PHYS 427 - Thermal and Statistical Physics - Discussion 09 - Solutions

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1. **Non-interacting fermions**: Consider a system of identical non-interacting fermions. (This is a good model for the free electrons roaming around inside a metal.) Each fermion can occupy many different **single-particle quantum states** which are labelled by an index $m = 0, 1, 2, \ldots$. The energy of a fermion in the single-particle state m will be denoted ε_m.

   In order to specify a microstate state of the whole system, we just have to specify N_m, the number of particles occupying the m^{th} single-particle state. Then, for example, the energy of the microstate is $\sum_m \varepsilon_m N_m$. Note that N_m can only be 0 or 1, because of the Pauli exclusion principle.

   (a) Show that the grand partition function becomes

   $$\mathcal{Z} = \prod_m \left(1 + e^{-\beta(\varepsilon_m - \mu)}\right). \tag{1}$$

   (b) Using the result from part (a), show that the number of particles in the system is

   $$N = \sum_m f(\varepsilon_m), \tag{2}$$

   where

   $$f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1} \tag{3}$$

   is the **Fermi-Dirac** distribution function.

   (c) Sketch the Fermi-Dirac distribution function at some positive temperature.

   i. Is the function consistent with the Pauli-exclusion principle?

   ii. What happens to the graph of the function if you change the value of the chemical potential?

   iii. Which single-particle states have a greater than 50% chance of being occupied?

   (d) Using the result from part (a), show that the energy of the system is

   $$U = \sum_m \varepsilon_m f(\varepsilon_m). \tag{4}$$

(e) Suppose you have actually created a gas of N^* non-interacting fermions in the lab which is in equilibrium at a temperature T (perhaps these are electrons in a metal). Convince yourself that you could use (2) to solve for μ (although in practice you would need to do it numerically, or make further approximations as in the next problem).

Note that you could plug this μ into (4), hence determining $U(T, N^*)$.

This gives another perspective on the meaning of μ. If you have the ability to choose (or measure) the number of particles in your system, μ can be thought of as a value which is tuned such that (2) correctly gives the chosen (or measured) number of particles in the system. Then all other thermodynamic quantities could in principle be expressed in terms of the number of particles instead of μ. However, it is typically much more convenient to continue working with μ.

(a) Refer to the solution of problem 1(a) in Discussion 8. We found

$$\mathcal{Z} = \left(\sum_{N_0} e^{-\beta(\varepsilon_0-\mu)N_0}\right)\left(\sum_{N_1} e^{-\beta(\varepsilon_1-\mu)N_1}\right)\left(\sum_{N_2} e^{-\beta(\varepsilon_2-\mu)N_2}\right)\cdots \tag{5}$$

This time, however, the particles are fermions. They obey the Pauli exclusion principle—for each state m, the number of particles in that state can only be $N_m = 0$ or $N_m = 1$. So

$$\sum_{N_0=0}^{1} e^{-\beta(\varepsilon_0-\mu)N_0} = 1 + e^{-\beta(\varepsilon_0-\mu)}, \tag{6}$$

and similarly for the other factors in (5). This proves the desired result.

(b) Recall in the grand-canonical ensemble the number of particles can be computed from

$$N = \frac{1}{\beta}\left(\frac{\partial}{\partial\mu}\ln\mathcal{Z}\right)_\beta \tag{7}$$

$$= \frac{1}{\beta}\left[\frac{\partial}{\partial\mu}\sum_m \ln\left(1 + e^{-\beta(\varepsilon_m-\mu)}\right)\right]_\beta \qquad \ln(ab) = \ln a + \ln b \tag{8}$$

$$= \frac{1}{\beta}\sum_m \frac{1}{1 + e^{-\beta(\varepsilon_m-\mu)}}(0 + e^{-\beta(\varepsilon_m-\mu)}\beta) \tag{9}$$

$$= \sum_m \frac{1}{e^{\beta(\varepsilon_m-\mu)} + 1} \tag{10}$$

$$= \sum_m f(\varepsilon_m) \tag{11}$$

(c) Figure 1 shows the Fermi-Dirac distribution function at a few different (positive) temperatures.

(c)i. The answer to (b) suggests that $f(\varepsilon_m)$ is the average number of particles in the single-particle state m. This is in fact true, as a slightly more refined calculation would show (see lecture notes).

Suppose we look into the single-particle state m. Either we'll see zero particles in that state or we'll see one particle—no more, due to the Pauli exclusion principle. Therefore the *average* number of particles in the single-particle state m must be somewhere between

0 and 1. Inspecting Figure 1, we find that $f(\varepsilon_m)$ is always between 0 and 1, so it's consistent with this requirement. (As it must be, because we didn't make any mistakes in our derivation!)

(c)ii. Increasing μ shifts the graph of $f(\varepsilon)$ toward the right, as seen in Figure 1. Likewise decreasing μ shifts it to the left. This doesn't change the "shape" of the graph, though.

(c)iii. If we plug in $\epsilon = \mu$, then $f = 1/2$. That means any single-particle state m whose energy ε_m happens to be equal to the chemical potential will have exactly 50% chance of being occupied. If $\varepsilon_m < \mu$, then the average occupation of m is greater than $1/2$, because in that case $f > 1/2$. Similarly, states above μ have less than 50% occupation.

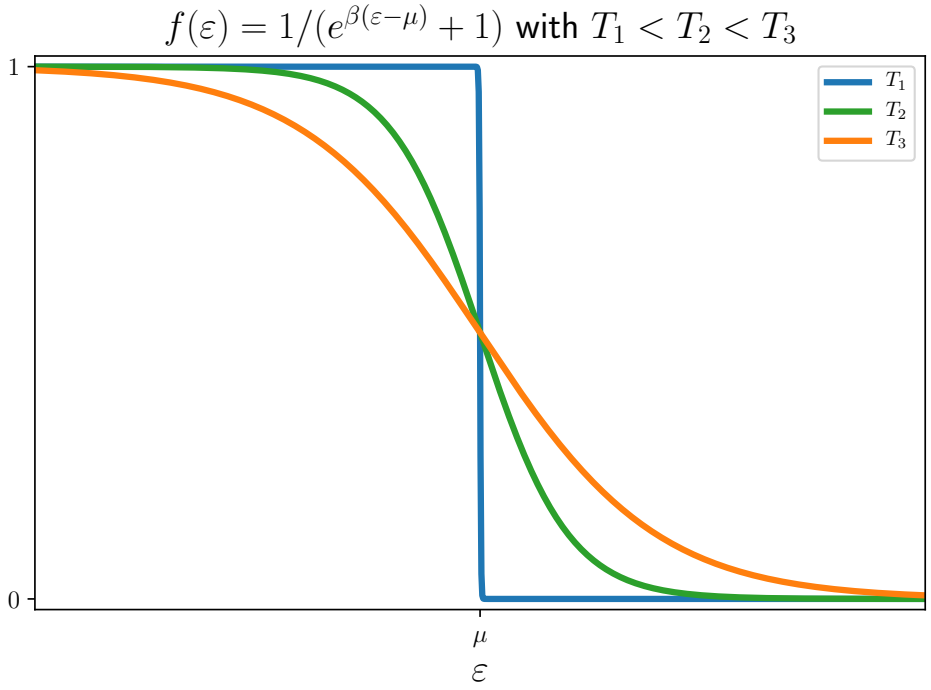

Figure 1

(d) Recall in the grand-canonical ensemble the energy is given by:

$$E = -\left(\frac{\partial}{\partial\beta}\ln\mathcal{Z}\right)_\mu + \mu N \tag{12}$$

$$= -\left[\frac{\partial}{\partial\beta}\sum_m \ln\left(1+e^{-\beta(\varepsilon_m-\mu)}\right)\right]_\mu + \mu\sum_m f(\varepsilon_m) \tag{13}$$

$$= \sum_m \left[\frac{-1}{1+e^{-\beta(\varepsilon_m-\mu)}}(0-(\varepsilon_m-\mu)e^{-\beta(\varepsilon_m-\mu)}) + \mu f(\varepsilon_m)\right] \tag{14}$$

$$= \sum_m \left[(\varepsilon_m-\mu)\frac{1}{e^{\beta(\varepsilon_m-\mu)}+1} + \mu f(\varepsilon_m)\right] \tag{15}$$

$$= \sum_m (\varepsilon_m - \mu + \mu) f(\varepsilon_m) \tag{16}$$

$$= \sum_m \varepsilon_m f(\varepsilon_m) \tag{17}$$

2. **Non-interacting ultra-relativistic gas**: Consider a collection of massive spin–3/2 particles in three dimensions confined to a square of volume $V = L^3$. Suppose the particles are moving very close to the speed of light; in this so-called "ultra-relativistic" limit, the relation between a particle's energy and wavevector is $\varepsilon_{\vec{k}} = c\hbar|\vec{k}|$, where c is the speed of light and the wavevector is quantized as $\vec{k} = \pi\vec{n}/L$ with $n_x, n_y, n_z = 1, 2, \ldots, \infty$.

   (a) Show that when L is sufficiently large we can approximate a sum over single-particle eigenstates by an integral over energy, i.e. show

   $$\sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \frac{2}{\pi^2} \frac{L^3}{(\hbar c)^3} \int_0^\infty d\varepsilon\, \varepsilon^2 F(\varepsilon) \tag{18}$$

   for any function F. It is customary to define the so-called *density of states*

   $$\mathcal{D}(\varepsilon) = \frac{2}{\pi^2} \left(\frac{L}{\hbar c}\right)^3 \varepsilon^2, \tag{19}$$

   so that the result can be written as

   $$\sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \int_0^\infty d\varepsilon\, \mathcal{D}(\varepsilon) F(\varepsilon). \tag{20}$$

   Explain why $\mathcal{D}(\varepsilon)$ is called the density of states.

   Note: you have calculated the density of states of ultrarelativistic massive spin-3/2 particles in 3 dimensions. For other dispersion relations in different number of dimensions, the expression for $\mathcal{D}(\varepsilon)$ will look different from (19).

   (b) Consider cooling down the system to absolute zero, $T = 0$. By inspecting the Fermi-Dirac distribution function, convince yourself that all single-particle states with energy less than μ are occupied, while all single-particle states with energy greater than μ are unoccupied. The Fermi energy ε_F is defined as the highest-energy single-particle state occupied at $T = 0$. In other words, $\varepsilon_F = \mu(T = 0)$.

   (c) Using (2) and (20), compute the Fermi energy as a function of the particle density $n = N/V$. *Hint: remember $T = 0$; use the result from (b) to simplify the integral. Answer:* $\varepsilon_F = \hbar c(3\pi^2 n/2)^{1/3}$

   (d) Compute the ground state energy of the system using (4) and (20). Write your answer in terms of the number of particles and Fermi energy. *Answer:* $U = \frac{3}{4} N\varepsilon_F$. *Does this make physical sense?*

   (e) Using $p = -(\partial F/\partial V)_{T,N}$ and noting that $F = U$ when $T = 0$, use your answer from part (d) to compute the pressure of the fermi gas at absolute zero. *Answer:* $p = U/3V$.

   Note: it may seem weird for the gas to have non-zero pressure at absolute zero temperature, because we expect things to stop "jiggling" at $T = 0$. The remnant pressure at $T = 0$ is called the *degeneracy pressure*, and it is ultimately a consequence of the Pauli exclusion principle. The degeneracy pressure of cold systems of identical fermions is the reason large numbers of particles can form long-lived macroscopic objects. This includes compact astrophysical objects (white dwarfs, neutron stars), which would otherwise collapse into black holes under gravity, but also the ordinary materials found in this room.

(a) We worked through this procedure last discussion (but in 2-dimensions). Recalling the wavevectors are quantized as $\vec{k} = (\pi/L)\vec{n}$ we have that smallest spacing between two wavevectors is $\Delta k_i = \pi/L$ for $i = x, y, z$. Then inserting a fancy version of 1 gives

$$\sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) = 4 \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \times 1 \qquad , \qquad 1 = \frac{L}{\pi}\Delta k_x = \frac{L}{\pi}\Delta k_y = \frac{L}{\pi}\Delta k_z \tag{21}$$

$$= 4\left(\frac{L}{\pi}\right)^3 \sum_{k_x} \Delta k_x \sum_{k_y} \Delta k_y \sum_{k_z} \Delta k_z \, F(\varepsilon_{\vec{k}}) \tag{22}$$

$$\to 4\left(\frac{L}{\pi}\right)^3 \int_0^\infty dk_x \int_0^\infty dk_y \int_0^\infty dk_z \, F(\varepsilon_{\vec{k}}) \qquad , \qquad \text{as } L \to \infty \tag{23}$$

If we then use the fact that the dispersion is **isotropic** (i.e. it only depends on the magnitude of $\vec{k}$) we can write this as an integral over all of $\mathbb{R}^3$:

$$\sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to 4\left(\frac{L}{2\pi}\right)^3 \int_{-\infty}^\infty dk_x \int_{-\infty}^\infty dk_y \int_{-\infty}^\infty dk_z \, F(\varepsilon_{|\vec{k}|}) \tag{24}$$

$$= 4\left(\frac{L}{2\pi}\right)^3 4\pi \int_0^\infty dk \, k^2 F(\varepsilon_k) \tag{25}$$

where in the last line we went to spherical coordinates and integrated over the solid angle. Making a change of variables to $\varepsilon = c\hbar k$ gives the final result:

$$\sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} F(\varepsilon_{\vec{k}}) \to \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) F(\varepsilon) \tag{26}$$

where the density of states is

$$\boxed{\mathcal{D}(\varepsilon) = 2\pi \frac{L^3}{(\pi\hbar c)^3} \varepsilon^2} \tag{27}$$

(b) As shown in Fig. 1, as $T \to 0$ the Fermi-Dirac distribution $f(\varepsilon)$ approaches a step function:

$$f(\varepsilon) \underset{T=0}{\to} \begin{cases} 1, & \text{if } \varepsilon < \mu(T=0) \\ 0, & \text{if } \varepsilon > \mu(T=0). \end{cases} \tag{28}$$

(c) From (2), the number of particles is given by

$$N = \sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} f(\varepsilon_{\vec{k}}) \to \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) f(\varepsilon). \tag{29}$$

(Note that the abstract label m in (2) refers to whatever collection of quantum numbers have to specified to specify the single-particle quantum state. In the context of this problem, those quantum numbers are the wavevector $\vec{k}$ and the spin m_s.)

Using (27), we have

$$N = \int_0^{\varepsilon_F} d\varepsilon \, 2\pi \frac{V}{(\pi\hbar c)^3} \varepsilon^2 = 2\pi \frac{V}{(\pi\hbar c)^3} \frac{\varepsilon_F^3}{3} \tag{30}$$

Therefore

$$\boxed{\varepsilon_F = \hbar c \left(\frac{3\pi^2 n}{2} \right)^{1/3}.} \tag{31}$$

(d) From (4),

$$U = \sum_{m_s=-3/2}^{3/2} \sum_{\vec{k}} f(\varepsilon_{\vec{k}}) \varepsilon_{\vec{k}} \to \int_0^\infty d\varepsilon \, \mathcal{D}(\varepsilon) f(\varepsilon) \varepsilon \tag{32}$$

At $T = 0$, the system will be in the ground state, and again the Fermi-Dirac distribution function is a step-function. Following the same procedure as part (b) one obtains

$$\boxed{U(T=0) = \frac{3}{4} N \varepsilon_F.} \tag{33}$$

Let's think about this result for a moment. If each of the N particles in the system had energy equal to the Fermi energy, then we would have $U = N\varepsilon_F$. But most particles have energy less than ε_F, and no particles have energy greater than ε_F because $T = 0$. So the actual ground state energy is lower.

(e) Using $U = \frac{3}{4} N \varepsilon_F$ and $F = U$, we have

$$p = -\left(\partial F / \partial V\right)_{T,N} \tag{34}$$

$$= -\left(\partial U / \partial V\right)_{T,N} \tag{35}$$

$$= \frac{3}{4} N \left(\partial \varepsilon_F / \partial V\right)_{T,N}. \tag{36}$$

From (31), we have

$$\left(\partial \varepsilon_F / \partial V\right)_{T,N} = -\frac{1}{3} \frac{\varepsilon_F}{n}. \tag{37}$$

Inserting this gives

$$p = \frac{3}{4} N \frac{1}{3} \frac{\varepsilon_F}{n} = \frac{U}{3V}. \tag{38}$$