Fys2160 – 2013 – Oblig 8

Density of states in one and two dimensions

The energy states of a particle in a box of size L are given as

$$\epsilon_n = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\left(n_x^2+n_y^2+n_z^2\right) , \tag{1}$$

for a three dimensional system. For a two and one dimensional system, the states have similar forms, but with only n_x for the one-dimensional case

$$\epsilon_{1d} = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\left(n_x^2\right) , \tag{2}$$

and with only n_x and n_y for the two-dimensional case:

$$\epsilon_{2d} = \frac{\hbar^2}{2m}\left(\frac{\pi}{L}\right)^2\left(n_x^2+n_y^2\right) . \tag{3}$$

(a) Show that the density of states $D_{1d}(\epsilon)$ for a free particle with spin 1/2 in one dimension is:

$$D_{1d}(\epsilon) = \left(\frac{L}{\pi}\right)\left(\frac{2m}{\hbar^2\epsilon}\right)^{1/2} . \tag{4}$$

(b) Show that the density of states $D_{12}(\epsilon)$ for a free particle with spin 1/2 in two dimensions is:

$$D_{2d}(\epsilon) = \frac{mL^2}{\pi\hbar^2} , \tag{5}$$

which is independent of ϵ.

(c) Plot or sketch the density of state as a function of energy in one, two, and three dimensions.

(d) (For discussion in class) Explain graphically why the initial curvature of $\mu(T)$ is upward in 1d and downward in 3d. (Hint: Set upt the integral for N and use the graphs to consider the behavior of the integrand from $T = 0$ to a finite temperature.)

Relativistic Fermi Gas

For relativistic electrons – that is for electrons where $\epsilon \gg mc^2$ – the energy is given as $\epsilon \simeq pc$, where p is the momentum. For a particle in a square box of size $L \times L \times L$, the momentum is

$$p = \frac{\pi\hbar}{L}\left(n_x^2+n_y^2+n_z^2\right)^{1/2} , \tag{6}$$

just as for non-relativistic electrons.

(a) Show that the density of states has the form

$$D(\epsilon) = \frac{\pi}{a^3}\epsilon^2 , \tag{7}$$

where $a = c\pi\hbar/L$.

(b) Show that the Fermi energy of a gas of N electrons is

$$\epsilon_F = \hbar c\pi\left(3n/\pi\right)^{1/3} , \tag{8}$$

where $n = N/V$.

(c) Show that the total energy when $T = 0$ is

$$U_0 = \frac{3}{4} N \epsilon_F \ . \tag{9}$$

Chemical potential in a Fermi Gas

For a Fermi-gas with N particles and volume V we can define the chemical potential μ by solving the following equation with respect to μ:

$$N = \int_0^\infty D(\epsilon) f(\epsilon, \mu, T)\, d\epsilon \ , \tag{10}$$

where the density of states, $D(\epsilon)$ for particles with spinn $1/2$ is given as

$$D(\epsilon) = \frac{3N}{2\epsilon_F^{3/2}} \epsilon^{1/2} = \frac{4V}{\sqrt{\pi}} \left(\frac{2\pi m}{h^2}\right)^{3/2} \epsilon^{1/2} \ , \tag{11}$$

and f is given as

$$f(\epsilon, \mu, T) = \frac{1}{1 + \exp\left(\frac{\epsilon - \mu}{kT}\right)} \ . \tag{12}$$

Equation 10 can be solved numerically to find $\mu(T)$, and we will here show how to proceed to do this.

In order to solve the equations numerically, it is useful to non-dimensionalize the equations. We do this by introducing a characteristic energy, ϵ_F, corresponding to the Fermi energy:

$$\epsilon_F = \frac{h^2}{8m} \left(\frac{3N}{\pi V}\right)^{2/3} \ . \tag{13}$$

Based on this energy, we introduce new dimensionless variables $t = kT/\epsilon_F$, $c = \mu/\epsilon_F$ and $x = \epsilon/\epsilon_F$.

(a) Show that equation 10 can be written as

$$1 = \frac{3}{2} \int_0^\infty \frac{x^{1/2}}{\exp((x - c)/t) + 1}\, dx \ , \tag{14}$$

using the dimensionless variables.

(b) What happens when $t = 0$? What is c in this case? Explain.

(c) Now we will find $c(t)$ numerically by varying c while holding t fixed until the integral gives the desired value. You should do this for t in the range from 0.1 to 2 and plot the results. (Hint: You can use the function `Integrate(F,0,Inf)` to find the integral of the function for a given set of values for t and c. You then need to adjust c until the integral becomes $2/3$.)

(d) Use your calculated values for $\mu(T)$ to find the energy $U(T)$ numerically for temperatures up to $t = 2$. Plot the result.

(e) Find the heat capacity as a function of temperature from your numerical calculation of the energy as a function of temperature.

(f) Plot the distribution function $f(\epsilon, \mu(T), T)$ as a function of ϵ for a range of values of T using your calculated values for $\mu(T)$. Comment on the results.

(g) (For discussion in class) Explain graphically why the initial curvature of $\mu(T)$ is upward in 1d and downward in 3d. (Hint: Use the integral for N and use the graphs to consider the behavior of the integrand from $T = 0$ to a finite temperature. You have found the density of states in 1d previously.)

End of Oblig 8