Oblig 4 - FYS2160

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a)

From Schroeder's equation (7.20) we have that the probability of a single-particle state being occupied by n particles from the Gibbs factor:

$$P(n) = \frac{1}{Z} \exp(-n(\epsilon-\mu)/kT) \tag{1}$$

where Z is the grand partition function which is the sum of all the Gibbs factors for all possible n:

$$Z = \sum_n \exp(-n(\epsilon-\mu)/kT) \tag{2}$$

To derive the Fermi-Dirac distribution we take a look at fermions (e.g. electrons). The Pauli exclusion principle tells us that no more than one fermion can occupy the same state at the same time, so the possible n values are just zero or one, we can then write the grand partition function as

$$Z_F = P(0) + P(1) = 1 + \exp(-(\epsilon-\mu)/kT) \tag{3}$$

Now we can derive the Fermi-Dirac distribution by calculating the occupancy of the state which is the average number of particles of the state by finding the average n, but again we only have $n = 0$ and $n = 1$:

$$\begin{aligned}
\bar{n}_F &= \sum_n P(n) = 0p(0) + 1P(1) \\
&= \frac{1}{Z} \exp(-(\epsilon-\mu)/kT) \\
&= \frac{\exp(-(\epsilon-\mu)/kT)}{1 + \exp(-(\epsilon-\mu)/kT)} \\
&= \underline{\frac{1}{\exp(\epsilon-\mu/kT) + 1}}
\end{aligned}$$

and this is the Fermi-Dirac distribution function

$$f(\epsilon, \mu, T) = \frac{1}{1 + \exp(\epsilon-\mu/kT)} \tag{4}$$

At $T = 0$ the distribution becomes the step function as shown in figure 1, and at $T > 0$ the function looks as shown in figure 2 where increasing T increases the curvature of the graph.

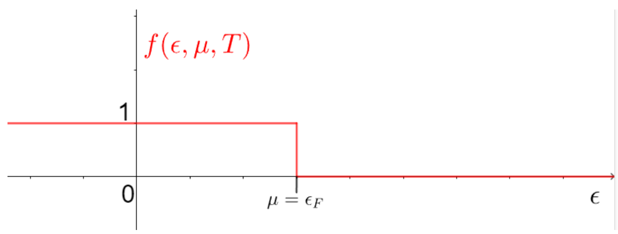

Figure 1: The Fermi-Dirac distribution function $f(\epsilon, \mu, T)$ for $T = 0$, which becomes a step function.

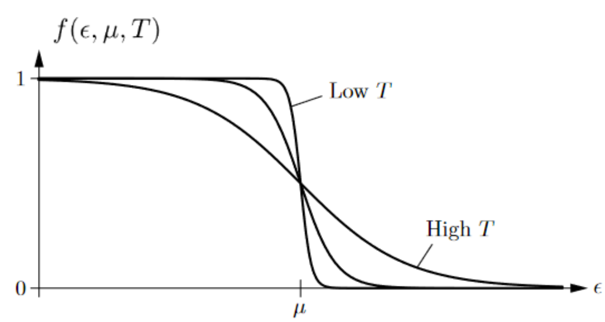

Figure 2: The Fermi-Dirac distribution function $f(\epsilon, \mu, T)$ for $T > 0$.

b)

To find the density of states $D(\epsilon)$ which is the number of single-particle states per unit energy we first take a look at the total energy U. We can write this as a sum or integral of all unit energies ϵ multiplied with the density of each state:

$$U = \int_0^{\epsilon_F} \epsilon D(\epsilon) d\epsilon \tag{5}$$

where ϵ_F is the Fermi energy.

Using Schroeder's expression (7.40) for the total energy we can write it for two dimensions and the convert it to circular coordinates like so

$$\begin{aligned} U &= 2 \int\int \epsilon(\vec{n})\ dn_x dn_y \\ &= 2 \int_0^{n_{max}} \int_0^{\pi/2} \epsilon(n)\ n\ dn d\theta \end{aligned}$$

where n_{max} is the highest n_i-value.

We integrate a quarter of a full circle since we are interested in non-negative n_x, n_y values

$$= \pi \int_0^{n_{max}} \epsilon(n)\ n\ dn$$

now we convert the integral from dn to $d\epsilon$ using the following expressions we have:

$$\begin{aligned} \epsilon(n_x, n_y) &= \frac{\hbar^2\pi^2}{2mA}(n_x^2 + n_y^2) \\ \Rightarrow \epsilon(n) &= \frac{\hbar^2\pi^2}{2mA} n^2 \\ \Rightarrow n &= \sqrt{\frac{2mA}{\hbar^2\pi^2}}\sqrt{\epsilon} \\ \Rightarrow \frac{dn}{d\epsilon} &= \sqrt{\frac{2mA}{\hbar^2\pi^2}}\frac{1}{2\sqrt{\epsilon}} \end{aligned}$$

we put this last expression into our integral and change it to integrate over ϵ:

$$\begin{aligned} U &= \pi \int_0^{\epsilon_F} \epsilon \sqrt{\frac{2mA}{\hbar^2\pi^2}}\sqrt{\epsilon}\ sqrt\frac{2mA}{\hbar^2\pi^2}\frac{1}{2\sqrt{\epsilon}}\ d\epsilon \\ &= \int_0^{\epsilon_F} \epsilon \left[\pi\sqrt{\frac{2mA}{\hbar^2\pi^2}}\sqrt{\epsilon}\ \sqrt{\frac{2mA}{\hbar^2\pi^2}}\frac{1}{2\sqrt{\epsilon}}\right]\ d\epsilon \\ &= \int_0^{\epsilon_F} \epsilon \left[\frac{mA}{\hbar^2\pi}\right]\ d\epsilon \end{aligned}$$

we recognize the bracketed part as $D(\epsilon)$ from (5):

$$\begin{aligned} \Rightarrow D(\epsilon) &= \frac{mA}{\pi\hbar^2} \\ &= bA \end{aligned} \tag{6}$$

with $b = {}^{m}/_{\pi\hbar^2}$.

c)

The chemical potential at $T = 0$ is also called the Fermi Energy ϵ_F which we can derive from the thermodynamic potential

$$dU = TdS - PdV + \mu dN$$

$$dU = TdS - \sigma dA + \mu dN \tag{7}$$

$$\Rightarrow = \mu = \left(\frac{dU}{dN}\right)_{S,A} \tag{8}$$

for the total energy we go back to our integral

$$\begin{aligned} U &= \pi \int_0^{n_{max}} \epsilon(n)\ n\ dn \\ &= \pi \int_0^{n_{max}} \frac{\hbar^2\pi^2}{2mA}\ n^3\ dn \\ &= \pi \frac{\pi}{2bA} \int_0^{n_{max}} n^3\ dn \\ &= \frac{\pi^2}{8bA} n_{max}^4 \end{aligned}$$

Now we want to write U as a function of N, we can write N as twice the area of the quarter-circle (see Schroeder chapter 7.3 page 273-274):

$$\begin{aligned} N &= 2 \cdot \frac{1}{4}\pi n_{max}^2 \\ &= \frac{\pi}{2} n_{max}^2 \\ \Rightarrow n_{max}^4 &= \frac{4}{\pi^2}N^2 \end{aligned}$$

combining these two expressions we can write $U(N)$ as

$$U(N) = \frac{N^2}{2bA} \tag{9}$$

this can also be calculated from $U = \int_0^\infty \epsilon D(\epsilon) f(\epsilon, \mu, T = 0)\ d\epsilon$ by using the fact that the FD distribution f becomes the step function/becomes piecewise at $T = 0$ and split the integral into the sum of two integrals.

From the above expression we can differentiate and derive $\mu(T = 0) = \epsilon_F$:

$$\begin{aligned}\mu(T=0) &= \left(\frac{dU}{dN}\right)_{S,A} \\ &= \frac{d}{dN}\left(\frac{N^2}{2bA}\right) \\ &= \frac{N}{Ab}\end{aligned} \tag{10}$$

d)

We first use Schroeder's equation (7.53) to find N:

$$\begin{aligned}N &= \int_0^\infty D(\epsilon) f(\epsilon, \mu, T > 0)\ d\epsilon \\ &= bA \int_0^\infty \frac{1}{1 + \exp(\epsilon - u/kT)}\ d\epsilon \\ &= bA \ln(\exp(\mu/kT) + 1)kT \\ \ln(\exp(\mu/kT) + 1) &= \frac{N}{bAkT} \\ \exp(\mu/kT) + 1 &= \exp\left(\frac{N}{bAkT}\right) \\ \frac{\mu}{kT} &= \ln\left(\exp\left(\frac{N}{bAkT}\right) - 1\right) \\ \mu(N, A) &= kT \ln\left(\exp\left(\frac{N}{bAkT}\right) - 1\right)\end{aligned} \tag{11}$$

e)

Using (11) we get that μ is zero for

$$\begin{aligned}\ln\left(\exp\left(\frac{N}{bAkT}\right) - 1\right) &= 0 \\ \exp\left(\frac{N}{bAkT}\right) - 1 &= 1 \\ \frac{N}{bAkT} &= \ln(2) \\ T &= \underline{\frac{N}{Abk \ln(2)}}\end{aligned}$$

f)

The classical limit is where the number of particles in a given state is much smaller than one. This also means that:

$$\begin{aligned}f(\epsilon, \mu, T) &\ll 1 \\ \frac{1}{1 + \exp(\epsilon - \mu/kT)} &\ll 1 \\ \Rightarrow \exp(\epsilon - \mu/kT) &\gg 1 \\ \Rightarrow f(\epsilon, \mu, T) = \frac{1}{1 + \exp(\epsilon - \mu/kT)} &\simeq \frac{1}{\exp(\epsilon - \mu/kT)}\end{aligned}$$

g)

We start off by holding S, N constant such that their differentials become zero which gives us

$$\begin{aligned}0 &= dU + \sigma dA - 0 \\ \Rightarrow \sigma &= -\left(\frac{\partial U}{\partial A}\right)_{S,N}\end{aligned} \tag{12}$$

Expressing σ as a derivative of Helmholtz free energy F we do the same, but we derive the identity for F by putting in the dU identity:

$$\begin{aligned}F &= U - TS \\ dF &= dU - TdS - SdT \\ dF &= dU - (dU + \sigma dA - \mu dN) - SdT \\ dF &= \underline{-\sigma dA + \mu dN - SdT}\end{aligned}$$

now we again hold the other two variables N, T constant such that we get

$$\begin{aligned}dF &= -\sigma dA + 0 - 0 \\ \Rightarrow \sigma &= -\left(\frac{\partial F}{\partial A}\right)_{T,N}\end{aligned} \tag{13}$$

h)

We begin with

$$
\begin{aligned}
dU &= TdS \\
dS &= \frac{dU}{T} \\
\int_0^S dS' &= \int_0^T \frac{dU}{T'} \\
S(T) &= \int_0^T \frac{1}{T'}\left(\frac{\partial U}{\partial T'}\right) dT' \\
S(T) &= \int_0^T \frac{1}{T'}\left(\frac{\partial U}{\partial T'}\right)_{A,N} dT' \\
S(T) &= \int_0^T \frac{C_A(T')}{T'} dT' \\
S(T) &= \frac{\pi^2}{3}k^2 bA\int_0^T \frac{T'}{T'} dT' \\
S(T) &= \frac{\pi^2}{3}k^2 bAT \\
S(T) &= M(b)AT \qquad (14)
\end{aligned}
$$

where we introduced the constant $M(b) = \frac{\pi^2}{3}k^2 b$.

i)

We use the identity, and I choose to hold N and A constant:

$$
\begin{aligned}
TdS &= dU \\
\int dU &= \int TdS \\
\int dU &= \int T\left(\frac{\partial S}{\partial T}\right)_{N,A} dT
\end{aligned}
$$

here we put in (14):

$$
\begin{aligned}
\int dU &= \int TM(b)AdT \\
\int_{U(0)}^{U(T)} dU &= M(b)A\int_T^0 T'dT' \\
U(T) - U(T=0) &= \frac{1}{2}MAT^2 \\
U(T) &= U(T=0) + \frac{1}{2}MAT^2
\end{aligned}
$$

To find $U(T=0)$ we use (8) and (10) to get

$$
\begin{aligned}
\mu &= \left(\frac{\partial U}{\partial N}\right)_{S,A} \\
\Rightarrow U(T=0) &= \int \mu(T=0)dN \\
U(T=0) &= \int \frac{N}{Ab}dN \\
U(T=0) &= \frac{N^2}{2Ab}
\end{aligned}
$$

Which gives us

$$U(T,A,N) = \frac{N^2}{2Ab} + \frac{1}{2}MAT^2 \qquad (15)$$

j)

Here we can't use (12) on (**??**) they don't have the same variables. Therefore I want to use (13):

$$
\begin{aligned}
F(N,A,T) &= U(N,A,T) - TS \\
&= \frac{N^2}{2Ab} + \frac{1}{2}MAT^2 - T\ MAT \\
&= \frac{N^2}{2Ab} - \frac{1}{2}MAT^2 \\
\Rightarrow \sigma &= -\frac{\partial}{\partial A}\left[\frac{N^2}{2Ab} - \frac{1}{2}MAT^2\right] \\
&= \frac{N^2}{2A^2b} + \frac{1}{2}MT^2
\end{aligned}
$$

$$\sigma = \frac{N^2}{2A^2b} + \frac{1}{2}MT^2 \qquad (16)$$

k)

We use the first law

$$
\begin{aligned}
\Delta U &= Q + W \\
&= Q + \sigma\Delta A \\
&= Q \\
\Rightarrow Q &= Q_{12} = U_2 - U_1
\end{aligned}
$$

Now we use the definition

$$
\begin{aligned}
C_A &= \left(\frac{\partial U}{\partial T}\right)_A \\
\Rightarrow C_A dT &= dU \\
\Rightarrow \int_{U_1}^{U_2} dU &= \int_{T_1}^{T_2} C_a dT \\
U_2 - U_1 = Q_{12} &= \int_{T_1}^{T_2} \frac{\pi^2}{3} k^2 bAT dT
\end{aligned}
$$

$$
Q_{12} = \frac{\pi^2}{6} k^2 bA(T_2^2 - T_1^2) \tag{17}
$$