

# 1 Electrons I (FEG)

(a)

For a system at temperature  $T$  the free energy is given by

$$G(p, T) = E + pV - TS$$

where the pressure  $p$ , the volume  $V$  and the temperature  $T$  are connected through a state equation of the type  $\phi(p, V, T) = 0$  that depends on the system.

For  $T = 0$  equation 1 reduces to

$$G(p, T) = E + pV \quad (1)$$

where  $E$  is the energy of the system.

In the Free Fermi Electron Gas model the energy can be computed as

$$E(T) = \int_{E_{min}}^{E_{max}} d\epsilon \text{ DOS}(\epsilon) f_{FD}(\epsilon, T) \epsilon \quad (2)$$

where  $f_{FD}(\epsilon)$  is the Fermi-Dirac distribution

$$f_{FD}(\epsilon) = \frac{1}{e^{(\epsilon - \mu)/k_B T} + 1}$$

and indicates the average number of fermions in a single-particle state.

In the limit of zero temperature one gets

$$\lim_{T \rightarrow 0} E(T) = \int_{E_{min}}^{E_{max}} d\epsilon \lim_{T \rightarrow 0} \text{DOS}(\epsilon) f_{FD}(\epsilon, T) \epsilon \quad (3)$$

The 3D density of states function

$$\text{DOS}(\epsilon) = \frac{V}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon^{1/2} \quad (4)$$

does not depend on the temperature, while the Fermi-Dirac distribution function in the limit  $T \rightarrow 0$  reduces to

$$\lim_{T \rightarrow 0} f_{FD}(\epsilon) = \begin{cases} 1 & \text{if } \epsilon < \mu \\ \frac{1}{2} & \text{if } \epsilon = \mu \\ 0 & \text{if } \epsilon > \mu \end{cases} \quad (5)$$

so that 3 becomes

$$E \equiv E(T = 0) = \frac{V}{2\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \int_{E_{min}}^{E_{max}} \epsilon^{3/2} d\epsilon$$

In the last integral the extrema are  $E_{min} = 0$  and  $E_{max} = \epsilon_F$ ,.  $E_F$  is the Fermi energy which is, by definition, the energy of the last occupied state. Hence

$$E = \frac{V}{5\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon_F^{5/2} \quad (6)$$

and using the relation

$$\epsilon_F = \frac{\hbar^2}{2m} \left( \frac{3\pi^2 N}{V} \right)^{1/3}$$

one obtains

$$E = \frac{V}{5\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon_F^{5/2}$$

The pressure can then be calculated by the Maxwell relation

$$p = -\frac{\partial E}{\partial V} = \frac{2}{3} \frac{1}{5\pi^2 V^{2/3}} \frac{\hbar^2}{2m} (3\pi^2 N)^{5/3} = \frac{2}{3} \frac{E}{V}$$

so that

$$G = E + pV = \frac{5}{3} E = \frac{2}{3} \frac{V}{5\pi^2} \left( \frac{2m}{\hbar^2} \right)^{3/2} \epsilon_F^{5/2}$$

which can be rearranged as

$$G = N\epsilon_F$$

Equating this result to the formula given in the text of the exercise  $G = N\mu$  one concludes that at temperature  $T = 0$

$$\epsilon_F = \mu \quad (7)$$

(b)

By looking at figure 1, one can notice that for  $T = 0.01 T_F$  and  $T = 0.1 T_F$  (blue and green lines) the dashed curves overlap with the continuous lines. This means that the approximation  $\mu = \epsilon_F$  in the Fermi-Dirac distribution is legitimate. On the other side for  $T = T_F/2$  one can see that the dashed line does not overlap with the continuous one and in particular the maximum difference occurs at  $\epsilon = \epsilon_F$ , where the approximated function ( $\mu = \epsilon_F$ ) is always 1/2 and the true function is not. This means that the approximation is not anymore valid.

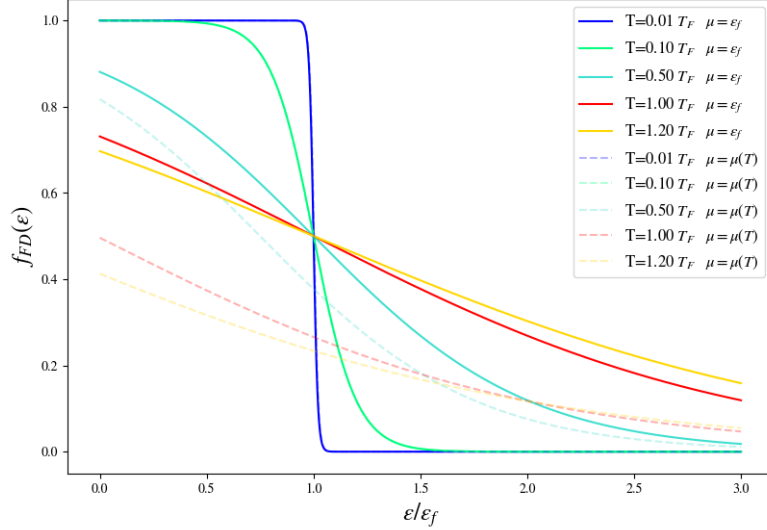


Figure 1: Fermi-Dirac distribution for various temperature values. The continuous lines correspond to the distribution drawn by keeping the chemical potential constant at  $\mu = \epsilon_F$ , while the dashed lines represent the true relations.

(c)

The number of orbitals whose energy is less than or equal to  $\epsilon$  is given by

$$N = \frac{V}{3\pi^2} \left( \frac{2m\epsilon}{\hbar^2} \right)^{3/2} \quad (8)$$

At  $T = 0$  all the electrons lie in the lowest-energy orbitals and the Fermi energy  $\epsilon_F$  corresponds to the energy of the last filled orbital. Hence in this particular case equation 8 gives exactly the number of electrons divided by 2 (there are 2 electrons for each orbital). By indicating with  $n$  the number of electrons, one has that

$$n = 2 \frac{V}{3\pi^2} \left( \frac{2m\epsilon_F}{\hbar^2} \right)^{3/2} \quad (9)$$

but on the other side

$$n = \int_0^{+\infty} 2DOS(\epsilon) f_{FD}(\epsilon) d\epsilon$$

One can now impose the equality between 9 and 1: in particular expression 1 is a function of the chemical potential  $\mu$  and the temperature  $T$  and the equation can be written as

$$N_0 = g(\mu, T)$$

where  $N_0$  is given by 9 and  $g(\mu, T)$ .

The equation can be solved numerically using the following procedure:

1. Fix a value for the temperature  $T_1$
2. The equation is now an equation in one variable  $\mu$  and can be solved via traditional numerical methods to obtain a corresponding value  $\mu_1$ .

3. Store the values  $(T_1, \mu_1)$

4. Select a value  $T_1$  and repeat from point 1)

In this way we obtain multiple couples  $(T_i, \mu_i)$  that can be plotted to give a graphical representation of the function  $\mu(T)$  (see figure 2)

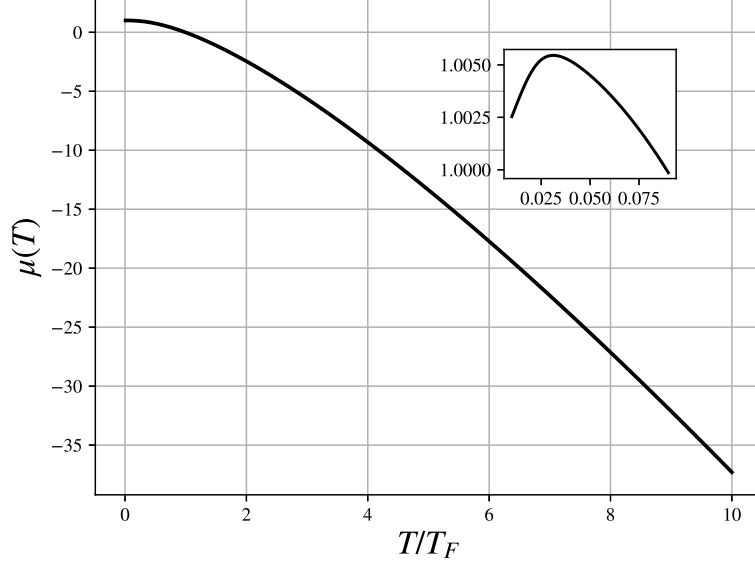


Figure 2: Chemical potential as a function of temperature. The small window on top right is a zoom on the low-temperature area. It shows that for low temperature the chemical potential dependence on the temperature can be well approximated by a parabola of the type  $\mu(T) = \mu(T=0) - \alpha T^2 = \epsilon_F - \alpha T^2$

(d)

The curves are already reported in figure 1 as dashed lines, but I report them here alone for clarity

(e)

The energy of the system can be computed as

$$E = \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, T) \epsilon d\epsilon$$

The electrons' heat capacity contribution is

$$C = \frac{dE}{dT} = \int_0^{+\infty} DOS(\epsilon) \frac{\partial f_{FD}(\epsilon, T)}{\partial T} \epsilon d\epsilon$$

Since the number of electrons is independent of the temperature the last expression is equivalent to

$$C = \frac{dE}{dT} - \epsilon_F \frac{dN}{dT} = \int_0^{+\infty} DOS(\epsilon) \frac{\partial f_{FD}(\epsilon, T)}{\partial T} (\epsilon - \epsilon_F) d\epsilon$$

Let us now consider the quantum limit  $k_B T \ll \epsilon_F$ : it can be easily seen from figure (REFFF) that  $\frac{df_{FD}}{d\epsilon}$  is significantly different from zero only in a small region of width  $2k_B T$  centered in  $\epsilon = \epsilon_F$ . Hence

$$C \approx DOS(\epsilon_F) \int_0^{+\infty} \frac{\partial f_{FD}(\epsilon, T)}{\partial T} (\epsilon - \epsilon_F) d\epsilon = DOS(\epsilon_F) k_B^2 T \int_{-\epsilon_F/k_B T}^{+\infty} \frac{e^x}{(e^x + 1)^2} dx$$

where I made the change of variable  $x = (\epsilon - \epsilon_F)/k_B T$  and I used the fact that

$$\frac{\partial f_{FD}(\epsilon, T)}{\partial T} = \frac{\epsilon - \epsilon_F}{k_B T^2} \frac{\exp((\epsilon - \epsilon_F)/k_B T)}{[\exp((\epsilon - \epsilon_F)/k_B T) + 1]^2}$$

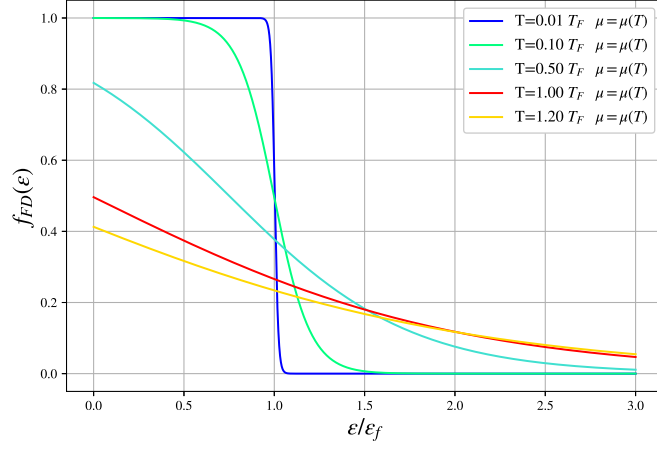


Figure 3: Fermi-Dirac distribution for various value of temperature. The dependence of the chemical  $\mu$  on the temperature is taken into account.

that is I used the approximation  $\mu \approx \epsilon_F$  (valid for the low temperature range). Since we assumed  $k_B T \ll \epsilon_F$  the lower extrema can be approximated to  $-\infty$ . The integral is now a known integral and the value is  $\pi^2/3$ . Using the fact that  $DOS(\epsilon_F) = \frac{3N}{2\epsilon_F}$  the estimated specific heat is

$$C \approx \frac{\pi^2}{2} N k_B^2 \frac{T}{E_F} = \frac{\pi^2}{2} N k_B \frac{T}{T_F}$$