

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.

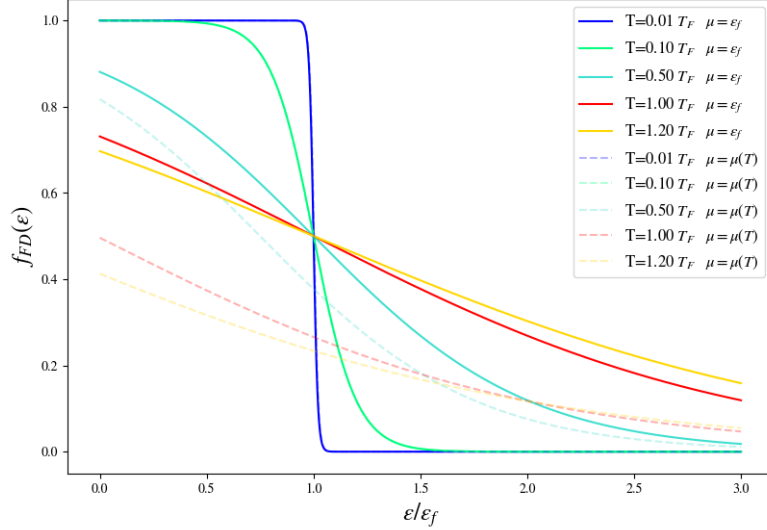


Figure 1: Fermi-Dirac distribution for various temperature values. The continuous lines correspond to the distribution drawn by keeping the chemical potential constant at $\mu = \epsilon_F$, while the dashed lines represent the true relations.

(c)

The number of orbitals whose energy is less than or equal to ϵ 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 ϵ_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 μ 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 μ and can be solved via traditional numerical methods to obtain a corresponding value μ_1 .

3. Store the values (T_1, μ_1)

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

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

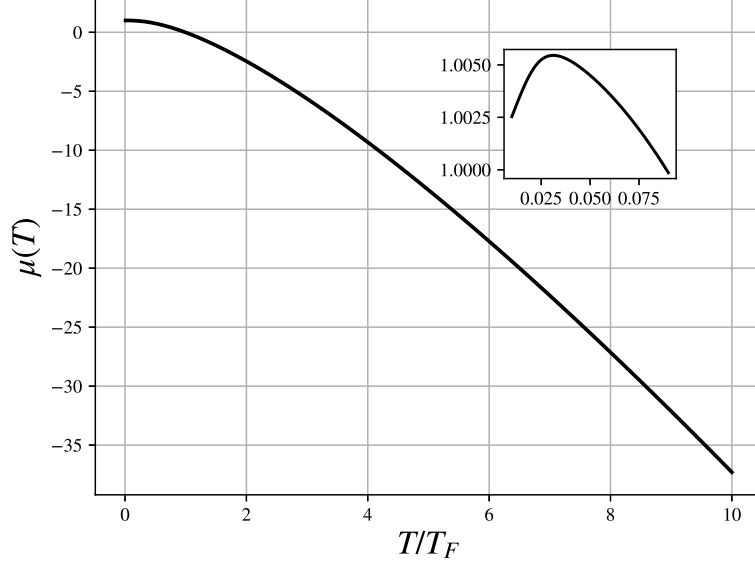


Figure 2: Chemical potential as a function of temperature. The small window on top right is a zoom on the low-temperature area. It shows that for low temperature the chemical potential dependence on the temperature can be well approximated by a parabola of the type $\mu(T) = \mu(T=0) - \alpha T^2 = \epsilon_F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

(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

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

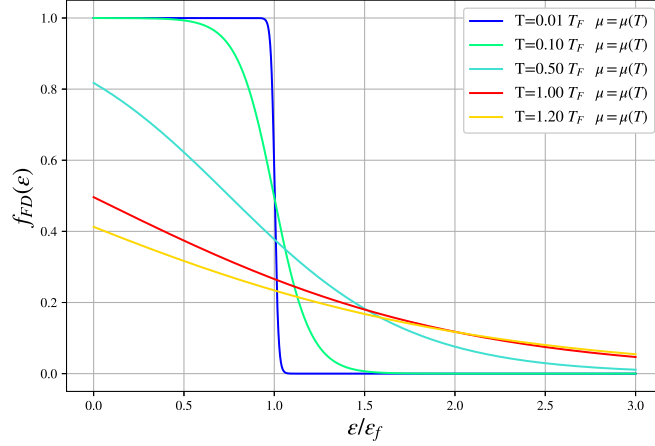


Figure 3: Fermi-Dirac distribution for various value of temperature. The dependence of the chemical μ on the temperature is taken into account.

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

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

2 Exercise II

Let us first consider a simple delta potential $V(x) = V_0 \delta(x)$ and the Schroedinger equation

$$-\frac{\hbar^2}{2m} \psi''(x) + V(x) \psi(x) = E \psi(x)$$

Let us integrate both members between $-\epsilon$ and $+\epsilon$ and let $\epsilon \rightarrow 0$, we obtain (in approximation for small ϵ)

$$\lim_{\epsilon \rightarrow 0} -\frac{\hbar^2}{2m} (\psi'(\epsilon) - \psi'(-\epsilon)) + V_0 \int_{-\epsilon}^{+\epsilon} \delta(x) \psi(x) = \lim_{\epsilon \rightarrow 0} 2\epsilon E \psi(0)$$

or

$$\psi'(0^+) - \psi'(0^-) = \frac{2mV_0}{\hbar^2} \psi(0)$$

This equation can be read as a condition on the discontinuity of the derivative of the function $\psi(x)$ across the δ .

Now let us return to the Dirac delta comb potential $V(x) = \sum_{n=-\infty}^{+\infty} \delta(x+na)$. The potential is clearly periodic with period a . Hence one can make use of the Bloch's theorem which states that the wavefunctions satisfy the conditions

$$\psi(x) = e^{iQx} u(x)$$

where $Q = \frac{2\pi}{na}$ and $u(x)$ satisfies in turn

$$u(x+na) = u(x)$$

One can now restrict the domain to $0 < x < a$ and solve the problem in this interval, imposing then the Bloch condition to obtain the solution to the complete theorem. For $0 < x < a$ the solution is a plane wave

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

By using the Bloch's theorem one can relate the solution for $a < x < 2a$

$$\frac{\psi(x)}{\psi(x+a)} = \frac{u(x) e^{iQx}}{u(x+a) e^{iQx} e^{iQa}} = e^{-iQa}$$

So that $\psi(x+a) = e^{iQa} \psi(x)$ Let us now impose the continuity of $\psi(x)$ and the discontinuity of $\psi'(x)$ on the edge between the two zones at $x = a$

$$\begin{cases} eq1 \end{cases}$$

which can be reduced

$$\cos(Qa) = \cos(ka) + \frac{V_0}{2ka} \sin(ka)$$

The admitted values of k for the system are those that satisfy the above equation. The corresponding energies are then $E_k = \frac{\hbar^2 k^2}{2m}$. The last equation has solution only if $|\cos(ka) + \frac{V_0}{2ka} \sin(ka)| < 1$. For $|\cos(ka) + \frac{V_0}{2ka} \sin(ka)| > 1$ there are no solutions: this means that therethose k -vectors are admitted by the system, hence those energies are not admitted.