdots\delta'*\delta$ (n δ' are convoluted) (this is well defined →**??**(2)). This and (12.96) immediately imply (12.102).

28.35 Fourier transform of sign function.

$$s\hat{g}n(k) = \frac{2}{i} P\frac{1}{k}, \tag{28.103}$$

where P denotes the Cauchy principal value (→**??**).
[Demo] We have demonstrated (→**??**)

$$\frac{d}{dx} sgn(x) = 2\delta(x). \tag{28.104}$$

Fourier-transforming this, we get (→(12.100) and $\hat{\delta} = 1$)

$$+ik\mathcal{F}(sgn)(k) = 2. \tag{28.105}$$

With the aid of (2) in **??**, we can solve this equation for $s\hat{g}n$ as

$$s\hat{g}n(k) = 2iP\frac{1}{k} + c\delta(k), \tag{28.106}$$

where c is a constant not yet determined. To fix this constant we apply this equality to an even test function, say e^{-k^2}. Since sgn is an odd generalized function, and since the Fourier transform of a Gaussian function is again Gaussian,

$$(s\hat{g}n, e^{-k^2}) \propto (sgn, e^{-x^2}) = 0. \tag{28.107}$$

$P(1/k)$ is also an odd function, so that this implies $c = 0$.

28.36 Plemelj formula.

$$w\text{-}\lim_{\epsilon \to +0} \frac{1}{x \pm \epsilon i} = P\frac{1}{x} \mp i\pi\delta(x), \tag{28.108}$$

where $w\text{-}\lim_{\epsilon\to+0}$ is the weak limit, that is, the limit is taken *after* integration in which the function appears is completed (→**??**).
[Demo] Obviously,

$$\lim_{\epsilon \to 0+} e^{-\epsilon x}\Theta(x) = \Theta(x), \tag{28.109}$$

If we interpret this equation as an equation for generalized functions, then integration and the limit can be freely exchanged. Therefore, we get

$$\hat{\Theta}(k) = w\text{-}\lim_{\epsilon \to 0+} \int_0^\infty e^{-(ik-\epsilon)x} = \lim_{\epsilon \to 0+} \frac{1}{ik + \epsilon}. \tag{28.110}$$

Since $sgn(x) = 2\Theta(x) - 1$, (12.103), (12.90) and (12.110) imply

$$2iP\frac{1}{k} = \lim_{\epsilon \to 0+} \frac{-2}{ik - \epsilon} - 2\pi\delta(k). \tag{28.111}$$

28.D Radon Transformation

Radon transformation is a theoretical basis of various tomographies. Its inverse transformation is constructed with the aid of Fourier transformation. Radon transformation allows us to solve the Cauchy problem of the wave equation in any dimensional space. The explicit formula clearly demonstrates the marked difference of even and odd dimensional spaces.

Key words: Radon's problem, Radon transform, modified Radon transform, tomography, wave equation, afterglow.

Summary:
(1) The mathematical principle of tomography is Radon transformation (**28.39**) whose inverse transformation is essentially calculable by Fourier transformation (**28.40**-**28.41**).
(2) Radon transform gives a general method to solve d-wave equation (**28.45**). The resultant solution clearly exhibits the afterglow effect in even dimensional spaces (**28.46**).

28.37 Radon's problem. Radon (1917) considered the following problem: Reconstruct a function $f(x, y)$ on the plane from its integral along all lines in the plane. That is, the problem is to reconstruct the shape of a hill from the areas of all its vertical cross-sections.

28.38 Radon transform. Let f be a function defined on a region in $\boldsymbol{R}^2$.[323]

$$\mathcal{R}f(s, \boldsymbol{\omega}) \rightleftharpoons \int_{\boldsymbol{R}^2} d\boldsymbol{x}\delta(\boldsymbol{x} \cdot \boldsymbol{\omega} - s)f(\boldsymbol{x}) \tag{28.112}$$

is called the *Radon transform* of f, where $\boldsymbol{\omega}$ is the directional vector $|\boldsymbol{\omega}| = 1$ specifying a line normal to it, and $s \in \boldsymbol{R}$ is the (signed) distance between the line and the origin. The Radon problem **28.37** is to find f from $\mathcal{R}f$.

That (12.112) is the integral of f along the line specified by $\boldsymbol{\omega}\cdot\boldsymbol{x} = s$ can easily be seen if we introduce the rotated Cartesian coordinate system O-x_1x_2 such that the x_2 axis is parallel to the line and x_1 perpendicular to it. The integral now reads $\int \delta(x_1 - s)f(x_1, x_2)dx_1dx_2 = \int f(s, x_2)dx_2$.

[323] The definition given here can easily be extended to general d-space. See **28.43**-**28.44**. A good introduction to the topic may be found in I. M. Gel'fand, M. I. Graev and N. Ya. Vilenkin, *Generalized Functions*, vol.5 *Integral Geometry and Representation Theory* (Academic Press, 1966). See also R. S. Strichartz, Am. Math. Month. 1982 June-July.

28.39 Some properties of Radon transform. Note that
(1) $\mathcal{R}f(s,\boldsymbol{\omega})$ is an even homogeneous function (→**??**) of s and $\boldsymbol{\omega}$ of degree -1:

$$\mathcal{R}f(\lambda s,\lambda\boldsymbol{\omega})=|\lambda|^{-1}\mathcal{R}f(s,\boldsymbol{\omega}). \tag{28.113}$$

(2) The Radon transform of a convolution (→**??**) is a convolution of Radon transforms:

$$\left(\mathcal{R}\left[\int_{\boldsymbol{R}^2} f_1(\boldsymbol{y})f_2(\boldsymbol{x}-\boldsymbol{y})d\boldsymbol{y}\right]\right)(s,\boldsymbol{\omega})=\int_{-\infty}^{\infty}dt\left[\mathcal{R}f_1(t,\boldsymbol{\omega})\right]\left[\mathcal{R}f_2(s-t,\boldsymbol{\omega})\right]. \tag{28.114}$$

28.40 Fourier transform of Radon transform.

$$\hat{f}(\rho\boldsymbol{\omega})=\mathcal{F}(\mathcal{R}f)(\rho,\boldsymbol{\omega})\rightleftharpoons\int_{-\infty}^{\infty}\mathcal{R}f(s,\boldsymbol{\omega})e^{-i\rho s}ds. \tag{28.115}$$

That is, the Fourier transform of $Rf(s,\boldsymbol{\omega})$ with respect to s is the Fourier transform of the function f itself with the '$\boldsymbol{k}$-vector' parallel to $\boldsymbol{\omega}$.
[Demo] Using the definition (12.112), we have only to perform a straightforward calculation:

$$\int_{-\infty}^{\infty}\mathcal{R}f(s\boldsymbol{\omega})e^{-i\rho s}ds=\int_{-\infty}^{\infty}ds\int d\boldsymbol{x}f(\boldsymbol{x})\delta(s-\boldsymbol{x}\cdot\boldsymbol{\omega})e^{-i\rho s}=\int d\boldsymbol{x}f(\boldsymbol{x})e^{-i\rho\boldsymbol{\omega}\cdot\boldsymbol{x}}. \tag{28.116}$$

Thus f can be reconstructed by

$$f(\boldsymbol{r})=\frac{1}{(2\pi)^d}\int\hat{f}(\rho\boldsymbol{\omega})e^{i\rho\boldsymbol{\omega}\cdot\boldsymbol{r}}d\rho d\boldsymbol{\omega}. \tag{28.117}$$

28.41 Theorem [Radon inversion formula]. Let f be a piecewise C^1-function defined on a region in $\boldsymbol{R}^2$. Then

$$f(\boldsymbol{x})=\int\tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega},\boldsymbol{\omega})d\sigma(\boldsymbol{\omega}), \tag{28.118}$$

where $d\sigma$ is the arc length element of the unit circle, and $\tilde{\mathcal{R}}f$ is the *modified Radon transform* defined by

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega})\rightleftharpoons\frac{1}{8\pi^2}\int_{-\infty}^{\infty}d\rho e^{-i\rho s}\rho\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega}). \tag{28.119}$$

28.42 X-ray tomography. The Radon transformation is the theoretical underpinning of the particle beam tomographies. These are applied not only medically, but also, e.g., to the anatomical study of fossils such as trilobites.

28.43 *d*-space version. In d-space the Radon transform is defined as

$$\mathcal{R}f(s,\boldsymbol{\omega}) = \int_{\boldsymbol{R}^d} f(\boldsymbol{x})\delta(s-\boldsymbol{\omega}\cdot\boldsymbol{x})d\boldsymbol{x}, \tag{28.120}$$

where $\boldsymbol{\omega}$ is the position vector on the unit $d-1$-sphere S^{d-1} (the skin of the d-unit ball). The d-dimensional version of **28.41** reads:

28.44 Theorem.

$$f(\boldsymbol{x}) = \int_{S^{d-1}} d\sigma(\boldsymbol{\omega})\tilde{R}f(\boldsymbol{x}\cdot\boldsymbol{\omega},\boldsymbol{\omega}), \tag{28.121}$$

where

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) \equiv \frac{1}{2(2\pi)^d}\int_{-\infty}^{\infty} e^{-i\rho s}|\rho|^{d-1}\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega})d\rho, \tag{28.122}$$

$$\hat{\mathcal{R}}f(\rho,\boldsymbol{\omega}) \equiv \int_{-\infty}^{\infty}\mathcal{R}f(s,\boldsymbol{\omega})e^{i\rho s}ds\,(=\hat{f}(\rho\boldsymbol{\omega})\,) \tag{28.123}$$

with σ being the area element of S^{d-1}.

28.45 Solving *d*-wave equation using Radon transform. Consider a wave equation in the whole d-space

$$(\partial_t^2-\Delta)u = 0 \tag{28.124}$$

with the initial condition $u=f$ and $\partial_t u = g$ at $t=0$. If the initial data are constant on all the hyperplanes perpendicular to the direction $\boldsymbol{\omega}$, i.e., $f(\boldsymbol{x}) = F(\boldsymbol{x}\cdot\boldsymbol{\omega})$ and $g(\boldsymbol{x}) = G(\boldsymbol{x}\cdot\boldsymbol{\omega})$, where F and G are functions defined on $\boldsymbol{R}$, then we can apply the method to solve the 1-space problem (→**??**) to get the solution as

$$u(\boldsymbol{x},t) = \frac{1}{2}[F(\boldsymbol{x}\cdot\boldsymbol{\omega}+t)+F(\boldsymbol{x}\cdot\boldsymbol{\omega}-t)] + \frac{1}{2}\int_{\boldsymbol{x}\cdot\boldsymbol{\omega}-t}^{\boldsymbol{x}\cdot\boldsymbol{\omega}+t} G(s)ds. \tag{28.125}$$

Therefore, if we can decompose the initial data into a superposition of data depending only on $\boldsymbol{x}\cdot\boldsymbol{\omega}$, the superposition principle (→**??**) allows us to reconstruct the solution from the pieces like (12.125). As can be seen from (12.121), d-dimensional Radon transformation is the very tool to accomplish the desired decomposition.
The strategy is as follows:
(1) Calculate the modified Radon transform (12.123) for f and g,
(2) Solve the wave equation for $\tilde{\mathcal{R}}u$.
(3) Use (12.121) to reconstruct u:

$$u(\boldsymbol{x},t) = \frac{1}{2}\int_{S^{d-1}} d\sigma(\boldsymbol{\omega})\left\{\frac{1}{2}[\tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega}+t,\boldsymbol{\omega})+\tilde{\mathcal{R}}f(\boldsymbol{x}\cdot\boldsymbol{\omega}-t,\boldsymbol{\omega})] + \frac{1}{2}\int_{\boldsymbol{x}\cdot\boldsymbol{\omega}-t}^{\boldsymbol{x}\cdot\boldsymbol{\omega}+t}\tilde{\mathcal{R}}g(s,\boldsymbol{\omega})\right\}ds. \tag{28.126}$$

28.46 Waves in odd and even dimensional spaces behave very differently. Let us calculate the modified Radon transform (12.123) explicitly. If d is odd, then $|\rho|^{d-1} = \rho^{d-1}$, so that multiplying ρ can be interpreted as differentiation with respect to s as

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) = \frac{1}{2}(-1)^{(q-1)/2}\left(\frac{1}{2\pi}\right)^{d-1}\frac{\partial^{d-1}}{\partial s^{d-1}}\mathcal{R}f(s,\boldsymbol{\omega}). \tag{28.127}$$

In contrast, if d is even then the non-analyticity of $|\rho|$ must be dealt with as $|\rho|^{d-1} = sgn(\rho)\rho^{d-1}$, so that

$$\tilde{\mathcal{R}}f(s,\boldsymbol{\omega}) = \frac{1}{2}(-1)^{(q-1)/2}\left(\frac{1}{2\pi}\right)^{d-1} H\left[\frac{\partial^{d-1}}{\partial s^{d-1}}\mathcal{R}f(s,\boldsymbol{\omega})\right], \tag{28.128}$$

where H is the *Hilbert transform* (→**??**) defined by

$$Hf(x) = P\int \frac{f(s)}{x-s}ds, \tag{28.129}$$

where P denotes the Cauchy principal value (→**??**). This can be obtained from the convolution formula and the Fourier transform of *sgn* (→**12.40**).

Look at the use of the modified Radon transform in the solution (12.126) when the initial velocity is everywhere zero. This applies to the case of an instantaneous flash of light emitted from a point (that is, $f = \delta(x)$). If $\tilde{\mathcal{R}}f(s\boldsymbol{\omega})$ is determined by $\mathcal{R}f(s,\boldsymbol{\omega})$ only, then the observer at distance sees only a flash of light. That is, the wave is localized in time in odd-dimensional (≥ 3) spaces. On the other hand, if the spatial dimensionality is even, then the Hilbert transform implies that the wave is not localized in time. Thus, after watching a flash, the observer must feel that the world becomes brighter (the *afterglow effect* in even dimensional spaces) (→**??**).

APPENDIX a32 Bessel Transform

28.47 Theorem [Hankel]. Let $f \in L_1([0,\infty), r)$ and be piecewise continuous. Then

$$\frac{1}{2}[f(r+0)+f(r-0)] = \int_0^\infty J_\nu(\sigma r)\sigma d\sigma \int_0^\infty f(\rho)J_\nu(\sigma\rho)\rho d\rho \quad (28.130)$$

for $\nu \geq 1/2$. This may also be expressed as

$$\int_0^\infty J_\nu(\sigma r)J_\nu(\sigma r')\sigma d\sigma = \delta(r-r')/r. \quad (28.131)$$

Notice that the RHS is the delta function adapted to the weight r (i.e., $\delta_r(r-r') \rightarrow$**??**).[324] □

[Demo] Here (12.130) is proved for continuous L_1 (→**15.9**) functions and integer $\nu = n$. Let

$$F(x,y) = f(r)e^{in\varphi}, \quad (28.132)$$

where $x = r\cos\varphi$ and $y = r\sin\varphi$. With the aid of the Fourier expression of the delta function (→**??**), we can write

$$F(x,y) = \frac{1}{(2\pi)^2}\int dk_x \int dk_y \int d\xi \int d\eta F(\xi,\eta)e^{ik_x(x-\xi)+ik_y(y-\eta)}. \quad (28.133)$$

Introduce polar coordinates as

$$\xi = r'\cos\psi, \quad \eta = r'\sin\psi, \quad (28.134)$$

$$k_x = k\cos\theta, \quad k_y = k\sin\theta. \quad (28.135)$$

(12.133) is rewritten as ($F(\xi,\eta) = f(r')e^{in\psi}$)

$$f(r)e^{in\varphi} = \int_0^\infty dk k \int_0^\infty dr' r' f(r') \left\{ \frac{1}{2\pi}\int_{-\pi}^{\pi} d\theta e^{ikr\cos(\theta-\varphi)} \frac{1}{2\pi}\int_{-\pi}^{\pi} d\psi e^{in\psi}e^{-ikr'\cos(\psi-\theta)} \right\}. \quad (28.136)$$

Setting $\psi - \theta = t$, we get

$$\frac{1}{2\pi}\int_\pi^\pi e^{in\psi}e^{-ikr'\cos(\psi-\theta)}d\psi = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ikr'\cos t}e^{in(t+\theta)}dt \quad (28.137)$$

$$= e^{in\pi/2}e^{in\theta}J_n(-kr') = e^{in\pi/2+in\theta}(-1)^n J_n(kr'). \quad (28.138)$$

Here the generating function of Bessels functions (→**23.5**) has been used. Analogously, we have

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{ikr\cos(\theta-\varphi)}e^{in\theta}d\theta = e^{in\pi/2+in\varphi}J_n(kr). \quad (28.139)$$

Hence, (12.136)–(12.139) implies (12.130) for $\nu = n$.

A more convenient formulas may be

[324] More generally, f may be of bounded variation. See G. N. Watson, *A Treatise on the Theory of Bessel Function* (Cambridge UP, 1962) p456–.

28.48 Bessel transform and its inverse.

$$g(r) = \int_0^\infty h(r')J_\nu(r'r)r'dr', \tag{28.140}$$

$$h(r) = \int_0^\infty g(r')J_\nu(r'r)r'dr'. \tag{28.141}$$

Note that these are the formulas for the Fourier sine (or cosine) transform (→**28.8**) for $\nu = \pm 1/2$ (→**23.19**).

28.49 Examples. See **23.15**.

$$\int_0^\infty e^{-ax}J_0(xy)dx = \frac{1}{\sqrt{a^2+y^2}} \leftrightarrow \int_0^\infty \frac{y}{\sqrt{a^2+y^2}}J_0(xy)dy = \frac{e^{-ax}}{x}. \tag{28.142}$$

$$\int_0^\infty \cos axJ_0(xy)dx = \frac{1}{\sqrt{y^2-a^2}} \leftrightarrow \int_0^\infty \frac{y}{\sqrt{y^2-a^2}}J_0(xy)dy = \frac{\cos ax}{x}. \tag{28.143}$$

$$\int_0^\infty e^{-a^2x^2}x^{\nu+1}J_\nu(xy)dx = \frac{y^\nu}{(2a^2)^{\nu+1}}e^{-y^2/4a^2} \leftrightarrow \int_0^\infty \frac{y^{\nu+1}}{(2a^2)^{\nu+1}}e^{-y^2/4a^2}J_\nu(xy)dy = e^{a^2x^2}x^\nu. \tag{28.144}$$

29 Laplace Transformation

Laplace transformation is a disguised Fourier transformation for causal functions (the functions that are zero in the past), and is a very useful tool to study transient phenomena. The inverse transformation is often not easy, but clever numerical tricks may be used to invert the transforms. Appendix **a33** discusses a disguised Laplace transformation, Mellin transformation, which is useful when we wish to solve problems on fan shaped domains.

Key words: Laplace transform, fundamental theorem, convolution, time-delay, fast inverse Laplace transform.

Summary:
(1) Laplace transformation **29.2** allows one to solve many ODE algebraically with the aid of tables (**33.14**).
(2) Basic formulas like the convolution theorem, delay theorem, etc should be known to this end (**29.7**-**29.10**).

29.1 Motivation. Due to causality, we often encounter functions of time t that are zero for $t < 0$ (or often so for $t \leq 0$ due to continuity). Then, the so-called one-sided Fourier transform

$$F[\omega] = \int_0^\infty f(t)e^{i\omega t}dt \tag{29.1}$$

appears naturally. However, if $f(t)$ grows as e^{at} $(a > 0)$, then this does not make sense even in the sense of generalized functions ($\rightarrow$**??**). Even in this case, if we choose sufficiently large $c > 0$, the one-sided Fourier transform of $e^{-ct}f(t)$ exists in the ordinary sense. If $f(t)e^{-ct}\Theta(t)$ ($\Theta(t)$ is the Heaviside step function $\rightarrow$**??**) is absolutely integrable, and f' is piecewise continuous for $t > 0$, then from the Fourier transform of this function, $f(t)$ for $t > 0$ can be recovered.

29.2 Definition of Laplace transform. The following transformation $\mathcal{L}_s$ is called the *Laplace transformation*:

$$\mathcal{L}_s[u(t)] = \int_0^\infty e^{-st}u(t)dt, \tag{29.2}$$

where $s = c - i\omega$ and c is chosen sufficiently large so that the integral exists. $\mathcal{L}_s[u]$ is called the *Laplace transform* of u.[325]

[325] For a history, see M. F. Gardner and J. L. Barnes, *Transients in Linear Systems* vol.I (Wiley, 1942) Appendix C.

Discussion.
(A) A discrete counterpart is the so-called *z-transformation*: The z-transform $A(z)$ of $\{a_n\}$ is defined by

$$A(z) = \sum_{n=0}^{\infty} a_n z^n. \tag{29.3}$$

This is also called the *generating function* of the sequence $\{a_n\}$. The inverse transform is given by

$$a_n = \frac{1}{2\pi i} \int_{\partial D} dz \frac{A(z)}{z^{n+1}}, \tag{29.4}$$

where D is a disc containing the origin but excluding all the singularities of $A(z)$.
(B) z-transform is a convenient way to solve linear difference equation:

$$a_0 x_{n+r} + a_1 x_{n+r-1} + \cdots + a_{r-1} x_{n+1} + a_r x_n = 0. \tag{29.5}$$

For example, let us solve

$$x_{n+2} - 2x_{n+1} + x_n = 0 \tag{29.6}$$

with the 'initial conditions' $x_0 = 1$, and $x_1 = 0$. The z-transform $X(z)$ obeys

$$X(z) - 1 + 2z(X(z) - 1) + z^2 X(z) = 0. \tag{29.7}$$

From this we can solve $X(z)$. The inverse transform gives $x_n = 1 - n$.
(C) An inhomogeneous linear difference equation is given by

$$a_0 x_{n+r} + a_1 x_{n+r-1} + \cdots + a_{r-1} x_{n+1} + a_r x_n = f_n \tag{29.8}$$

The general solution to this equation is given by the sum of the general solution of (13.5) and a special solution to (13.8) just as the linear differential equation. If we can compute the z-transform of $\{f_n\}$, then at least $X(z)$ can be obtained. However, to obtain x_n from X may not be very easy.

29.3 Who was Laplace (1749-1827) ? The 'Newton of France' was born into a cultivated provincial bourgeois family in Normandy (Beaumont-en-Auge) in 1749. After his secondary school education he attended University of Caen n 1766 to study the liberal arts, but two of his professors (Gadbled and LeCanu) urged this gifted student to pursue mathematics. With LeCanu's letter to d'Alembert (→**??**) he left for Paris at age 18 in 1768. He impressed d'Alembert, who secured a position for him at the Ecole Militaire. In 1773 he demonstrated that the acceleration observed in Jupiter and Saturn was not cumulative but periodic. This was the principal advance in dynamical astronomy since Newton toward establishing the stability of the solar system. This work won him election to the Paris Academy in 1773.

Between 1778 and 1789 he was at his scientific prime. Laplace introduced his transformation in 1779, which was related to Euler's work. In 1780 he worked together with Lavoisier to make a calorimeter to establish that respiration is a form of combustion. Although he played

a decisive role to design the metric system in 1790, he wisely avoided Paris when the Jacobins dominated until 1794. In the late 1790s with three well received books (one of which, *Systéme du Monde*, was not only a fine science popularizer but also a model of French prose), he became a European celebrity.

Laplace advanced applied mathematics and theory of probability substantially. He based his theory on generating functions, and extended Jakobi Bernoulli's work on the law of large numbers. He was amply honored by Napoleon and by Louis XVIII. During his final years he lived at his country home in Arceuil, next to his friend chemist Berthollet, surrounded by the adopted children of his thoughts, Arago, Poisson, Biot, Gay-Lussac, von Humboldt and others.

29.4 Fundamental theorem of Laplace transform.

(1) The Laplace transform of f (13.2) exists for s such that $e^{-(Re\, s)t} f(t) \in L_1([0,\infty))$.
(2) There is a one-to-one correspondence between $f(t)$ and its Laplace transform $\mathcal{L}_s[f]$. More explicitly, we have

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{st} \mathcal{L}_s[f] ds, \tag{29.9}$$

where c is a real number larger than the convergence coordinate c^* such that all the singularities of $\mathcal{L}_s[f]$ lie on the left side of $z = c^*$ in $\boldsymbol{C}$.[326]
[Demo] (1) is obvious. At least formally, (2) follows from the motivation **29.1**. Fourier inverse transform of $\mathcal{L}_s[f]$ gives

$$f(t) = e^{ct} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega t} \mathcal{L}_{c-i\omega}[u(t)] d\omega. \tag{29.10}$$

Since $d\omega = ids$, (13.10) becomes

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} \mathcal{L}_s[f(t)] e^{st} ds. \tag{29.11}$$

For this integral to be meaningful, we need the following theorem:

Discussion.
(1) $f(t) = \exp(t^\sigma)$ with $\sigma > 1$ does not have Laplace transforms.
(2) The minimum real number r making $f(t)e^{-rt} \in L_2([0,+\infty))$ is called the *convergence coordinate*.
Exercise.
Although practically, there is almost no need (→**29.14**) of calculating the integral

[326] This was formally shown by Riemann by 1859. Mellin proved this in Acta Soc. Sci. Fenn. **21**, 115 (1896). Hence, there is absolutely no justification to call this integral the 'Bromwitch integral.' History must not be distorted due to national interests.

(13.9), still it is a good exercise of complex integration. Demonstrate the following inverse transform relations with the aid of the residue theorem (→**8B**).
(1)

$$\mathcal{L}_s^{-1}\frac{1}{(s+\alpha)^n} = \frac{t^{n-1}}{(n-1)!}e^{-\alpha t}, \tag{29.12}$$

where $\alpha > 0$ and n is a positive integer.
(2) How can we do a similar thing, if n is not an integer? In this case, $s = 0$ is a branch point (→**??**-**??**). If $n \in (0, 1)$, then a straightforward contour integration along the contour in the figure works. The contribution from the small circle vanishes in the small radius limit, and the contribution from the large circle is zero thanks to the Jordan lemma **??**. We need **14.4** to streamline the formula. If n is larger, then probaly the cleverest way is to use **29.7**(5) and reduce the problem to the case of $n \in (0, 1)$.

29.5 Theorem. $\mathcal{L}_s[f]$ is holomorphic (→**??**) where $\mathcal{L}_s[f]$ exists. □[327] Therefore, if $\mathcal{L}_s[f]$ exists for $c > c^*$, then $\mathcal{L}_s[f]$ has no singularity on the half plane $Re\, z \geq c$.

This implies that
(1) $\mathcal{L}_s[f]$ is differentiable with respect to s,
(2) $\mathcal{L}_s[f]$ is determined by its behavior on the portion of the real axis $x > c^*$ through analytic continuation (→**??**).

29.6 Theorem. If s goes to s_0 along a curve lying inside the convergence domain, then

$$\lim_{s\to s_0} \mathcal{L}_s[f] = \mathcal{L}_{s_0}[f]. \tag{29.13}$$

Especially,

$$\lim_{s\to\infty} \mathcal{L}_s[f] = 0. \tag{29.14}$$

[Demo] (13.14) follows from (13.13), which follows trivially from an elementary property of the Lebesgue integral.

29.7 Some properties of Laplace transform.
(1) $a\mathcal{L}_s[f(at)] = \mathcal{L}_{s/a}[f(t)]$, where a is a positive constant. This can be shown by a straightforward calculation.
(2) $\mathcal{L}_s[e^{-bt}f(t)] = \mathcal{L}_{s+b}[f(t)]$. This is straightforward, too.
(3) $\mathcal{L}_s[t^n f(t)] = (-1)^n(d/ds)^n\mathcal{L}_s[f(t)]$. In particular, $\mathcal{L}_s[tf(t)] = -d/ds\mathcal{L}_s[f(t)]$.

[327] To prove this we need the following elementary theorem about Lebesgue integration
Theorem. Suppose
(1) $f(x, s)$ is integrable (→**15.9**) for each s as a function of x,
(2) $f(x, s)$ is holomorphic for almost all x as a function of s,
(3) There is an integrable function Φ such that $|f(x, s)| \leq \Phi(x)$.
Then, $\int dx f(x, s)$ is holomorphic as a function of s. □

(4) $\mathcal{L}_s[f^{(n)}(t)] = s^n\mathcal{L}_s[f(t)] - s^{n-1}f(0) - s^{n-2}f'(0) - \cdots - s^{n-k}f^{(k-1)}(0) - \cdots - sf^{(n-2)}(0) - f^{(n-1)}(0)$. In particular,

$$\mathcal{L}_s[f'(t)] = s\mathcal{L}_s[f(t)] - f(0). \tag{29.15}$$

This is due to integration by parts.
(5) $\mathcal{L}_s\left[\int_0^t f(t')dt'\right] = s^{-1}\mathcal{L}_s[f(t)]$.
(6) $\mathcal{L}_s[t^{-1}f(t)] = \int_s^\infty ds\mathcal{L}_s[f(t)]$.
(3) - (6) imply that calculus becomes algebra through the Laplace transformation. This is the most important and useful property facilitating the solution of linear ODE.

Discussion
The following equation is called the *Airy equation* (→**23.23** Exercise (3))

$$\frac{d^2y}{dt^2} - ty = 0. \tag{29.16}$$

Since the coefficient is only a linear function of t, Laplace transformation is advantageous. Let z be a function of s that is the Laplace transform of y with respect to t. Then,

$$\frac{dz}{ds} - s^2z = 0, \tag{29.17}$$

which can be solved easily as

$$z = e^{s^3/3}. \tag{29.18}$$

Hence, a solution to can be written as

$$Ai(t) = \frac{1}{2\pi i}\int_C \exp\left(st - \frac{1}{3}t^3\right)ds. \tag{29.19}$$

Here C can be a path as shown in the figure. The integral is called the *Airy integral* .
Show that

$$Ai(0) = 3^{-1/6}\Gamma(1/3)/2\pi. \tag{29.20}$$

29.8 Convolution. If we adapt the ordinary definition of convolution **??** to functions that are zero for $t < 0$, we get

$$(f_1 * f_2)(t) = \int_0^t f_1(t-u)f_2(u)du. \tag{29.21}$$

A straightforward calculation gives

$$\mathcal{L}_s[f_1 * f_2] = \mathcal{L}_s[f_1]\mathcal{L}_s[f_2]. \tag{29.22}$$

Exercise.

$$\int_0^x \sin(x-y)u(y)dy + u(x) = \cos x. \tag{29.23}$$

29.9 Time-delay.

$$\mathcal{L}_s[f(at-b)\Theta(at-b)] = \frac{1}{a}e^{-bs/a}\mathcal{L}_{s/a}[f(t)] \tag{29.24}$$

This is also demonstrated by a simple calculation. $e^{-\tau s}$ is often called a delay factor.

29.10 Periodic functions. If f is a function with period T, then

$$\mathcal{L}_s[f(t)] = (1-e^{-sT})^{-1}\int_0^T e^{-st}f(t)dt. \tag{29.25}$$

[Demo] Thanks to the periodicity, we get

$$\int_0^\infty e^{-st}f(t)dt = \int_0^\infty e^{-st}f(t+T)dt = \int_T^\infty e^{-s\tau}f(\tau)d\tau e^{sT}, \tag{29.26}$$

where $t=\tau-T$. This implies that

$$\mathcal{L}_s[f(t)] = \left\{\mathcal{L}_s[f(t)] - \int_0^T e^{-st}f(t)dt\right\}e^{sT}. \tag{29.27}$$

Solving this equation for $\mathcal{L}_s[f]$, we get the desired formula.

29.11 Examples.
(1) $\mathcal{L}_s[1] = 1/s$ is obvious by definition.
(2) This with (2) of **29.7** implies $\mathcal{L}_s[e^{-bt}] = 1/(s+b)$.
(3) Linearity of the Laplace transformation and (2) give, for example,

$$\mathcal{L}_s[\cos\omega t] = \frac{1}{2}(\mathcal{L}_s[e^{i\omega t}] + \mathcal{L}_s[e^{-i\omega t}]) = \frac{s}{s^2+\omega^2}. \tag{29.28}$$

Analogously, we get $\mathcal{L}_s[\cosh at] = s/(s^2-a^2)$, $\mathcal{L}_s[\sin\omega t] = \omega/(s^2+\omega^2)$, etc.
(4) (3) with (2) of **29.7** gives for example

$$\mathcal{L}_s[e^{-bt}\cos\omega t] = \frac{s+b}{(s+b)^2+\omega^2}. \tag{29.29}$$

(5) (1) and (3) of **29.7** imply

$$\mathcal{L}_s\left[\frac{t^n}{n!}\right] = \frac{1}{s^{n+1}}. \tag{29.30}$$

More generally, for $\nu > -1$

$$\mathcal{L}_s\left[\frac{t^\nu}{\Gamma(\nu+1)}\right] = \frac{1}{s^{\nu+1}}. \tag{29.31}$$

This can be shown immediately by the definition of the Gamma function (→**9**).
(6) Combining (13.30) and (2) of **29.7** gives

$$\mathcal{L}_s[e^{-bt}t^n] = \frac{n!}{(s+b)^{n+1}}. \tag{29.32}$$

(7) An application of **29.10** is

$$\mathcal{L}_s[|\sin t|] = \frac{1}{s^2+1}\coth\frac{\pi s}{2}. \tag{29.33}$$

(8) Applying the convolution theorem **29.8** we can demonstrate

$$\int_0^t J_0(\tau)J_0(t-\tau)d\tau = \sin t \tag{29.34}$$

This follows from (→**23.15**)

$$\mathcal{L}_s[J_0(t)] = \frac{1}{\sqrt{s^2+1}}. \tag{29.35}$$

Exercise.
(A) Show

$$\mathcal{L}_s\frac{1}{\sqrt{t}} = \frac{\sqrt{\pi}}{\sqrt{s}}. \tag{29.36}$$

(B) Find
(1) $\mathcal{L}_s \cos^2 \omega t$.
(2) For $\tau > 0$ and $a > 0$ $\mathcal{L}_s(t-t_1)E^{-a(t-t_2}\Theta(t-\tau)$.

29.12 Laplace transform of delta function. We can define Laplace transforms of generalized functions. We will not discuss this, since the relation between Fourier and Laplace transformations **29.1** explains virtually everything we need practically. A subtlety may remain in the definition of the Laplace transformation of $\delta(x)$, since the definition **29.2** requires an integration from 0. That is, we must consider the product of $\delta(x)$ and $\Theta(x)$, which is meaningless (→**??**) as generalized functions. Without any ambiguity for $a > 0$

$$\mathcal{L}_s[\delta(t-a)] = e^{-as}. \tag{29.37}$$

This means the Laplace transform of the weak limit $\lim_{\epsilon\to 0+}\delta(t-\epsilon)$ is 1. Hence, as a generalized function it is sensible to define (→**??**)

$$\mathcal{L}_s[\delta(t)] = 1. \tag{29.38}$$

From this (13.37) is obtained with the aid of the time delay formula **29.9**.

29.13 Short time limit.

$$\lim_{t\to 0+} f(t) = \lim_{s\to\infty} s\mathcal{L}_s[f(t)]. \tag{29.39}$$

[Demo] **29.7**(4) with $n = 1$ reads $\mathcal{L}_s[f'(t)] = s\mathcal{L}_s[f(t)] - f(0)$. Apply **29.6** to f', and we get $\lim_{s\to\infty} \mathcal{L}_s[f'(t)] = 0$.

29.14 Practical calculation of Laplace inverse transformation: Use of tables. Although the fundamental theorem **29.4**(2) gives a method to compute the inverse transforms, practically, an easier method is to use a table of Laplace transforms of representative functions. The uniqueness of the transforms (→**29.4**(2)) guarantees that once we can find an inverse transform, that is the inverse transform of a given function of s. Also numerical fast Laplace inverse transform is available.

Exercise.

(1) Solve the following differential equation with the aid of Laplace transformation

$$\frac{d^2y}{dt^2} + 2a\frac{dy}{dt} + (a^2 + b^2)y = e^{-at}\sin bt.$$

Here a and b are positive constants, and the initial condition is $y(0) = y'(0) = 0$.

(2) Using Laplace transformation, solve the following integrodifferential equation

$$y(t) = y'(t) + t + 2\int_0^t (t-u)y(u)du$$

with the initial condition $y(0) = 0$.

29.15 Heaviside's expansion formula.[328] Let $F(s)$ be a rational function[329] $F(s) = P(s)/Q(s)$, where P and Q are mutually prime polynomials, and the order of Q is higher than that of P. If $Q(s) = A(s-a_1)\cdots(s-a_n)$ and $a_1, \cdots, a_n$ are all distinct, then

$$\frac{P(s)}{Q(s)} = \sum_{s=1}^{n} \frac{c_k}{s-a_k} \tag{29.40}$$

with $c_k = P(a_k)/Q'(a_k)$. □

This is obvious, and implies that

$$\mathcal{L}_s^{-1}[P(s)/Q(s)] = \sum_{k=1}^{n} P(a_i)e^{a_k t}/Q'(a_k) \tag{29.41}$$

[328] Heaviside (1850–1925) introduced an algebraic method to solve ODEs, which can be understood as the Laplace transform method explained below. The method, which requires generalized functions like the Heaviside step function, and even the delta function, was never accepted by mathematicians of his day. According to an anecdote, he said that we could eat even though we did not know the mechanism of digestion. This story is often told as a story of a triumph of a self-educated genius. **However**, the method was actually invented by Cauchy long ago. Therefore the story must be quoted as a failure of premature ossification of mathematics due to mediocre mathematicians.

[329] A rational function is a ratio of two polynomials.

29.16 Examples.

$$\mathcal{L}_s^{-1}\left[\frac{s^2+s+1}{(s^2+1)^3}\right] = \frac{1}{8}(4+t)\sin t - \frac{1}{8}(4t+t^2)\cos t. \tag{29.42}$$

$$\mathcal{L}_s^{-1}\left[\frac{2s+3}{2s^3+3s^2-2s}\right] = -\frac{3}{2} - \frac{1}{10}e^{-2t} + \frac{8}{5}e^{t/2}. \tag{29.43}$$

$$\mathcal{L}_s^{-1}\left[\frac{s^2+1}{2(s^4+s^2+1)}\right] = 1-\frac{\sqrt{3}}{3}\left[e^{t/2}\cos\left(\frac{\sqrt{3}}{2}t+\frac{\pi}{6}\right) + e^{-t/2}\cos\left(\frac{\sqrt{3}}{2}t-\frac{\pi}{6}\right)\right]. \tag{29.44}$$

Exercise.
(1) Find the inverse transform of

$$g(s) = \frac{s^2-\omega s+\omega^2}{s(s^2+\omega^2)}. \tag{29.45}$$

(Answer: $\Theta(t) - \sin\omega t$).

$$g(s) = \frac{1+e^{\pi s}}{s(s^2+1)}. \tag{29.46}$$

29.17 Fast inverse Laplace transform. T. Hosono, "Numerical inversion of Laplace transform and some applications to wave optics," Radio Science **16**, 1015 (1981); *Fast Laplace transform in Basic*, (Kyoritsu Publ., 1984)

Table

Appendix a33 Mellin Transformation

29.18 Mellin transformation. The *Mellin transform* $\breve{f}$ of $f(r)$ is defined as

$$\breve{f}(p) = \int_0^\infty f(r) r^{p-1} dr. \tag{29.47}$$

This is well-defined for p satisfying $\sigma_1 < Re\, p < \sigma_2$, where

$$\int_0^1 r^{\sigma_1 - 1} |f(r)| dr < +\infty, \quad \int_1^\infty r^{\sigma_2 - 1} |f(r)| dr < +\infty. \tag{29.48}$$

29.19 Theorem [Fundamental theorem of Mellin transformation].
(1)

$$\breve{f}(p) = \int_0^\infty f(r) r^{p-1} dr \tag{29.49}$$

is analytic in the strip $\sigma_1 < Re\, p < \sigma_2$.
(2) Inverse transformation:

$$f(r) = \frac{1}{2\pi i} \int_\Gamma \breve{f}(p) r^{-p} dp, \tag{29.50}$$

where Γ is a straight line in the above strip.□
[Demo] (1) is shown just as the counterpart for the Laplace transformation (→). (2) is also a disguised version of the inversion formula for the Laplace transformation (→**29.2**). Introduce t as $r = e^{-t}$. Then (13.47) reads

$$\breve{f}(p) = \int_0^\infty e^{-pt} f(e^{-t}) dt \tag{29.51}$$

This is the Laplace transformation (→**29.3**). Therefore, we can apply the inverse transformation formula to obtain

$$f(e^{-t}) = \frac{1}{2\pi i} \int_{\sigma - i\infty}^{\sigma + i\infty} \breve{f}(p) e^{pt} dp. \tag{29.52}$$

In terms of r, this is just what we wanted.

29.20 Applications to PDE. If the region of the problem is fan-shaped, then the Mellin transformation is particularly useful. 2-Laplace problem in the cylindrical coordinates is

$$r^2 \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) u + \frac{\partial^2}{\partial \varphi^2} u = 0. \tag{29.53}$$

Melling transforming this, we get

$$p^2 \breve{u} + \frac{d^2}{d\varphi^2} \breve{u} = 0, \tag{29.54}$$

which can be solved easily. The rest is to compute the inverse transform. To calculate it as the Laplace transform (13.52) may be advantageous, since there is the so-called fast Laplace transform algorithm (→**29.17**).

30 Linear Operators

A linear partial differential operator is understood as a linear map from a function space into another function space. The most important case for physicists may be the linear map on a Hilbert space. We will discuss the meaning of self-adjointness of an operator in conjunction to quantum mechanics in Part A. Part B discusses spectral decomposition of an operator. Part C is a short summary of spectrum theory.

Key words: linear operator (symmetric, self-adjoint), operator extension, observable, spectral decomposition, decomposition of unity, spectral measure, semibound operator, spectrum (essential, point, discrete, absolute continuous), compact operator, Hilbert-Schmidt theorem.

Summary:
(1) In quantum mechanics, self-adjoint linear operators are regarded as observables. The reason why self-adjointness is required can be glimpsed in **30.2**-**30.5**. [Notice that the explanation is probably very different from the one given in physics courses, because in the ordinary quantum mechanics courses self-adjointness is never explained correctly.]
(2) Spectral decomposition is a generalization of diagonalization of matrices, and is the theoretical underpinning of separation of variables (**30.8**, **30.11**).
(3) Whether we may apply the spectral decomposition to a partial differential operator can be checked very formally (**30.10**).
(4) Spectrum of an operator is often directly related to physical observables as electronic and phonon spectra. A clear definition of spectrum must be recognized (**30.13**). Physicists call absolutely continuous spectrum band spectrum, and point spectrum discrete spectrum (**30.19**). Cantor-set like spectrum has also become relevant to physics, which is the singular continuous spectrum.

30.A Self-Adjointness

30.1 Linear operator.[330] As discussed in **??** the superposition principle requires that the quantum mechanical state is described by a vector in a vector space (→**16.1**) (Hilbert space →**16.3**) V. A linear operator A is a linear map from a subspace $D(A)$ of V into V. $D(A)$ is called the *domain* of A, and $AD(A) \equiv \{Az : z \in D(A)\}$ is called the *range* of A. In quantum mechanics it is assumed that a linear operator (with appropriate properties) A corresponds to a dynamical variable (*observable*), and that for a state $|x\rangle$, the expectation value of the observable A is given by $\langle x|A|x\rangle$.[331]

Example. The domain of d/dx in $L_2([a,b])$ (→**16.5**(2)) is not the whole space, because d/dx cannot be operated on non-differentiable functions.[332] However, since $C^1([a,b])$ is dense in $L_2([a,b])$, the domain of d/dx is dense in $L_2([a,b])$.

30.2 When can a linear operator be an observable?

(1) Let A be a linear operator on a Hilbert space V (→**16.3**). If $D(A)$ is dense in V and Hermitian (i.e., $\langle x|Ay\rangle = \langle Ax|y\rangle$[333]), we say A is *symmetric*. Since this is a necessary and sufficient condition for $\langle x|A|x\rangle$ to be real, physical observables must at least be symmetric.

(2) However, this is not enough, because the extension of A may not be symmetric. An operator $\tilde{A}$ such that $D(\tilde{A}) \supset D(A)$ and $A = \tilde{A}$ on $D(A)$ is called an *extension* of A. Unfortunately, indeed some symmet-

[330] The most authoritative (and accessible) reference is T. Kato, *Perturbation Theory for Linear Operators* (Springer, 1966).

[331] Dirac explicitly assumes these, while Landau and Lifshitz use spectral decomposition to justify the assumption. However, all the assumptions have come from the observations based on finite dimensional linear algebra.

[332] More precisely, $df/dx \in L_2([a,b])$ is required.

[333] Of course, this means

$$\int \overline{x(t)}(Ay)(t)dt = \int \overline{(Ax)(t)}y(t)dt.$$

ric operators are extended to non-symmetric operators.[334] The whole Hilbert space should be physically meaningful, so that symmetry is not enough to characterize a respectable observable.
(3) It is important that a symmetric operator A which corresponds to a 'physical observable' should not be extended further. A condition is the self-adjointness. To understand this statement, we need the following entries.

30.3 Adjoint operator. Let A be an operator on a Hilbert space V whose domain is dense. Let $D(A^*)$ be the totality of $x \in V$ such that

$$\langle x|Ay\rangle = \langle z|y\rangle \tag{30.3}$$

for all $y \in D(A)$ for some $z \in V$. For $x \in D(A^*)$ z is unique: if there were two z_1 and z_2, then $\langle z_1 - z_2|y\rangle = 0$ for $\forall y \in D(A)$. Since $D(A)$ is dense, this implies $z_1 = z_2$. Thus there is a unique map $x \to z$. We will write this as $z = A^*x$, defining a linear map A^*. This is called the *adjoint* of A.

For example $-id/dx$ defined on C_0^1[335] is self-adjoint:

$$\int d\tau \overline{f(x)} \left(-\frac{d}{dx}\right) g(x) = \int d\tau \left\{\overline{-i\left(\frac{d}{dx}\right)}\right\} g(x), \tag{30.4}$$

so that indeed $(-id/dx)^* = -id/dx$.

30.4 Self-adjoint operator. If A is a linear operator with a dense domain and $A = A^*$ (i.e., $D(A) = D(A^*)$ and symmetric), then A is called a *self-adjoint operator*.

[334] An example from H. Ezawa, *Quantum Mechanics III* (Iwanami, 1972) p26. follows. Let $V = L_2(\boldsymbol{R})$. The operator Z is defined by

$$Z\psi(x) = -i\left(x^3\frac{d}{dx} + \frac{d}{dx}x^3\right)\psi(x) \tag{30.1}$$

with the dense domain spanned by $\{H_n e^{-x^2/2}\}$ (→**17.20**). It is easy to check that Z is symmetric. However, if this is applied to

$$\varphi(x) = x^{-3/2}e^{-1/4x^2}, \text{ for } x > 0; \quad \text{otherwise } \varphi(x) = 0, \tag{30.2}$$

we know $Z\varphi(x) = -i\varphi(x)$ (except at $x = 0$; this exception may be ignored, because we are in a L_2-space), so that $\langle\varphi|Z|\varphi\rangle = -i$, the expectation value is purely imaginary!

[335] C^1 functions with compact supports, i.e., they vanish outside sufficieintly large sphere centeres at the origin.

30.5 Observable should be at least self-adjoint. We know that an observable must be a symmetric operator. However, A^* is obviously its extension, so it is natural to interpret that A^* is 'the' observable. However, we know that this may not be symmetric. This strongly suggests that observables must be self-adjoint, so that we will never encounter imaginary eigenvalues. Later, we will learn that for a self-adjoint operator, we can unambiguously determine (define) the probability of observing a particular value (or a particular range of the values) for any state in the state space thanks to the spectral decomposition theorem (→**34B.3**). This justifies the identification.

30.B Spectral Decomposition

30.6 Spectral decomposition in finite dimensional space. Consider a normal linear operator[336] A on a finite dimensional vector space. Let $\{\lambda\}$ be its eigenvalues, and $|\lambda\rangle$ be the corresponding normalized eigenkets. Then, we have the following *spectral decomposition* formula

$$A = \sum_\lambda |\lambda\rangle\lambda\langle\lambda| = \sum_\lambda \lambda P(\lambda), \tag{30.5}$$

where $P(\lambda)$ is the orthogonal projection (→**16.18**) to the eigenspace belonging to λ.

$$1 = \sum_\lambda |\lambda\rangle\langle\lambda| = \sum_\lambda P(\lambda) \tag{30.6}$$

is called a *decomposition of unity* (→**16.15**). If we can have this decomposition, we can spectral decompose the operator. How can we generalize this to the operators on a Hilbert space (→**16.3**)?

30.7 Decomposition of unity in Hilbert space. This is, for physicists, just (→**16.23**)

$$1 \equiv \int_{-\infty}^{\infty} |\nu\rangle w(\nu) d\nu \langle\nu|, \tag{30.7}$$

where $|\nu\rangle$ is an eigenket or *improper eigenket* (because it may not be normalizable), and w is a weight function (let us call $w(\nu)$ a *spectral weight*). To find improper eigenkets is called the *generalized eigenvalue problem* (**31.5** solves the problem.)

[336] If a linear operator A satisfies $A^*A = AA^*$, then we say A is a *normal* operator. Its matrix representation is a *normal matrix* and is diagonalizable with a unitary transformation. Actually, a necessary and sufficient condition for a matrix A to be diagonalizable with a unitary transformation is that A is normal.

30.8 Theorem. Let A be a self-adjoint operator (→**30.4**) on a Hilbert space V. Then, there is a unique decomposition of unity

$$1 = \int |\nu\rangle w(\nu) \langle \nu| \tag{30.8}$$

such that

$$A = \int_{-\infty}^{\infty} \nu \, |\nu\rangle w(\nu) d\nu \langle \nu|. \tag{30.9}$$

30.9 Why do we pay attention to spectral decomposition? It is a fundamental tool to understand operators, and is a very useful tool for quantum mechanics. In our current partial differential equation context, the spectral decomposition is of superb importance with respect to, as the reader should have already guessed, the separation of variables (→**18**, **23**). However, to understand the justification of the method in general, we need almost all the machineries of elementary functional analysis. First of all, most partial differential operators are not self-adjoint. For example, the Laplacian with a homogeneous Dirichlet condition is only symmetric. Hence, to use the operator theory, we must consider the self-adjoint extension (→**30.2**) of the differential operator. Rather heavy tools are required to obtain it, but the result boils down to:

30.10 Practical conclusion. The following is a practical conclusion about differential operators:
(1) If $P(x, D)$ is formally self-adjoint, i.e.,

$$\int_\Omega f(x) P(x, D) g(x) dx = \int \left(P^T(x, D) f(x) \right) g(x) dx, \tag{30.10}$$

where

$$P^T(x, D) f(x) = \sum_{|\alpha| \le m} (-D)^\alpha (a_\alpha(x) f(x)), \tag{30.11}$$

for

$$P(x, D) f(x) = \sum_{|\alpha| \le m} a_\alpha(x) D^\alpha, \tag{30.12}$$

(This guarantees that the operator is symmetric (→**30.2**)) and
(2) if $P(x, D)$ is *semibounded*, i.e., for any sufficiently differentiable $f \in L_2(\Omega)$, there is a positive α such that

$$\pm \int_\Omega f(x) P(x, D) f(x) dx \le \alpha \|f\|^2 \tag{30.13}$$

for + or −, then (thanks to Friedrichs-Freudenthal's theorem[337]), then P can be extended to a self-adjoint operator and,
(A) The totality of normalized eigenfunctions $\{u_n\}$ of the operator:

$$P(x, D)u_n(x) = \lambda_n u_n(x), \tag{30.14}$$

makes an orthonormal basis for $L_2(\Omega)$,
and
(B) we may justify the separation of variables:

30.11 Justification of separation of variables. Let Ω be a region and P be a partial differential operator (with appropriate boundary conditions) on $L_2(\Omega)$ satisfying the consitions (1) and (2) in **30.10**. Then there is an appropriate weight w (→**30.8**) such that the solution to

$$L_t u = P(x, D)u, \tag{30.15}$$

where L_t is a differential operator with respect to time, is given by φ such that

$$L_t\langle\lambda|\varphi\rangle = \int \mu\langle\lambda|\mu\rangle w(\mu)d\mu\langle\mu|\varphi\rangle \ \ [= \lambda\langle\lambda|\varphi\rangle]. \tag{30.16}$$

The formula inside [ ] holds if the spectrum is discrete (if not, the formula is not simple as we will see in **32.5**).

Discussion.
(A) The extension may be understood formally as follows. Let L^* be the formal adjoint of L. Then the operator $\hat{L}$ introduced as follows is the extension of L (that is, $\hat{L}^* = \hat{L} \supset L$).

$$\langle u|\hat{L}v\rangle = \langle L^*u|v\rangle. \tag{30.17}$$

(B) We have encountered the following equation in **19.9** (2)

$$\left[\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} + \frac{m^2}{r^2}\right] R = -\lambda^2 R \tag{30.18}$$

with the boundary conditions $R(a) = R(b) = 0$ $(a < b)$. The eigenfunctions are written in terms of the following 'esoteric' functions $I_{im}(x)$ and $K_{im}(x)$. We wish to demonstrate that the eigenfunctions of this problem makes a complete system. We wish to use the 'high-tech' functional analytic weapon. That is:
(1) Demonstrate that the operator is formally self-adjoint.
(2) Demonstrate that the operator is semibounded (→**??**).
(C) With the aid of the same argument as above demonstrate that the totality of spherical harmonics makes a complete set of functions. That is, demonstrate that

$$L^2 \equiv \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \tag{30.19}$$

[337] See K. Yosida, *Functional Analysis* (Springer, 1980 Sixth edition), Chapter XI, Section 7, Theorem 2.

is formally self-adjoint and semibounded.[338]

30.C Spectrum

30.12 Introduction to spectrum. Physicists usually write for a linear operator

$$L|\lambda\rangle = \lambda|\lambda\rangle \tag{30.20}$$

and say that λ is an eigenvalue. However, if L is a linear operator acting on a subset of a Hilbert space, then the equation makes sense, strictly speaking, only when $|\lambda\rangle$ is in the Hilbert space (That is, $|\lambda\rangle$ is normalizable →**16.3**). We know this is not always the case. If we rewrite (30.20) as

$$(L-\lambda)|\lambda\rangle = 0, \tag{30.21}$$

we realize that what we wish to mean by (30.20) is that $(L-\lambda)^{-1}$ is not a bounded operator: a linear operator A is a *bounded operator*, if its operator norm (→**??**) is bounded: $\|A\| \equiv \sup_{a\in D(A)} \|Aa\|/\|a\| < +\infty$.

30.13 Resolvent, resolvent set. Let L be a linear operator on a Hilbert space V with a dense domain (→**30.1**). The operator

$$R(\lambda) \equiv (L-\lambda I)^{-1} \tag{30.22}$$

is called the *resolvent* of L. If the domain of $R(\lambda)$ is dense, and $R(\lambda)$ is bounded on its domain, then λ is called a *regular point*. The totality of the regular points of L is called the *resolvent set* of L and is denoted by $\rho(L)$.

Notice that if $\lambda, \mu \in \rho(L)$, then

$$R(\lambda) - R(\mu) = (\lambda-\mu)R(\lambda)R(\mu). \tag{30.23}$$

This is called the *resolvent equation*.

Exercise.

(1) Demonstrate the resolvent equation.

(2) Construct the resolvent kernel (i.e., $R(x,y;\lambda) \equiv \langle x|(L-\lambda)^{-1}|y\rangle$) for $L = -d^2/dx^2$ with the boundary condition $u'(0) = u'(1) = 0$. Cf. **16.28**, **16.29**.

30.14 Spectrum. Let L be a linear operator whose domain is dense in a Hilbert space V. Then $\sigma(L) \equiv \boldsymbol{C} \setminus \rho(L)$ is called the *spectrum* of L. In other words, λ is a point in the spectrum of L, if $(L-\lambda)^{-1}$ is not defined, or even if it is defined, its domain is not dense in V, or even if dense, it is not a bounded operator.

[338] Do not forget an appropriate weight when you perform integration. This also applies to (B).

30.15 Classification of spectrum. Let T be a linear operator whose domain is dense in a Hilbert space V.
(1) If $T-\lambda$ is not one to one, that is, there is a nonzero ket $|u\rangle$[339] such that $A|u\rangle = \lambda|u\rangle$, we say λ is an eigenvalue. The totality of such λ is called the *point spectrum* of T.
(2) If $T-\lambda$ is one to one, but if $R(\lambda)$ is not a bounded linear operator, and
(21) if the domain of $R(\lambda)$ is dense, then we say λ belongs to the *continuous spectrum*.
[(22) if the domain of $R(\lambda)$ is not dense, then we say λ belongs to the residual spectrum.]

30.16 Discrete and essential spectrum. The totality of eigenvalues is called the *point spectrum* σ_p. The union of the continuous spectrum and the set of eigenvalues of infinite multiplicity is called the *essential spectrum* and is denoted by $\sigma_{ess}(L)$. $\sigma(L) \setminus \sigma_{ess}(L)$ is called the *discrete spectrum* and is denoted by $\sigma_{disc}(L)$.

30.17 Classification of continuous spectrum. Let L be a linear operator whose domain is in a Hilbert space V with a continuous spectrum $\sigma_c(L)$. It is classified as follows:

Let $w(\lambda)$ be the spectral weight (→**30.7**). If for any set $A \subset \sigma_c(L)$ with measure zero (→**15.4**) $\int_A |\lambda\rangle w(\lambda) d\lambda \langle\lambda| V = \{0\}$, we say the spectrum is absolutely continuous, and the continuous spectrum is called an *absolutely continuous* spectrum. The definition applies to a subset of $\sigma_c(L)$, so we may say the operator L has an absolutely continuous spectrum in $[a,b]$, if $\int_a^b |\lambda\rangle w(\lambda) d\lambda \langle\lambda| VV$ is a nontrivial subspace of the Hilbert space V, but for any measure zero subset Q of $[a,b]$ $\int_Q |\lambda\rangle w(\lambda) d\lambda \langle\lambda| V = \{0\}$. Otherwise, we say L has a *singular continuous spectrum* (like the one concentrated on a Cantor set).

30.18 Pure point spectrum. Let L be a linear operator whose domain is dense in a Hilbert space V. If the linear hull of the eigenspaces for all $\lambda \in \sigma_p(L)$ is dense in V, then we say L has a *pure point spectrum*.

30.19 Are the above classification relevant to physics?.
(1) The Hamiltonian of 1D harmonic oscillator has a pure point spectrum. $\sigma = \sigma_p = \sigma_{disc}$.
(2) The Hamiltonian of a particle in a 1D periodic potential has an absolutely continuous spectrum, which physicists call a band spectrum.
(3) Consider a random 1d harmonic lattice. For example, the value of the spring constant is k or $k'(\neq k)$ chosen randomly for each spring, or a harmonic lattice with a uniform spring constant but two kinds of

[339] Of course, the ket must be in the Hilbert space. That is, it must be normalizable.

mass points m and $M(\neq m)$ randomly placed on the lattice points. In this case all the harmonic modes are localized (i.e., in l_2 →**16.5**(1)) and its spectrum is pure point (→**30.18**). The reason for the localization is not very hard to understand intuitively; if there is a cluster of lighter atoms, then they tend to behave differently from the rest. If the reader solve a finite size lattice system, then the mode localization lengths may be larger than the system size, so she would see clear localization for higher frequency modes only as illustrated below:

(4) The problem in (3) is mathematically the same as the random Frenkel model; that is, the discrete Schrödinger equation with random hopping or with random site potential energy can be cast into the harmonic lattice problem. In this case localization is called the *Anderson localization.*
(5) If the spring constant or hopping probability above is chosen to be almost periodic (that is, it behaves like $\sin kx$ with k being irrational),[340] then the spectrum becomes self-similar.

In this case the eigenfunctions are not localized in the standard sense (i.e., not in l_2), but very different from the ordinary delocalized wave functions. If the largest peak is normalized, then in many cases the slow algebraic decay is observed. Experimentally, now we can fabricate almost periodic layered structures on which we can perform optical experiments. Numerically, the behavior above can be observed most easily with the most irrational $k = 1/(1 + 1/(1 + /(1 + 1/(\cdots$.

[340] Physicists say a function $f(x)$ is almost periodic if $f(x)$ is a sum of periodic functions with incommensurate (not rationally related) periods.

(6) If the system exhibits only a point spectrum, then there cannot be any transport of phonons or electrons, because all the eigenfunctions are spatially localized.

Discussion.
If the system exhibits only a point spectrum, then there cannot be any transport of phonons or electrons, because all the eigenfunctions are spatially localized.

30.20 Compact operator. If a linear operator A has a sequence of finite-dimensional operator[341] converging[342] to it, we say A is a *compact operator*. If A is self-adjoint, then, roughly speaking, we can write $A \sim \sum_{k=1}^{N} |k\rangle\lambda_k\langle k|$.

30.21 Integral operator, Fredholm integral equation. Formally we can introduce a linear operator by the following integral[343]

$$(\Gamma u)(x) = \int_a^b dy\, w(y)K(x,y)u(y), \tag{30.24}$$

where we assume $u \in L_2([a,b],w)$ (→**16.19**), and K is an integrable function. Γ is often called a *Fredholm operator*, and K is called its *kernel*.

$$u = \Gamma u + f \tag{30.25}$$

for some function $f \in L_2([a,b],w)$ is called a *Fredholm integral equation*.

30.22 Theorem [Hilbert-Schmidt]. Γ in **30.21** is a compact operator, if

$$\int_a^b dx\, w(x) \int_a^b dy\, w(y)|K(x,y)|^2 < \infty. \tag{30.26}$$

Exercise.
The inverse operator of the regular Sturm-Liouville operator is compact. Demonstrate this statement. Cf. **??**.

30.23 Spectral theorem for compact self-adjoint operator [Hilbert-Schmidt]. Let A be a compact self-adjoint operator (→**30.15**) on a Hilbert space V. Then,
(1) V has an orthonormal basis $\{|e_n\rangle\}$ consisting of eigenvectors of A.
(2) Let $A|e_n\rangle = \lambda_n|e_n\rangle$. Then $\lambda_n \to 0$ as $n \to \infty$.
(3) If $|x\rangle = \sum c_n|e_n\rangle$, then $A|x\rangle = \sum c_n\lambda_n|e_n\rangle$. □
Thus, almost everything true for a finite dimensional Hermitian matrix is true. The only caution we need is that we cannot freely change the order of the vectors in the basis (→**16.17**). □
Compactness implies $A \sim \sum_{k=1}^{N} |k\rangle\lambda_k\langle k|$, so intuitively, the theorem is plausible.

[341] A linear operator B is said to be finite dimensional, if its non-zero spectrum is point (→**34C.4**) and the total dimension of its eigenspaces is finite.
[342] with respect to the operator norm.
[343] Mathematicians introduce a measure $d\mu$ instead of w. Cf. **a19**.

30.24 Variational Principle for compact self-adjoint operator. Let A be a compact ($\rightarrow$**28.32**: do not forget that the theorem is NOT for any self-adjoint operator) self-adjoint linear operator on a Hilbert space V. The unit vector $|f\rangle$ which maximizes $\langle f|A|f\rangle$ is an eigenvector of A belonging to the eigenvalue with the largest modulus which is identical to $|\langle f|A|f\rangle|$. $\square$

30.25 Finding eigenvalues with the aid of variational principle. With the aid of **30.24** we can determine the largest modulus eigenvalue λ_1 of a compact self-adjoint linear operator A, and a vector maximizing $F(x)$ to be denoted by $|\lambda_1\rangle$. Let V_1 be the perpendicular subspace to $|\lambda_1\rangle$. Since

$$\langle\lambda_1|A|y\rangle = \lambda_1\langle\lambda_1|y\rangle = 0, \tag{30.27}$$

if $|y\rangle \in V_1$, so is $A|y\rangle \in V_1$. Hence we can apply the same argument to A restricted to V_1. In this way we can construct the nonincreasing sequence (in modulus) of eigenvalues $\lambda_1, \lambda_2, \cdots$.

31 Spectrum of Sturm-Liouville Problem

Eigenvalues for a regular Sturm-Liouville problem can be studied more conveniently through its Green's function which is a Hilbert-Schmidt kernel. We need a more general theory to go beyond the regular case – the Weyl-Stone-Titchmarsh-Kodaira theorem, which is also briefly introduced.

Key words: Sturm-Liouville eigenvalue problem, fundamental theorem, Weyl-Stone-Titchmarsh-Kodaira theorem

Summary:

(1) Remember that the inverse operator of the regular Sturm-Liouville operator is compact. All the fundamental properties of its spectrum follows from this fact (→**31.3**).
(2) Details of the Weyl-Stone-Titchmarsh-Kodaira theorem **31.5** need not be understood, but remember that there is a general way to expand a function in terms of functions in a fundamental system of solutions of a formally self-adjoint differential operator.

31.1 Rewriting of the eigenvalue problem as integral equation. The Sturm-Liouville eigenvalue problem is to find λ for

$$\mathcal{L}_{ST}u \rightleftharpoons \left[\frac{d}{dx}p(x)\frac{d}{dx} + q(x)\right]u = \lambda w(x)u \tag{31.1}$$

(with $p > 0$) under the following boundary condition:

$$B_a[u] \equiv Ap(a)u'(a) - Bu(a) = 0, \tag{31.2}$$
$$B_b[u] \equiv Cp(b)u'(b) - Du(b) = 0, \tag{31.3}$$

The problem can be rewritten with the aid of the Green's function (→**??**) as

$$u(x) = \lambda \int dy\, w(y)G(x|y)u(y) = \lambda(\mathcal{G}u)(x) \tag{31.4}$$

G is called the *kernel* of the integral operator $\mathcal{G}$.

31.2 Formal theory. [**16.28** repeated] (31.4) can be written as

$$|u\rangle = \lambda\mathcal{G}|u\rangle, \tag{31.5}$$

where bras and kets are defined with the weight function w (→**16.22**, **16.23**). Let $|i\rangle$ be an eigenket belonging to the eigenvalue λ_i:

$$\lambda_i \mathcal{G}|i\rangle = |i\rangle. \tag{31.6}$$

If $\{|i\rangle\}$ is an orthonormal basis of $L_2([a,b],w)$ (→**16.19**), then from (31.5) we get

$$\mathcal{G} = \sum_i |i\rangle \lambda_i^{-1} \langle i|. \tag{31.7}$$

That is, the Green's function can be written as

$$G(x|y) = \langle x|\mathcal{G}|y\rangle = \sum_i \lambda_i^{-1} u_i(x)\overline{u_i(y)}. \tag{31.8}$$

We must justify this result.

31.3 Theorem [Fundamental theorem of Sturm-Liouville eigenvalue problem]. The eigenfunctions of a regular Sturm-Liouville problem (→**??**) form an orthogonal basis of $L^2([a,b],w)$ (→**16.19**), and the sequence of eigenvalues satisfies $|\lambda_n| \to \infty$ as $n \to \infty$.□

[Demo] We can explicitly construct the Green's function for this problem as in **??**, which is a continuous function of x and y, so that $\mathcal{G}$, whose kernel is given by **??**, is a compact operator (→**30.20**) thanks to Hilbert and Schmidt **30.22**. Its self-adjointness is also easy to demonstrate. Hence, we can apply **30.23**. Note that the eigenvalues here are the reciprocals of those in **30.23**.

Discussion.

(A) **Classical approach due to Prüfer**.

Our demonstration heavily relied on functional analytic methods. The facts were known before functional analytic methods were widely available. Here a classical proof of the theorem due to Prüfer is given. The argument may seem more complicated and more artful, but more delicate results than those obtained by a high-tech functional analysis may be obtained.

(1) Suppose there is a solution $u \not\equiv 0$ to (31.1). Then, pu' and u do not vanish simultaneously.

Hence, we can introduce a polar coordinate system such as

$$u(x) = \rho(x)\sin\theta(x), \tag{31.9}$$
$$p(x)u'(x) = \rho(x)\cos\theta(x). \tag{31.10}$$

(2) Our eigenvalue problem can be rewritten as follows:

$$\rho'(x) = (p(x)^{-1} + q(x) + \lambda w(x))\rho\sin\theta\cos\theta \tag{31.11}$$
$$\theta' = p(x)^{-1}\cos^2\theta + (-\lambda w(x) - q(x))\sin^2\theta. \tag{31.12}$$

The second equation does not contain ρ, so we can integrate this for $\theta(x)$ with an arbitrary initial condtion $\theta(0) = \alpha$.

(3) A necessary and sufficient condition for λ to be an eigenvalue of **31.1** is that

$\theta(x)$ with the initial condtion $\theta(a) = \alpha$ satisfies $\theta(b) = \beta + n\pi$, where n is a positive integer. Here the angles α and β are determined as

$$\tan\alpha = A/B, \quad \tan\beta = C/D \tag{31.13}$$

with $\alpha, \beta \in [0, \pi)$.
(4) **Prüfer's comparison theorem**. Let $\theta(x, \lambda)$ be the solution of (2) with the initial condition $\theta(a) = \alpha$. Then, for $x \in (\alpha, \beta]$

$$\lambda_1 < \lambda_2 \Rightarrow \theta(x, \lambda_1) < \theta(x, \lambda_2). \tag{31.14}$$

This tells us that the eigenfunction corresponding to a larger eigenvalue oscillates faster. θ is monotonically increasing as a function of λ. In particular,
(5)

$$\lim_{\lambda \to -\infty} \theta(b, \lambda) \leq 0, \tag{31.15}$$

$$\lim_{\lambda \to +\infty} \theta(b, \lambda) = +\infty. \tag{31.16}$$

This implies
(6) The Sturm-Liouville eigenvalue problem has a discrete set of eigenvalues such that

$$\lambda_1 < \lambda_2 < \cdots < \lambda_n \to +\infty. \tag{31.17}$$

(7) Furthermore, the eigenfunction corresponding to the n-th largest eigenvalue has exactly $n-1$ simple zeros in (a, b). See **20.13** (Discussion) for the simplicity of the zeros (non-degeneracy of eigenstates). For nodal sets, see **33.4**. Also note that this proves the statement about the positions of the zeros of orthogonal polynomials **21A.11** (2) (see **17.7**).
(8) Completeness of the eigenfunctions: If a continuous function $h(x)$ satisfies

$$\int_a^b dx w(x) h(x) \phi_n(x) dx = 0, \tag{31.18}$$

for all $n \in \boldsymbol{N}$, then $h \equiv 0$, where ϕ_n is an eigenfunction belonging to λ_n.
Its proof depends on the fact that if (31.18) is true, then the solution to

$$\mathcal{L}_{ST} y = w(x) h(x) \tag{31.19}$$

with the homogeneous boundary condtion has a continuous solution for any real λ. However, this cannot be true if $h \equiv 0$.
(9) (8) gives us a generalized Fourier expansion: If

$$f(x) \sum f_n \phi_n(x) \tag{31.20}$$

is uniformly and absolutely convergent, then the coefficient can be computed as a Fourier coefficien.
(10) Let f be piecewisely C^1. The formal series (31.20) is actually uniformly and absolutely convergent.
(B) Prüfer's technique allows us to prove the following theorem about the distribution of zeros of a Schödinger equation:

$$u'' + q(x) u = 0. \tag{31.21}$$

Suppose

$$m^2 \leq q(x) \leq M^2. \tag{31.22}$$

Then, for any solution $u \not\equiv 0$, the spacing of the zeros δ satisfies

$$\frac{\pi}{M} \leq \delta \leq \frac{\pi}{m}. \tag{31.23}$$

Exercise.
Suppose (31.21) is considered on $[a, b]$ with the Dirichlet condition. Demonstrate that the magnitude of the eigenvalue λ_n increases asymptotically as n^2.
Discussion.
(C) Find the eigenvalues and eigenfunctions of the operator $d^2/dx^2 + \lambda$ on $[-1, 1]$ with the following boundary conditions:
(1) $du/dx(-1) = du/dx(1) = 0$.
(2) $u - du/dx = 0$ at $x = \pm 1$.
(D) What happens if the regularity condition is dropped?[344]
Consider

$$\frac{d}{dt}\left(t^2 \frac{d}{dt} x\right) + \lambda x = 0, \tag{31.24}$$

with the following boundary conditions.
(1) $x(-1) + x'(-1) = x(1) + x'(1) = 0$ (no eigenvalue).
(2) $x(-1) + x'(-1) = 0$ and $x(1) - x'(1) = 0$ (-2 is the only eigenvalue. The corresponding eigenfunction is t.)
(C) Irrespective of the boundary conditions, the n-th eigenvalue of a Sturm-Liouville problem is a continuous function of the coefficients of the equation (Courant-Hilbert).

31.4 Justification of separation of variables. When the region of the problem is finite, very often the separated problems are regular Sturm-Liouville eigenvalue problem. Hence, **31.3** is the key (if the reader does not wish to use less elementary Friedrichs extension (→**30.10**)). However, notice that **31.3** is <u>not</u> enough to justify what we wish to do on unbounded regions. Friedrichs extensions work even in such cases. Here, however, a more constructive theory is posted.

31.5 Theorem [Weyl-Stone-Titchmarsh-Kodaira]. Let L be a second order linear differential operator which is formally self-adjoint:

$$L = -\frac{d}{dx} p(x) \frac{d}{dx} + q(x), \tag{31.25}$$

where p and q are C^∞ on (a, b).[345] For $\lambda \in \boldsymbol{R}$, consider

$$Lu = \lambda u. \tag{31.26}$$

[344] N
[345] a could be $-\infty$ and b ∞.

Let $\{\psi_1(x;\lambda), \psi_2(x;\lambda)\}$ be a fundamental system of solutions (→**20.11**) of this equation. Then, there is a matrix measure ρ_{ij} $(i,j \in \{1,2\})$[346] such that we can make the following decomposition of unity

$$\delta(x-y) = \int_{-\infty}^{\infty} \sum_{i,j} \psi_i(x;\lambda) d\rho_{ij}(\lambda) \psi_j(y;\lambda). \tag{31.27}$$

The equality here is in the L_2-sense.[347] Here the so-called density matrix ρ_{ij} can be constructed from the resolvent (→**30.13**) of L.□
(31.27) implies the following:

$$f(x) = \int_{-\infty}^{\infty} \sum_{i,j} \psi_i(x;\lambda) d\rho_{ij}(\lambda) \hat{f}_j(\lambda), \tag{31.28}$$

and

$$\hat{f}_j(\lambda) = \int_a^b dy \psi_j(y;\lambda) f(y). \tag{31.29}$$

Thus $\hat{f}_i(\lambda)$ is a kind of generalized Fourier transform of f.

Discussion.
(A) Let us consider

$$Lu(x;\lambda) + \lambda w(x) u(x;\lambda) = -f(x)w(x) \tag{31.30}$$

with the standard homogeneous boundary conditions as in **31.1**. If we may assume that the homogeneous eigenvalue problem allows us to construct a complete set of orthonormal eigenfunction set $\{\varphi_n\}$, then we can expand as

$$u(x;\lambda) = \sum_{n=1}^{\infty} c_n(\lambda) \varphi_n(x), \tag{31.31}$$

when $\lambda \neq \lambda_n$ for any n.
(1) Putting this into (31.30), show that

$$\sum_{n=1}^{\infty} (\lambda - \lambda_n) w(x) \varphi_n(x) = -w(x) f(x), \tag{31.32}$$

(2) Using the orthonormal relation, obtain

$$c_n(\lambda) = -\frac{f_n}{\lambda - \lambda_n}, \tag{31.33}$$

where $f_n = \langle \varphi_n | f \rangle$ (→**16.19** for the notational convention). Thus,

$$u(x;\lambda) = -\sum_{n=1}^{\infty} \frac{f_n}{\lambda - \lambda_n} \varphi_n(x). \tag{31.34}$$

[346] That is, any component of the matrix $Matr\{\rho_{ij}(\lambda)\}$ is a measure.
[347] That is, when it is applied to a ket, the difference of RHS and LHS measured in terms of the L_2-norm is zero.

(3) Hence,

$$\frac{1}{2\pi i}\int_C u(x;\lambda)d\lambda = \sum_{n=1}^{\infty}\varphi_n(x)f_n = -f(x), \tag{31.35}$$

where C is a closed path encircling all the eigenvalues (which are all on the real axis) ($\rightarrow$**??**).
(4) This implies that if we could obtain $u(x;\lambda)$ as a meromorphic function[348]

[348] a

32 Green's Function: Laplace Equation

The Green's function method to solve the general boundary value problem for the Laplace equation is given. Neumann conditions need special care.

Key words: fundamental solution, Kirchhoff's formula, Neumann function

Summary:
(1) The reader must be able to explain the general idea of Green to her friend, and how to use Green's formula (→**32.6**).
(2) The Neumann function needs a special care, because homogeneous boundary conditions and the unit source are not compatible (→**32.7**, **33.9**).

32.1 Summary up to this point. Definition of Green's functions and fundamental solutions can be found in **??**. An intuitive idea was explained in **??**. Green's formula is in **??** and some examples of Green's functions are in **16**.

32.2 Fundamental solution. The fundamental solution of the Laplace equation is a solution to

$$-\Delta\psi = \delta(x-y). \tag{32.1}$$

It is customary to put $-$ in front of the Laplacian, because $-\Delta$ is a positive definite operator (→**28.3**). In d-space the following w is a fundamental solution. For $d \geq 3$ the function vanishes at infinity, so it is also a Green's function for free space $\boldsymbol{R}^d$ with the vanishing condition at infinity (→**??**)

$$w(x|y) = \begin{cases} \frac{1}{S_{d-1}(d-2)|x-y|^{d-2}} & \text{for } d \geq 3, \\ -\frac{1}{2\pi}\ln|x-y| & \text{for } d = 2, \end{cases} \tag{32.2}$$

where S_{d-1} is the surface volume of the $(d-1)$-unit sphere.[349]

Notice that d-space function w can be obtained from the $(d+1)$-space counterpart through integrating along one coordinate direction (→**??**).

Discussion Double layer.

[349] $S_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$.

(1) Consider two parallel surfaces with their spacing d. We assume that the surfaces are orientable[350] and let ν denote the outward normal direction. Let us assume that the outer surface has a uniformly distributed charge of area density $+\rho$, and the inner surface has the same distribution of the charge but of oppoisite sign. $p = \rho d$ is the area density of the dipole moment. We take the limit of $d \to 0$ while keeping p. The resultant double surface is called (electrical) *double layer*.
(1) Show that the electrical potential (assuming 0 potential at infinity) is given by (in 3-space) (ignore numerical coefficients)

$$V(\mathrm{P}) = \int_S d\sigma p \frac{\partial}{\partial \nu}\left(\frac{1}{r}\right), \tag{32.3}$$

where S is the surface, r is the distance between the point on the surface and the point P where we measure the potential.
(2) Let us introduce the angle θ between the outward normal and the line connecting the point on the surface and the point P. Then notice that

$$-\cos\theta = \frac{dr}{d\nu}, \tag{32.4}$$

so that (32.3) can be written as

$$V(\mathrm{P}) = \int_S \frac{p\cos\theta}{r^2} d\sigma. \tag{32.5}$$

(3) Notice that the solid angle of $d\sigma$ seen from P is given by

$$d\Omega = \pm \frac{d\sigma \cos\theta}{r^2}, \tag{32.6}$$

where the sign convention is $+$, if P is on the positive side of the double layer,[351] and $-$, if P is on the negative side. Hence, we have

$$V = \pm \int_S p d\Omega. \tag{32.7}$$

(4) This implies that, when $p = \text{const.}$, if P is outside a closed double layer S, then $V = 0$. If P is inside, then $V = -4\pi p$.

32.3 Theorem [Unique existence of Dirichlet problem Green's function]. For any well behaved[352] surface $\partial\Omega$ enclosing an open region Ω, there exists the unique Green's function $G_D(x|y)$ for $-\Delta$ which vanishes on $\partial\Omega$.□

[350] that is, there are two sides unlike the Möbius strip.
[351] This does not mean that P is located outside the layer even when the layer is closed. Simply, we draw a tangent plane on the shell and we ask on which side P exists.
[352] This vague statement will not be made precise here to avoid the technicality. Piecewise smooth surfaces are admissible. Cf. **??**(2) Discussion.

[Demo] The Green's function for the homogeneous Dirichlet problem is the solution to

$$-\Delta G_D(x|y) = \delta(x-y) \tag{32.8}$$

with $G_D = 0$ for $x \in \partial\Omega$. Here y is in Ω.[353] The problem can be rewritten as $G_D(x|y) = w(x|y) + u(x|y)$, where w is a fundamental solution in **32.2** and u satisfies

$$-\Delta u(x|y) = 0 \tag{32.9}$$

with the Dirichlet boundary condition $u(x|y) = -w(x|y)$ for $x \in \partial\Omega$. We have discussed that this problem has a unique solution at least informally (→**??**, **25.9**).

32.4 Symmetry of Dirichlet Green's function. In Green's formula (→**??**) set $u(x) = G_D(x|y)$ and $v(x) = G_D(x|z)$. Then, we get

$$\int [G_D(x|y)\Delta G_D(x|z) - G_D(x|z)\Delta G_D(x|y)]dx = 0. \tag{32.10}$$

If we use (32.8), this immediately gives

$$G_D(y|z) = G_D(z|y), \tag{32.11}$$

the symmetry of the Green's function. We have already discussed this (formally in **31.2**, **??**) (→**33.7**).

32.5 Free space Green's function is the largest. Let $G_D(x|y)$ be the Green's function for a region D. Then,

$$G_D(x|y) \le w(x|y). \tag{32.12}$$

Here w is the fundamental solution given in **32.2**, that is, the Coulomb potential.

This follows easily from the maximum principle **25.6**.

32.6 Solution to Dirichlet problem in terms of Green's function (**??** repeated). The solution to the following Dirichlet problem on an open region Ω

$$-\Delta u = \varphi, \quad u|_{\partial\Omega} = f, \tag{32.13}$$

where φ and f are integrable functions, is given by

$$u(x) = \int_\Omega G_D(x|y)\varphi(y)dy - \int_{\partial\Omega} f(y)\partial_{n(y)}G_D(x|y)d\sigma(y). \tag{32.14}$$

Here $\partial_{n(y)}$ is the outward normal derivative at y, τ is the volume element, and σ is the surface volume element.

Discussion

The Discussion in **32.2** allows us to understand (**??**) in terms of the charge distribution in Ω and the double layer $\partial\Omega$. That is, Dirichle conditions can be understood as appropriately distributed layers.

[353] Impossible if y is an external point of Ω, since it is open.

32.7 Special feature of homogeneous Neumann condition. For a Neumann problem we do not know u but $\partial_n u$ on the boundary. We need the Green's function satisfying the homogeneous Neumann condition. However, we cannot impose a homogeneous boundary condition on a closed surface $\partial\Omega$ as seen below. Let G_N satisfy

$$-\Delta G_N(x|y) = \delta(x-y). \tag{32.15}$$

Then, Gauss' theorem (→**??**) tells us that

$$\int_{\partial\Omega} \frac{\partial G_N}{\partial n} d\sigma = -1. \tag{32.16}$$

Therefore, the homogeneous Neumann condition cannot be imposed.[354] The simplest boundary condition compatible with (32.15) is

$$\frac{\partial G_N}{\partial n} = -1 \Big/ \int_{\partial\Omega} d\sigma = \frac{-1}{(\text{surface area of } \Omega)}. \tag{32.17}$$

32.8 Neumann function. The function satisfying (32.15) and (32.17) is called the *Neumann function*. In terms of the Neumann function, the solution to the following Neumann problem

$$-\Delta u = \varphi, \quad u|_{\partial\Omega} = h \tag{32.18}$$

reads

$$u(x) = \int_\Omega G_N(x|y)\varphi(y)dy + \int_{\partial\Omega} G_N(x|y)h(y)d\sigma(y). \tag{32.19}$$

Note that the solution to a Neumann problem is unique only up to an additive constant (→**??**(3)).

[Demo] In Green's formula let u be the solution and v be the Neumann function G_N. Then we have

$$\begin{aligned} u(x) &= \int_\Omega G_N(x|y)\varphi(y)dy + \int_{\partial\Omega} \left[G_N(x|y)h(y) + u(y) \Big/ \int_{\partial\Omega} d\sigma(y) \right] d\sigma(y), \\ &= \int_\Omega G_N(x|y)\varphi(y)dy + \int_{\partial\Omega} G_N(x|y)h(y)d\sigma(y) + const. \end{aligned} \tag{32.20}$$

The constant can be ignored, because we need the solution up to an additive constant.

32.9 Method of images. (→**??**, **??**, **??**) With the aid of the superposition principle and the conformal invariance (say, the reflection principle) (→**??**), we can construct Green's functions for special cases. For example, the half 3-space Green's function can be obtained by **??**. Analogous half 2-space Green's function can be obtained. Notice that this Green's function vanishes at infinity in contrast to the free space counterpart.

[354] If we wish to keep the homogeneous Neumann boundary condition, we must modify (32.15). This will be discussed in **33.9**.

33 Spectrum of Laplacian

The spectrum of Laplacian gives the energy level of quantum mechanical billiards. It is important to grasp its general feature to understand the general spectrum of a particle in a potential well. One of the most interesting questions was to determine the shape of the domain from the spectrum: Can you here the shape of the drum? Now, we know that this is impossible even in 2-space.

Key words: Fundamental theorem, nodes, eigenfunction expansion of Green's function

Summary:
(1) Understand the eigenfunction expansion of Green's functions (→**33.7**, **33.9**).
(2) Remember the general features of the spectrum and eigenfunctions of the Laplacian with the Dirichlet condition on a bounded domain (→**37.1**). (Theoreticians) This is an example of the spectrum of compact operators.
(3) We cannot hear the shape of the drum (→**33.6**).

33.1 Theorem [Fundamental theorem].[355] Let Ω be a bounded open region, and $\partial\Omega$ be smooth. Then, the following eigenvalue problem

$$-\Delta u = \lambda u, \quad u|_{\partial\Omega} = 0 \tag{33.1}$$

has the following properties:
(1) There are countably many eigenvalues $\{\lambda_n\}$ such that $0 \le \lambda_1 \le \lambda_2 \le \cdots$, and $\lim_{n\to\infty} \lambda_n = +\infty$.
(2) There is no finite accumulation point for $\{\lambda_n\}$.
(3) Let φ_n be an eigenfunction belonging to λ_n. Then, $\{\varphi_n\}$ is an orthogonal basis of $L_2(\Omega)$.□

Physically, if we consider the eigenmodes of a drumhead, at least (1) and (2) are understandable. There should not be any upper limit in its frequency for an ideal continuum drumhead. For a finite frequency there cannot be infinitely many independent modes.
[Demo for 3-space] With the aid of the Green's function (→**32.3**), we can convert (33.1) into an integral equation problem:

$$u(x) = \lambda \int_\Omega G(x|y)u(y)dy \equiv \lambda(\mathcal{G}u)(x). \tag{33.2}$$

[355] Actually, much more general theorems are known, since the Laplacian can be defined on any Riemann manifold.

Since $G(x|y) - w(x|y)$ is everywhere finite on Ω, if we can show

$$\int_\Omega |w(x|y)|^2 dx < +\infty \quad \text{for } \forall y \in \Omega, \tag{33.3}$$

the Hilbert-Schmidt theorem (→**30.22**) tells us that $\mathcal{G}$ is a compact (self-adjoint) operator (→**30.20**). Let B_ϵ be a ball of radius ϵ centered at y. On $\Omega \setminus B_\epsilon$ the integral is finite, so we have only to consider

$$\int_{B_\epsilon} |w(x|y)|^2 dx. \tag{33.4}$$

But this is finite as can be seen from the order $w^2 = O[|x-y|^{-2}]$. Hence, Theorem **30.23** tells us (1)-(3) except nonnegativity of the eigenvalue. We know $-\Delta$ is non-negative, so eigenvalues cannot be negative.

Discussion.
According to the variational principle for the eigenvalues of self-adjoint operators, **30.24**, we can say that the fundamental frequency of a drum goes up if the drum head is constrained; in contrast, if the drum head is torn, then its fundamental frequency goes down.

33.2 Theorem [Monotonicity]. Let there be two open regions such that $\Omega \supset \Omega'$. Consider the eigenvalue problems $-\Delta u = \lambda u$ on Ω with the condition $u|_{\partial\Omega} = 0$, and that with Ω replaced by Ω'. Let the n-th eigenvalue (arranged in the increasing order) for the problem with the region Ω be λ_n, and that for the region Ω' be λ'_n. Then, $\lambda_n \leq \lambda'_n$.□
[Demo] We use the variational principle for the eigenvalues of compact self-adjoint operators **30.24**. Notice, however, the eigenvalue there is the reciprocal of the eigenvalues in our present context. That is, the variational principle gives us the eigenvalue with the *smallest* modulus. Due to the non-negativity of the eigenvalues, actually the variational principle gives us the smallest eigenvalue λ_1. More generally, the minimum of $\langle\varphi| - \Delta|\varphi\rangle$ under the condition $\langle\varphi|\varphi\rangle = 1$ is λ_n in the orthogonal complement V_n of the direct sum of the eigenspaces for $\lambda_1, \cdots, \lambda_{n-1}$. For any n the minimum value of $\langle\varphi| - \Delta|\varphi\rangle$ on V_n with the condition $\varphi|_{\partial\Omega} = \varphi|_{\partial\Omega'} = 0$ cannot be smaller than that with the condition $\varphi_{\partial\Omega} = 0$.

33.3 Theorem. Eigenvalues depend on Ω continuously.□[356]

33.4 Theorem [Courant]. Let u_n be the eigenfunction belonging to the n-th smallest eigenvalue of $-\Delta$ on Ω under the condition $u|_{\partial\Omega} = 0$. Then the *nodal set*:

$$\mathcal{N}(u_n) \rightleftharpoons \{x \,:\, u_n(x) = 0, x \in \Omega\} \tag{33.5}$$

[356] See Courant-Hilbert, vol. I Chapter 6, Section 2 Theorem 10.

separates Ω into <u>at most</u> n disjoint components.$\square$[357]

Discussion.
Consider the Laplace eigenvalue problem in a bounded closed domain with a homogeneous Dirichlet boundary condition in 2-space. The curves on which the eigenfunction vanishes is called the *nodal curve*. Demonstrate that a nodal curve is perpendicular to the boundary curve, when the former touches the latter where the latter is smooth.

33.5 Vibrating drumhead. The eigenmodes of a 2-dimensional drumhead of shape D obey

$$-\Delta u = \omega^2 u, \quad u|_{\partial D} = 0. \tag{33.6}$$

If D is a disk of radius a, then the eigenfunctions (modes) are given by

$$u_{mn} = \begin{cases} J_m(r_n^{(m)} r/a)\cos m\varphi, \\ J_m(r_n^{(m)} r/a)\sin m\varphi, \end{cases} \tag{33.7}$$

where $\omega = r_n^{(m)}/a$ with $r_n^{(m)}$ being the n-th zero of J_m ($\rightarrow$**??**). Illustration of low frequency modes can be found in Wyld p164-5.[358]

33.6 Can one hear the shape of the drum? Suppose the set of all the eigenvalues of $-\Delta$ on Ω_1 and that on Ω_2 are identical. Can we conclude that the shapes of the domains are congruent: $\Omega_1 \equiv \Omega_2$? If yes, we can hear the shape of a drum. Now, we know this is not true even for 2-d drums.[359] However, we can hear quite a lot. For example, we can here the area of the drumhead: Let $N(\lambda)$ be the number of eigenvalues less than λ. Then,

$$N(\lambda)/(\mu(\Omega)\lambda/4\pi) \to 1 \tag{33.8}$$

asymptotically for large λ, where $\mu(\Omega)$ is the volume of Ω (conjectured by Lorentz who gave a lecture on this at Göttingen. This was later proved by Weyl). We can also here the number of holes.

[357] See Courant-Hilbert, Chapter 6, Section 6 for a proof.
[358] Excellent pictures of modes of a kettledrum can be found in T. D. Rossing, "The Physics of Kettledrums," Sci. Am. **247** (5) (1982) [November 1982].
[359] A readable account can be found in M A Shubin (ed.) *Partial Differential Equations VII* (Springer, 1994) Section 16.7 (p165-). However, the counter examples are all on the domains with non-smooth boundaries. No smooth counterexample is known. This is still a major problem. Historically, the first negative answer to the question was given in 16-space by Smale.

33.7 Eigenfunction expansion of Green's function. The formal theory in **31.2** can be justified exactly as in the regular Sturm-Liouville problem (→**31.3**) thanks to **33.1**. Hence we have:
Theorem. The Green's function for the Laplacian in a compact domain Ω can be written as

$$G(x|y) = \sum_{i=1}^{\infty} \lambda_i^{-1} u_i(x)\overline{u_i(y)}, \tag{33.9}$$

where u_i is the normalized eigenvector belonging to the eigenvalue λ_i of $-\Delta$.□
From this, the symmetry of Green's functions (→**32.4**) is obvious.

33.8 Examples.
(1) The Green's function for a rectangular domain $[0,a]\times[0,b]$. The eigenvalues and the corresponding normalized eigenfunctions are given by

$$u_{mn} = \frac{2}{\sqrt{ab}} \sin\frac{m\pi x}{a} \sin\frac{n\pi y}{b}, \quad \lambda_{mn} = \left(\frac{m\pi}{a}\right)^2 + \left(\frac{n\pi}{b}\right)^2 \tag{33.10}$$

for positive integers m and n. Hence, the Green's function for the present problem is, according to (33.9)

$$G(x,y|x',y') = \frac{4}{\pi^2 ab} \sum_{m,n>0} \frac{\sin\frac{m\pi x}{a}\sin\frac{m\pi x'}{a}\sin\frac{n\pi y}{b}\sin\frac{n\pi y'}{b}}{(m/a)^2+(n/b)^2}. \tag{33.11}$$

(2) Cylindrically symmetric Green's function for 3-space. In this case it is sensible to define the L_2-space with weight r, because the volume element is $2\pi r dr dz$. Hence, the delta function with the same weight (→**16.25**) is convenient (that is, $\delta(r-r')\delta(z-z')/r$ →**16.26**). The Green's function is the solution to

$$-\Delta u = -\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}\right) u = \delta(z-z')\frac{\delta(r-r')}{r} \tag{33.12}$$

with the vanishing condition at infinity. We first solve the eigenvalue problem

$$-\left(\frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}\right) u = \kappa^2 u. \tag{33.13}$$

We get the eigenvalues and the corresponding normalized eigenfunctions as (→**23.21**)

$$u_{\kappa,k} = \frac{1}{\sqrt{2\pi}} e^{i\kappa z} J_0(kr), \quad \lambda_{\kappa,k} = \kappa^2 + k^2. \tag{33.14}$$

Here, $\kappa \in \boldsymbol{R}$ and k is any positive real. Thus **37.7** (or its natural extension) tells us that the Green's function for our problem is

$$G(r, z|r', z') = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\kappa \int_0^{\infty} dk \frac{e^{i\kappa(z-z')} J_0(kr) J_0(kr')}{\kappa^2 + k^2}. \qquad (33.15)$$

Exercise.
Construct the Green's functions for the Laplace equation with the following boundary conditions:
(1) On $[0, \pi] \times [0, 2\pi]$ with a homogeneous Dirichlet boundary condition along $x = 0$, $x = \pi$ and $y = 2\pi$, and a homogeneous Neumann boundary condition on $y = 0$.
(2) On the same domain with a periodic boundary condition.

33.9 Neumann function in terms of eigenfunctions. Under the homogeneous Neumann boundary condition any constant is an eigenfunction belonging to the zero eigenvalue. Hence, as can clearly be seen in (33.9), we cannot construct the Green's function. However, still the following 'generalized Green's function' works:

$$\hat{G}_N(x|y) = \sum_i{}' \lambda_i u_i(x) \overline{u_i(y)}, \qquad (33.16)$$

where $'$ implies that zero eigenvalue is excluded from the summation, and u_i is the normalized eigenfunction belonging to the eigenvalue λ_i. The solution to **33.8** can be written as

$$u(x) = \int_\Omega \hat{G}_N(x|y) \varphi(y) dy + \int_{\partial\Omega} \hat{G}_N(x|y) h(y) d\sigma(y). \qquad (33.17)$$

(This is essentially (32.19). The difference is a constant which we may ignore.)
[Demo] First we find the equation for $\hat{G}_N$

$$-\Delta \hat{G}_N(x|y) = \sum_i{}' u_i(x) \overline{u_i(y)} = \sum_i u_i(x) \overline{u_i(y)} - V^{-1}, \qquad (33.18)$$

where V is the volume of Ω. We have used that the normalized eigenfunction belonging to zero is $1/\sqrt{V}$. Since the eigenfunctions are with the homogeneous Neumann condition

$$\frac{\partial \hat{G}_N}{\partial n} |_{x \in \partial\Omega} = 0. \qquad (33.19)$$

This is compatible with the equation (33.18). Now put $v = \hat{G}_N$ in Green's formula **??**, and we get (33.17), ignoring an additive constant.

34 Green's Function: Diffusion Equation

The Green's function method to solve the general initial-boundary value problem for diffusion equations is given. The Markovian property of the free-space Green's function (= heat kernel) is the key to construct Feynman-Kac path integral representation of Green's functions.

Key words: reciprocity, general solution formula, eigenfunction expansion, Markovian property, Feynman-Kac formula, path integral.

Summary:
(1) The reader should roughly remember the strategy for constructing Green's function, and its use (→**34.9**, **34.7**).
(2) The relation between the heat kernel and random walk is extremely important.[360] Many important properties of the heat kernel can be derived and/or understood with the aid of this interpretation.
(3) The Markovian property (→**34.10**) of the heat kernel is crucial in developing path integrals (→**34.11**).
(4) Functional integrals are staple for theoreticians. Cf. Glimm and Jaffe.[361]

34.1 Summary up to this point. We have constructed the free-space Green's function, and used it to solve the initial value-problem in **??**, **??**. The image source method is explained in **??** to construct Green's functions for various simple regions.

34.2 The most general diffusion problem. The general form of the problem on the region Ω is

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) \quad \text{on } \Omega \tag{34.1}$$

with the boundary condition, a Dirichlet or a Neumann condition on $\partial\Omega$ for $t > 0$, and the initial condition $u(0,x) = f(x)$. It is a standard trick that the initial condition can be written as a source term as (→**??**)

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) + f(x)\delta(t) \quad \text{on } \Omega. \tag{34.2}$$

Hence we have only to solve the inhomogeneous initial value problem.

[360] See, **??**. An elementary (and classic) introduction is: S. Chandrasekhar, Rev. Mod. Phys. **15**, 1 (1943). This does not use δ-function at all. If you use it, you can rewrite the review in a more concise way. To make a modern version is a good exercise (was good to the lecturer as an undergrad).

[361] J. Glimm and A. Jaffe, *Quantum Physics, a functional integral point of view*, (Springer, 1987). However, the book is not recommended to a casual reader.

34.3 Green's function. The solution to

$$(\partial_t - D\Delta)G(x,t|y,s) = \delta(t-s)\delta(x-y) \tag{34.3}$$

with the homogeneous boundary condition is called the *Green's function.*

34.4 Existence of Dirichlet Green's function. We have constructed the Green's function G_0 for the free space in **16B.1**. Now we wish to determine the Green's function for the homogeneous Dirichlet problem. Note that $u \rightleftharpoons G(x,t|x',t') - G_0(x,t|x',t')$ obeys the diffusion equation with the boundary condition

$$u(t,x|t',x') = -w(x,t|x',t') \quad \text{on } \partial\Omega, t > t' \tag{34.4}$$

and the initial condition $u = 0$ for $t = t'$ (or $t \leq t'$). The unique existence of the solution has been discussed (heuristically **??**; **24.3**). Hence, the existence of Green's functions is guaranteed at least for a compact domain.

The Neumann condition can also be treated analogously.

34.5 Counterpart of Green's formula. Let $\mathcal{L} \equiv \partial_t - D\Delta$ and $\mathcal{L}^+ \equiv -\partial_t - D\Delta$. Then for u which is zero for $t \leq 0$[362] and also $u \to 0$ in the $t \to \infty$ limit we have

$$\int_0^\infty dt \int_\Omega dx[(\mathcal{L}u)v - u\mathcal{L}^+ v] = -D\int_0^\infty dt \int_{\partial\Omega} d\sigma \cdot (v\nabla u - u\nabla v). \tag{34.5}$$

This is essentially Green's theorem and can be proved quite analogously ($\to$**??**).

Exercise. Prove this.

34.6 Reciprocity relations. Notice that the Green's function is a function of $t-s$ (time translational symmetry), so that $G(x,t-\tau|y,s-\tau) = G(x,t|y,s)$. If we choose $\tau = t+s$, we get

$$G(x,t|y,s) = G(x,-s|y,-t). \tag{34.6}$$

We have

$$\left(-\frac{\partial}{\partial t} - D\Delta_x\right) G(x,-t|y,-s) = \delta(x-y)\delta(t-s) \tag{34.7}$$

[362] Since the solution to the diffusion equation is very smooth, we may put the initial condition at $t = 0+$ instead of $t = 0$.

as can easily be seen from the change of variables $t \to -t$ and $s \to -s$. Hence, (34.6) implies

$$\mathcal{L}^+ G = \left(-\frac{\partial}{\partial t} - D\Delta_x \right) G(x,s|y,t) = \delta(x-y)\delta(t-s). \tag{34.8}$$

If we set $u = G(z,\tau|y,s)$ and $v = G(z,t|x,\tau)$ in (34.5), we obtain, regarding u and v as functions of z and τ

$$\int_0^\infty d\tau \int_\Omega dz[(\mathcal{L}G(z,\tau|y,s))G(z,t|x,\tau) - G(z,\tau|y,s)\mathcal{L}^+ G(z,t|x,\tau)] = 0. \tag{34.9}$$

(Here the operators act on the functions of z and τ.) That is, with the aid of (34.8)

$$G(y,t|x,s) = G(x,t|y,s). \tag{34.10}$$

34.7 Solution to general boundary value problem. In terms of the Green's function the solution to

$$(\partial_t - D\Delta)u(x,t) = \varphi(x,t) \tag{34.11}$$

under the initial condition $u(x,0) = f(x)$ and an appropriate boundary condition (inhomogeneous Dirichlet or Neumann that may depend on time) reads

$$\begin{aligned} u(t,x) &= \int_0^t ds \int_\Omega dy\, G(x,t|y,s)\varphi(y,s) + \int_\Omega dy G(x,t|y,0)f(y) \\ &+ D\int_0^t ds \int_{\partial\Omega} d\sigma(y) \left[G(x,t|y,s)\frac{\partial u(y,s)}{\partial n(y)} - u(y,s)\frac{\partial}{\partial n(y)}G(x,t|y,s) \right]. \end{aligned} \tag{34.12}$$

Here the surface term simplifies if we specialize the formula to Dirichlet or Neumann cases.

[Demo] In the analogue of Green's theorem **34.5** we set u to be the solution to the problem, and G to be the Green's function for the corresponding homogeneous boundary condition. We know $\mathcal{L}^+ G(x,s|y,t) = \mathcal{L}^+ G(y,s|x,t) = \mathcal{L}^+ G(x,t|y,s) = \delta(x-y)(t-s)$ ($\to$**34.6**).

34.8 Steady source problem, recurrence of random walk. Let us assume that the source term $\varphi(x,t)$ is time-independent point source $\delta(x)$, and the problem is in the free space with 0 initial condition. Then, (34.12) gives

$$u(x,t) = \int_0^t G(x,t|0,s)ds, \tag{34.13}$$

which is increasing without limit for $d \leq 2$ and finite for $d > 2$. This distinct behaviors for $d > 2$ or not can be understood as the recurrence property of the random walks.

34.9 Eigenfunction expansion of Green's function. (cf. **??**) Let λ_n be the n-th eigenvalue of $-\Delta$ on Ω with a homogeneous boundary condition (Dirichlet or Neumann), and u_n be the corresponding normalized eigenfunction. Then the Green's function for the diffusion equation with the same boundary condition $G(x,t|x',t')$ reads

$$G(x,t|x',t') = \sum_n u_n(x)\overline{u_n(x')}e^{-\lambda_n(t-t')}\Theta(t-t'). \tag{34.14}$$

Notice that in this case the zero eigenvalue existing for the Neumann condition is not excluded (this is required by the conservation of the total mass).

Exercise.
Find the Green's function for the following equation on the unit 3-cube $[0,1]\times[0,1]\times[0,1]$

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta u - cu, \tag{34.15}$$

where c is a positive constant, with a homogeneous Dirichlet boundary condition.

34.10 Markov property revisited. ($\rightarrow$**??**) For the heat kernel G_0 ($\rightarrow$**??**),

$$G_0(x,t|x_0,t_0) = \int_{\boldsymbol{R}^d} dx_1 G_0(x,t|x_1,t_1)G_0(x_1,t_1|x_0,t_0), \tag{34.16}$$

[Demo] Note the 'translation symmetry' (34.6) allows (34.16) to be rewritten with the introduction of $g(x,t) = G_0(x,t|0,0)$ as

$$g(x,t) = \int_{\boldsymbol{R}^d} dy\, g(x-y,t-s)g(y,s). \tag{34.17}$$

(There is NO integral with respect to time.) Introducing the Fourier transform $\hat{g}$ of g with respect to x, this reads $\hat{g}(k,t) = \hat{g}(k,t-s)\hat{g}(k,s)$ ($\rightarrow$**29.8**). This is obvious from

$$\hat{g}(k,t) = e^{-Dk^2t}. \tag{34.18}$$

which is directly obtainable from $(\partial_t - D\Delta)g(x,t) = \delta(t)\delta(x)$.[363]

34.11 Feynman-Kac formula for the heat kernel. Using (34.16) repeatedly to divide the time axis into pieces, we get

$$g(x,t) = \prod_{i=1}^{N-1}\int_{\mathbf{R}^d} dx_i \prod_{i=1}^{N} g(x_i - x_{i-1}, t_i - t_{i-1}), \tag{34.19}$$

[363] We can invert this to get

$$g(x,t) = (4\pi Dt)^{-3/2}e^{-x^2/4Dt}.$$

.

where $t_N \equiv t$, $t_0 \equiv 0$, $x_N \equiv x$ and $x_0 \equiv 0$. Let us choose the equal spacing of the time axis $\Delta t = t_i - t_{i-1}$ for all i, and let $\Delta x_i \rightleftharpoons x_i - x_{i-1}$. Then (34.19) and (363) imply

$$g(x,t) = \prod_{i=1}^{N-1} \int dx_i (4\pi D\Delta t)^{-3/2} \exp[-\sum_{i=1}^{N} (\Delta x_i)^2/4D\Delta t]. \tag{34.20}$$

If Δt is sufficiently small, then, formally,

$$\sum_{i=1}^{N} \frac{(\Delta x_i)^2}{\Delta t} \to \int_0^t dt \left(\frac{dx}{dt}\right)^2. \tag{34.21}$$

Therefore, formally, (34.20) converges to

$$g(x,t) = \int_{x(0)=0}^{x(t)=x} \mathcal{D}[x(\cdot)] \exp\left[-\frac{1}{4D}\int_0^t dt \left(\frac{dx}{dt}\right)^2\right], \tag{34.22}$$

where $\mathcal{D}$ is the 'uniform measure'[364] on the set of continuous functions $[0,t] \to \boldsymbol{R}^3$. This is the *Feynman-Kac formula* for the heat kernel.

34.12 Feynman-Kac path integral. The Green's function for

$$(\partial_t - D\Delta + V)\, u = 0 \tag{34.23}$$

with $u \to 0$ in the $|x| \to \infty$ limit can be written as

$$g(x,t) = \int_{x(0)=0}^{x(t)=x} \mathcal{D}[x(\cdot)] \exp\left[-\int_0^t dt \left(\frac{1}{4D}\left(\frac{dx}{dt}\right)^2 + V(x(t))\right)\right], \tag{34.24}$$

where V is a function bounded from below.[365]

[364] This is a very delicate object, but is definable in a certain sense. However, in these days. mathematicians seem to avoid this altogether. Cf. **16.2** Discussion (1).

[365] A good introductory book on this subject may be R. P. Feynman, *Statistical Mechanics*, Chapter 3 (Benjamin, 1972). This path integral is well defined as a Lebesgue integral on the set of continuous functions. For Schrödinger equation, we must replace t with it. This replacement completely destroys the currently available justification of the formula as a Lebesgue integral.

35 Green's Function: Helmholtz Equation

The Helmholtz equation results from diffusion and wave equations. Its Green's functions are constructed with the aid of generalized function theory. To single out physically meaningful solution, we need an extra condition (radiation condition).

Key words: Helmholtz equation, radiation condition, analogue of Green's formula

Summary:
(1) If the region is finite, then there is no special difficulty compared with the Laplace case (→**35.2**).
(2T) Juggling of generalized functions in **35.4**-**35.6** seems to be the simplest way to obtain physically meaningful Green's function. If the reader can follow the logic, that is enough. However,
(3) She must understand that a special condition is needed to guarantee the causality in the solution (Sommerfeld's radiation condition) (→**35.6**).

35.1 Helmholtz equation. The Helmholtz equation (→**23.24**, **??**)

$$-(\Delta + \kappa^2)\psi = 0 \tag{35.1}$$

appears when we Laplace transform (→**33**) the diffusion equation, or when we Fourier transform the wave equation (in this case $\kappa^2 = c^2/\omega^2$).
Convention. We will use the time Fourier transform with $e^{i\omega t}$. That is,

$$\psi(t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \psi(\omega) e^{-i\omega t}. \tag{35.2}$$

35.2 Green's function for Helmholtz equation on bounded domain. The formal formula for the Green's function is immediately obtained from the formal solution in, say, **31.2** or **33.7**. Let us solve

$$-(\Delta + \kappa^2)G = 1 \tag{35.3}$$

on a region D under the homogeneous boundary condition at the boundary ∂D. We know that the Laplacian has a set of eigenkets $\{|\lambda\rangle\}$ which makes an orthonormal basis (→**33.1** $\sum |\lambda\rangle\langle\lambda| = 1$ →**16.15**). Sandwiching (35.3) with an eigenket and bra

$$(\lambda - \kappa^2)\langle\lambda|G|\lambda'\rangle = \delta_{\lambda,\lambda'}, \tag{35.4}$$

so that we obtain

$$G = \sum |\lambda\rangle(\lambda - \kappa^2)^{-1}\langle\lambda|. \tag{35.5}$$

35.3 Example: Neumann condition on a rectangular region. The Green's function under a homogeneous Neumann condition (i.e., Neumann's function) for the Helmholtz equation in the rectangular domain $[0,a]\times[0,b]$ can be obtained as

$$N(x,y|x',y')=\frac{4}{ab}\sum_{n\geq 0,m\geq 0,nm\neq 0}\frac{\cos(n\pi x/a)\cos(n\pi x'/a)\cos(m\pi y/b)\cos(m\pi y'/b)}{(n\pi/a)^2+(m\pi/b)^2-\kappa^2}-\frac{1}{ab\kappa^2}. \tag{35.6}$$

35.4 Green's function for the whole space. We wish to solve

$$-(\Delta+\kappa^2)G(\boldsymbol{r}|\boldsymbol{r}_0)=\delta(\boldsymbol{r}-\boldsymbol{r}_0) \tag{35.7}$$

with the boundary condition $|u|\to 0$ as $|\boldsymbol{r}|\to\infty$. We interpret this equation in the generalized function sense (→**14**). After Fourier transforming this (→**28.32**), we obtain

$$(k^2-\kappa^2)\hat{u}=e^{ikr_0}. \tag{35.8}$$

Recalling **??**(2), we can solve this equation as

$$\hat{u}=\hat{h}(k)e^{ikr_0}, \tag{35.9}$$

$$\hat{h}(k)=P\frac{1}{k^2-\kappa^2}+C\delta(k^2-\kappa^2), \tag{35.10}$$

where C is a constant, but may depend on κ. This can be rewritten as (→**28.36**, **??**)

$$\hat{h}(k)=\frac{1}{2\kappa}\left\{\left[P\left(\frac{1}{k-\kappa}\right)+C\delta(k-\kappa)\right]-\left[P\left(\frac{1}{k+\kappa}\right)-C\delta(k+\kappa)\right]\right\}. \tag{35.11}$$

The Fourier inverse transform of u is given by the convolution of $h(\boldsymbol{r})$ and $\delta(\boldsymbol{r}-\boldsymbol{r}_0)$ (→**28.2**),

$$h(\boldsymbol{r})=\frac{1}{4\pi^2 r}\frac{\partial}{\partial r}\int_{-\infty}^{+\infty}dk\frac{e^{ikr}}{2\kappa}\left\{\left[P\left(\frac{1}{k-\kappa}\right)+C\delta(k-\kappa)\right]-\left[P\left(\frac{1}{k+\kappa}\right)-C\delta(k+\kappa)\right]\right\}. \tag{35.12}$$

Here the angular integral has already been performed.

35.5 How to interpret the formal solution (35.11)? Using the Plemelj formula (→**28.36**), we can rewrite

$$P\left(\frac{1}{k-\kappa}\right)+C\delta(k-\kappa)=\lim_{\epsilon\to+0}\frac{1}{k-\kappa\pm i\epsilon}+(C\pm i\pi)\delta(k-\kappa), \tag{35.13}$$

and

$$P\left(\frac{1}{k-\kappa}\right)-C\delta(k-\kappa)=\lim_{\epsilon\to+0}\frac{1}{k-\kappa\pm i\epsilon}-(C\mp i\pi)\delta(k-\kappa). \tag{35.14}$$

Thus, there are four combinations of + and − for (35.11). Consequently, we need an extra condition to select a solution.

35.6 Radiation condition (Ausstrahlungsbedingung). The extra condition to single out the physically meaningful solution from (35.11) is

$$\left|\frac{\partial}{\partial r}h - i\kappa h\right| \to 0. \tag{35.15}$$

for $r \to \infty$ This condition is called the Ausstrahlungsbedingung (out radiating condition due to Sommerfeld). This requires that $-$ must be chosen in (35.13) and $+$ in (35.14): the integrand in (35.11) now reads

$$\left\{\frac{1}{k-\kappa-i\epsilon} - \frac{1}{k+\kappa+i\epsilon} + (C-i\pi)[\delta(k-\kappa)+\delta(k+\kappa)]\right\} e^{ikr}. \tag{35.16}$$

Choosing $C = i\pi$, we can remove unwanted $e^{-i\kappa r}$. Thus, we can get

$$h(\boldsymbol{r}) = -\frac{2\pi i}{8\pi^2 r\kappa}\frac{\partial}{\partial r}e^{i\kappa r} = \frac{e^{i\kappa}r}{4\pi r}. \tag{35.17}$$

That is,

$$G(\boldsymbol{r}|\boldsymbol{r}_0) = \frac{\exp(i\kappa|\boldsymbol{r}-\boldsymbol{r}_0|)}{4\pi|\boldsymbol{r}-\boldsymbol{r}_0|}, \tag{35.18}$$

which is called the *retarded Green's function* (cf. **36.1**, **9.30**).

35.7 Green's functions for 2 and 1-spaces. With the aid of an analogous consideration, we can write down G in 2 and 1-space. For 2-space ($\to$**23.20** for $H_0^{(1)}$)

$$G(\boldsymbol{r}|\boldsymbol{r}_0) = \frac{i}{4}H_0^{(1)}(\kappa|\boldsymbol{r}-\boldsymbol{r}_0|). \tag{35.19}$$

For 1-space

$$G(\boldsymbol{r}|\boldsymbol{r}_0) = \frac{i}{2\kappa}\exp(i\kappa|\boldsymbol{r}-\boldsymbol{r}_0|). \tag{35.20}$$

The difference comes only from the angular integration.

35.8 Analogue of Green's formula. The equation corresponding to Green's formula **??** is immediately obtained from Green's formula for the Laplace equation as

$$\int_D d\tau[u(\Delta+\kappa^2)v - v(\Delta+\kappa^2)u] = \int_{\partial D} d\sigma\left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\right). \tag{35.21}$$

How to use it should now also be obvious ($\to$**??**).

36 Green's Function: Wave Equation

The Green's functions of wave equations are constructed directly or from those of Helmholtz equation. The radiation condition implies the specification of the time arrow.

Key words: retarded and advanced Green's function, propagator, afterglow effect, Helmholtz formula, causality, time arrow

Summary:
(1) If we use the retarded Green's function for the Helmholtz equation, we can obtain the retarded Green's function (→**36.1**).
(2) For wave equations the tiem arow is selected by the radiation condition.

36.1 Fundamental solution. A fundamental solution to the wave equation satisfies

$$\Box w(t,\boldsymbol{x};t',\boldsymbol{x}') = \delta(t-t')\delta(\boldsymbol{x}-\boldsymbol{x}'), \tag{36.1}$$

where

$$\Box \rightleftharpoons c^{-2}\partial_t^2 - \Delta \tag{36.2}$$

is called the *D'Alembertian*. Fourier-transforming this with respect to time, we obtain (→**35.1**, **23.24**)

$$-(\Delta+\kappa^2)\hat{w}(\omega,\boldsymbol{x};t',\boldsymbol{x}') = e^{-i\omega t'}\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{36.3}$$

with $\kappa = \omega/c$. Thus basically this is the same as the problem of finding a fundmental solution for the Helmholtz equation in the whole space. If we use the retarded Green's function for the Helmholtz equation (→**35.6**), then inverse Fourier transformation gives

$$w(t,\boldsymbol{x};t',\boldsymbol{x}') = w(t-t',\boldsymbol{x}-\boldsymbol{x}';0,0) = \frac{1}{2\pi}\int d\omega \frac{e^{i\omega|\boldsymbol{x}-\boldsymbol{x}'|/c - i\omega(t-t')}}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|} \tag{36.4}$$

This can easily be integrated to give (→**??**)

$$w(t,\boldsymbol{x};t',\boldsymbol{x}') = \frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{x}'|}\delta(t-t'-|\boldsymbol{x}-\boldsymbol{x}'|/c). \tag{36.5}$$

Note that this is zero for any $t < t'$. This function is the Green function for 3-space, and is called the *retarded Green function*.

Discussion.
In terms of the retarded Green's function, the inhomogeneous wave equation

$$\Box u = q \tag{36.6}$$

can be solved as

$$u(t, \boldsymbol{x}) = \frac{1}{4\pi} \int_{|\boldsymbol{x}-\boldsymbol{y}|\leq ct} \frac{q(t, \boldsymbol{y})}{|\boldsymbol{y} - \boldsymbol{x}|} d\boldsymbol{y}. \tag{36.7}$$

The formula is called the *Duhamel's formula*.

36.2 Advanced Green's function. We see above that the radiation condition (→**35.6**) imposes time reversal asymmetry (causality). Since the wave equation itself is time-reversal symmetric, the time reversed (36.5) should also be a solution to (36.1):

$$w_A(t, \boldsymbol{x}; t', \boldsymbol{x}') = \frac{1}{4\pi|\boldsymbol{x} - \boldsymbol{x}'|} \delta(t - t' + |\boldsymbol{x} - \boldsymbol{x}'|/c). \tag{36.8}$$

Note that this is zero for $t > t'$ everywhere. This is anti-causal, and is called the *advanced Green's function*.

36.3 Propagator. A fundamental solution $K(t, \boldsymbol{x}; t', \boldsymbol{x}')$ satisfying the boundary condition and symmetric in time is called the *propagator* of the problem. Its existence should be clear from the advanced and retarded Green's functions discussed above. The retarded Green's function is related to the propagator as

$$G(t, \boldsymbol{x}; t'\boldsymbol{x}') = \Theta(t - t')K(t, \boldsymbol{x}; t', \boldsymbol{x}'), \tag{36.9}$$

The fundamental solution satisfying the boundary condition and causality is called the retarded Green's function.

36.4 Symmetry of propagator.

$$K(t, \boldsymbol{x}|t', \boldsymbol{x}') = K(t - t', \boldsymbol{x}|0, \boldsymbol{x}'). \tag{36.10}$$

This time translation symmetry directly follows from **??**. This formula implies

$$K(t, \boldsymbol{x}|t', \boldsymbol{x}') = K(-t', \boldsymbol{x}| - t, \boldsymbol{x}'). \tag{36.11}$$

and consequently

$$\partial_t K(t, \boldsymbol{x}|t', \boldsymbol{x}') = -\partial_{t'} K(t, \boldsymbol{x}|t', \boldsymbol{x}'). \tag{36.12}$$

They imply that

$$K(t, \boldsymbol{x}|t', \boldsymbol{x}') = -K(t', \boldsymbol{x}|t, \boldsymbol{x}'). \tag{36.13}$$

Analogously

$$K(t, \boldsymbol{x}|t', \boldsymbol{x}') = K(t, \boldsymbol{x}'|t', \boldsymbol{x}), \tag{36.14}$$

so that we get

$$K(t, \boldsymbol{x}|t', \boldsymbol{x}') = -K(t', \boldsymbol{x}'|t, \boldsymbol{x}). \tag{36.15}$$

36.5 Eigenfunction expansion of propagator. Introducing the eigenfunction of the Laplacian with an appropriate homogeneous boundary condition (Dirichlet, Robin or Neumann condition) $\{|\lambda_n\rangle\}$ such that $-\Delta|\lambda_n\rangle = \lambda_n|\lambda_n\rangle$, we can separate the wave equation, to get

$$K(t,\boldsymbol{x}|t',\boldsymbol{x}') = \langle \boldsymbol{x}| \left\{ \sum_{n=0}^{\infty} |\lambda_n\rangle \frac{c\sin[c^2\sqrt{\lambda_n}(t-t')]}{\sqrt{\lambda_n}} \langle\lambda_n| \right\} |\boldsymbol{x}'\rangle. \quad (36.16)$$

Here, if $\lambda_0 = 0$ (this happens only when the Neumann condition is imposed), the sine term is computed with the aid of l'Hospital's rule.

36.6 Propagator in infinite space. From (38.4) and the symmetry we can easily guess that[366]

$$K(t,\boldsymbol{x}|0,\boldsymbol{0}) = \frac{1}{4\pi x}[\delta(t-x/c) - \delta(t+x/c)]. \quad (36.17)$$

This is indeed the right answer as can be computed from the continuum version of (36.16) to obtain

$$K(t,\boldsymbol{x}|0,\boldsymbol{0}) = \frac{c}{(2\pi)^3}\int d^3k \frac{\sin(ckt)}{ck} e^{i\boldsymbol{k}\cdot\boldsymbol{x}} = \frac{c}{(2\pi)^3}\frac{4\pi}{x}\int_0^\infty dk \sin(ckt)\sin(kx). \quad (36.18)$$

See **??** Exercise.

36.7 Propagator in 2- and 1-spaces. For 2-space,

$$K^{(2)}(t,\boldsymbol{x}|0,\boldsymbol{0}) = sgn(t)\frac{1}{2\pi}\frac{\Theta(|t|-x/c)}{(t^2-x^2/c^2)^{1/2}}, \quad (36.19)$$

and for 1-space

$$K^{(1)}(t,\boldsymbol{x}|0,\boldsymbol{0}) = sgn(t)\frac{c}{2}\Theta(t^2-x^2/c^2). \quad (36.20)$$

Of course, they can be obtained by integrating unnecessary coordinates out from the 3-space version (→**??**).

36.8 Afterglow revisited. We can see explicitly from $G^{(2)}$ obtainable from $K^{(2)}$ that for $|\boldsymbol{x}| < tc$ $G^{(2)} > 0$, but this does not happen for 3-space. This is the afterglow in even dimensional spaces. (→**??**, **28.46**)

[366] $|\boldsymbol{x}| = x$.

36.9 Helmholtz formula. The solution in 3-space to

$$\Box\psi(t,\boldsymbol{x}) = \varphi(t,\boldsymbol{x}) \tag{36.21}$$

can be written as

$$\begin{aligned}\psi(t,\boldsymbol{x}) &= \int_{T_1}^{t} dt' \int_\Omega d\boldsymbol{x} G(t,\boldsymbol{x};t',\boldsymbol{x}')\varphi(t',\boldsymbol{x}') \\ &- \int_{T_1}^{t} dt' \int_{\partial\Omega} d\sigma(\boldsymbol{x}') \left[G(t,\boldsymbol{x};t',\boldsymbol{x}') \frac{\partial\psi}{\partial n(\boldsymbol{x}')} - \psi \frac{\partial}{\partial n(\boldsymbol{x}')} G(t,\boldsymbol{x};t',\boldsymbol{x}') \right] \\ &+ \frac{1}{c^2} \int_\Omega d\boldsymbol{x}' [G\partial_t\psi - \psi\partial_t G]_{t=T_1}. \end{aligned} \tag{36.22}$$

Just as in the case of the Helmholtz equation (→**35.8**), this is *not* the formula describing ψ in terms of the initial and boundary values.
[Demo] Just as a proof of Green's formula (→**??**), we get

$$\int_{T_1}^{T_2} dt \int_\Omega d\boldsymbol{x}[(\Box f)g - f\Box g] = -\int_{T_1}^{T_2} dt \int_{\partial\Omega} d\boldsymbol{S}\cdot[f\nabla g - g\nabla f] + \int_\Omega d\boldsymbol{x} \frac{1}{c^2}[f\partial_t g + g\partial_t f]_{t=T_1}^{t=T_2}. \tag{36.23}$$

Take f to be the retarded Green's function (→**36.1**), and g to be the solution to (36.21), then this can be rewritten as the desired formula.

36.10 General causal solution. In (36.22) the surface integrals of the 4-volume $\Omega \times [T_1, t]$ describes the effects of the incoming waves into Ω from the past. Hence this can be rewritten as

$$\psi(t,\boldsymbol{x}) = \psi_{in}(t,\boldsymbol{x}) + \int_{T_1}^{t} dt' \int_\Omega d\boldsymbol{x}' G(t,\boldsymbol{x};t',\boldsymbol{x}')\varphi(t',\boldsymbol{x}'). \tag{36.24}$$

Here ψ_{in} denotes the incoming wave. The Ausstrahlungsbedingung (→**35.6**) on ψ implies that $\psi_{in} \to 0$ when $\Omega \to \boldsymbol{R}^3$ and $T_1 \to -\infty$.

37 Colloquium: What Is Computation?

The section contains several deep examples of conceptual analysis – of computer, computation, algorithm, randomness, etc. In **A** Church's idea on computation is outlined. Turing's idea in **B** made this idea convincing. Here Turing machines are outlined. With these preparations, decision problems are briefly discussed in **C**. With the aid of one of the main results of this part, computability and non-computability in elementary calculus is outlined in **D**. Part **E** explains the basic idea of the algorithmic randomness. In the final part **F**, the algorithmic randomness is reconsidered from a more fundamental point of view. The concepts in **A**-**C** and **E** at least must be a part of elementary knowledge of any civilized person.

Keywords: computer, algorithm, recursive function, Church's thesis, Turing machine, universal Turing machine, Turing computability, decision problem, halting problem, recursive set, recursively enumerable set, effectiveness, computable real, computable function, Myhill's theorem (on differentiability).

Summary
(1) The basic content of this section should be a rudimentary knowledge of every intellectual person.
(2) The reader must be able to explain to her lay friends what computation is (**37.11**-**37.12**) and Turing machines **37.16**.
(2) The concept of effectiveness must be understood (**??**).
(3) The reader must be able to explain algorithmic randomness (**37.49**).

37.A Recursive Functions and Church Thesis

37.1 What is a computer? It is a device to perform computation. Then, what do we mean by 'computation'? Intuitively, a computation is a transformation of a finite sequence of symbols by a finite number of applications of finitely many well-defined rules (algorithms). This aspect does not change even if we wish to consider the so-called quantum computation. Since we consider precise computations only, i.e., computations without any roundoff errors, we have only to consider

procedures to transform a nonnegative integer into another nonnegative integer (i.e., $\boldsymbol{N}$ into itself).[367]

37.2 Arithmetic function. A function which maps $\boldsymbol{N}$ into itself is called an *arithmetic function* or a *number theoretic function*. Thus we have only to consider the computation of arithmetic functions.

37.3 Remark. A trivial fact should be kept in mind that we cannot understand the crucial concept 'computer' by analyzing the material basis of an actual computer. There are important things about the physical world on which materialistic physics cannot say anything meaningful.

37.4 Obviously computable functions. To characterize precisely the procedure we call 'computation',[368] we must start with intuitively obviously computable arithmetic functions S, U and C:
(A) $S(x) = x + 1$,
(B) $U_i^n(x_1, \cdots, x_n) = x_i$,
(C) $C_m^n(x_1, \cdots, x_n) = m$.
S is the function giving the successor (in $\boldsymbol{N}$) to x, and U_i^n is the projection operator selecting the i-th coordinate out of n coordinates. C_m^n assigns a constant $m(\in \boldsymbol{N})$ to $\{x_1, \cdots, x_n\}$. These are the functions probably everybody thinks computable.

37.5 Basic operations on functions. Combining these elementary functions, we can produce more complicated functions. What kind of procedures should we allow as obviously doable?[369] The following three **37.6-??** procedures are regarded unambiguously doable and elementary:

[367] When we consider the computability of, e.g., irrational numbers, we must carefully treat the computational errors. Roughly speaking, something is computable if there is an algorithm which gives it within any specified error bar (→**37.36**). See M. B. Pour-El and J. I. Richards, *Computability in Analysis and Physics* (Springer, 1989). Recently, Blum et al. have developed a theory of computation over reals: L. Blum, M. Shub and S. Smale, "On a theory of computation and complexity over the real numbers: NP-completeness, recursive functions and universal machines," Bull. Amer. Math. Soc., **21**, 1-46 (1989). In the theory of computation we use here, that is, in the traditional theory of computation, a real number is considered as a string of bits. In contrast, in the new theory a real number is not viewed as its decimal or binary expansion, but rather as a mathematical entity.

[368] An extremely efficient exposition can be found in the beginning part of R. I. Soare, *Recursively Enumerable Sets and Degrees – a study of computable functions and computability generated sets* – (Springer, 1987). A classic may be M. Davis, *Computability and Unsolvability* (Dover, 1982).

[369] In the following, in contrast to the ordinary definition of functions in analysis, they are *partial functions*, i.e., $f(x_1, \cdots, x_n)$ need not make sense (need not be defined) for all n-tuples $\{(x_1, \cdots, x_n)\}$. We simply stop assigning a value to f when it is not defined. If f is defined for all $(x_1, \cdots, x_n)$, we say the function is a *total function*.

37.6 Composition. The first admissible procedure (I) is: Suppose we already have functions $g_1, \cdots, g_m$ and h. From this we can make

$$f(x_1, \cdots, x_n) = h(g_1(x_1, \cdots, x_n), \cdots, g_m(x_1, \cdots, x_n)), \tag{37.1}$$

where h is a function of m variables, and g_i are functions of n variables. There should not be any difficulty to accept this.

37.7 (Primitive) Recursion (II). Suppose we have functions of $n+1$ variables f and a function of n variables such that

$$f(x_1, \cdots, x_n, 0) = g(x_1, \cdots, x_n). \tag{37.2}$$

Then, starting with this function we can recursively construct $f(x_1, \cdots, x_n, m)$ for $m \in \boldsymbol{N}$ as follows:

$$f(x_1, \cdots, x_n, m) = h(x_1, \cdots, x_n, m-1, f(x_1, \cdots, x_n, m-1)), \tag{37.3}$$

where functions h is a function of $n+2$ variables.

This is allowed for any $m \in \boldsymbol{N}$. This may cause some practical problem, but if we are patient enough, for any fixed m there should not be a problem.

37.8 Minimalization (or unbounded search) (III). Let $f(x_1, \cdots, x_n)$ be a total function.[370] Then, we can make a function $h(x_1, \cdots, x_{n-1})$ which gives the smallest x_n satisfying $f(x_1, \cdots, x_n) = 0$ for each $\{x_1, \cdots, x_{n-1}\}$. (Here f being a total function is crucial.)

(I)-(II) and (III) are markedly different, because while it is guaranteed that the procedures (I) and (II) end within finite number of procedures, (III) is not guaranteed to end; there may not be any solution (→**37.10**).

37.9 Partial recursive functions. The functions generated by applying the basic operations I–III finite times on the basic functions [A]–[C] are called *partial recursive functions*.

37.10 Algorithm and partial recursive functions. Algorithms is a finite set of well defined finite means. We may say partial recursive functions are the functions we have algorithms to compute them (disregarding whether we can complete the procedure).

The operation III (minimalization) is a very tricky procedure. Certainly, we can compute the value of $f(x_1, \cdots, x_{n-1}, m)$ for a fixed choice of the set $\{x_1, \cdots, x_{n-1}\}$ for any m, because f is a total function. Putting m into f one by one in the increasing order starting from $m = 0$,

[370] That is, it is defined for any $x_1, \cdots x_n \in \boldsymbol{N}$.

we can ask whether $f(x_1, \cdots, x_{n-1}, m)$ vanishes or not. If f vanishes for the first time with $m = q$, then we know $h(x_1, \cdots, x_{n-1}) = q$.

However, we do not know whether such integer ever exists. Thus. although we have an algorithm to perform the recursive procedures (we explicitly know each step), we do not know whether we can ever finish it, since there is no guarantee of the existence of the solution. For partial recursive functions, the fact that the procedure has not yet been completed can imply either that the function is not defined for the given instance of variables (that is, no solution exists for $f(x_1, \cdots, x_{n-1}, m) = 0$) or that the function has a value for the given instance but further computation is required to obtain it.

37.11 Recursive functions. More convenient functions should be the ones for which not only each step of construction is explicitly known, but also there is a guarantee that its construction (computation) ends with finite number of steps. They are the recursive functions:
Definition. Total partial recursive functions are called *recursive functions.*

Notice that there are only countably many recursive functions, but of course uncountably many non-recursive functions.

37.12 Church's Thesis. Church proposed: *Computable functions are recursive functions.* □[371]

We may say that Church proposed a definition of the word 'computable.'

37.13 Remark. The crucial elements of the thesis is an explicit description of construction procedures,[372] and the guarantee that the procedure always ends with finite steps ('finitary dogma').

37.14 The thesis was not well accepted initially. Church's thesis was not recognized as a really convincing definition of computability when it was first proposed. The reason for this is that there was no clear feeling about explicitly describable construction procedures. There may be a completely novel type of algorithm which is not recursive, so that the thesis may be under the limitation of the contemporary mathematics. A more general objection was: even apparently intuitively obvious concepts such as 'continuity' requires its definitive characterization by

[371] Some people identifies computable functions and partial recursive functions, and call this identification Church's thesis. For example, M. Li and P. Vitànyi, *An Introduction to Kolmogorov Complexity and Its Applications* (Springer, 1993); J. E. Hopcroft and J. D. Ullman, *Introduction to Automata Theory, Languages and Computation* (Addison Wesley, 1979) are among them.

[372] Church's thesis implies that logical inference is possible only when the procedure can be made purely syntactic. It is a sort of ultimate reductionism.

the axioms of topological spaces; one must be cautious when one says 'so-and-so' is intuitively obvious.[373]

37.15 Turing machine was crucial. The thesis became really convincing after the work of Turing (Turing machine, see the next subsection), who started with the analysis of the limitations of our sensory and mental apparatus. Church himself wrote that Turing-computability has the advantage of making the identification with effectiveness in the ordinary sense evident immediately without any preliminary theorems.

37.B Turing Machine

37.16 Turing machine. A Turing machine consists of a two-way infinite tape divided into cells, a read-write head which can scan one cell of the tape at a time, and a 'black box' with finite number of internal states. A Turing machine may essentially be identified with its program:

37.17 Turing program. A *Turing program* is a finite set of the following four-tuples, $(q, S, *, q')$. Here
(1) q and q' are the internal states of the (black box of the) Turing machine,
(2) S is the symbol in the cell currently being scanned by the head, and
(3) $*$ is R, L or S': R (L) implies that at the next step the head moves one cell to the right (resp. left), and S' implies that the head replaces the tape symbol S with S' without moving.

Thus $(q, S, *, q')$ implies that if the Turing machine reads S when its internal state is q, then the head does $*$ and the internal state becomes q'. Usually the symbol in a cell is either blank B or 1. □

37.18 Turing's motivation. Turing arrived at the concept of Turing machine, analyzing the limitations of our sensory and mental apparatus. The restrictions required are:
(i) finite symbols are allowed to each cell,
(ii) the computer can see only a finite number of cells at a time,
(iii) at each time step the computer may alter the contents of a single cell,
(iv) scan can be finite range,
(v) there is an upper bound to the number of states of mind, only fixed finite set of instructions can be performed.

In short, Turing conceived our brains as finite machine (finite number of distinguishable symbols, finite number of rules or procedures, finite number of distinguishable internal states, etc).

[373] R. Gandy, "Church's thesis and principles for mechanisms" in *The Universal Turing Machine, a half-century survey* (Oxford UP, 1988) : Gödel as well as Post did not accept the thesis.

37.19 How to operate Turing machine. We begin with the machine in its starting state q_I with its head at the leftmost 1 on the tape where x is coded[374] . There is a special state q_H called the halting state. The number y of 1's left on the tape when the Turing machine comes to q_H is the output of the Turing machine. That is, the Turing machine defines a function $x \to y$.

37.20 Turing computable function. The Turing machine operated as in the previous entry may never halt, so that a Turing machine generally defines a partial function. If a Turing machine always halts for any input, the Turing machine defines a total function. In this case we say the total function is a *Turing computable function*.

37.21 Turing computability ≡ Church computability. A Turing machine which halts for all the inputs defines a recursive function, and any recursive function can be realized as a Turing machine which halts for all the inputs.□.[375]

That is, the set of all the functions computable by Turing machine is the totality of recursive functions.

37.22 Remark. The identity of the Turing computability and computability due to Church made the Church's thesis convincing to many (→**37.14-37.15**). However, one might not accept all five restrictions for the human thinking ability stated by Turing (→**41B.3**). Gödel and Post always believed that a true account – an acceptable theory – of human mathematical intelligence must be nonmechanical. In particular Gödel has argued that in our ability to handle abstract concepts we are not subject to the restrictions described by Turing. These only apply when we are dealing with (potentially) concrete objects such as strings or symbols; they believed that satisfactory theory of mathematical intelligence must take account of nonfinitary creative reasoning.

37.23 Universal Turing machine. As is clear from the definition of Turing machines, each machine which halts for all the inputs defines a single recursive function. Turing machines are, so to speak, single-function computers. Notice, however, that any Turing program can be coded in terms of positive integers (the Gödel number of the Turing machine program **37.17**). Hence we can imagine a 'master' computer which compiles the program in Gödel numbers into a set of (Turing executable) four-tuples to emulate the corresponding particular Turing machine. That is, there is a Turing machine which can emulate all the Turing machine. Such a Turing machine is called a *universal Turing machines*. Universal Turing machines may be regarded as idealized digital computers with infinite memory space.

[374] There are many different ways to code x. Choose one and fix it.

[375] A proof may be found in Davis or Soare *op. cit.*

37.24 Universality of universal Turing machine. Universal Turing machines are not unique, but the following theorem guarantees that in essence all the universal Turing machines have the same computational power:
Theorem [**Kolmogorov-Solomonov**]. Let M and M' be two universal Turing machines, and $\ell_M(x)$ be the length (in bits) of the shortest program for M to print out the output x. Then

$$\ell_M(x) \preceq \ell_{M'}(x), \tag{37.4}$$

where $A(x) \preceq B(x)$ implies that there is an x-independent positive constant c such that $A(x) \leq B(x) + c$ for all x. □

37.25 Absoluteness of Turing machine. What is impossible for a universal Turing machine cannot be done by any computer (or brain, if we accept Turing's analysis **37.18**). This statement is unaltered even if we consider quantum computation. However, if a computer or a machine can have an access to a large oracle set (solution sets), the situation could be very different. This may be the reason for Gödel's and Post's objection to Turing's characterization of our brain function.

37.C Decision Problem

37.26 Decision problem. Given a set of problems (or a set of instances of a problem, e.g., whether a polynomial has 0 as its root or not), we ask whether there is an algorithm to answer all the problems in the set. This problem is called a *decision problem*. If there is such an algorithm, we say the set (or the problem) is *decidable*. If not, we say it is *undecidable*. The word 'algorithm' was unclear before Turing, but now we can clearly state that 'algorithm = existence of Turing program.'

37.27 Remark. If a set is finite, or the problem has only finite instances, then it is trivially decidable, because we can check all of them one by one blindly. The decision problem becomes nontrivial only if the problem has infinite instances like the one due to Diophantus (**37.28**(1)).

37.28 Examples.
(1) Hilbert's 10th problem. Decide whether a polynomial $P(x_1, x_2, \cdots, x_n)$ with integer coefficients (Diophantine equations) has an integer root. This is decidable if $n = 2$,[376] but is undecidable for general n.[377]

[376] A. Baker, Phil. Trans. Roy. Soc. London A 263 (1968).
[377] Ju. V. Matyasevich, 1970.

(2) Is $\exists x_1 \exists x_2 \exists x_3 \forall y_1 \cdots \forall y_m \mathcal{U}$ true ($m \in \boldsymbol{N}$)? Here, $\mathcal{U}$ is any logical formula within the first order logic[378] without including $\exists$, $\forall$ and free object variables. This is undecidable.

37.29 Halting problem of Turing machine. Suppose we have a Turing machine T. We feed programs to it, and ask whether it ever stops (that is, the solution is given within a finite time or not (→**37.19**)). Certainly, we can run the program on T, but that the machine has not yet stopped does not mean anything about its final result. Is there any algorithm to judge that a program α ever gives a solution when run on T? This is called the *halting problem*.

37.30 Halting problem is undecidable. Suppose there is a desired algorithm which works on a universal Turing machine (→**37.23**) X. The meaning of the statement is this. In order to decide (T, α) (α is run on T) halts or not, we feed the Gödel number of T (or a code for the Turing program of T) and α to X. X stops after printing 1, if (T, α) halts.[379] Otherwise, X stops after printing 0 (or B). Now we demonstrate that the existence of such UT leads us to absurdity.
(1) We construct another universal Turing machine Y as follows: if X halts after printing 1, Y keeps moving its head to the right; otherwise Y stops after printing 0.
(2) Now we make the third universal Turing machine Z such that if Z is fed a program β, Z make (β, β) and then does what Y does.
(3) Suppose Z stops with a program Z. Then Y must halt with the input (Z, Z). That is, X halts with (Z, Z), printing 0. However, this means that Z does not halt with the program Z.
(4) Suppose Z does not stop with the program Z. Then Y keeps running with the input (Z, Z). Hence X halts after printing 0 when fed (Z, Z), but then Y must halt after printing 0. That is Z must halt with the program Z.
Hence, we cannot decide whether (T, α) halts or not.

37.31 Recursive set. A set whose characteristic function is a recursive function (→**37.11**) is called a *recursive set*.

What this means is: if a set is a recursive set, then we have an algorithm to tell whether a given number is in the set or not. In this sense, we can tell the member of the set without referring to how to generate the set.

[378] I recommend H. D. Ebbinghaus, J. Flum and W. Thomas, *Mathematical Logic* (Springer Undergraduate Texts in Mathematics, 1984; there is a new edition).
[379] Here we identify T with its program or its Gödel number, so program (T, α) on a universal Turing machine means that the machine reads the program and emulates the machine T and then interpret α as T does.

In other words, if we can construct a Turing machine (or a program for a universal Turing machine) such that it can print 1 if the element[380] is in the set and 0 otherwise with finite steps.

37.32 Recursively enumerable set. A set which is a range of a recursive function is called a *recursively enumerable set*.

Hence, if a set is a recursively enumerable set, we know how to produce the set (there is a computer program which generates the set). We simply feed the elements of $\boldsymbol{N}$ one by one to the recursive function, and collect its outcomes.[381]

In other words, we feed all the possible Turing programs into a Turing machine (we must demand that the machine surely stops for all the programs) and collect all the outputs.

37.33 Theorem: There exists a recursively enumerable but not recursive (RENR) set. This is important, so a demonstration is given here.

Let $\phi_x(y)$ be the output (if any) of the Turing machine whose Gödel number is x (remeber that there are only countably many Turing machines), when its input is y. Here, both x and y are in $\boldsymbol{N}$. Make a set

$$K \equiv \{\, x : \phi_x(x) \text{ is defined}\}. \tag{37.5}$$

That is, K is the set of all the numbers x such that the corresponding Turing machine halts with the input x. Certainly, this is a recursively enumerable set, because we know how to perform each step needed to compute $\phi_x(x)$, although we do not know whether it actually gives a number or not. Now define a function f such that

$$f(x) \equiv \begin{cases} \phi_x(x) + 1, & \text{if } \phi_x(x) \text{ is defined,} \\ 0, & \text{otherwise.} \end{cases} \tag{37.6}$$

That is,

$$f(x) \equiv \begin{cases} \phi_x(x) + \chi_K(x), & \text{if } \phi_x(x) \text{ is defined,} \\ \chi_K(x), & \text{otherwise,} \end{cases} \tag{37.7}$$

where χ_K is the characteristic function of K. If K is recursive, then χ_K is recursive, so there must be a Turing machine which reproduces f. However, there cannot be such a Turing machine; if any, there must be an x such that $f(z) = \phi_x(z)$ for any $z \in \boldsymbol{N}$, but obviously this is untrue for $z = x$. Thus we cannot assume that χ_K is a recursive function. (This is an example of the famous diagonal argument).

[380] Of course, this must be suitably encoded so that the machine can understand it.

[381] In this case it is known that the enumeration can be done without repetition. See e.g., Zvonkin and Levine, *op. cit.* Theorem 0.4.

37.34 Theorem. A set Q is recursive if and only if both Q and Q^c are recursively enumerable. □
This should be obvious from the explanation in **37.31**.

37.D Computable Analysis

37.35 Computable rational sequence. We say a rational number sequence $\{r_k\}$ is a *computable rational number sequence*, if for any $k \in \boldsymbol{N}$ there are recursive functions (→**37.11**) a, b and s ($b \neq 0$) such that

$$r_k = (-1)^{s(k)} \frac{a(k)}{b(k)}. \tag{37.8}$$

37.36 Effective convergence. Let $\{r_k\}$ be a computable rational sequence. We say it converges effectively to $x \in \boldsymbol{R}$, if there is a recursive function $e(N)$ such that

$$k \geq e(N) \Rightarrow |r_k - x| \leq 2^{-N}. \tag{37.9}$$

That is, if $\{r_k\}$ converges to x in the ordinary sense of this word and if there is an algorithm to estimate error, we say $\{r_k\}$ converges effectively to x.

37.37 Computable real number. x is a *computable real number*, if there is a computable rational number sequence effectively converging to x.

37.38 Remark: Effectiveness. We say we can do something effectively, if we have an algorithm. We say a concept is effective, if we can define it with an algorithm (for example, whether it is correct or not can be decided). An asymptotic object such as irrational numbers is said to be an effective object when its construction and the distance (error) from the asymptotic limit can be estimated effectively. Thus, 'effectiveness' is a precise formalization of 'constructibility.'

37.39 How to destroy effectiveness. Let $A = \{a(n)\}$ be a RENR set without repetition (i.e., $a(n) \neq a(m)$, if $n \neq m$). We can compute each $a(n)$, but we cannot effectively tell whether, say, 10 appears in A or not. Hence, if we can construct a procedure whose error estimate is bounded by $2^{-a(m)}$, then effective estimation is destroyed.

37.40 Waiting lemma. Let $A = \{a(n)\}$ be a RENR set (→**37.33**) without repetition (i.e., $a(n) \neq a(m)$ if $n \neq m$). Let

$$w(n) \equiv \max\{m | a(m) \leq n\}. \tag{37.10}$$

Then, there is no recursive function (→**37.11**) $c(n)$ such that

$$w(n) \leq c(n). \tag{37.11}$$

That is, there is no algorithm to estimate the needed m so that $\{1, \cdots, n\} \subset \{a(1), \cdots, a(m)\}$. □

If $c(n)$ were recursive, then we could tell whether $n \in A$ or not with a finite number of steps. First, compute $c(n) = m$, then check all $a(m')$ for m' up to m. If we could find n among the output, certainly $n \in A$; if we could not, then $n \neq A$. Hence, A would be a recursive set, a contradiction.

37.41 Theorem. There is a bounded monotone increasing series consisting of computable rational numbers that does not converge effectively (that is, although its convergence is guaranteed, we have no means to compute its value for sure). □.

Take A in the above and construct

$$S = \sum_{n=0}^{\infty} 2^{-a(n)}. \tag{37.12}$$

This is a desired example of the series claimed in the theorem. Since, for example, we do not know whether 2 is in A or not effectively, we cannot estimate S (which must be less than 2) better than the error of 1/4.

37.42 Computable function. We say a function from $\boldsymbol{R}$ into itself is computable, if its values at computable reals are computable reals. Pour-El and Richards impose further the following *effective uniform continuity*. There is a recursive function d such that for any $n \in \boldsymbol{N}$

$$|x - y| \leq 1/d(n) \Rightarrow |f(x) - f(y)| < 2^{-n}. \tag{37.13}$$

37.43 'Ordinary functions' are computable. sin, cos, exp, J_n, etc., are computable. Behind this statement lies the following 'effective Weierstrass' theorem.'

If we can find a recursive function $D(n)$ such that

$$p_n(x) = \sum_{i=0}^{D(n)} r_{nj} x^j, \tag{37.14}$$

where r_{nj} are computable rationals, we say $\{p_n\}$ is a *computable sequence of rational polynomials*.

Effective Weierstrass. If we can find a recursive function $e(n)$ such that

$$m \geq e(N) \Rightarrow |f(x) - p_n(x)| < 2^{-N}, \tag{37.15}$$

then f is a computable function.[382]

[382] See Pour-El and Richards, Chapter 0, Section 5 and 7.

37.44 Computable operations on functions. Composition $f \circ g$, sum $f \pm g$, multiplication fg, and many other elementary operations preserve computability. Integration also preserves computability. Hence, it is not hard to guess that the derivatives of computable analytic functions are again computable. However,

37.45 Theorem [Myhill]. Even if f is a computable C^1 function, f' may not be computable. □

The following is the counterexample. Let

$$\varphi(x) = \begin{cases} \exp(-x^2/(1-x^2)) \text{ for } |x| < 1, \\ 0 \text{ otherwise,} \end{cases} \tag{37.16}$$

which is a C^∞ function. Let $A = \{a(n)\}$ be the RENR set mentioned before. Define

$$\varphi_n(x) = \varphi[2^{n+a(n)+2}(x - 2^{-a(n)})]. \tag{37.17}$$

Construct

$$f(x) = \sum_{k=0}^{\infty} 4^{-a(k)} \varphi_k(x). \tag{37.18}$$

This is computable, but

$$f'(2^{-m}) = 4^{-m} \chi_A(m), \tag{37.19}$$

where χ_A is the characteristic function of A, which cannot be computed.

37.46 PDE and computabilty.
(1) Laplace and diffusion equations preserve the computability of the auxiliary conditions.
(2) In $d(\geq 2)$-space, the wave equation cannot preserve computability. More explicitly, even if the initial data is computable, the solution at time, say, $t = 1$ is not computable. It is not hard to understand this, if we notice that the Radon transformation formula (→**??** $d \geq 2$) involves differentiation (cf. **37.45**).

37.E Algorithmic Randomness

37.47 Regularity in sequence. If something (e.g., a sequence) is 'random', then we would not discern any feature in it. Therefore, to communicate it to someone else, the simplest way is to send its faithful copy. If we could discern a certain characteristic feature or regularity in the sequence, we can exploit the feature to shorten its description. For example, the sequence 11235831459437077415617 85... is produced

by the rule $a_n = a_{n-1} + a_{n-2} \pmod{10}$ with $a_1 = a_2 = 1$. Thus to send million numbers $a_1, \cdots, a_{10^6}$, we send the rule, the initial two numbers, and the total number of digits $N = 10^6$. If one has to send extremely many terms, the length of the message is dominated by the length of N. Hence, we may expect the message length is asymptotically proportional to $\log N$.

37.48 Another example. Consdier another example: 33057270365759 59195309218611738193261179310511854807446237996274956735188575272 4. This may look random, but this is the 1001st to 1100th digits from the decimal expansion of π. Hence, the statement "the 1001st to 1100th digits in the decimal expansion of π" is already shorter than the sequence itself. Certainly, this would be the case if one wishes to send million digits from the decimal expansion of π starting from the one millionth digit. Again, in this example, the length of the message would be dominated by the number specifying the total number of digits as in the preceding example. This example gives us another important lesson. It is almost impossible to compress the length of the message by only looking at the message (in this case a sequence). This implies that there is no general fool-proof method to compress the message (to tell whether the sequence is random or not) (→**37.52**).

37.49 Intuitive introduction to algorithmic randomness. A formalization of the above idea of randomness = information incompressibility is the intuitive essence of algorithmic randomness due to Solomonov, Kolmogorov and Chaitin. If there is a much shorter program for a computer to print out the sequence than the printout itself, then the sequence cannot be random, because some order or discernible structure must have been used to information compress the sequence. Thus the idea seems to capture our intuition about the 'lawlessness' of the random sequence[383] (but see**41E.2**).

37.50 A definition of randomness. The *randomness* $K(\omega)$ of a binary sequence $\omega \in \{0,1\}^{\boldsymbol{N}}$ is defined by

$$K(\omega) \equiv \limsup_{n\to\infty} \ell_M(\omega[n])/n, \tag{37.20}$$

where $\omega[n]$ denotes the first n letters of ω. □
Notice that this does not depend on the choice of the universal Turing machine M thanks to Kolmogorov and Solomonov (→**37.24**).

[383] To clearly define lawlessness itself is a challenging endeavor. Within the ordinary classical logic it is impossible, because due to the exclusion of middle, if a sequence does not have some property, then it can be characterized by the lack of the same property. Thus excluding one law implies admitting the negation of that law.

37.51 Random sequence. A binary sequence ω is *(algorithmically) random* if $K(\omega) > 0$. □

37.52 Noncomputability of randomness. Notice that $K(\omega)$ is not computable as can easily be guessed from the appearance of the words such as the *shortest program* for a machines, etc. This is the difficulty we have already encountered with π. It is usually extremely hard (virtually impossible) to discern an order even if it exists which can be exploited to compress the sequence. Thus except for very obvious cases we may not be able to tell whether a given sequence is random or not. It is generally impossible to quantify the randomness of a particular sequence in terms of K.[384]

37.53 Examples.
(1) There are only countably many algorithmically non-random sequences, so the 01 sequences obtained from the binary expansion of almost all numbers in [0,1] with respect to the Lebesgue measure are algorithmically random.
(2) All the binary expansions of algebraic numbers are nonrandom.
(3) π is not random algorithmically, although its decimal expansion sequence exhibits all the good characteristics of a random sequence statistically.[385] Such a fact will be crucial in trying to understand what complexity is.[386]

37.54 Randomness and chaos. Chaos in dynamical systems can be characterized by the algorithmic random trajectories.[387]

37.F Randomness as a Fundamental Concept

37.55 Why do we discuss randomness further? A mathematical reason is stated below. Here a physical motivation is given. Every one

[384] My math mentor told me, "A random number is like God. If you are told that this is God, you would be extremely suspicious."
[385] In practice, random number evolves. The random number of today is the sequence which passes all the statistical test available today.
[386] There are attempts to make a measure of randomness which is actually computable. One approach is to use finite automatons instead of universal Turing machine. However, these approaches may be fundamentally flawed, because the concept 'random' may naturally be transcendental. That is, whether a given instant is random or not cannot be judged within the mathematical (or logical) framework we are working in (→**37.50**).
[387] A. A. Brudno, "Entropy and the complexity of the trajectories of a dynamical system," Trans. Moscow Math. Soc. Issue **2**, 127-151 (1983).

knows that the basic principle of statistical mechanics is the principle of equal probability. That is, the sampling measure for the equilibrium state is the Liouville measure (or the Riemann volume of the phase space). It is in principle impossible to justify this with the aid of mechanics, because this is a statement about the initial condition of the closed systems. Hence, this is a principle beyond any physical law,[388] and dictates how we observe Nature. When we sample randomly, statistical mechanics holds. Thus at the heart of statistical mechanics and thermodynamics, which are the only means to relate microscopic and macroscopic observables, there is a characterization of randomness. Thus randomness is of central importance in physics.

37.56 Mathematization of 'randomness'. In the algorithmic characterization of randomness, 'randomness,' which is an intuitive concept, is mathematized by identifying it with 'the lack of computable regularity.' One may well argue that there is no guarantee that all the regularities are 'computable regularities'; some inspiration or revelation might tell us the existence of a different kind of regularity in the sequence. This is not an outrageous statement, if mathematical intelligence is, as supposed by Gödel and Post, nonfinitary (→**37.22**). Furthermore, 'random sampling' may be done by Nature herself. In this case, why do we have to assume that Her capability is restricted to computation?

37.57 Why Axiomatization of Randomness? Fundamental concepts should not have unique and privileged interpretations. That is, if X is very fundamental, we should not be able to answer the question, "What is X?", because we need understanding of more fundamental concepts to answer the question. Thus, axiomatization in which X appears as primitive is the only way to formalize our thought on fundamental objects or foundational issues.

37.58 Van Lambargen Axioms. Van Lambalgen's independence axioms are informally as follows. He introduces a relation R such that $R(x, y)$ may be interpreted as 'y has no information about x,' or 'x cannot be information-compressed even with the extra information y (or 'oracle y'). This relation R is specified by the following axioms, which are put informally here:[389]
R1. There is a sequence which cannot be information-compressed without any 'external information (or oracle). [$\exists x R(x, \emptyset)$.]

[388] However, you could imagine that a special initial condition was imposed as time $t = 0$ of the Universe.

[389] There are slightly different versions of axioms given in van Lambalgen's papers. Also here the exposition is informal, so the numbering of the axioms are different from the original versions. Probably the latest paper is, "Independence, randomness and the axiom of choice," J. Symbolic Logic **57**, 1274-1304 (1992).

R2. If x cannot be information-compressed with the information of y and z, then it cannot be done so with the information of z alone. [$R(x, yz) \Rightarrow R(x, z)$.] (Here y and z may be understood as sets, and yz their joint set.)
R3. If x cannot be information-compressed by the information of y, then x and y are different. [$R(x, y) \Rightarrow x \neq y$.]
R4. If there ia a ϕ-relation between y and x, and x cannot be information -compressed with the aid of y, then there is a more random sequence w such that there is a ϕ-relation between w and y, and w cannot be information-compressed with th aid of not only y but of z. [$\exists x(R(x, y) \bigwedge \phi(x, y)) \Rightarrow \exists w(R(w, zy) \bigwedge \phi(w, y))$. Here ϕ should not have any parameters other than listed in y.] (In a certain sense, w satisfying $R(w, y)$ is 'more random (lawless)' than x satisfying $R(x, \emptyset)$, because **R2** implies that w satisfies $R(w, \emptyset)$. That is, w is not only information-*in*compressible without any extra information, but also incompressible even with the extra-information y. Thus this axiom demands that there always exists a 'more' random sequence than a given one; Indeed, **R4** implies, when no relation ϕ is chosen, $\exists x R(x, y) \Rightarrow \exists w(R(w, zy)$. Hence, $xR(x, \emptyset)$ implies that x is in a certain sense with the lowest level randomness.
R5. If y cannot be information-compressed with the information z, and, simultaneously, x cannot be information-compressed with the aid of y, then y cannot be information-compressed with the aid of x. [$R(y, z) \bigwedge R(x, yz) \Rightarrow R(y, xz)$.][390] [391]

37.59 Grave consequences of R. There is a very grave consequence of van Lambalgen's axioms of randomness. If we add these axioms **R** to the usual Zermelo-Fraenkel axioms of sets, then Axiom of Choice does not hold.

[390] The following axiom is also sometimes required. R6. In the ordinals, there is no element of randomness. [$R(x, y) \Rightarrow R(x, \alpha y)$, where α is an ordinal.]
[391] The axioms of independence and Friedman's quantifier 'almost all' Q have an intimate relation. $Qx\phi(x)$ can be interpreted as: if x is randomly generated, then it is practically certain that $\phi(x)$. Thus we can translate $Qx\phi(x)$ as $\forall x(R(x, \emptyset) \Rightarrow \phi(x))$.

APPENDIX A. Rudiments of Analysis

Warning. This is not a substitute of a standard textbook of elementary calculus, but covers most topics every undergraduate analysis course must cover. This is only a summary or a check list of the reader's knowledge. Scan the titles of the numbered entries, and if she finds a somewhat unfamiliar concept, read the entry. Try to form vivid mental image of defined concepts. Try to be able to explain why the statements are plausible intuitively. If you feel a theorem to be obvious, you need not prove it. The following material heavily relies on K. Kodaira, *Introductory Calculus* I-IV (Iwanami 1986), and *Encyclopedic Dictionary of Mathematics* (Iwanami 1985, 3rd edition). J. D. DePree and C. W. Swartz, *Introduction to Real Analysis* (Wiley, 1988) may be recommended as an introductory textbook.

Table of Standard Symbols

$\forall$	all, any, arbitrary.
$\exists$	there exist(s)
$\Rightarrow$	$A \Rightarrow B$ means A implies B.
$\Longleftrightarrow$	if and only if (iff)
$\rightleftharpoons$	$A \rightleftharpoons B$ means "A is defined by B."
$\in$	$a \in A$ implies that a is an element of A.
$\boldsymbol{C}$	the set of all complex numbers.
$\boldsymbol{N}$	the set of all nonnegative integers
$\boldsymbol{Q}$	the set of all rational numbers
$\boldsymbol{R}$	the set of all real numbers.
$\boldsymbol{Z}$	the set of all the integers
C^r	the set of all the C^r-class functions (r-times continuously differentiable functions).
C^0	the set of all the continuous functions
C^∞	the set of all the infinite times differentiable functions.
C^ω	the set of all (real) analytic functions
$L^1(A, \rho)$	Lebesgue integrable functions on A with weight ρ.
$L^2(A, \rho)$	Square Lebesgue integrable functions on A with weight ρ.
inf	infimum
sup	supremum
supp	support
L(R)HS	Left (right) hand side

38 Point Set and Limit

The properties of reals (=real numbers) such as their continuity are assumed to be known.

A1.1 Sequence. Let a_1, a_2, $\cdots$ be reals. $a_1, a_2, a_3, \cdots$ is called a *sequence* and is denoted as $\{a_n\}$. Each real in the sequence $\{a_n\}$ is called a *term*.

A1.2 Convergence, limit. A sequence is said to *converge* to α if for any positive ϵ, there is a positive integer $N(\epsilon)$ such that

$$n > N(\epsilon) \Rightarrow |a_n - \alpha| < \epsilon. \tag{38.1}$$

α is called the *limit* of the sequence $\{a_n\}$, and is often written as $a_n \to \alpha$.

A1.3 Theorem [Cauchy]. A necessary and sufficient condition for a (real) sequence $\{a_n\}$ to converge is that for any positive number ϵ there is a positive integer $N(\epsilon)$ such that

$$n > N(\epsilon), \;\; m > N(\epsilon) \Rightarrow |a_n - a_m| < \epsilon. \tag{38.2}$$

□
Such a sequence is called a *Cauchy sequence*. [In an infinite dimensional space, a Cauchy sequence may not converge.]

A1.4 Symbol 'O' and 'o'.
(1) $f = O[g]$ means that the quantity f is of order g in the appropriate limit in the context. That is $\lim f/g$ is not divergent. For example, $1 - \cos x = O[x^2]$ in the $x \to 0$ limit. That is, $\lim_{x\to 0}(1 - \cos x)/x^2 < +\infty$, which is, of course, correct.
(2) $f = o[g]$ means that the quantity f is 'much smaller' than g in the appropriate limit in the context. For example, $\sin(x^2) = o[x]$ in the $x \to 0$ limit.

A1.5 Limit and arithmetic operations commute. Let $a_n \to \alpha$ and $b_n \to \beta$. Then,
(i) If $a_n \geq b_n$ for infinitely many n, then $\alpha \geq \beta$.
(ii) $a_n \pm b_n \to \alpha \pm \beta$.
(iii) $a_n b_n \to \alpha\beta$.
(iv) If $a_n \neq 0$ and $\alpha \neq 0$, then $b_n/a_n \to \beta/\alpha$.

A1.6 Lower and upper bound, supremum and infimum. Let $S \subset \boldsymbol{R}$. If any element in S does not exceed a real μ (i.e., $s \leq \mu$ for any $s \in S$) [resp., is not exceeded by a real number μ (i.e., $s \geq \mu$ for any $s \in S$)], we say S is *bounded to the above* [resp., *bounded to the below*] and μ is called an *upper bound* [resp., *lower bound*] of S. The smallest upper bound [resp., the largest lower bound] of S is called the *supreme* [resp., *infimum*] of S, and is written as $\sup_{s\in S} s$ [resp., $\inf_{s\in S} s$]. If S is bounded to the above and to the below, S is said to be *bounded*.

A1.7 Monotone sequences. If $a_1 < a_2 < \cdots < a_n < \cdots$ [resp., $a_1 > a_2 > \cdots > a_n > \cdots$], $\{a_n\}$ is called a *monotone increasing* [resp., *monotone decreasing*] sequence. If $a_1 \geq a_2 \geq \cdots \geq a_n \geq \cdots$ [resp.,

$a_1 \le a_2 \le \cdots \le a_n \le \cdots]$, $\{a_n\}$ is called a *monotone non-decreasing* [resp., *monotone non-increasing*] sequence.

A1.8 Theorem [Bounded monotone sequences converge].
A monotone non-decreasing [resp., non-increasing] sequence bounded to the above [resp., to the below] converges to its supremum [resp., its infimum]. □

A1.9 Divergence to ± infinity. If a monotone non-decreasing sequence [resp., non-increasing sequence] is not bounded to the above [resp., to the below], we say it diverges to positive infinity [resp., negative infinity] and write $\lim_{n\to\infty} a_n = +\infty$ [resp., $\lim_{n\to\infty} a_n = -\infty$].

A1.10 Limsup and liminf. Suppose $\{a_n\}$ is a bounded sequence. Let $\sup_n a_{n+m} = \alpha_m$ for $m = 1, 2, 3, \cdots$. Then $\{\alpha_n\}$ is a bounded monotone non-increasing sequence. Hence, Theorem **A1.8** tells us that $\lim_{n\to\infty} \alpha_n$ exists. This is called the *superior limit* of the sequence $\{a_n\}$, and is written as $\limsup_{n\to\infty} a_n$. Analogously, the limit $\lim_{m\to\infty} \inf_n a_{n+m}$ exists, which is called the *inferior limit* of the sequence $\{a_n\}$, and is written as $\liminf_{n\to\infty} a_n$.
(i) For any positive ϵ there are only finitely many a_n larger than $\limsup_{n\to\infty} a_n + \epsilon$, but there are infinitely many a_n larger than $\limsup_{n\to\infty} a_n - \epsilon$.
(ii) For any positive ϵ there are only finitely many a_n smaller than $\liminf_{n\to\infty} a_n - \epsilon$, but there are infinitely many a_n smaller than $\liminf_{n\to\infty} a_n + \epsilon$.
(iii) A necessary and sufficient condition for $\{a_n\}$ to converge is $\limsup a_n = \liminf a_n$.

A1.11 Infinite series. For a sequence $\{a_n\}$, $a_1 + a_2 + a_3 + \cdots + a_n + \cdots$ is called an *infinite series*, and is often written as $\sum_{n=1}^{\infty} a_n$. The convergence of the series is defined by the convergence of the sequence $\{s_n\}$ consisting of its *partial sums*: $s_n \rightleftharpoons a_1 + \cdots + a_n$. $\lim_{n\to\infty} s_n$, if it converges, is called the *sum* of the infinite series $\sum_{n=1}^{\infty} a_n$. If $\{s_n\}$ does not converge, the series is said to be divergent.
If $\sum_{n=1}^{\infty} a_n$ converges, then a_n converges to zero.

A1.12 Absolute convergence. If $\sum_{n=1}^{\infty} |a_n|$ converges, $\sum_{n=1}^{\infty} a_n$ is said to be *absolutely convergent*.
(i) If $\{a_n\}$ converges absolutely, $\{a_n\}$ converges.
(ii) Suppose $\sum_{n=1}^{\infty} r_n$ is convergent and $r_n \ge 0$. If $|a_n| \le r_n$ for all n larger than some integer m, then $\sum_{n=1}^{\infty} a_n$ converges absolutely.

A1.13 Power series. A series of the form $\sum_{n=0}^{\infty} a_n (x-b)^n$ is called a *power series*, where b is a constant.

A1.14 Conditional convergence, alternating series. If a convergent series is not absolutely convergent, it is said to *converge conditionally*. If positive and negative terms appear alternatingly, the series is called an *alternating series*.
If $\{a_n\}$ $(a_n > 0)$ is a monotone decreasing sequence converging to zero, then the alternating series $a_1 - a_2 + a_3 - a_4 + \cdots$ converges ($\rightarrow$[AV7]).

A1.15 Theorem [Nested sequence of intervals shrinking to a point share the point]. If a sequence of closed intervals $\{I_n\}$ such that $I_n = [a_n, b_n]$ satisfies (i) $I_1 \supset I_2 \supset \cdots \supset I_n \supset \cdots$ and (ii) $\lim_{n\to\infty}(b_n - a_n) = 0$, then there is a unique real c which is in all I_n.□
For this theorem it is crucial that I_n are closed intervals.

A1.16 Denumerability. An infnite set for which we can make a one-to-one correspondence with nonnegative integers $\boldsymbol{N}$ is called a *countable set* or *denumerable set*. An infinite set which is not countable is called an *uncountable set* or *nondenumerable set*.
The set of rational numbers $\boldsymbol{Q}$ is countable.

A1.17 Cantor's Theorem [Continuum is not denumerable]. A closed interval $I = [a, b]$ is nondenumerable. □

A1.18 n-space, distance, ϵ-neighborhood. The totality of the n-tuples $(x_1, x_2, \cdots, x_n)$ is a direct product set $\boldsymbol{R} \times \cdots \times \boldsymbol{R} \equiv \boldsymbol{R}^n$ and is called the *n-space*. The (Euclidean) distance between two points $(x_1, \cdots, x_n)$ and $(y_1, \cdots, y_n)$ is defined by $[(x_1-y_1)^2+\cdots+(x_n-y_n)^2]^{1/2}$. The (Euclidean) distance between point P and Q is denoted by $|PQ|$. The totality of the points which are within the distance ϵ of point P is called the *ϵ-neighborhood* (ϵ-nbh) of P (and is denoted by $U_\epsilon(P)$ in this Appendix).

A1.19 Inner point, boundary, accumulating point, closure, open kernel. Let S be a subset of $\boldsymbol{R}^n$.
Inner point: P is an *inner point* of S if there is $\epsilon > 0$ such that $U_\epsilon(P) \subset S$.
Boundary point: If for any $\epsilon > 0$ $U_\epsilon(P) \subset_{\neq} S$ and $U_\epsilon(P) \cap S \neq \emptyset$, P is called a *boundary point* of S.
Boundary: The totality of the boundary points of S is called the *boundary* of S and is denoted by ∂S.
Closure: $S \cup \partial S$ is called the *closure* of S and is denoted by $[S]$. If $T \subset S$, then $[T] \subset [S]$.
Open kernel: $S \setminus \partial S$ is called the *open kernel* of S and is denoted by

S°.
Dense: Let T be a subset of S. If $[T] \supset S$, T is said to be *dense* in S.
Accumulating point: If $U_\epsilon(P) \cap S$ contains infinitely many points of S for any positive ϵ, we say P is an *accumulating point* of S.
Isolated point: If a point in S is not an accumulating point of S, the point is called an *isolated point*.
(i) A necessary and sufficient condition for a point Q to be in $[S]$ is that for any positive ϵ $U_\epsilon(Q) \cap S \neq \emptyset$.
(ii) The totality of rational numbers $\boldsymbol{Q}$ has no inner point and $[\boldsymbol{Q}] = \boldsymbol{R}$.
(iii) All the inner points of S are accumulating points of S. An accumulating point of S is its inner point or its boundary point. If a boundary point of S is not in S, it is an accumulating point of S.
(iv) A necessary and sufficient condition for a point P to be an isolated point of S is that there is a positive ϵ such that $U_\epsilon(P) \cap S = \emptyset$.

A1.20 Open set, closed set. If S contains only its inner points, that is, if $S = S^\circ$, then S is called an *open set*. If all the boundary points are included in S, that is, if $S = [S]$, S is called a *closed set*. The empty set $\emptyset$ is simultaneously open and closed, so is $\boldsymbol{R}$.
(i) The intersection of finite or infinite closed sets is a closed set.
(ii) The union of finite or infinite open sets is an open set.
(iii) The intersection of finitely many open sets is an open set.
(iv) The union of finitely many closed sets is a closed set.

A1.21 Limit of point sequence. A sequence of points $\{P_n\}$ ($P_n \in \boldsymbol{R}^n$) is called a *point sequence*. If there is a point A such that $\lim_{n\to\infty} |P_nA| = 0$, we say the point sequence $\{P_n\}$ converges to A. and write $\lim_{n\to\infty} P_n = A$.

A1.22 Bounded set, diameter. If the distance between any point $P \in S$ and the origin O is bounded to the above ($\rightarrow$**A1.6**), then the set S is called a *bounded set*. When S is a bounded set we can define its diameter $\delta(S)$ as $\delta(S) \equiv \sup_{P,Q\in S} |PQ|$. There is a theorem analogous to **A1.15**:

A1.23 Theorem [Shrinking nested sequence of bounded closed sets]. If a sequence of nonempty bounded closed sets $\{S_n\}$ satisfies the following two conditions (i) and (ii), then there is a unique point P shared by all of the closed sets S_n: (i) $S_1 \supset S_2 \supset \cdots \supset S_n \supset \cdots$, (ii) $\lim_{n\to\infty} \delta(S_n) = 0$.

A1.24 Covering. Let $\mathcal{U}$ be a set of sets. The joint set of all the members of $\mathcal{U}$ is written as $\cup_{U\in\mathcal{U}} U$. If a set S satisfies $S \subset \cup_{U\in\mathcal{U}} U$, then $\mathcal{U}$ is called a *covering* of S. If all the elements of $\mathcal{U}$ is open, it is called

an *open covering* of S. If a covering $\mathcal{U}$ contains only a finite number of elements, $\mathcal{U}$ is called a *finite covering*. If a subset $\mathcal{V}$ of $\mathcal{U}$ is also a covering of S, $\mathcal{V}$ is called a *subcovering* of $\mathcal{U}$.

A1.25 Compact set. If any open covering of S has a finite subcovering, S is called a *compact set*.

A1.26 Theorem [Compactness is equivalent to bounded closedness]. S is compact if and only if S is a bounded closed set.□
The only-if part is called the *Heine-Borel covering theorem*. This is true only if the space is finite dimensional.

[27] Theorem [Bolzano and Weierstrass]. A bounded infinite set must have an accumulating point(→**A1.19**).□
Theorem. A bounded point sequence has a converging subsequence.□[392]

39 Function

A2.1 Function, domain, range, independent and dependent variables. Let $D \subset \boldsymbol{R}$. A rule f corresponding a single real η to each $\xi \in D$ is called a *function* f.[393] $\eta = f(\xi)$ is called the *value* of f at ξ. D is called its *domain* and $f(D) \equiv \{f(\xi)|\xi \in D\}$ is called the *range* of f. Usually, f is described as $f(x)$, and x is called the *variable*, and $f(x)$ is called a function of x. When we write $y = f(x)$, x is called the *independent variable* and y the *dependent variable*.

A2.2 Limit of function. Let $f(x)$ be a function whose domain is D. We say $f(x)$ converges to α in the limit $x \to a$, if for any positive ϵ, there is a positive number $\delta(\epsilon)$ such that

$$|x - a| < \delta(\epsilon),\ x \in D \Rightarrow |f(x) - \alpha| < \epsilon.$$

and we write $\lim_{x \to a} f(x) = \alpha$. $\lim_{x \to a}$ and arithmetic operations are commutative as **A1.5**. We have a theorem analogous to **A1.3**:

[392] These theorems assume that we can always choose one point from each member of a family of infinitely many sets. From the constructive point of view, this is not always possible. That is, we may not be able to write a computer program to do so. In the usual mathematics, we postulate this possibility as an axiom called the Axiom of Choice.
[393] This is often called a *map* as well.

A2.3 Cauchy's criterion. Let f be a function whose domain is D. A necessary and sufficient condition for f to be convergent in the $x \to a$ limit is: For any positive ϵ there is a positive $\delta(\epsilon)$ such that for $x, y \in D$

$$|x - a| < \delta(\epsilon),\ |y - a| < \delta(\epsilon) \Rightarrow |f(x) - f(y)| < \epsilon.$$

□

A2.4 Graph of a function. The graph G_f of a function f is a set $G_f = \{(x, f(x))|x \in D\}$.

A2.5 Continuity. A function f is *continuous* at a, if $\lim_{x\to a} f(x) = f(a)$.
If the definition of the limit is spelled out completely as in **A2.2**, we say: f is continuous at a, if for $x \in D$ and for any positive ϵ there is a positive $\delta(\epsilon)$ such that

$$|x - a| < \delta(\epsilon) \Rightarrow |f(x) - f(a)| < \epsilon.$$

Theorem. If the domain of a continuous function f is a closed interval, then its range is again a closed interval. □

A2.6 Left and right continuity. When taking the $x \to a$ limit, if x is always smaller (resp., larger) than a, we write this limiting procedure as $\lim_{x\to a-0}$ (resp., $\lim_{x\to a+0}$) and is called the *left limit* (resp., right limit). If $\lim_{x\to a-0} f(x) = f(a)$ (resp., $\lim_{x\to a-0} f(x) = f(a)$), we say f is *left (resp., right) continuous* at a.

A2.7 Theorem of middle value. Let a function f be continuous in a closed interval $[a, b]$, and $f(a) \neq f(b)$. There is a real c such that $a < c < b$ and $f(c) = \mu$ for any μ between $f(a)$ and $f(b)$. □
The image of a finite interval by a continuous map is again a finite interval.

A2.8 Uniform continuity. A function f is *uniformly continuous* in D if for any positive ϵ, there is a positive constant $\delta(\epsilon)$ such that

$$|x - y| < \delta(\epsilon), x \in D, y \in D \Rightarrow |f(x) - f(y)| < \epsilon.$$

Theorem. A continuous function defined on a closed interval is uniformly continuous on the interval. □

A2.9 Maximum and minimum. Let f be a function whose domain is D. If $f(D)$ is bounded, we say f is bounded. If there is a maximum (resp., minimum) value in $f(D)$, then it is called the *maximum* (resp.,

minimum) of f.
Theorem [**Maximum value theorem**]. A continuous function defined on a closed interval has a maximum and minimum values. □

A2.10 Composite function. Let f be a function whose domain is D, and g is a function whose domain is in the range of f, $f(D)$. Then $h(x) = g(f(x))$ is called the *composite function* of f and g, and is denoted by $g \circ f$.

A2.11 Monotone function. Let f be a function whose domain is D. If for any $x, y \in D$ $x < y$ implies $f(x) < f(y)$ (resp., $f(x) > f(y)$), f is called a *monotone increasing function* (resp., *monotone decreasing function*). If for any $x, y \in D$ $x < y$ implies $f(x) \leq f(y)$ (resp., $f(x) \geq f(y)$), f is called a *monotone non-decreasing function* (resp., *monotone non-increasing function*).

A2.12 Inverse function. Let f be a function whose domain is D. If there is only one x such that $f(x) = y$ for each $y \in f(D)$, the correspondence $y \to x$ defines a function. This function, denoted by f^{-1}, is called the *inverse function* of f.
The symbol f^{-1} is used generally to denote the *preimage* of a point. Thus $f^{-1}(x) = \{y | f(y) = x, y \in D\}$, where D is the domain of f. f^{-1} becomes the inverse function, if $f^{-1}(x)$ is a single point for all x in the range of f.
Theorem. If f is a monotone increasing (resp., decreasing) function defined on an interval, then f has the inverse function which is monotone increasing (resp., decreasing). □

A2.13 Even and odd functions. If a function f has a domain invariant under $x \to -x$, and
(i) $f(x) = f(-x)$, we say f is an *even function*,
(ii) $f(x) = -f(-x)$, we say f is an *odd function*.

40 Differentiation

A3.1 Differentiability, derivative. Let f be a function defined on an interval I, and $a \in I$. If the following limit, denoted by $f'(a)$, exists, we say f is *differentiable* at a:

$$f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a}.$$

$f'(a)$ is called the *differential coefficient* of f at a. If f is differentiable for any $x \in I$, we say that f is differentiable in I, and $f'(x)$ becomes a function on I. f' is called the *derivative* of f. To obtain f' from f is said to *differentiate* f. Recognize that the existence of the limit implies that the limit does not depend on how the point a is reached.

A3.2 Theorem [Differentiability implies continuity]. If f is differentiable at a, then f is continuous there. If f is differentiable in an interval I, it is continuous in the interval. □
Warning. However, continuity does not guarantee differentiability. See **A3.12**.

A3.3 Increment, differential quotient]. Let f be as in **A3.1** and write $y = f(x)$, and $\Delta y \equiv f(x + \Delta x) - f(x)$. Δx and Δy are called *increments*. Then

$$f'(x) = \lim_{\Delta x \to 0} \frac{\Delta y}{\Delta x},$$

so that the derivative is also called the *differential quotient* and is denoted by dy/dx. If f is differentiable, then we may write

$$\Delta y = \frac{dy}{dx}\Delta x + o[\Delta x],$$

For o see **A1.4**.

A3.4 Right or left differentiable. If the right limit (→**A2.6**) $\lim_{x \to a+0}(f(x) - f(a))/(x - a)$ exists, then we say f is *right differentiable* at a, and the limit, called *right differential coefficient* at a, is denoted by $D^+f(a)$. Analogously the left differential coefficient $D^-f(a)$ can be defined.

A3.5 Differentiation and arithmetic operations commute. Let f, g be differentiable in some interval, and c_1, c_2 be constants. Then 'arithmetic operations do not destroy differentiability':
(i) $\frac{d}{dx}(c_1 f(x) + c_2 g(x)) = c_1 f'(x) + c_2 g'(x)$.
(ii) $\frac{d}{dx}(f(x)g(x)) = f'(x)g(x) + f(x)g'(x)$.
(iii) If g is not zero, then $\frac{d}{dx}\frac{f(x)}{g(x)} = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2}$.

A3.6 Derivative of composite function. Let f be a differentiable function on an interval I, and g be a differentiable function on an interval J containing $f(I)$. Then, $g \circ f$ (→**A2.10**) is differentiable and

$$\frac{d}{dx}g(f(x)) = g'(f(x))f'(x).$$

A3.7 Derivative of inverse function. Let f be a differentiable

monotone function on an interval I. Then its inverse function (→**A2.12**) is differentiable and

$$\frac{d}{dx}f^{-1}(x) = 1/f'(f^{-1}(x)).$$

A3.8 Theorem [Mean-value theorem]. Let f be a continuous function on the closed interval $[a, b]$. If f is differentiable in (a, b), then there is $\xi \in (a, b)$ such that

$$f'(\xi) = \frac{f(b) - f(a)}{b - a}.$$

□
A special case of this theorem is:

A3.9 Theorem [Rolle's theorem]. Let f be continuous in $[a, b]$. If f is differentiable in (a, b) and $f(a) = f(b)$, then there is $\xi \in (a, b)$ such that $f'(\xi) = 0$. □

A3.10 Theorem [Generalization of mean-value theorem]. Let f and g be continuous functions on a closed interval $[a, b]$, and are differentiable on (a, b). If f' and g' do not simultaneously vanish in (a, b) and $g(a) \neq g(b)$, then there is $\xi \in (a, b)$ such that

$$\frac{f'(\xi)}{g'(\xi)} = \frac{f(b) - f(a)}{g(b) - g(a)}.$$

□

A3.11 Theorem [Condition for monotonicity]. A necessary and sufficient condition for a differentiable function defined on an interval I is monotone increasing (→**A2.11**) is that $f'(x) \geq 0$ on I and $f'(x) > 0$ on a dense (→**A1.19**) subset of I. □

A3.12 Counterexamples.
(i) $f(x) = x \sin(1/x)$ is continuous at $x = 0$ but not differentiable there.
(ii) $f(x) = \sum_{n=1}^{\infty} 2^{-n} |\sin(\pi n! x)|$ is continuous on $\boldsymbol{R}$, but not differentiable on $\boldsymbol{Q}$.
(iii) $f(x) = \sum_{n=1}^{\infty} 2^{-n} \cos(k^n \pi x)$ (k is an odd integer larger than 13) is continuous on $\boldsymbol{R}$, but is nowhere differentiable.

A3.13 Higher order derivatives. Suppose f is a differentiable function on an interval I. If f' is again differentiable on I, then we can define the second derivative df'/dx. If the function f is sufficiently smooth,

then we can define higher-order derivatives like the *n-th derivative*, which is denoted by $f^{(n)}(x)$, $d^n f/dx^n$, $D^n f(x)$ or $(d/dx)^n f(x)$. Arithmetic operations do not destroy higher order differentiability as **A3.5**. The composite function of n-times differentiable functions is n-times differentiable as [6].

A3.14 Leibniz' formula.

$$\begin{aligned}\frac{d^n}{dx^n}(f(x)g(x)) &= f^{(n)}(x)g(x) + \binom{n}{1} f^{(n-1)}(x)g'(x) + \cdots \\ &\quad + \binom{n}{k} f^{(n-k)}(x)g^{(k)}(x) + \cdots + f(x)g^{(n)}(x).\end{aligned}$$

A3.15 Taylor's formula, remainder. Let f be a n-times differentiable function on an interval I, and $a \in I$. Then for any $x \in I$ there is a point ξ between a and x such that

$$f(x) = f(a) + \sum_{k=1}^{n-1} \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{f^{(n)}(\xi)}{n!}(x-a)^n. \tag{40.1}$$

The last term is called the *remainder*, and is written as R_n. □
For $n = 1$ this is the mean-value theorem (→**A3.8**), and this theorem is regarded as an extension of the mean-value theorem.
The remainder can be written as follows: Let $\xi = a + \theta(x-a)$ $(0 < \theta < 1)$.
(i) Schlömilch's remainder: Choosing an integer q $(0 \le q \le n-1)$,

$$R_n = \frac{f^{(n)}(\xi)(1-\theta)^q}{(n-1)!(n-q)}(x-a)^n.$$

(ii) Cauchy's remainder. This is a special case of (i) with $q = n-1$:

$$R_n = \frac{f^{(n)}(\xi)}{(n-1)!}(1-\theta)^{n-1}(x-a)^n.$$

(iii) The remainder in (40.1) is another special case of (i) with $q = 0$, and is called Lagrange's remainder.

A3.16 Taylor's series. If f is infinite times differentiable, and $\{R_n\}$ in **A3.15** converges to zero, then f can be expanded in a *Taylor series* about a:

$$f(x) = f(a) + \sum_{k=1}^{\infty} \frac{f^{(k)}(a)}{k!}(x-a)^k.$$

A3.17 Convex and concave function. Let f be a function whose domain is I. Let $x_1, x_2 \in I$ and λ and μ be positive reals satisfying $\lambda + \mu = 1$. If

$$f(\lambda x_1 + \mu x_2) \leq \lambda f(x_1) + \mu f(x_2), \tag{40.2}$$

we say f is *convex* on I, and f is called a *convex function*. If there is no equality in (40.2), then we say f is *strictly convex*, and f is called a *strictly convex function*. If $-f$ is (strictly) convex, we say f is (strictly) *concave*, and f is called a (strictly) concave function.

A3.18 Theorem [Convexity and second derivative]. Let f be a twice differentiable function on an interval I.
(i) A necessary and sufficient condition that f is convex on I is that $f''(x) \geq 0$ for all the inner points of I.
(ii) If $f''(x) > 0$ for all the inner points of I, then f is strictly convex. □
An analogous theorem for concave functions should be self-evident. Simply switch f to $-f$.
Remark. (i) assumes that f is twice differentiable. Convex functions must be continuous, but need not even be differentiable once.

A3.19 Local maximum, minimum. Let f be a continuous function on an interval I, and a be an inner point of I. $f(a)$ is a *local maximum* (resp., *local minimum*), if for some positive number ϵ $0 < |x - a| < \epsilon$ implies $f(x) < f(a)$ (resp., $f(x) > f(a)$). These are collectively called *local extrema*.
Theorem. If f is a differentiable function on an interval I, and has a local extremum at $a \in I^\circ$,[394] then $f'(a) = 0$.□
Theorem. Let f be a function which is n-times ($n \geq 2$) differentiable and $f'(a) = f''(a) = \cdots = f^{(n-1)}(a) = 0$ at some inner point of I.
(i) If n is odd, then $f(a)$ is not an extremum of f.
(ii) If n is even, and $f^{(n)}(a) > 0$, then $f(a)$ is a local minimum of $f(x)$.
(iii) If n is even, and $f^{(n)}(a) < 0$, then $f(a)$ is a local maximum of $f(x)$.□

A3.20 Stationary value. Suppose f is n-times differentiable in an interval I, and for some inner point a of I $f'(a) = f''(a) = \cdots = f^{(n-1)}(a) = 0$ but $f^{(n)}(a) \neq 0$. If $n \geq 3$ and odd, $f(a)$ is called a *stationary value* of f, and a is called a *stationary point* of f.
Theorem. For the f in this item,
(i) If $f^{(n)}(a) > 0$, then there is a positive number ϵ such that f is strictly convex in $[a, a + \epsilon]$ and strictly concave in $[a - \epsilon, a]$.

[394] For $^\circ$ see **A1.19**.

(ii) If $f^{(n)}(a) < 0$, then there is a positive number ϵ such that f is strictly concave in $[a, a+\epsilon]$ and strictly convex in $[a-\epsilon, a]$.□

A3.21 Class C^n. Let f be a function defined on an interval I. If f is n-times differentiable and $f^{(n)}$ is continuous on I, then f is called a *function of class* C^n (or a C^n*-function*). If f is infinite-times differentiable, it is called a C^∞*-function*.
Theorem. Let f and g be C^n-functions on an interval I.
(i) Arithmetic operations do not destroy C^n-functions.
(ii) $g \circ f$ is again a C^n-function.
(iii) If for all $x \in I$ $f'(x) \neq 0$, and f is monotone, then its inverse function f^{-1} is a monotone C^n-function.□
These statements hold for C^∞ functions as well.

A3.22 Class C^ω. Let f be a C^∞-function in an open interval I. If f can be Taylor-expanded (→**A3.16**) in the neighborhood of each $a \in I$, then f is said to be *real analytic* in I and is called a *real analytic function* or a C^ω-function.
Warning. A C^∞-function need not be a real analytic function. A typical example is

$$\begin{aligned} \psi(x) &= 0 \text{ for } x \leq 0, \\ &= e^{-1/x} \text{ for } x > 0. \end{aligned}$$

Its derivatives at $x = 0$ all vanish, so that Taylor series formally constructed becomes identically zero, but this contradicts the fact that $\psi(x) > 0$ for positive x. Hence, this function is not real analytic.
This is an important function to be used to 'mollify' functions through convolution.

A3.23 Theorem [Existence of mollifier]. Let a and b be two arbitrary points $(a < b)$ in $\boldsymbol{R}$. There is a C^∞-function $\rho(x)$ on $\boldsymbol{R}$ such that $\rho(x) = 0$ for $x \leq a$, $\rho(x) = 1$ for $x \geq b$ and $0 \leq \rho(x) \leq 1$.□
Corollary. Let f and g be C^∞-functions on $\boldsymbol{R}$, and a and b are the same as in the theorem. There is a C^∞-function h such that $h(x) = f(x)$ for $x \leq a$, $h(x) = g(x)$ for $x \geq b$ (and h interpolates f and g between a and b). □
Thus C^∞-functions can be deformed freely. In contradistinction, C^ω-functions cannot be deformed freely as shown in the following

A3.24 Theorem [Identity theorem]. Let f and g be C^ω-functions defined on an open set I. If f and g coincide in some neighborhood of a point $a \in I$, then f and g are identical on I.□

A3.25 Complex analysis. Real analytic functions are best under-

stood as special complex-valued functions defined on the complex plain. "The shortest path between two truths in the real domain passes through the complex domain." (J. Hadamard). H. A. Priestley, *Introduction to Complex Analysis* (Oxford UP, 1990, revised edition) is a convenient introduction to the topic. See also my notes for Physics 413, which is much more complete than the book with a sizable chapter on conformal mapping and its application to boundary value problems.

41 Integration

A4.1 Definite integral (Riemann integral). Let f be a continuous function defined on a closed interval $I = [a, b]$. Let $a = x_0 < x_1 < x_2 < \cdots < x_k < \cdots < x_{m-1} < x_m = b$, and partition $[a, b]$ into m intervals $[x_{k-1}, x_k]$ $(k = 1, 2, \cdots, m)$. The partion determined by the set $\Delta \equiv \{x_0, x_1, \cdots, x_m\}$ is called the *partition* Δ. Let the maximum of $|x_k - x_{k-1}|$ $(k = 1, 2, \cdots, m)$ be $\delta(\Delta)$. The following limit exists (remember that f is assumed to be continuous) and called the *definite integral* of f on $[a, b]$:

$$\int_a^b f(x)dx \equiv \lim_{\delta(\Delta)\to 0} \sum_k f(\xi_k)(x_k - x_{k-1}),$$

where $\xi_k \in [x_{k-1}, x_k]$. The limit does not depend on the choice of ξ_k. f is called the *integrand*, x the *integration variable*, and b (resp., a) the *upper limit* (resp., *lower limit*) of integration. The integration variable x is a dummy variable in the sense that we may freely replace it with any letter.
We define for $b > a$ $\int_b^a f(x)dx \equiv -\int_a^b f(x)dx$, and $\int_a^a f(x)dx = 0$.
Sometimes, the definite integral is written as

$$\int_a^b dx\, f(x).$$

This notation clearly shows that integration is an operation applied to f.

A4.2 Riemann-integrability. Integration can be defined even if f is not continuous. Let f be a bounded function on $[a, b]$. For the partition Δ in **A4.1**, define

$$S_\Delta \equiv \sum_{k=1}^m M_k(x_k - x_{k-1}), \quad s_\Delta \equiv \sum_{k=1}^m m_k(x_k - x_{k-1}),$$

where M_k (resp., m_k) is the maximum (resp., minimum) value of f in $[x_{k-1}, x_k]$. Let $S \equiv \sup_\Delta S_\Delta$ and $s \equiv \inf_\Delta s_\Delta$ (Here the supremum (infimum) is looked for over all the possible finite partitions of $[a, b]$. If $S = s$, we say f is *Riemann integrable* on $[a, b]$. In this case, $S = s$ is the definition of $\int_a^b f(x)dx$. Even if f has finitely many discontinuous points in I, f is Riemann-integrable.

A4.3 Basic properties of definite integral. Let f and g be Riemann-integrable on the closed interval $[a, b]$.
(i) For $c \in (a, b)$

$$\int_a^b f(x)dx = \int_a^c f(x)dx + \int_c^b f(x)dx.$$

(ii) For arbitrary constant c_1 and c_2,

$$\int_a^b [c_1 f(x) + c_2 g(x)]dx = c_1 \int_a^b f(x)dx + c_2 \int_a^b g(x)dx.$$

(iii) If $f \geq 0$ on $[a, b]$, then $\int_a^b f(x)dx \geq 0$. If, furthermore, f is continuous and is not identically zero, then the integral is strictly positive.
(iv)

$$\left| \int_a^b f(x)dx \right| \leq \int_a^b |f(x)|dx.$$

A4.4 Theorem [Mean value theorem].
(1) If f is a continuous function defined on a closed interval $[a, b]$, there exists a point $\xi \in (a, b)$ such that

$$\frac{1}{b-a} \int_a^b f(x)dx = f(\xi).$$

(2) If f and g are continuous on the closed interval [a,b], and if $g > 0$ on the open interval (a, b), then there exists $\xi \in (a, b)$ such that

$$\int_a^b f(x)g(x)dx = f(\xi) \int_a^b g(x)dx.$$

□

A4.5 Fundamental theorem of calculus, primitive function, indefinite integral. If f is integrable on a closed interval $I = [a, b]$, then for $x \in [a, b]$, we can define the definite integral of f on $[a, x]$:

$$F(x) = \int_a^x f(t)dt$$

which is a function of x on I.
Theorem [**Fundamental theorem of calculus**].

$$\int_a^b f(x) = F(b) - F(a)$$

or $F'(x) = f(x)$.□
Any function such that $F'(x) = f(x)$ on I is called a *primitive function* of f. A primitive function for f, if any, is not unique; it is unique up to an additive constant. Thus any primitive function of f, if any, can be written as

$$F(x) = \int_a^x f(t)dx + C,$$

where C is called the *integration constant*.
The *indefinite integral* of f is defined as a primitive function of f, and is denoted by

$$\int f(x)dx.$$

A4.6 Integration by parts. Let f and g be C^1-functions (→**A3.21**) on an interval I. Then

$$\int_a^b f(x)g'(x)dx = f(x)g(x)|_a^b - \int_a^b f'(x)g(x)dx,$$

where $h(x)|_a^b \equiv h(b) - h(a)$.

A4.7 Improper integral. When

$$\lim_{c\to b} \int_a^c f(x)dx$$

exists, we write this $\int_a^b f(x)dx$ even if f is not integrable on $[a, b)$ in the sense of **A4.2**, and call it an *improper integral*. b may be a discontinuous point of f or $\pm\infty$. It is easy to construct the Cauchy convergence criterion (→**A1.3**) for improper integrals.
Improper integrals satisfy **A4.3** (i) and (ii), and if the improper integral of $|f|$ is definable (we say f is *absolutely integrable*; absolutely integrable functions are integrable.), (iii) holds as well.
Also the fundamental theorem of calculus (→**A4.5**), and the mean value theorem (→**A4.4**) are valid.

A4.8 Change of integration variables. Let f be a continuous function on an interval $I = [a, b]$, $\varphi(t)$ be a continuous function defined on

an interval J whose range is in I. $\alpha, \beta \in J$ ($\alpha \neq \beta$), $a = \varphi(\alpha)$ and $b = \varphi(\beta)$. Then

$$\int_a^b f(x)dx = \int_\alpha^\beta f(\varphi(t))\varphi'(t)dt.$$

If f is an even function (→[AII13]), then

$$\int_a^b f(x)dx = \int_{-b}^{-a} f(x)dx.$$

If f is an odd function (→AII13]), then

$$\int_a^b f(x)dx = -\int_{-b}^{-a} f(x)dx.$$

42 Infinite Series

A5.1 Changing the order of summation in infinite series. Absolutely convergent series and conditionally convergent series (→**A1.12**, **A1.14**) have diametrically different properties with respect to the rearrangement of the terms in the summation:
Theorem.
(i) The sum of an absolutely convergent series does not depend on the order of summation of the terms in the series.
(ii) If a series $\sum_{n=1}^\infty a_n$ is conditionally convergent, then for any given real ξ there is a reordering of the series $\{a_{\gamma(n)}\}$ such that

$$\sum_{n=1}^\infty a_{\gamma(n)} = \xi.$$

There is also a reordering to make the series divergent to $\pm\infty$. □

A5.2 Product of two series. The product of two absolutely convergent series (→**A1.12**) can be computed via distributive law: Let $s = \sum a_n$ and $t = \sum b_n$, and both are absolutely convergent. Then

$$st = a_1b_1 + a_2b_1 + a_1b_2 + a_3b_1 + a_2b_2 + a_1b_3 + \cdots.$$

This is not necessarily true for conditionally convergent series, e.g., consider $a_n = b_n = (-1)^n/\sqrt{n}$.

A5.3 Theorem [Comparison theorem I. comparison with improper integral]. Let $r(x) > 0$ be a continuous monotone decreasing function ($\rightarrow$**A2.11**) on $[k, +\infty)$ with k being a positive integer such that $\lim_{x\to\infty} r(x) = 0$. Let $r_n \equiv r(n)$. $\sum_{n=k}^{\infty} r_n$ converges (resp., diverges), if $\int_k^{\infty} r(x)dx$ converges (resp., diverges). □
Examples:
(i) $\sum_{n=1}^{\infty} n^{-s}$ $(s > 0)$ converges for $s > 1$ and diverges for $s \geq 1$.
(ii) $\sum_{n=2}^{\infty}\{1/[n(\log n)^s]\}$ $(s > 0)$ converges for $s > 1$ and diverges for $s \geq 1$.
(iii) $\sum_{n=3}^{\infty}\{1/[n \log n(\log\log n)^s]\}$ $(s > 0)$ converges for $s > 1$ and diverges for $s \geq 1$.

A5.4 Theorem [Comparison theorem II. comparison of series]. Let $\sum_{n=1}^{\infty} u_n$ and $\sum_{n=1}^{\infty} v_n$ be positive term series, and there is a positive integer n_0 such that for $n > n_0$

$$u_n/u_{n+1} \geq v_n/v_{n+1}.$$

Then
(i) If $\sum v_n$ converges, then so is $\sum u_n$.
(ii) If $\sum u_n$ diverges, then so is $\sum v_n$. □
From this theorem, we get useful convergence criteria:

A5.5 Cauchy's convergence criterion. Let $\sum a_n$ be a positive term series. Suppose the limit $\rho = \lim_{n\to\infty}(a_n/a_{n+1})$ exists. If $\rho < 1$, then the series converges, and if $\rho \geq 1$, the series diverges.

A5.6 Gauss' convergence criterion. For a positive term series $\sum a_n$ with

$$\frac{a_n}{a_{n+1}} = 1 + \frac{\sigma}{n} + O\left[\frac{1}{n^{1+\delta}}\right],$$

where δ is positive.[395] Then the series converges if $\sigma > 1$, and diverges if $\sigma \leq 1$.

A5.7 Abel's formula. Let the partial sums $s_m = \sum_{n=1}^{m} a_n$ and $t_m = \sum_{n=1}^{m} b_n$. Then

$$\sum_{n=k}^{m} a_n t_n = [s_m t_m - s_{k-1}t_k] - \sum_{n=k}^{m} s_n b_{n+1}.$$

This is a discrete analogue of integration by parts ($\rightarrow$**A4.6**).
This transformation implies the following criteria:
(i) If $\sum_{n=1}^{\infty} a_n$ converges and $\sum_{n=2}^{\infty}(t_n - t_{n-1})$ converges absolutely, then

[395] For the symbol O see **A1.4**.

$\sum_{n=1}^{\infty} a_n t_n$ converges.
(ii) The sequence $\{s_n\}$ is bounded and $\{t_n\}$ is a monotone decreasing positive sequence converging to zero, then $\sum a_n t_n$ converges.
For example, (ii) implies that $\sum t_n \cos(nx)$ and $\sum t_n \sin(nx)$ converge, if $\{t_n\}$ is a monotone decreasing positive sequence converging to zero. This is an extension of [AI14] on alternating series.

A5.8 Function sequence, convergence. A sequence of functions $\{f_n(x)\}$ is called a *function sequence* defined on I, if the domains of all the functions in the sequence are identically I. For a fixed $x = \xi \in I$, if the sequence $\{f_n(\xi)\}$ converges, we say the function sequence converges at $x = \xi$. If the function sequence converges at every point of I, we say that the sequence converges on I. The limit for each x may be written as $f(x)$, which is regarded as the limit function of the function sequence, and we say the function sequence $\{f_n(x)\}$ converges to $f(x)$. More formally, we say that the function sequence $\{f_n(x)\}$ converges to $f(x)$ if for each $x \in I$ and for any positive number ϵ, there is a positive integer $n_0(\epsilon, x)$ such that

$$n > n_0(\epsilon, x) \Rightarrow |f_n(x) - f(x)| < \epsilon. \tag{42.1}$$

A5.9 Uniform convergence. Let $\{f_n(x)\}$ be a function sequence defined on an interval I. If in (42.1) $n_0(\epsilon, x)$ is independent of $x \in I$, we say the function sequence $\{f_n\}$ is *uniformly convergent* to f on I. That $\{f_n\}$ is uniformly convergent to f on I is equivalent to

$$\lim_{n\to\infty} \sup_{x\in I} |f_n(x) - f(x)| = 0.$$

A5.10 Theorem [Cauchy's criterion for uniform convergence]. Let $\{f_n(x)\}$ be a function sequence defined on an interval I. A necessary and sufficient condition for the sequence to be uniformly convergent is that there is a positive integer $n_0(\epsilon)$ such that for any $x \in I$

$$n > n_0(\epsilon), \;\; m > n_0(\epsilon) \Rightarrow |f_n(x) - f_m(x)| < \epsilon.$$

□

A5.11 Function series, convergence, uniform convergence, maximal convergence. $\sum_{n=1}^{\infty} f_n(x)$ is called a function series. Let its partial sum be $s_m(x) \equiv \sum_{n=1}^{m} f_n(x)$. If the function sequence $\{s_n(x)\}$ (uniformly) converges to $s(x)$, we say the series $\sum_{n=1}^{\infty} f_n(x)$ (uniformly) converges to $s(x)$, which is called the *sum* of the series. If $\sum_{n=1}^{\infty} f_n(x)$ is uniformly and absolutely convergent, we say the series is *maximally convergent*.

A5.12 Theorem [Uniform convergence preserves continuity]. Let $\{f_n(x)\}$ be a function sequence of continuous functions defined on an interval I.
(i) If the sequence uniformly converges to f on I, then f is continuous in I.
(ii) If the series $\sum_{n=1}^{\infty} f_n(x)$ converges uniformly, then its sum is a continuous function on I.□

A5.13 Theorem [Dini's theorem]. Let $\{f_n(x)\}$ be a sequence of continuous functions defined on the closed interval $[a, b]$. Suppose the sequence is monotonically decreasing: for any $x \in [a, b]$ $f_1(x) \geq f_2(x) \geq \cdots \geq f_n(x) \geq \cdots$. If the sequence $\{f_n(x)\}$ converges on $[a, b]$ to a continuous function $f(x)$, then the sequence uniformly converges to f on $[a, b]$. □.
A5.14 Theorem [Comparison theorem]. Let $\sum_{n=1}^{\infty} a_n$ be a convergent positive term series. For a sequence of $\{f_n(x)\}$, suppose $|f_n(x)| \leq a_n$ for all n on an interval I. Then the infinite sum $\sum_{n=1}^{\infty} f_n(x)$ is maximally convergent.□

A5.15 Theorem [Exchange of limit and integration]. Let $\{f_n(x)\}$ be a sequence of continuous functions defined on $[a, b]$, uniformly convergent to $f(x)$ there. Then

$$\int_a^b f(x)dx = \lim_{n\to\infty} \int_a^b f_n(x)dx.$$

□
A more general theorem (Arzelá's theorem) will be given in **A5.17**.
The theorem implies that a uniformly convergent series of continuous functions is termwisely integrable:

$$\int_c^x \sum_{n=1}^{\infty} f_n(x)dx = \sum_{n=1}^{\infty} \int_c^x f_n(x)dx.$$

A5.16 Theorem [Exchange of limit and differentiation]. Let $f_n(x)$ be a C^1-function (→**A3.21**). If $\sum_{n=1}^{\infty} f_n(x)$ converges on I, and $\sum_{n=1}^{\infty} f_n'(x)$ converges uniformly on I, then the sum of the series is differentiable and

$$\frac{d}{dx} \sum_{n=1}^{\infty} f_n(x) = \sum_{n=1}^{\infty} f_n'(x)$$

□

A5.17 Theorem [Arzelá's theorem]. Let $f_n(x)$ be a continuous

function defined on a closed set [a,b] (actually this need not be a closed interval) and uniformly bounded, i.e., there is a positive number M independent of n such that $|f_n(x)| < M$ on the interval. If the function sequence $\{f_n(x)\}$ converges to a continuous function $f(x)$ on [a,b], then

$$\int_a^b f(x)dx = \lim_{n\to\infty} \int_a^b f_n(x)dx.$$

□

A5.18 Majorant. For a function sequence $\{f_n(x)\}$ defined on an interval I, a function $\sigma(x)$ such that $|f_n(x)| < \sigma(x)$ is called a *majorant* of the sequence.
Theorem. If a majorant $\sigma(x)$ is integrable on the interval, then the order of integration and $\lim_{n\to\infty}$ can be exchanged.□

A5.19 Convergence radius of power series. For a power series $\sum_{n=0}^{\infty} a_n x^n$,

$$r \equiv \frac{1}{\limsup_{n\to\infty} |a_n|^{1/n}}$$

is called the *convergence radius* of the power series (the reason for the name is seen from the following theorem **A5.20**. The formula is called the *Cauchy-Hadamard formula*). Here, if the lim sup diverges to $+\infty$, then we define $r = 0$, and if lim sup converges to zero, then we define $r = +\infty$.

A5.20 Theorem [Power series is termwisely differentiable]. The power series $\sum_{n=0}^{\infty} a_n x^n$ is absolutely convergent for $|x| < r$, and is divergent for $|x| > r$, where r is the convergence radius (→**A5.19**). For any $0 < \rho < r$, the series is uniformly convergent (→**A5.11**) in $[-\rho, \rho]$ to a continuous function (*cf.* **A5.12**), so that the series is termwisely differentiable there. □

A5.21 Theorem [Power series defines a real analytic function]. The power series $\sum_{n=0}^{\infty} a_n x^n$ whose convergence radius is r uniquely determines a C^ω-function (→**A3.22**) f in the open interval $(-r, r)$. Actually, the power series is the Taylor series (→**A3.16**) for f. □

A5.22 Theorem [Continuity at $x = r$ or $-r$]. Let r be the convergence radius of the power series $\sum_{n=0}^{\infty} a_n x^n = f(x)$. If $\sum_{n=0}^{\infty} a_n r^n$ is convergent, then $f(x)$ is continuous in $(-r, r]$. If $\sum_{n=0}^{\infty} a_n (-r)^n$ is convergent, then $f(x)$ is continuous in $[-r, r)$. □

A5.23 Infinite product. For a sequence $\{a_n\}$ $(a_n \neq 0)$ $a_1 a_2 \cdots a_n \cdots$ is called an *infinite product*, and is denoted by $\prod_{n=1}^{\infty} a_n$. $p_n = a_1 a_2 \cdots a_n$

is called the *partial product*.

A5.24 Convergence of infinite product. Let $\prod_{n=1}^{\infty} a_n$ be an infinite product and its partial product sequence be $\{p_n\}$. If this sequence converges, and $p = \lim_{n\to\infty} p_n$ is not zero, we say the infinite product *converges* to p: $p = \prod_{n=1}^{\infty} a_n$. Else, we say the infinite product is *divergent*.

A5.25 Theorem [Convergence condition for infinite product].
(i) A necessary and sufficient condition for the infinite product $\prod_{n=1}^{\infty}(1+u_n)$ $(u_n > -1)$ to be convergent is that the infinite series $\sum_{n=1}^{\infty} \log(1+u_n)$ converges.
(ii) If $\sum_{n=1}^{\infty} u_n$ $(u_n > -1)$ converge absolutely, then $\prod_{n=1}^{\infty}(1+u_n)$ converges. (In this case we say the infinite product converges absolutely, and the product does not depend on the order of its terms.)
(iii) If $\sum u_n$ $(u_n > -1)$ and $\sum u_n^2$ both converges, then the infinite product $\prod_{n=1}^{\infty}(1+u_n)$ converges. □

A5.26 Conditional convergence of infinite product. If an infinite product $\prod_{n=1}^{\infty}(1+u_n)$ converges but does not converge absolutely (→**A5.25**(ii)), we can reorder the product to converge to any positive number. □
This is quite parallel to a similar theorem for conditionally convergent series (→A5.1(ii)).

43 Function of Two Variables

Since real valued-functions of two variables illustrate complications due to the existence of many independent variables, in this rudimentary part, we discuss only a function defined on a point set D in $\boldsymbol{R}^2$.

A6.1 Rudiments of topology.
(i) If an open set $U \in \boldsymbol{R}^2$ is not a join of two open sets, U is said to be *connected*.
(ii) **Theorem**. A necessary and sufficient condition for an open set U to be connected is that any points $P, Q \in U$ can be connected by a piecewise straight curve in U. □
(iii) A connected open set is called a *region*, and its closure (→**A1.19**) is called a *closed region*.

(iv) Distance $\rho(x, y)$ of two points x and y in $\boldsymbol{R}^2$ is defined as

$$\rho(x, y) = |x - y| = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2},$$

where x (or y) is identified with its coordinate expression, say, (x_1, x_2).

A6.2 Function, domain, range. Let D be a point set in $\boldsymbol{R}^2$. A rule which defines a correspondence of each $x \in D$ to some real is called a function from $D \subset \boldsymbol{R}^2$ to $\boldsymbol{R}$. D is called its *domain* and $f(D) \subset \boldsymbol{R}$ is called its *range*.[396] We write $f : D \to \boldsymbol{R}$.

A6.3 Limit. Let D be a point set in $\boldsymbol{R}^2$. For $f : D \to \boldsymbol{R}$, we say $\lim_{P \to A} f(P) = \alpha \in \boldsymbol{R}$, if for any positive number ϵ there is a positive number $\delta(\epsilon)$ such that

$$\rho(P, A) < \delta(\epsilon) \Rightarrow |f(P) - \alpha| < \epsilon.$$

Notice that the limit should not depend on how P approaches A.
It is easy to write down Cauchy's criterion for the convergence (*cf.* **A1.3**).

A6.4 Continuity. Let D be a point set in $\boldsymbol{R}^2$. A function $f : D \to \boldsymbol{R}$ is continuous at an accumulation point ($\to$**A1.19**) $P \in D$, if $\lim_{Q \to P} f(Q) = f(P)$. (To discuss the continuity on the point of D which are not accumulating points of D is uninteresting.)
Uniform continuity can also be defined quite analogously as in the one-variable function case (*cf.* **A2.8**).

A6.5 Theorem [**Maximum value theorem**]. A real-valued continuous function defined on a bounded closed set $D \subset \boldsymbol{R}^2$ has a maximum and minimum values on D. The range of f is a closed interval. □
(*cf.* [AII9]).

A6.6 Partial differentiation. Let $f(x, y)$ be a real-valued function defined in a region $D \subset \boldsymbol{R}^2$, and $(a, b) \in D$. If $f(x, b)$ is differentiable at a with respect to x, we say that $f(x, y)$ is *partially differentiable* with respect to x at (a, b), and the derivative is denoted by $f_x(a, b)$. More generally, if f is partial differentiable in D with respect to x, we may define $f_x(x, y)$:

$$f_x(x, y) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h}.$$

If we write $z = f(x, y)$, $f_x(x, y)$ is written as $\partial z / \partial x$. $f_x(x, y)$ is called the *partial derivative* of f with respect to x. We say that we *partial-differentiate* f with respect to x to obtain $f_x(x, y)$. Similarly, we can

[396] The set $\{f(x) : x \in D\}$ is often written as $f(D)$.

define the partial derivative with respect to y of f. Analogously, we can define higher-order (mixed) partial derivatives like f_{xxy}.
Warning. Even if f_x and f_y exists at a point, f need not be continuous at the point. □
This implies that the 'differentiability' of f must be defined separately from its partial differentiability.

A6.7 Differentiability, total differential. Let $f(x, y)$ be a real-valued function defined in a region $D \subset \boldsymbol{R}^2$, and $(a, b) \in D$. We say f is *differentiable* at (a, b) if there is constants A and B such that

$$f(x, y) = f(a, b) + A(x - a) + B(y - b) + o[\sqrt{(x - a)^2 + (y - b)^2}].$$

Theorem. If f above is differentiable at (a, b), then f is continuous there, and is partially differentiable with respect to x and y with $A = f_x(a, b)$, $B = f_y(a, b)$. □.
$dz = f_x dx + f_y dy$ is called the *total differential* of f.
We say that f is differentiable in D, if f is differentiable at every point in D.
Intuitively, if a local linear approximation is reliable, we say the function is differentiable.
A6.8 Theorem [Partial differentiability and differentiability]. Let f be a function defined in a region $D \subset \boldsymbol{R}^2$. If f_x and f_y exist and are continuous in D, then f is differentiable in D. □

A6.9 Theorem [Order of partial differentiation]. Let f be a function defined in a region $D \subset \boldsymbol{R}^2$. If partial derivatives f_x, f_y, f_{xy} and f_{yx} exist and if f_{xy} and f_{yx} are continuous, then $f_{xy} = f_{yx}$. □

A6.10 Theorem [Young's theorem]. Let f be a function defined in a region $D \subset \boldsymbol{R}^2$. If f_x and f_y exist and f is differentiable, then $f_{xy} = f_{yx}$. □

A6.11 Theorem [Schwarz' theorem]. Let f be a function defined in a region $D \subset \boldsymbol{R}^2$. If partial derivatives f_x, f_y and f_{xy} exist and if f_{xy} is continuous, then f_{yx} exists and $f_{xy} = f_{yx}$. □

A6.12 $f_{xy} = f_{yx}$ is not always correct. Let $f(x, y) = xy(x^2 - y^2)/(x^2 + y^2)$ except for $(0, 0)$, where f is defined to be 0. Then $f_{xy}(0, 0) \neq f_{yx}(0, 0)$; the left-hand-side is -1, and the right-hand-side is 1.

A6.13 C^n-class function. If f has all the partial derivatives of order n, which are all continuous, we say that f is a *C^n-function*. If derivatives of any order exists, we say that the function is a C^∞-function.

A6.14 Composite function. Let $\varphi(t)$ and $\psi(t)$ be continuous functions defined on an interval I such that $(\varphi(t), \psi(t)) \in D$ for all $t \in I$. If $f(x, y)$ is a continuous function defined on D, then $f(\varphi(t), \psi(t))$ is continuous.
If $\varphi(t)$ and $\psi(t)$ are differentiable with respect to t, and $f(x, y)$ is differentiable in D, then $f(\varphi(t), \psi(t))$ is differentiable with respect to t, and

$$\frac{d}{dt} f(\varphi(t), \psi(t)) = f_x(\varphi(t), \psi(t))\varphi'(t) + f_y(\varphi(t), \psi(t))\psi'(t).$$

If $\varphi(t)$ and $\psi(t)$ are C^n-functions of t, and $f(x, y)$ is C^n in D, then $f(\varphi(t), \psi(t))$ is again C^n.
These propositions hold even if we replace the function of t with functions of s and t. For example, If $\varphi(s, t)$ and $\psi(s, t)$ are C^n-functions of s and t in a domain D_1, $(\varphi(s, t), \psi(t, s)) \in D$, and $f(x, y)$ is C^n in D, then $f(\varphi(s, t), \psi(s, t))$ is again C^n in D_1.

A6.15 Taylor's formula. Let $f(x, y)$ be a C^n-class function defined on a region D, $(a, b) \in D$, and the line segment AP with $P = (a+h, b+k)$ be in D. Then

$$f(a + f, b + k) = f(a, b) + \sum_{m=1}^{n-1} \frac{1}{m!} \left(f\frac{\partial}{\partial x} + k\frac{\partial}{\partial y} \right)^m f(a, b) + R_n$$

with

$$R_n \equiv \frac{1}{n!} \left(f\frac{\partial}{\partial x} + k\frac{\partial}{\partial y} \right)^n f(a + \theta h, b + \theta k)$$

for some $\theta \in (0, 1)$. R_n is called the residue.
If f is a C^∞-function ($\rightarrow$[13]) in a region D and if in some subregion D_A of D $\lim_{n\to\infty} R_n = 0$, then we say f is *Taylor-expandable* in D_A:

$$f(x, y) = f(a, b) = \sum_{n=1}^{\infty} \sum_{p+q=n} \frac{\partial^{p+q} f(a, b)}{\partial x^p \partial y^q} (x - a)^p (y - b)^q.$$

If f is Taylor-expandable, we say f is a real analytic function (C^ω-function) of two variables.
This is a double series, so we need some general theory of double series and double sequences.

A6.16 Limit of double sequence. Let $\{a_{nm}\}$ be a double sequence. If for any positive ϵ, there is a positive integer $N(\epsilon)$ such that

$$m > N(\epsilon),\ n > N(\epsilon) \Rightarrow |a_{mn} - \alpha| < \epsilon,$$

then we say the double sequence converges to α, and write $\lim_{m,n\to\infty} a_{mn} = \alpha$. It is easy to state Cauchy's convergence criterion ($\to$**A1.3**) for a double series.

A6.17 Warning. $\lim_{m,n\to\infty}$ and $\lim_{m\to\infty}\lim_{n\to\infty}$ or $\lim_{m\to\infty}\lim_{n\to\infty}$ are distinct. For example, if $a_{mn} = 2mn/(m^2+n^2)$, $\lim_{m\to\infty}\lim_{n\to\infty} a_{mn} = 0$ and $\lim_{n\to\infty}\lim_{m\to\infty} a_{mn} = 0$, but $\lim_{m,n\to\infty} a_{mn}$ does not exist. If $a_{mn} = (-1)^n/m + (-1)^m/n$, then $\lim_{m,n\to\infty} a_{mn} = 0$ but the other limits do not exist.

A6.18 Theorem [**Exchange of limits**]. Suppose $\lim_{m,n\to\infty} a_{mn} = \alpha$ exists. If for each n $\lim_{m\to\infty} a_{mn}$ exists, then $\lim_{n\to\infty}\lim_{m\to\infty} a_{mn} = \alpha$. If for each m $\lim_{n\to\infty} a_{mn}$ exists, then $\lim_{m\to\infty}\lim_{n\to\infty} a_{mn} = \alpha$. □

A6.19 Double series, convergence. For a double sequence $\{a_{mn}\}$, $\sum_{m,n=1}^{\infty} a_{mn}$ is called a *double series*. We say that the double series *converges* if the double sequence $\{s_{mn}\}$ of its partial sums $s_{mn} = \sum_{p=1}^{m}\sum_{q=1}^{n} a_{pq}$ converges. Its absolute convergence can also be defined analogously as in the ordinary series case ($\to$**A1.12**).
Theorem. If a double sequence $\sum_{m,n=1}^{\infty} a_{mn}$ converges absolutely, then $\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} a_{mn} = \sum_{m,n=1}^{\infty} a_{mn}$. □

A6.20 Power series of two variables. The set G such that $\sum_{m,n=0}^{\infty} a_{mn}x^m y^n$ for $\forall(x,y) \in G$ is absolutely convergent is called the convergence domain of the double power series.
Theorem. If for $(\xi,\eta) \neq (0,0)$ the double series $\sum a_{mn}\xi^m\eta^n$ is bounded, then for $|x| < |\xi|$ and $|y| < |\eta|$ the double power series $\sum_{m,n=0}^{\infty} a_{mn}x_m y_n$ is absolutely convergent.□

A6.21 Exchange of order of limits, uniform convergence. If for any positive ϵ there is $N(\epsilon)$ independent of m such that

$$n > N(\epsilon) \Rightarrow |a_{mn} - \alpha_m| < \epsilon,$$

we say $\{a_{mn}\}$ converges to α_m *uniformly* with respect to m.
Theorem. If $\{a_{mn}\}$ converges to α_m uniformly with respect to m in the $n \to \infty$ limit, and if α_m converges to α in the $m \to \infty$ limit, then $\lim_{m,n\to\infty} a_{mn} = \alpha$. □
Theorem. If $\lim_{n\to\infty}\lim_{m\to\infty} a_{mn}$ exists, $\{a_{mn}\}$ converges to α_m uniformly with respect to m in the $n \to \infty$ limit, and if α_m converges to α in the $m \to \infty$ limit, then $\lim_{m\to\infty}\lim_{n\to\infty} a_{mn} = \lim_{n\to\infty}\lim_{m\to\infty} a_{mn} = \alpha$. □
In contrast to **A6.18** here the existence of $\lim_{m,n\to\infty} a_{mn}$ is not assumed.

A6.22 Counterexample.
(i) For $a_{mn} = (-1)^n m/(m+n)$, $\lim_{m\to\infty} \lim_{n\to\infty} a_{mn} = 0$, $\lim_{n\to\infty} \lim_{m\to\infty} a_{mn}$ does not exist.
(ii) For $a_{mn} = m/(m+n)$ both limits exist but not identical.

A6.23 Theorem [Differentiation and integration within integration]. Let $f(x,y)$ be a bounded function defined on a rectangle $K = \{(x,y)|x \in [a,b], y \in [c,d]\}$. Assume that f is continuous as a function of x (resp., y) for each y (resp., x). Then
(i) $\int_a^b dx f(x,y)$ is a continuous function of y in $[c,d]$.
(ii) If $f(x,y)$ is partially differentiable with respect to y, and if $f_y(x,y)$ is bounded on K, and continuous as a function of x for each y, then

$$\frac{d}{dy}\int_a^b dx f(x,y) = \int_a^b dx \frac{\partial}{\partial y} f(x,y).$$

(iii)

$$\frac{d}{du}\int_a^u dx f(x,y) = f(u,y).$$

(iv)

$$\int_c^d dy \int_a^b dx f(x,y) = \int_a^b dx \int_c^d dy f(x,y).$$

□

A6.24 Theorem [Differentiation and integration within improper integration]. Let $f(x,y)$ be a bounded function defined on a rectangle $K = \{(x,y)|x > a, y \in [c,d]\}$. Assume that f is continuous as a function of x (resp., y) for each y (resp., x). Assume, furthermore, that there is a nonnegative continuous function $\sigma(x)$ such that $|f(x,y)| \leq \sigma(x)$ and $\int_a^{+\infty} dx \sigma(x) < +\infty$. Then
(i) $\int_a^{+\infty} dx f(x,y)$ is a continuous function of y in $[c,d]$.
(ii) If $f(x,y)$ is partially differentiable with respect to y and if there is a nonnegative continuous function $\sigma(x)$ such that $|f_y(x,y)| \leq \sigma_1(x)$ and $\int_a^{+\infty} dx \sigma_1(x) < +\infty$, then

$$\frac{d}{dy}\int_a^{+\infty} dx f(x,y) = \int_a^{+\infty} dx \frac{\partial}{\partial y} f(x,y).$$

(iii)

$$\int_c^d dy \int_a^{+\infty} dx f(x,y) = \int_a^{+\infty} dx \int_c^d dy f(x,y).$$

□

44 Fourier Series and Fourier Transform

In this section all the integrals are Riemann integrals [AIV1]. Thus integrable or absolutely integrable means Riemann-integrable and absolutely Riemann integrable.

A7.1 Fourier series.{Fourier series Let f be a function on $\boldsymbol{R}$ with period 2π.[397] Assume that the following integrals exist[398]

$$a_n = \frac{1}{\pi}\int_0^{2\pi} dx f(x)\cos nx \quad \text{for } n = 0, 1, 2, \cdots,$$

$$b_n = \frac{1}{\pi}\int_0^{2\pi} dx f(x)\sin nx \quad \text{for } n = 1, 2, 3, \cdots.$$

Then

$$S[f] = \frac{1}{2}a_0 + \sum_{n+1}^{\infty}(a_n \cos nx + b_n \sin nx)$$

is called the *Fourier series* of f. To construct $S[f]$ is said to *Fourier-expand* f.
Notice that the Fourier series converges uniformly ($\rightarrow$[AV11]) if $\sum_{n=0}^{\infty}|a_n|$ and $\sum_{n=0}^{\infty}|b_n|$ both converge.

A7.2 Theorem. Let f be a 2π periodic function which has at most finitely many discontinuities, and is absolutely integrable on $[0, 2\pi]$. If $S[f]$ converges uniformly, then $S[f](x_0)$ converges to $f(x_0)$ if f is continuous at x_0. Specifically, if f is 2π-periodic continuous function, then $S[f] = f$.□
This theorem uses the property of the Fourier series (its uniform convergence), so it is not very satisfactory. **A7.8** below tells us that we cannot remove of this extra condition from this theorem.

A7.3 Complex Fourier series. Let f be a function on $\boldsymbol{R}$ with period 2π. Assume that the following integrals exist

$$c_n = \frac{1}{2\pi}\int_0^{2\pi} dx f(x)e^{-ikx} \quad \text{for } k = \cdots, -2, -1, 0, 1, 2, \cdots.$$

Then

$$S[f] \rightleftharpoons \sum_{k=-\infty}^{\infty} c_n e^{ikx}$$

[397] That is, $f(x + 2\pi) = f(x)$ for any $x \in \boldsymbol{R}$.
[398] The integration range can be $[-\pi, \pi]$.

is called the *complex Fourier series* of f.
Needless to say, a theorem corresponding to **A7.2** holds.

A7.4 Theorem [Bessel's inequality]. If f is 2π-periodic and square integrable on $[0, 2\pi]$, then

$$2\pi \sum_{k=-\infty}^{\infty} |c_k|^2 \leq \int_{-\pi}^{\pi} dx |f(x)|^2.$$

□

A7.5 Theorem [Parseval's equality]. If f is a 2π-periodic continuous function, and f' is square integrable (especially f is a 2π-periodic C^1-function (→**A3.21**)), then $S[f]$ uniformly converges to f. In this case the following equality holds

$$2\pi \sum_{k=-\infty}^{\infty} |c_k|^2 = \int_{-\pi}^{\pi} dx |f(x)|^2,$$

which is called *Parseval's equality.*□
Warning. The continuity of f is not sufficient even for pointwise convergence of $S[f]$ to f. See **A7.8**.

A7.6 L^2-convergence. A function sequence f_n defined on $(-\pi, \pi)$ is said to *L^2-converge* to f (or to converge in the square mean), if

$$\int_{-\pi}^{\pi} dx |f_n(x) - f(x)|^2 \to 0$$

as $n \to \infty$.

A7.7 Theorem. If f is a 2π-periodic continuous function, then $S[f]$ L^2-converges to f, and Parceval's equality (→**A7.5**) holds. □

A7.8 Theorem [duBois-Reymond]. For a 2π-periodic function f, its continuity does not guarantee the pointwise convergence of $S[f]$ to f. [Counterexamples exist.] □
However,

A7.9 Theorem [Fejér]. Let S_n be the partial sum of the Fourier series up to the n-th term. Define

$$\sigma_n \equiv \frac{1}{n+1} \sum_{k=0}^{n} S_k.$$

If f is a 2π-periodic continuous function, then σ_n uniformly converges to f. □

A7.10 Piecewise C^1-function. A function f is said to be piecewise C^1, if there are finitely many points $\gamma_1 < \gamma_2 < \cdots < \gamma_m$ such that on each open interval (γ_l, γ_{l+1}) f and f' are continuous and bounded.
Notice that at each γ_l right and left limits (→**A2.6**) of f (denoted by $f(\gamma_l + 0)$ and $f(\gamma_l - 0)$) exist.

A7.11 Theorem. If f is piecewisely C^1, then $S[f]$ converges to $[f(x+0) + f(x-0)]/2$ for all x. The same holds if f' is piecewise continuous and square-integrable (i.e., its boundedness need not be assumed). The convergence is uniform except in the arbitrarily small neighborhood of the discontinuities of f. □

A7.12 Theorem. If f is a 2π-periodic function, integrable on $(-\pi, \pi)$ and is of bounded variation,[399] then the conclusion of **A7.11** holds. □

A7.13 Theorem [Locality of convergence]. Let f_1 and f_2 be piecewise 2π-periodic functions integrable on $(-\pi, \pi)$. If there is a neighborhood of x_0 such that $f_1 \equiv f_2$ on it, then $S[f_1]$ converges (resp., diverges) at x_0 if and only if $S[f_2]$ converges (resp., diverges) at x_0. When they converge, the limits are identical. □

A7.14 Fourier transform. Let f be an integrable function on $\boldsymbol{R}$. If the following integral exists

$$\hat{f} = \int_{-\infty}^{\infty} dx f(x) e^{-ikx},$$

it is called the *Fourier transform* of f. Mathematicians often multiply $1/\sqrt{2\pi}$ to this definition to symmetrize the formulas. However, this makes the convolution formula **A7.20**(iv) awkward. For physicists and practitioners, the definition here is the most convenient.
If a function $f : \boldsymbol{R} \to \boldsymbol{C}$ is continuous except for finitely many points, and absolutely integrable, then its Fourier transform $\hat{f} : \boldsymbol{R} \to \boldsymbol{C}$ is a bounded continuous function such that $\lim_{k\to\infty} f(\pm k) = 0$.
Also we have an important relation

$$\hat{f}' = ik\hat{f}.$$

A7.15 Rapidly decreasing function. A function $f : \boldsymbol{R} \to \boldsymbol{C}$ is

[399] That is, f can be written as a difference of two monotone increasing functions (→**A2.11**).

called a *rapidly decreasing function*, if the following two conditions hold:
(i) f is a C^∞-function ($\rightarrow$**A3.21**).
(ii) For any $k, l \in \boldsymbol{N}$, $x^l f^{(k)} \to 0$ in the $|x| \to \infty$ limit.
The function is also called a *Schwartz*-class function (or $\mathcal{S}$-function).

A7.16 Inverse Fourier transform. If f is a rapidly decreasing function, then the following *inversion formula* holds:

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \hat{f}(k) e^{ikx}.$$

□

A7.17 Theorem. If $f : \boldsymbol{R} \to \boldsymbol{C}$ is continuous (and bounded), and both f and $\hat{f}$ are absolutely integrable, then the inversion formula holds.
□

A7.18 Parseval's equality. If the inversion formula holds and if f is square integrable, we have

$$\int_{-\infty}^{\infty} dx |f(x)|^2 = 2\pi \int_{-\infty}^{\infty} dk |\hat{f}(k)|^2.$$

□

A7.19 Convolution. Let f and g be integrable function defined on $\boldsymbol{R}$. The following $h(x)$ is called the *convolution* of f and g and is denoted by $f * g$:

$$h(x) = (f * g)(x) \equiv \int_{-\infty}^{\infty} dy f(x-y) g(y).$$

A7.20 Properties of convolution.
(i) The definition is symmetric with respect to f and g, that is, $f * g = g * f$.
(ii) If f and g are rapidly decreasing, then so is h.
(iii) $h^{(k)} = f^{(k)} * g$
(iv) $\hat{f * g} = \hat{f}\hat{g}$.

A7.21 Theorem [Inversion formula for piecewise C^1-function]. Let f be piecewise C^1-function ($\rightarrow$**A7.10**) on $\boldsymbol{R}$. Then

$$\frac{1}{2}[f(x_0 - 0) + f(x_0 + 0)] = \frac{1}{2\pi} \text{p.v.} \int_{-\infty}^{\infty} dk e^{ikx_0} \hat{f}(k).$$

Here p.v. implies Cauchy's principal value of the integral. □
We can write the formula as

$$\frac{1}{2}[f(x_0 - 0) + f(x_0 + 0)] = \lim_{\lambda \to \infty} \int_{-\infty}^{\infty} d\xi \frac{\sin(\lambda(x_0 - \xi))}{x_0 - \xi} f(\xi).$$

□

A7.22 Multidimensional case. It is easy to generalize the rapidly decreasing property to multidimensional cases. If a function is rapidly decreasing, then formal generalization of the above results to multidimensional cases are legitimate.

45 Ordinary Differential Equation

Practical advice. See Schaum's outline series *Differential Equations* by R. Bronson for elementary methods and practice. To learn the theoretical side, V. I. Arnold, *Ordinary differential equations* (MIT Press 1973; there is a new version from Springer) is highly recommended.

A8.1 Ordinary differential equation. Let y be a n-times differentiable function of $x \in \boldsymbol{R}$. A funcitonal relation $f(x, y, y', \cdots, y^{(n)}) = 0$ among x,y, y', $\cdots$, $y^{(n)}$ is called an *ordinary differential equation* (ODE) for $y(x)$, and n is called its *order*, where the domain of f is assumed to be appropriate. Such $y(x)$ that satisfies $f = 0$ is called a *solution* to the ODE.

A8.2 General solution, singular solution. The solution $y = \varphi(x, c_1, c_2, \cdots, c_n)$ to $f = 0$ in **A8.1** which contains n arbitrary constants c_1, $\cdots$, c_n (which are called *integral constants*) is called the *general solution* of $f = 0$. A solution which can be obtained from this by specifying the arbitrary constants is called a *particular solution*. A solution which cannot be obtained as a particular solution is called a *singular solution*.

A8.3 Normal form. If the highest order derivative of y is explicitly solved as $y^{(n)}(x) = F(x, y', \cdots, y^{(n-1)})$, we say the ODE is in the *normal form*. Notice that not normal ODE's may have many pathological phenomena.

A8.4 Initial value problem of first order ODE. Consider the following first order ODE

$$\frac{dy}{dx} = f(x, y), \tag{45.1}$$

where f is defined in a region $D \subset \boldsymbol{R}^2$. To solve this under the condition that $y(x_0) = y_0$ ($(x_0, y_0) \in D$) is called a *initial value problem*.

A8.5 Theorem [Cauchy-Peano]. If for (45.1) f is continuous on a region $D \subset \mathbf{R}^2$, then for any $(x_0, y_0) \in D$ there is a solution $y(x)$ of (45.1) passing through this point whose domain is an open interval (α, ω) $(-\infty \leq \alpha < \omega \leq \infty)$, and in the limits $x \to \alpha$ and $x \to \omega$ $y(x)$ approaches the boundary of D or the solution becomes unbounded. □

A8.6 Lipschitz condition. Let $f(x, y)$ be a continuous function whose domain is a region $D \subset \mathbf{R}^2$. For any compact set (→[AI25]) $K \subset D$, if for any (x, y), $(x', y') \in K$ there is a positive constant L_K (which is usually dependent on K) such that

$$|f(x, y) - f(x', y')| \leq L_K |y - y'|,$$

then f is said to satisfy a *Lipschitz condition* on D for y.
If f and f_y are both continuous in D, then f satisfies a Lipschitz condition on D.

A8.7 Theorem [Cauchy-Lipschitz uniqueness theorem]. For (45.1), if f satisfies a Lipschitz condition on D for y, then if there is a solution passing through $(x_0, y_0) \in D$, it is unique. □

A8.8 Theorem. Let $f : \boldsymbol{R} \to \boldsymbol{R}$ be a continuous and monotone decreasing function. Then the initial value problem $dy/dx = f(y)$ (for $x > x_0$) with $y(x_0) = y_0$ has a unique solution for $x \geq x_0$. □

A8.9 Method of quadrature. To solve an ODE by a finite number of indefinite integrals is called the *method of quadrature*. Representative examples are given in **A8.10-A8.13**.

A8.10 Separation of variables. The first order equation of the following form

$$\frac{dy}{dx} = p(x)q(y),$$

where p and q are continuous functions, is solvable by the separation of variables: Let $Q(y)$ be a primitive function (→[AIV5]) of $1/q(y)$ and P that of p. Then $Q(y) = P(x) + C$ is the general solution, where C is the integration constant.

A8.11 Perfect differential equation, integrating factor. The first order ODE of the following form

$$\frac{dy}{dx} = -\frac{P(x, y)}{Q(x, y)},$$

where $Q \neq 0$. If there is a function Φ such that $\Phi_x = P$ and $\Phi_y = Q$, then $\Phi(x, y) = C$, C being the integral constant, is the general solution. Even if P and Q may not have such a 'potential' Φ, P and Q times some function I called *integrating factor* may have a 'potential.' However, it is generally not easy to find such a factor except for some special cases.

A8.12 Linear first order equation, variation of parameter. The first order equation

$$\frac{dy}{dx} = p(x)y + q(x)$$

is called a *linear equation*. The equation can be solved by the method of variation of parameters. Let $y(x) = C(x)e^{\int^x p(s)ds}$. Then the equation for C can be integrated easily. As we will see in **A8.14**, the method of variation of parameters *always* works for linear equations.

A8.13 Bernoulli equation. The first order equation of the following form is called a *Bernoulli equation*:

$$\frac{dy}{dx} = p(x)y + Q(x)y^n,$$

where n is a real number. Introducing the new variable $z(x) = y(x)^{1-n}$, we can reduce this equation to the case [12] for $z(x)$.

A8.14 Linear ODE with constant coefficients, characteristic equation. Consider

$$\frac{d^2y}{dx^2} + a\frac{dy}{dx} + by = 0, \tag{45.2}$$

where a and b are constants.

$$P(\lambda) = \lambda^2 + a\lambda + b$$

is called its *characteristic equation*, and its roots are called *characteristic roots*.

A8.15 Theorem [General solution to (4.80)]. If the characteristic roots of (4.80) are α and β ($\neq \alpha$), then its general solution is the linear combination of $\varphi_1(x) = e^{\alpha x}$ and $\varphi_2(x) = e^{\beta x}$. If $\alpha = \beta$, then the general solution is the linear combination of $\varphi_1(x) = e^{\alpha x}$ and $\varphi_2(x) = xe^{\alpha x}$ (the characteristic roots need not be real.) □
$\varphi_1(x)$ and $\varphi_2(x)$ are called *fundamental solutions* and $\{\varphi_1(x), \varphi_2(x)\}$ is called the *system of fundamental solutions* for (4.80).

A8.16 Inhomogeneous equation, Lagrange's method of variation of constants. An ODE

$$\frac{d^2y}{dx^2} + a\frac{dy}{dx} + by = f(x) \tag{45.3}$$

with nonzero f is called an *inhomogeneous* ODE (the one without nonzero f is called a homogeneous equation). The general solution is given by the sum of the general solution to the corresponding homogeneous equation and one particular solution to the inhomogeneous problem. A method to find one solution to (4.83) is the *Lagrange's method of variation of constants*. Let $\varphi_i(x)$ be the fundamental solutions and determine the functions $C_i(x)$ to satisfy (4.83):

$$u(x) = C_1(x)\varphi_1(x) + C_2(x)\varphi_2(x).$$

One solution can be obtained from

$$\frac{dC_1}{dx} = -\frac{f(x)\varphi_2(x)}{W(x)}, \quad \frac{dC_2}{dx} = \frac{f(x)\varphi_1(x)}{W(x)},$$

where $W(x) = \varphi_1(x)\varphi_2'(x) - \varphi_2(x)\varphi_1'(x)$, the Wronskian of the fundamental system. □
If the two characteristic roots α and β are distinct, then such a u is given by

$$u(x) = \frac{1}{\alpha - \beta}\left(\int_0^t dsf(s)e^{\alpha(t-s)} - \int_0^t dsf(s)e^{\beta(t-s)}\right).$$

46 Vector Analysis

A9.1 Gradient. Suppose we have a sufficiently smooth function $f : D \to \boldsymbol{R}$, where $D \subset \boldsymbol{R}^2$ is a region. We may imagine that $f(P)$ for $P \in D$ is the altitude of the point P on the island D. Since we assume the landscape to be sufficiently smooth, at each point on D there is a well defined direction $\boldsymbol{n}$ of the steepest ascent and the slope (magnitude) $s(\geq 0)$. That is, at each point on D, we may define the *gradient vector* $s\boldsymbol{n}$, which will be denoted by a vector field $grad\, f$.

A9.2 Coordinate expression of $grad\, f$. Although $grad\, f$ is meaningful without any specific coordinate system, in actual calculations, introduction of a coordinate system is often useful. Choose a Cartesian coordinate system O-xy. Then the vector has the following representation:

$$grad\, f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right),$$

or

$$grad\, f = \boldsymbol{i} \frac{\partial f}{\partial x} + \boldsymbol{j} \frac{\partial f}{\partial y}. \tag{46.1}$$

A9.3 Remark. Note that to represent $grad\, f$ in terms of numbers, we need two devices: one is the coordinate system to specify the point in D with two numbers, which allow us to describe f as a function of two independent variables, and two vectors to span the two dimensional vector '$grad\, f$' at each point on D. In principle any choice is fine, but practically, it is wise to choose these base vectors to be parallel to the coordinate directions at each point. In the choice **A9.2**, the coordinate system has globally the same coordinate direction at every point on D, and the basis vectors are chosen to be parallel to these directions, so again globally uniformly chosen. Nonuniformity in space of representation schemes may cause complications. Especially when we formally use operators as explained below, we must be very careful (→**A9.7**,**A9.9** for a warning).

A9.4 Nabla or del. (3.2) suggests that $grad$ is a map which maps f to the gradient vector at each point in its domain (if f is once partially differentiable). We often write this linear operator as ∇, which is called *nabla*,[400] but is often read 'del' in the US. We write $grad\, f = \nabla f$. ∇ has the following expression if we use the Cartesian coordinates (read [3])

$$\nabla \equiv \sum_{k=1}^{n} \boldsymbol{i}_k \frac{\partial}{\partial x_k}, \tag{46.2}$$

where x_k is the k-th coordinate and $\boldsymbol{i}_k$ is the unit directional vector in the k-th coordinate direction.

A9.5 Divergence. Suppose we have a flow field (velocity field) $\boldsymbol{u}$ on a domain $D \in \boldsymbol{R}^3$. Let us consider a convex domain[401] $V \subset \boldsymbol{R}^3$ which may be imagined to be covered by area elements $d\boldsymbol{S}$ whose area is $|d\boldsymbol{S}|$, and whose outward normal unit vector is $d\boldsymbol{S}/|d\boldsymbol{S}|$. Then $\boldsymbol{u} \cdot d\boldsymbol{S}$ is the

[400] 'Nabla' is a kind of harp (Assyrian harp).

[401] A set is said to be *convex* if the segment connecting any two points in the set is entirely included in the same set.

rate of the volume of fluid going out through the area element in the unit time. Hence the area integral

$$\int_{\partial V} d\boldsymbol{S} \cdot \boldsymbol{u}$$

is the total amount of the volume of the fluid lost from the domain V. The following limit, if exists, is called the *divergence* of the vector field $\boldsymbol{u}$ at point P and is written as $div\, \boldsymbol{u}$:

$$div\, \boldsymbol{u} \equiv \lim_{|V| \to 0} \frac{\int_{\partial V} \boldsymbol{u} \cdot d\boldsymbol{S}}{|V|}, \tag{46.3}$$

where the limit is taken over a nested sequence of convex volumes converging to a unique point P. Thus its meaning is clear: $div\, \boldsymbol{u}$ is the rate of loss of the quantity carried by the flow field $\boldsymbol{u}$ per unit volume.

A9.6 Cartesian expression of *div*. From (3.5) assuming the existence of the limit, we may easily derive the Cartesian expression for *div*. Choose as V a tiny cube whose surfaces are perpendicular to the Cartesian coordinates of O-xyz. We immediately get

$$div\, \boldsymbol{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z}. \tag{46.4}$$

A9.7 Operator *div*. (3.10) again suggests that *div* is an operator which maps a vector field to a scalar field. Comparing (3.3) and (3.10) allows us to write

$$div\, \boldsymbol{u} = \nabla \cdot \boldsymbol{u}.$$

This 'abuse' of the symbol is allowed only in the Cartesian coordinates. Generalization to n-space is straightforward.

A9.8 Curl. Let $\boldsymbol{u}$ be a vector field as in **A9.5**. Take a singly connected compact surface S in $\boldsymbol{R}^3$ whose boundary is smooth. The boundary closed curve with the orientation according to the right-hand rule is denoted by ∂S (see Fig.). Consider the following line integral along ∂S:

$$\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l},$$

where $d\boldsymbol{l}$ is the line element along the boundary curve. Ket us imagine a straight vortex line and take S to be a disc perpendicular to the line and its center is on the line. Immediately we see that the integral is the strength of the vortex whose center (singular point) goes through S. Thus the following limit, if exists, describes the 'area' density of

the $\boldsymbol{n}$-component of the vortex (as in the case of angular velocity, the direction of vortex is the direction of the axis of rotation with the right-hand rule):

$$\boldsymbol{n} \cdot curl\, \boldsymbol{u} = \lim_{|S|\to 0} \frac{\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l}}{|S|}, \tag{46.5}$$

where the limit is over the sequence of smooth surfaces which converges to point P with its orientation in the $\boldsymbol{n}$-direction. If the limit exists, then obviously there is a vector $curl\, \boldsymbol{u}$ called *curl* of the vector filed $\boldsymbol{u}$.

A9.9 Cartesian expression of curl. If we assume the existence of the limit (3.14), we can easily derive the Cartesian expression for $curl\, \boldsymbol{u}$. We have

$$curl\, \boldsymbol{u} = \left(\frac{\partial u_z}{\partial y} - \frac{\partial u_y}{\partial z}, \frac{\partial u_x}{\partial z} - \frac{\partial u_z}{\partial x}, \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \right), \tag{46.6}$$

or

$$curl\, \boldsymbol{u} = \begin{vmatrix} \boldsymbol{i} & \boldsymbol{j} & \boldsymbol{k} \\ \partial_x & \partial_y & \partial_z \\ u_x & u_y & u_z \end{vmatrix} = \nabla \times \boldsymbol{u}. \tag{46.7}$$

This 'abuse' of the nabla symbol is admissible only with the Cartesian coordinates.

A9.10 Potential field, potential, solenoidal field, irrotational field. If a vector field $\boldsymbol{u}$ allows an expression $\boldsymbol{u} = grad\, \phi$, then the field is called a *potential field* and ϕ is called its *potential*. A field without divergence $div\, \boldsymbol{u} = 0$ is called a divergenceless or *solenoidal field*. The field without curl $curl\, \boldsymbol{u} = 0$ is called an *irrotational field*.

A9.11.
(i) $curl\, grad\, \phi = 0$ (Potential fields are irrotational).
(ii) $div\, curl\, \boldsymbol{u} = 0$.
(iii) If a vector field is irrotational on a singly connected domain,[402] then the field is a potential field.
(iv) If a vector field $\boldsymbol{u}$ is solenoidal in a singly connected domain, then there is a vector field $\boldsymbol{A}$ on the domain such that $\boldsymbol{u} = curl\, \boldsymbol{A}$. $\boldsymbol{A}$ is called a *vector potential*.

A9.12 Theorem [Gauss-Stokes-Green's theorem]. From our definitions of divergence and curl, we have

[402] A domain is *singly connected*, if, for any given pair of points in the domain, any two curves connecting them are homotopic. That is, they can be smoothly deformed into each other without going out of the domain.

(i) Gauss' theorem.

$$\int_{\partial V} \boldsymbol{u} \cdot d\boldsymbol{S} = \int_V div\, \boldsymbol{u} d\tau, \tag{46.8}$$

where V is a domain in the 3-space and $d\tau$ is the volume element.
(ii) Stokes' theorem.

$$\int_{\partial S} \boldsymbol{u} \cdot d\boldsymbol{l} = \int_S curl\, \boldsymbol{u} \cdot d\boldsymbol{S}, \tag{46.9}$$

where S is a compact surface in 3-space.

A9.13 Laplacian. The operator Δ defined by $\Delta f \equiv div\, grad\, f$ is called the *Laplacian*, and is often written as ∇^2. Δ is defined for a scalar function.

A9.14 Laplacian for vector fields. If we formally calculate $curl\, curl\, \boldsymbol{u}$ in the Cartesian coordinates, then we have

$$curl\, curl\, \boldsymbol{u} = grad\, div\, \boldsymbol{u} - \nabla^2 \boldsymbol{u}.$$

Since the formal calculation treating ∇ as a vector is legitimate only in the Cartesian coordinate system, this calculation is meaningful only in the Cartesian system. Thus, in particular $\nabla^2 \boldsymbol{u} = (\Delta u_x, \Delta u_y, \Delta u_z)$ is meaningful only in this coordinate system. However, the other two terms are coordinate-free expressions. Hence, we *define* $\Delta \boldsymbol{u}$ as

$$\Delta \boldsymbol{u} \equiv grad\, div\, \boldsymbol{u} - curl\, curl\, \boldsymbol{u}. \tag{46.10}$$