

HW 6 Solutions Corrected (stupid error in 4F3) and augmented

1. [Very elementary problem]

There is a system with only three one-particle states with energies 0 , ϵ and 2ϵ ($\epsilon > 0$). There are two identical particles without spin.

Suppose both particles are fermions.

(F1) Write down the canonical partition function for the system.

(F2) What is the probability $P(N)$ to find N particles in the ground state? (Obtain $P(0)$, $P(1)$ and $P(2)$).

(F3) What is the average occupation number of the one particle ground state?

Suppose both particles are bosons. Repeat the above questions. That is:

(B1) Write down the canonical partition function for the system.

(B2) What is the probability $P(N)$ to find N particles in the ground state? (Obtain $P(0)$, $P(1)$ and $P(2)$).

(B3) What is the average occupation number of the one particle ground state?

Solution

(F1) The definition of the canonical partition function is sum of e^{-E} for all microstates, where E is the energy of the microstate. Therefore, we must itemize all the microstates allowed to this two-particle system.

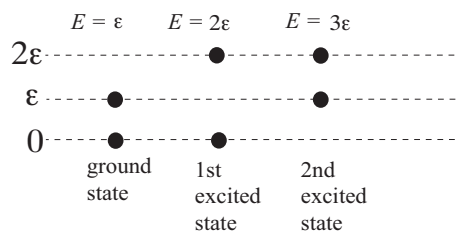


Figure 1: Three microstates

Therefore,

$$Z = e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon}.$$

(F2) From Fig. 1 we see the ground state and the first excited state have 1 particle in the 1P ground state, and the second excited state has 0 particle in the 1P ground state. Therefore,

$$P(0) = e^{-2\beta\epsilon} / (1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}), \quad P(1) = (1 + e^{-\beta\epsilon}) / (1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}),$$

and $P(n) = 0$ for any $n > 1$.

(F3) $\langle n \rangle = \sum_h nP(n)$, so $\langle n \rangle = P(1)$.

(B1) We repeat a very similar argument. The table of the microstates is in Fig. 2.

Therefore,

$$Z = 1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}.$$

(B2) From Fig. 2 we see $n = 2$ for $E = 0$, $n = 1$ for $E = \epsilon$ and 2ϵ , $n = 0$ for $E = 2\epsilon$, 3ϵ and 4ϵ . Therefore,

$$P(0) = \frac{e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}}{1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}},$$

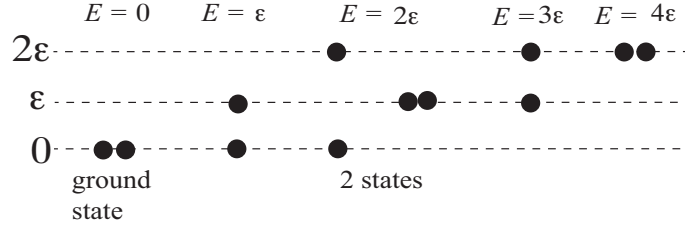


Figure 2: Six microstates: for non-interacting particles each microstate (= eigenstate of the system (many-body) Hamiltonian) corresponds to a unique combination of one-particle (1P) state occupation numbers.

$$P(1) = \frac{e^{-\beta\epsilon} + e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}},$$

$$P(2) = \frac{1}{1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}}$$

For other n $P(n) = 0$.

(B3) Therefore,

$$\langle n \rangle = \frac{2 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + 2e^{-2\beta\epsilon} + e^{-3\beta\epsilon} + e^{-4\beta\epsilon}}.$$

2. [Very elementary problem]

There are 300 spinless bosons whose k -th one particle excited state has an energy $(2k - 1)\epsilon$ ($\epsilon > 0$, $k \in \{1, 2, \dots\}$); the energy origin is the one-particle ground state.

- (1) How many microstates does the system have whose energy is less than or equal to 4ϵ ?
- (2) Suppose the systems is attached to a chemostat whose temperature is T and chemical potential μ . On the average 298 particles occupy the one-particle ground state, and 2 particles occupy the one-particle first excited state. The remaining one-particle states are not appreciably occupied. Obtain $\beta = 1/k_B T$ and μ in terms of ϵ .

Solution

- (1) Seven microstates: the table of the low-lying microstates is as follows

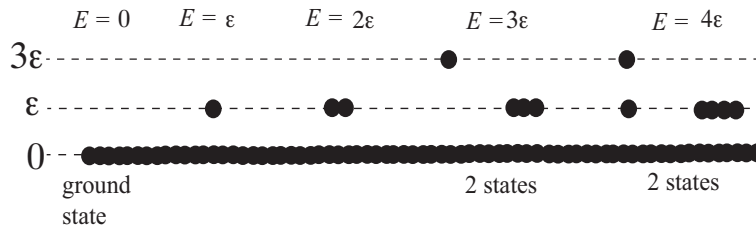


Figure 3: Seven microstates with $E \leq 4\epsilon$.

- (2) We simply write down the expected values in terms of μ and β as

$$\langle n_0 \rangle = 298 = \frac{1}{e^{-\beta\mu} - 1}, \quad \langle n_1 \rangle = 2 = \frac{1}{e^{\beta(\epsilon-\mu)} - 1}.$$

That is, [Since we can expect μ to be small, you should keep sufficiently many digits.]

$$e^{-\beta\mu} = 299/298, \quad e^{\beta(\epsilon-\mu)} = 3/2,$$

or

$$\beta\mu = \log(298/299) = -0.00335, \quad \beta\mu - \beta\epsilon = -0.405465.$$

Therefore,

$$\beta = (0.405465 - 0.00335)/\epsilon = 0.402115/\epsilon, \quad \mu = -(0.00335/0.402115)\epsilon = -0.0087\epsilon < 0.$$

Confirm that $\mu < 0$.

3. [Very elementary problem]

(1) We have an ideal gas mixture consisting of ideal fermions and ideal bosons in a volume V . What is the relation between the total pressure and the total internal energy of the system?

(2) Explicitly demonstrate with the aid of the expression of the total number of particles N that μ decreases as temperature goes up if N and the total volume are maintained.

Solution

(1) Note: Many people simply quoted that $PV = (2/3)E$ is true for both fermions and bosons, and concluded without any argument that $PV = (2/3)E$. The answer is correct, but I wish you to explain why this is also true for mixtures. You must be conscious about the fundamental laws (properties) you rely on. In this case, you need the *extensivity of internal energy* and the *law of partial pressures for ideal gases*.

The partial pressure of the bosons is $P_B V = (2/3)E_B$, where E_B is the total internal energy carried by the bosons. For the fermions we have a similar formula $P_F V = (2/3)E_F$. The system is non-interacting, so the total pressure must be $P = P_B + P_F$ due to the law of partial pressures. The total internal energy $E = E_B + E_F$ due to extensivity, so $PV = (2/3)E$.

If you wish, we can honestly start with the grand-canonical formalism, but we have two different chemical species, so we need two distinct chemical potentials μ_B and μ_F (each determined from the numbers of bosons and fermions, separately), which are determined by the total numbers of particles. Fermions and bosons do not interact, so (with obvious notations)

$$\Xi = \Xi_F \Xi_B.$$

Therefore, obviously, $PV = \beta \log \Xi = P_F V + P_B V$. Thus, our intuitive approach has been vindicated.

When you conclude something, you must provide a justifying argument.

(2) We know

$$N = \sum_i \frac{1}{e^{\beta(\epsilon - \mu)} \mp 1}.$$

If $T \nearrow$, $\beta \searrow$. Since $\epsilon - \mu > 0$, if we fix μ , $e^{\beta(\epsilon - \mu)} \searrow$, so $1/(e^{\beta(\epsilon - \mu)} \mp 1) \nearrow$. That is, if we maintain μ and $T \nearrow$, then $N \nearrow$, but we wish to keep N . Since $e^{\beta(\epsilon - \mu)}$ is a decreasing function of μ , $1/(e^{\beta(\epsilon - \mu)} \mp 1)$ is an increasing function of μ . Hence, to keep N despite $T \nearrow$, we must reduce μ .

A simplified argument is: Since we wish to maintain N despite decreasing β , we must at least increase $\epsilon - \mu$ for any ϵ . This means we must decrease μ .

However, these arguments do not show that N is indeed maintained. In this sense the argument is not complete.

More formally, we know

$$dN = \left. \frac{\partial N}{\partial \mu} \right|_{\beta} d\mu + \left. \frac{\partial N}{\partial \beta} \right|_{\mu} d\beta = 0.$$

We can explicitly compute the partial derivatives in the above formula as¹

$$\left. \frac{\partial N}{\partial \mu} \right|_{\beta} = \sum \frac{\beta e^{\beta(\epsilon - \mu)}}{(e^{\beta(\epsilon - \mu)} \mp 1)^2}, \quad \left. \frac{\partial N}{\partial \beta} \right|_{\mu} = \sum \frac{(\mu - \epsilon) e^{\beta(\epsilon - \mu)}}{(e^{\beta(\epsilon - \mu)} \mp 1)^2}.$$

Therefore, we may write

$$\left. \frac{\partial N}{\partial \mu} \right|_{\beta} = A\beta, \quad \left. \frac{\partial N}{\partial \beta} \right|_{\mu} = A\mu - B,$$

where

$$A = \sum \frac{e^{\beta(\epsilon - \mu)}}{(e^{\beta(\epsilon - \mu)} \mp 1)^2}, \quad B = \sum \frac{\epsilon e^{\beta(\epsilon - \mu)}}{(e^{\beta(\epsilon - \mu)} \mp 1)^2}.$$

Let us assume that $D_t(\epsilon)$ is at most algebraic and bounded at $\epsilon = 0$. A and B are obviously finite for fermions. For bosons B is obviously finite; A is bounded from above by N^2 . Both are positive.

$$\beta d\mu + (\mu - B/A) d\beta = 0 \Rightarrow \left. \frac{\partial \mu}{\partial \beta} \right|_{N,V} = k_B T (B/A - \mu) > 0$$

Therefore, if $T \nearrow$, then $\mu \searrow$.

4. In a cylinder with a piston are N identical particles.

The fermion case: At $T = 0$ the volume is doubled reversibly and adiabatically.

(F1) What is the final temperature?

(F2) Suppose the initial internal energy is E . What is the work done by the system?

(F3) What is the ratio P_f/P_i of the initial P_i and the final P_f pressures? [no extra work is needed, if you do (2)]

The boson case:

(B1) When the volume is doubled reversibly and adiabatically, does the critical temperature of the system go up or down?

(B2) Let us assume that the temperature is always below T_c . What is the ratio of the initial T_i and the final T_f temperatures?

(B3) What is the work done by the system, if the initial internal energy is E ?

Solution

For simple problems you seem to use whatever logic you can manage to reach supposedly correct answers. I strongly dissuade you to do so.

First, try to use thermodynamics without any ad hoc or materials-specific assumptions.

(F1) The temperature is still $T = 0$, because particles ‘move’ with the energy levels; filled 1P states are still filled, and unoccupied states are still unoccupied if the change is adiabatic (see the note at the end).

¹The summation and the differentiation may be exchanged, because the series formally constructed from derivatives converges uniformly in $\epsilon - \mu$ (if D_t increases only algebraically).

More formally, we could use thermodynamics (+ the property of a free fermion system). Let us show

$$\left. \frac{\partial T}{\partial V} \right|_S \rightarrow 0$$

in the $T \rightarrow 0$ limit.

$$\left. \frac{\partial T}{\partial V} \right|_S = \frac{\partial(T, S)}{\partial(V, S)} = \frac{\partial(T, S)}{\partial(T, V)} \frac{\partial(T, V)}{\partial(V, S)} = \frac{T}{C_V} \frac{\partial(T, S)}{\partial(V, T)}.$$

We know C_V/T is finite for free fermions (this is not thermodynamic).

$$\frac{\partial(T, S)}{\partial(V, T)} = \frac{\partial(T, S)}{\partial(P, V)} \frac{\partial(P, V)}{\partial(V, T)} = - \left. \frac{\partial P}{\partial T} \right|_V \propto - \left. \frac{\partial E}{\partial T} \right|_V,$$

where the last step is due to $PV = (2/3)E$ for ideal gas. We know $E(T) = E(0) + O[T^2]$, so this goes to zero for $T \rightarrow 0$. We are done.

Some people claim that $E(0)$ scales as $V^{-2/3}$ as $E(T)$. so $T_f = 0$. This logic is not enough unless you show that the $O[T^2]$ is NOT proportional to $V^{-2/3}$. Also I found $dS = 0 \Rightarrow dT = 0$. This is not generally true.

(F2) Thus we need how the Fermi energy changes with the volume. We know $(N/V)^{2/3} \propto \mu$, so $\mu_i^{3/2}/2 = \mu_f^{3/2}$. That is, $\mu_f = 2^{-2/3}\mu_i$. Since $E = (3/5)\mu(0)N$ at $T = 0$, we have $E_f = 2^{-2/3}E$. Therefore, $W = (2^{-2/3} - 1)E (< 0)$. The system produces a positive work (the system energy must be reduced).

Perhaps, you do not like this. More ‘honestly,’ since $dS = 0$ (reversible and adiabatic), $dE = -PdV$ (use thermodynamics whenever you can!). We know $E = (3/2)PV$ (or $P = 2E/3V$), so

$$dE = -\frac{2E}{3V}dV$$

That is, $EV^{2/3}$ must be constant. This implies $EV^{2/3} = E_f(2V)^{2/3}$. That is, $E_f = 2^{-2/3}E$. The rest is the same as above.

In this second argument, did we use something peculiar to fermions? No. Thus you have also answered (B3) (partially, a merit of thermodynamics).

(F3) Use $PV \propto E$. $P_f/P_i = E_fV/2VE = 2^{-2/3}/2 = 2^{-5/3}$.

The point of the boson part is that below T_c many thermodynamic quantities are simple power functions of T , so you can answer many questions quantitatively. However, always try to use thermodynamics and intuitive arguments as much as possible.

(B1) $T_c(V)$ is a decreasing function of V , so T_c goes down. You could use $VT_c^{3/2} \propto N$. (In the problem it is said ‘reversible’, needless to say, such a condition is not needed.) An intuitive understanding is that the gap between the ground 1P-state and the first excited 1P-state is reduced if V is increased, so the ground state particles become easier to jump up to the excited state. That is, the condensate becomes less populated at the same temperature. Therefore, if you wish to keep the population of the condensate, you must cool the system. In particular, to create the condensate you need a lower temperature, so T_c lowers with the increase of V .

(B2) Adiabatic change implies that the number of the particles in the condensate does not change (see the note at the end). So $AVT^{3/2} = N_1$ is constant. (Notice that if the energy levels

are uniformly scaled as in the present case $\epsilon \rightarrow a\epsilon$, scaling T and μ can maintain the same occupation numbers for all the 1P states.) Therefore, $VT_i^{3/2} = 2VT_f^{3/2}$ or $T_f = 2^{-2/3}T_i$.

(B3) (If you do not use thermodynamics) The internal energy is $E \propto VT^{5/2}$. Therefore, $E = AVT_i^{5/2}$, and $E_f = A(2V)T_f^{5/2}$, where A is a constant. That is,

$$E_f/E = 2(T_f/T_i)^{5/2} = 2(2^{-2/3})^{5/2} = 2^{-2/3} \Rightarrow E_f = 2^{-2/3}E.$$

Therefore, the works done by the system is

$$-W = E - E_f = (1 - 2^{-2/3})E.$$

This is the same as above, but we already know this.

Comment on adiabaticity

In this problem, the systems are changed reversibly and adiabatically. Thermodynamically, this implies that the systems are modified very gently (avoiding any cause of dissipation²), so no ‘production’ of entropy occurs in the system. Since the systems are adiabatic (in the thermodynamic sense), no heat is imported to or exported from the systems. Hence, the system entropy does not change. This is the hallmark of thermodynamic adiabatic process.

In the solutions above, I used ‘quantum mechanical adiabatic change’ as a mechanical description of thermodynamic adiabatic process: each particle follows its already occupying energy level that moves along the energy axis. It is worth remembering that this type of argument works whenever a process is macroscopically gentle and without any heat exchange.

However, as stressed repeatedly in the lecture notes, thermodynamic reversible processes are far more violent processes than quantum-mechanical adiabatic processes. Since we know quantum mechanics does not contradict thermodynamics, you can use the mechanical interpretation of thermodynamic reversible adiabatic process to guess the results (as above), but never believe that actual thermodynamic reversible adiabatic processes can be described as quantum-mechanical adiabatic processes.

²Notice that the entropy production rate is proportional to (the changing rate)², so if the changing rate is small, entropy change may be ignored (according to the linear irreversible thermodynamics).