

Answers F

Problem 7.28

a) We consider a free Fermi gas of spin-1/2 particles in two dimensions. The single particle states have energies

$$\epsilon = \frac{h^2}{8mA} (n_x^2 + n_y^2), \quad n_x \in \{1, 2, 3, \dots\}, \quad n_y \in \{1, 2, 3, \dots\}.$$

The number of particles is

$$N = 2 \int_0^{\pi/2} d\phi \int_0^{n_{\max}} n dn = \frac{\pi}{2} n_{\max}^2 \quad \text{so} \quad n_{\max}^2 = \frac{2N}{\pi}.$$

The Fermi energy is hence

$$\epsilon_F = \frac{h^2}{8mA} n_{\max}^2 = \frac{h^2 N}{4\pi mA},$$

and the average energy per particle is

$$\frac{U}{N} = \frac{2}{N} \int_0^{\pi/2} d\phi \int_0^{n_{\max}} n \epsilon dn = \frac{\pi h^2}{8mA N} \int_0^{n_{\max}} n^3 dn = \frac{\pi h^2 n_{\max}^4}{32mA N} = \frac{h^2 N}{8\pi mA} = \frac{\epsilon_F}{2}.$$

b) Note that

$$N = \int_0^{\epsilon_F} g(\epsilon) d\epsilon = 2 \int_0^{\pi/2} d\phi \int_0^{n_{\max}} n dn = \pi \int_0^{n_{\max}} n dn.$$

We change variables utilizing

$$\epsilon = \frac{h^2 n^2}{8mA} \Leftrightarrow n = \sqrt{\frac{8mA\epsilon}{h^2}} \Rightarrow dn = \sqrt{\frac{8mA}{h^2}} \frac{1}{2\sqrt{\epsilon}} d\epsilon$$

and obtain

$$N = \int_0^{\epsilon_F} \frac{4\pi mA}{h^2} d\epsilon.$$

We hence conclude that

$$g(\epsilon) = \begin{cases} \frac{4\pi mA}{h^2} & \text{for } \epsilon > 0, \\ 0 & \text{otherwise.} \end{cases}$$

c) Let us first note that

$$\frac{1}{e^{\frac{\epsilon-\mu}{kT}} + 1} = \frac{e^{-\frac{\epsilon-\mu}{kT}}}{1 + e^{-\frac{\epsilon-\mu}{kT}}} = \frac{1 + e^{-\frac{\epsilon-\mu}{kT}}}{1 + e^{-\frac{\epsilon-\mu}{kT}}} - \frac{1}{1 + e^{-\frac{\epsilon-\mu}{kT}}} = 1 - \frac{1}{1 + e^{-\frac{\epsilon-\mu}{kT}}}.$$

This result means that the probability for a state at energy $\epsilon = \mu + \Delta$ to be occupied by a particle is the same as the probability for a state at energy $\epsilon = \mu - \Delta$ to be unoccupied.

As long as the temperature is small enough that the probability for a state at $\epsilon = 0$ to be occupied by a particle is practically unity, it follows that the number of particles we remove at energies below ϵ_F is equal to the number of particles we add at energies above ϵ_F , if we keep $\mu = \epsilon_F$ also at nonzero temperature. Therefore the chemical potential will remain unchanged and is hence independent of T .

When T gets sufficiently large, however, we begin to see that $g(\epsilon)$ is zero for negative ϵ . If we keep μ at ϵ_F , we will remove fewer particles below ϵ_F than we add above ϵ_F , giving an increase in the number of particles. To keep the number of particles fixed, we need the chemical potential to be smaller than ϵ_F for high T . The effect is larger, the larger the temperature is, and therefore the chemical potential decreases with temperature for high T .

d) We have

$$N = \int_0^\infty g(\epsilon) \frac{1}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon = \frac{4\pi mA}{h^2} \int_0^\infty \frac{1}{e^{\beta(\epsilon-\mu)} + 1} d\epsilon = \frac{4\pi mkTA}{h^2} \int_{-\frac{\mu}{kT}}^\infty \frac{1}{e^x + 1} dx.$$

Note that

$$\begin{aligned} \int_{-\frac{\mu}{kT}}^\infty \frac{1}{e^x + 1} dx &= \int_{-\frac{\mu}{kT}}^\infty \frac{e^{-x}}{1 + e^{-x}} dx = \sum_{n=0}^\infty \int_{-\frac{\mu}{kT}}^\infty e^{-x} (-e^{-x})^n dx \\ &= \sum_{n=0}^\infty (-1)^n \int_{-\frac{\mu}{kT}}^\infty e^{-(n+1)x} dx = \sum_{n=0}^\infty (-1)^n \left[-\frac{1}{n+1} e^{-(n+1)x} \right]_{-\frac{\mu}{kT}}^\infty \\ &= \sum_{n=0}^\infty (-1)^n \frac{1}{n+1} \left(e^{\frac{\mu}{kT}} \right)^{n+1} = \sum_{n=1}^\infty (-1)^{n+1} \frac{1}{n} \left(e^{\frac{\mu}{kT}} \right)^n = \ln \left(1 + e^{\frac{\mu}{kT}} \right) \end{aligned}$$

Inserting this into the expression for N , we obtain

$$N = \frac{4\pi mkTA}{h^2} \ln \left(1 + e^{\frac{\mu}{kT}} \right),$$

which we rearrange into

$$\mu = kT \ln \left(e^{\frac{Nh^2}{4\pi mkTA}} - 1 \right) = kT \ln \left(e^{\epsilon_F/(kT)} - 1 \right).$$

For $kT \ll \epsilon_F$, the exponential is large, and we can neglect the -1 . We hence obtain

$$\mu \approx \frac{Nh^2}{4\pi mA} = \epsilon_F.$$

The chemical potential is hence independent of T and equals the Fermi energy as expected.

For $kT \gg \epsilon_F$, we can Taylor expand the exponential to first order, which gives

$$\mu \approx kT \ln \left(\frac{Nh^2}{4\pi mkTA} \right) = kT \ln \left(\frac{\epsilon_F}{kT} \right).$$

When $kT \gg \epsilon_F$, the argument of the logarithm is less than one and the logarithm is therefore negative. Increasing T in the high temperature limit, therefore makes μ more

and more negative as expected.

e) Adapting equation (6.93) in Schroeder to two dimensions gives

$$\mu_{\text{ideal gas}} = -kT \ln \left(\frac{2\pi mkTA}{h^2 N} Z_{\text{int}} \right).$$

In our case the particles have two different spin states with the same energy. Therefore $Z_{\text{int}} = 2$ and we see that the result agrees with the chemical potential in the high temperature limit found above.

Problem F1

a) The possible system states are



The first three states have energy -2ϵ , the fourth state has energy 2ϵ , and the last two states have energy 0 , so the partition function is

$$Z = 3e^{2\beta\epsilon} + 2 + e^{-2\beta\epsilon}, \quad \beta = \frac{1}{kT}.$$

b) The partition function is now

$$Z = e^{2\beta\epsilon} + 2e^{-\beta(U-2\epsilon)} + 2 + e^{-\beta(U+2\epsilon)},$$

and the average energy is

$$E(T) = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = \frac{-2\epsilon e^{2\beta\epsilon} + 2(U-2\epsilon)e^{-\beta(U-2\epsilon)} + (2\epsilon+U)e^{-\beta(U+2\epsilon)}}{e^{2\beta\epsilon} + 2e^{-\beta(U-2\epsilon)} + 2 + e^{-\beta(U+2\epsilon)}}.$$

c) The entropy is

$$S(T) = \frac{E - F}{T} = \frac{E}{T} + k \ln(Z) = k \frac{-2\beta\epsilon e^{2\beta\epsilon} + 2\beta(U-2\epsilon)e^{-\beta(U-2\epsilon)} + \beta(U+2\epsilon)e^{-\beta(U+2\epsilon)}}{e^{2\beta\epsilon} + 2e^{-\beta(U-2\epsilon)} + 2 + e^{-\beta(U+2\epsilon)}} + k \ln(e^{2\beta\epsilon} + 2e^{-\beta(U-2\epsilon)} + 2 + e^{-\beta(U+2\epsilon)}).$$

In the high temperature limit, we obtain

$$\lim_{T \rightarrow \infty} S(T) = \lim_{\beta \rightarrow 0} S(T) = k \frac{0}{1+2+2+1} + k \ln(1+2+2+1) = k \ln(6).$$

In the high temperature limit, all six states are equally probable, since this maximizes the entropy of the system. The entropy is hence $k \ln(6)$.

We now consider the low temperature limit and $U < 0$. In this case the energy of the ground state is $-2\epsilon + U$. We therefore rewrite the entropy into

$$S(T) = k \frac{4\beta\epsilon e^{-4\beta\epsilon} - \beta U e^{\beta U} - 2\beta(U-2\epsilon)e^{\beta(U-2\epsilon)}}{e^{\beta U} + 2 + 2e^{\beta(U-2\epsilon)} + e^{-4\beta\epsilon}} + k \ln(e^{\beta U} + 2 + 2e^{\beta(U-2\epsilon)} + e^{-4\beta\epsilon}).$$

Since $xe^{-x} \rightarrow 0$ for $x \rightarrow \infty$, and remembering that $U < 0$, we conclude that

$$\lim_{T \rightarrow 0} S(T) = \lim_{\beta \rightarrow \infty} S(T) = k \frac{0 + 0 + 0}{0 + 2 + 0 + 0} + k \ln(0 + 2 + 0 + 0) = k \ln(2).$$

We obtain this limit, since the system is in the ground state for $T \rightarrow 0$, and the ground state has degeneracy 2 for $U < 0$.

Next we consider the low temperature limit, when $U > 0$. In this case, the ground state is the state with energy -2ϵ . We hence rewrite the entropy into

$$S(T) = k \frac{2\beta U e^{-\beta U} + 4\beta \epsilon e^{-2\beta \epsilon} + \beta(U + 4\epsilon)e^{-\beta(U+4\epsilon)}}{1 + 2e^{-\beta U} + 2e^{-2\beta \epsilon} + e^{-\beta(U+4\epsilon)}} + k \ln(1 + 2e^{-\beta U} + 2e^{-2\beta \epsilon} + e^{-\beta(U+4\epsilon)}).$$

From this we conclude that

$$\lim_{T \rightarrow 0} S(T) = \lim_{\beta \rightarrow \infty} S(T) = k \frac{0 + 0 + 0}{1 + 0 + 0 + 0} + k \ln(1 + 0 + 0 + 0) = 0.$$

We obtain this limit, since the system is in the ground state for $T \rightarrow 0$, and the ground state is nondegenerate for $U > 0$. This gives the entropy $k \ln(1) = 0$.

Summarizing,

$$\lim_{T \rightarrow 0} S(T) = \begin{cases} k \ln(2) & \text{for } U < 0, \\ 0 & \text{for } U > 0. \end{cases}$$

Problem F2

a) The grand partition function for a single binding point is

$$\mathcal{Z} = 1 + 2 \sum_{j=0}^{\infty} e^{-\beta(jhf - \mu)} = 1 + \frac{2e^{\beta\mu}}{1 - e^{-\beta hf}} \Rightarrow g(x) = \frac{2}{1 - e^{-x}}.$$

b) The average vibrational energy of bound electrons in a given binding point is

$$E(T) = \frac{2}{\mathcal{Z}} \sum_{j=0}^{\infty} jhf e^{-\beta(jhf - \mu)} = \frac{2hf e^{-\beta(hf - \mu)}}{\mathcal{Z}(1 - e^{-\beta hf})^2} = \frac{2hf e^{-\beta(hf - \mu)}}{(1 - e^{-\beta hf})(1 - e^{-\beta hf} + 2e^{\beta\mu})}.$$

c) The average number of electrons bound to the binding point is

$$N_b = \frac{2e^{\beta\mu} \frac{1}{1 - e^{-\beta hf}}}{1 + 2e^{\beta\mu} \frac{1}{1 - e^{-\beta hf}}} = \frac{2e^{\beta\mu}}{1 - e^{-\beta hf} + 2e^{\beta\mu}}.$$

When T goes to zero, the chemical potential approaches the Fermi energy, which is positive. The low temperature limit is therefore

$$\lim_{T \rightarrow 0} N_b = 1.$$

When T is large compared to the Fermi temperature, the chemical potential is given by (6.93) in Schroeder with $Z_{\text{int}} = 2$. This leads to

$$N_b \approx \frac{nV_Q}{1 - e^{-\beta hf} + nV_Q} \text{ for } T \gg T_F, \text{ where } V_Q = \left(\frac{h^2}{2\pi mkT} \right)^{3/2}.$$

Problem F3

a) The partition function for a single particle in the quantum well is

$$Z_1 = 1 + 2e^{-\beta\epsilon} + e^{-2\beta\epsilon}, \quad \beta = \frac{1}{kT},$$

and the average energy is

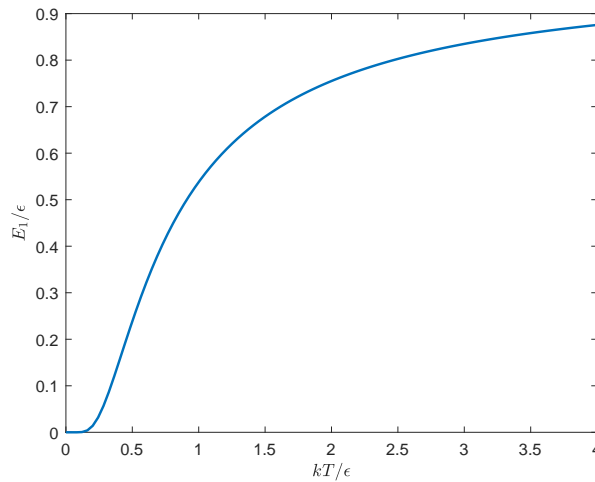
$$E_1 = -\frac{1}{Z_1} \frac{\partial Z_1}{\partial \beta} = 2\epsilon \frac{1 + e^{-\beta\epsilon}}{e^{\beta\epsilon} + 2 + e^{-\beta\epsilon}} = \frac{2\epsilon}{e^{\beta\epsilon} + 1}.$$

The limits are

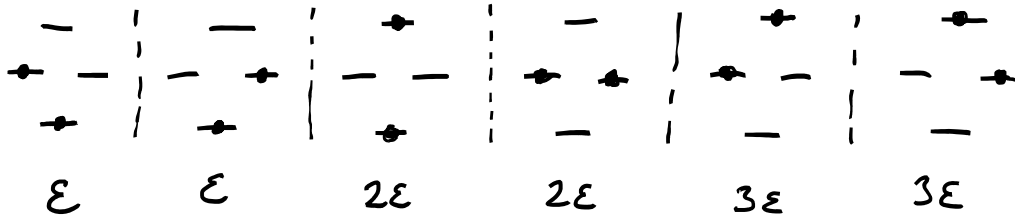
$$\lim_{T \rightarrow 0} E_1 = 0 \quad \text{and} \quad \lim_{T \rightarrow \infty} E_1 = \epsilon.$$

For $T = 0$, the particle sits in the ground state, which has energy 0, and for $T \rightarrow \infty$, the particle has equally large probability to sit in all 4 states, so the average energy is the average energy of the 4 states.

Plot of the energy E_1 as a function of the temperature



b) The possible system states and their energies are



This gives the partition function

$$Z_2 = 2(e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon}).$$

c) The average energy is

$$E_2 = -\frac{1}{Z_2} \frac{\partial Z_2}{\partial \beta} = \epsilon \frac{1 + 2e^{-\beta\epsilon} + 3e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}} = \epsilon + \epsilon \frac{e^{-\beta\epsilon} + 2e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}},$$

and the limits are

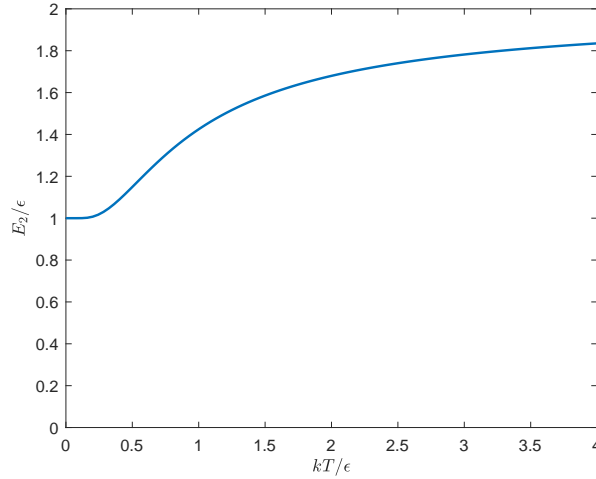
$$\lim_{T \rightarrow 0} E_2 = \epsilon + \epsilon \frac{0+0}{1+0+0} = \epsilon$$

and

$$\lim_{T \rightarrow \infty} E_2 = \epsilon + \epsilon \frac{1+2}{1+1+1} = 2\epsilon.$$

For $T = 0$, the system is in one of the two ground states with energy ϵ , and for $T \rightarrow \infty$, the system has equally large probability to sit in all 6 states, which gives an average energy of 2ϵ .

Plot of the energy E_2 as a function of the temperature



d) The entropy can be computed from

$$S_2 = \frac{E_2 - F}{T} = \frac{E_2}{T} + k \ln(Z_2).$$

This gives

$$S_2 = k\beta\epsilon \frac{1 + 2e^{-\beta\epsilon} + 3e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}} + k \ln [2(e^{-\beta\epsilon} + e^{-2\beta\epsilon} + e^{-3\beta\epsilon})].$$

We can also write this as

$$S_2 = k \frac{\beta\epsilon e^{-\beta\epsilon} + 2\beta\epsilon e^{-2\beta\epsilon}}{1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}} + k \ln(2) + k \ln(1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon}).$$

From this we obtain the limits

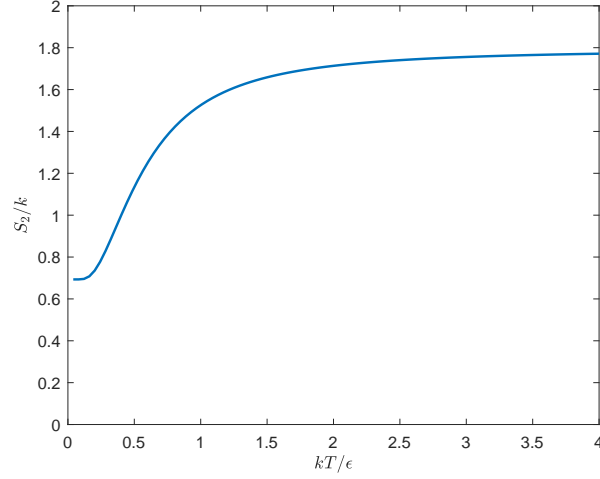
$$\lim_{T \rightarrow 0} S_2 = k \frac{0+0}{1+0+0} + k \ln(2) + k \ln(1+0+0) = k \ln(2)$$

and

$$\lim_{T \rightarrow \infty} S_2 = k \frac{0+0}{1+1+1} + k \ln(2) + k \ln(1+1+1) = k \ln(6).$$

The limits can be understood from $S = k \ln(\Omega)$. For $T = 0$, there are two ground states accessible for the system, that is $\Omega = 2$, and for $T \rightarrow \infty$ all 6 states are equally probably, so $\Omega = 6$.

Plot of the entropy S_2 as a function of the temperature



Problem Hand-in F

a) The grand partition function for the case of fermions is

$$Z = 1 + e^{\beta(\epsilon+\mu)} + e^{-\beta(\epsilon-\mu)} + e^{2\beta\mu} = (e^{\beta(\epsilon+\mu)} + 1) (e^{-\beta(\epsilon-\mu)} + 1), \quad \beta = \frac{1}{kT}.$$

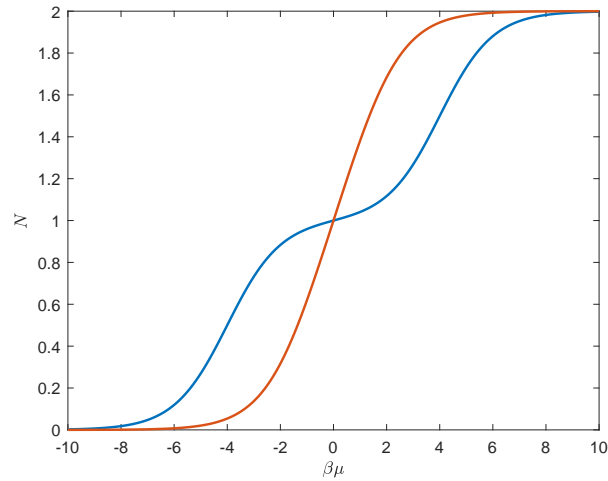
b) The average number of fermions in the system is

$$N = \frac{e^{\beta(\epsilon+\mu)} + e^{-\beta(\epsilon-\mu)} + 2e^{2\beta\mu}}{1 + e^{\beta(\epsilon+\mu)} + e^{-\beta(\epsilon-\mu)} + e^{2\beta\mu}} = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} + \frac{1}{e^{-\beta(\epsilon+\mu)} + 1},$$

and the limits are

$$\lim_{\mu \rightarrow -\infty} N = 0 \quad \text{and} \quad \lim_{\mu \rightarrow \infty} N = 2.$$

Plot of N as a function of $\beta\mu$ for $\beta\epsilon = 1$ (red curve) and $\beta\epsilon = 4$ (blue curve)



c) The grand partition function for the case of bosons is

$$Z = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} e^{-\beta((m-n)\epsilon - \mu(m+n))} = \sum_{n=0}^{\infty} e^{n\beta(\epsilon+\mu)} \sum_{m=0}^{\infty} e^{-m\beta(\epsilon-\mu)} = \frac{1}{1 - e^{\beta(\epsilon+\mu)}} \cdot \frac{1}{1 - e^{-\beta(\epsilon-\mu)}}.$$

d) According to the Bose-Einstein distribution, the number of bosons in a single particle state with energy x is

$$\bar{n}_{\text{BE}} = \frac{1}{e^{\beta(x-\mu)} - 1}.$$

The number of bosons in the system is the number of bosons in the single particle state with energy $-\epsilon$ plus the number of bosons in the single particle state with energy ϵ , that is

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

The limits are

$$\lim_{\mu \rightarrow -\infty} N = 0 \quad \text{and} \quad \lim_{\mu \rightarrow -\epsilon} N = \infty.$$

There can be infinitely many particles in the system, and this is achieved for μ approaching $-\epsilon$ from the left.

Plot of N as a function of $\beta\mu$ for $\beta\epsilon = 1$

