FEFG at T>0

and its heat capacity in 3D.

July 1, 2021

FEFG general overview

- To study what happens to a system of electrons when the temperature increases we need to introduce the Fermi-Dirac distribution:

$$f_{FD}(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1} \tag{1}$$

  where μ is the chemical potential, and in general it depends on the temperature. Nevertheless, at absolute zero ($T = 0$) μ is equal to ϵ_f, where ϵ_f is the fermi energy; defined as the energy of the topmost filled orbital at absolute zero.
- Intuitively the Fermi-Dirac distribution gives the probability that an orbital will be occupied.
- The number of fermions that occupy an energy states is given by:

$$< N >= \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, \mu, \beta) d\epsilon$$

Comparing FD distribution with $\mu = \epsilon_F$ assumption with real FD distribution

From the figures we notice that the approximation $\mu = \epsilon_F$ holds only at very low temperature

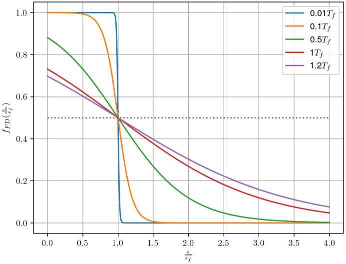

Figure 1: Fermi-Dirac distribution function (1) at the various labelled temperatures with the assumption of $\mu = \epsilon_f$. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature.

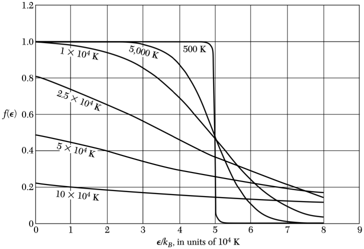

Figure 2: Fermi-Dirac distribution function (1) at the various labelled temperatures, for $T_f = \frac{\epsilon_F}{k_B} = 5 \times 10^4 K$. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature. The chemical potential μ at each temperature may be read off the graph as the energy at which $f_{FD} = 0.5$.

Real Fermi-Dirac distribution

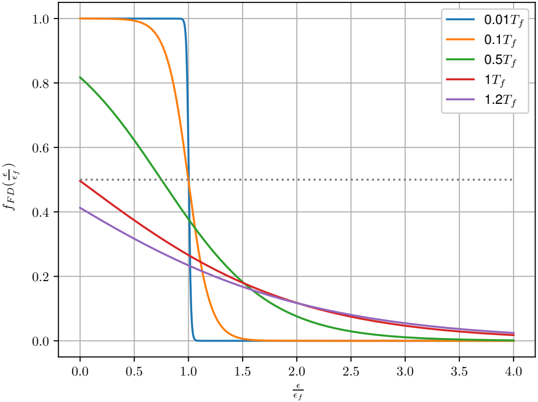

Figure 3: Fermi-Dirac distribution function (1) at the various labelled temperatures with $\mu(T)$ depending on the temperature. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature.

Schrödinger equation for a FEFG

- In order to study the fermi gas at $T > 0$ we need to find the density of states.
- To find this quantity we proceed as follow: solve the 3D Schrödinger equation for a FEFG:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(\vec{r}) = E\psi(\vec{r}) \tag{2}$$

- solving the Schrödinger equation we obtain:

$$E = \frac{\hbar^2}{2m}(k_x^2+k_y^2+k_z^2) = \frac{\hbar^2}{2m}k^2 \tag{3}$$

- This is a sphere in the k-space. In the ground state of a system of N free electrons, the occupied orbitals may be represented as points inside a sphere in k space
- Then find the fermi energy: the energy at the surface of the sphere is the Fermi energy; the wave-vectors at the Fermi surface have a magnitude k_F such that:

$$\epsilon_F = \frac{\hbar^2}{2m}k_F^2 \tag{4}$$

Density of states

- Thus in the sphere of volume $4\pi k_F^3/3$ we have the total number of orbitals N:
$$k_F = \left(\frac{3\pi^2 N}{V}\right)^{\frac{1}{3}} \tag{5}$$
which depends only on the particle concentration.
- On substituting (5) in (4) we have the total number of orbitals of energy $\leq \epsilon_f$.
$$N = \frac{V}{3\pi^2}\left(\frac{2m\epsilon}{\hbar^2}\right)^{3/2} \tag{6}$$
This equation is valid for every ϵ, not only for the fermi energy.
- The last step consist in derivating this respect the energy. Doing this we get the density of states:
$$D(\epsilon) \equiv \frac{dN}{d\epsilon} = \frac{\mathrm{V}}{2\pi^2} \cdot \left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \epsilon^{1/2} \tag{7}$$

Temperature dependence of chemical potential

- μ is not constant and it changes with temperature. The approximation $\mu = \epsilon_f$ holds only in the limit of $T \to 0$. We can estimate the trend of μ as a function of temperature.
- We can estimate the trend of μ as a function of temperature. As a starting point we observe that the total number of particles in the system N, it is not changing with the temperature. Hence, $N - N0 = 0, \forall T$
- At Temperature 0 the number of particle in the system is:
$$N_0 = \frac{V}{3\pi^2}\left(\frac{2m\epsilon_f}{\hbar^2}\right)^{\frac{3}{2}} \tag{8}$$
On the other hand, when the temperature increase the number of particle can be calculated as:
$$\begin{aligned} N &= \int_0^{+\infty} DOS(\epsilon) f_{FD}(\epsilon, \mu, \beta) d\epsilon \\ &= \int_0^{+\infty} \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}} \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon-\mu)}+1} d\epsilon \end{aligned} \tag{9}$$
- After all the calculations the dependence on temperature of μ it goes like $\epsilon_f - aT^2$, where a is fit constant.

Temperature dependence of chemical potential

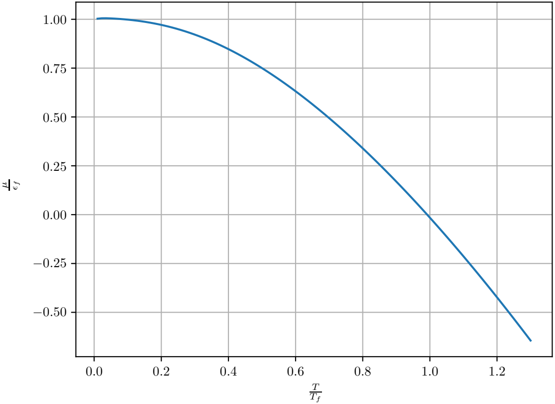

Figure 4: This plot shows the true dependence of the chemical potential μ as a function of T. From the plot we can see that the dependence on temperature of μ it goes like $\epsilon_f - aT^2$

Comparing FD distribution with $\mu = \epsilon_F$ assumption with real FD distribution

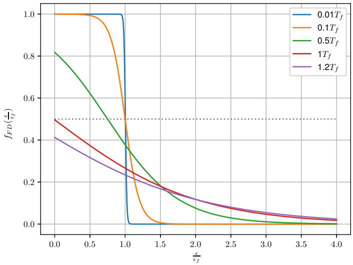

Figure 5: Fermi-Dirac distribution function (1) at the various labelled temperatures with $\mu(T)$ depending on the temperature. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature.

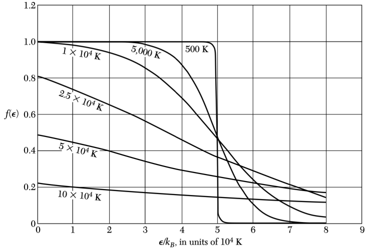

Figure 6: Fermi-Dirac distribution function (1) at the various labelled temperatures, for $T_f = \frac{\epsilon_F}{k_B} = 5 \times 10^{\mathbf{4}} K$. The results apply to a gas in three dimensions. The total number of particles is constant, independent of temperature. The chemical potential μ at each temperature may be read off the graph as the energy at which $f_{FD} = 0.5$.

Heat capacity 3D Fermi-Gas

- When we heat the crystal from $0K$, not every electron gains an energy $\approx k_B T$ as expected classically, but only the electrons within an energy range $k_B T$ of the Fermi level ϵ_f can be excited thermally.
- Only those electron near the fermi energy can absorb energy as heat and jump to a new energy level above ϵ_f. The higher is T, more electron can jump and occupy new energy levels.

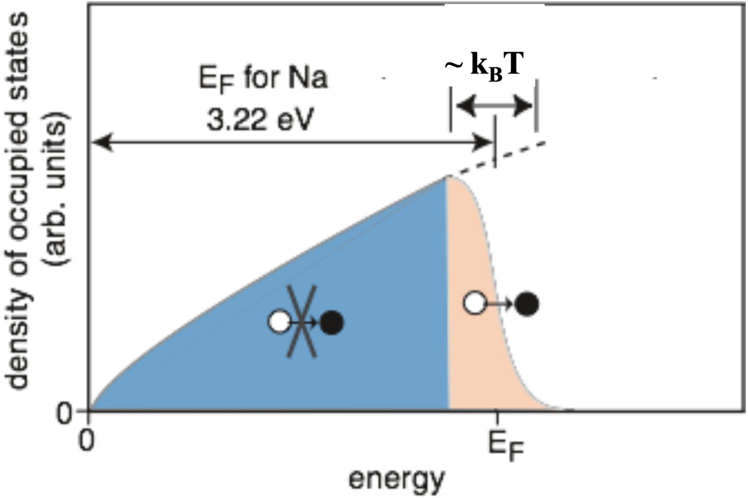
E_F for Na
3.22 eV
$\sim k_B T$
density of occupied states
(arb. units)
0
0
E_F
energy

Figure 7:

Heat capacity 3D Fermi-Gas

- If N is the total number of electrons, we expect that only a fraction of the order of $\frac{k_B T}{\epsilon_f}$ can be excited thermally at temperature T, only these lie within an energy range of the order of $k_B T$ around the fermi energy.
- Each of these $N \frac{k_B T}{\epsilon_f}$ contribute in the total kinetic thermal energy: $U \sim N \frac{k_B T}{\epsilon_f} k_B T$. The electronic heat capacity is given by: $C_v^{el} = \frac{\partial U}{\partial T}|_V \sim N \frac{k_B}{\epsilon_f} T$. From a qualitative analysis we see that the heat capacity of the FEFG is directly proportional to T
- More accurate calculations shown that the heat capacity is:

$$C_{el} \approx \frac{k_B}{\beta} \frac{3N}{2\epsilon_f} \frac{\pi^2}{3} = \frac{\pi^2}{2} \frac{k_B^2 N}{2\epsilon_f} T$$

Heat capacity 3D: Fermi-Gas vs Phonons

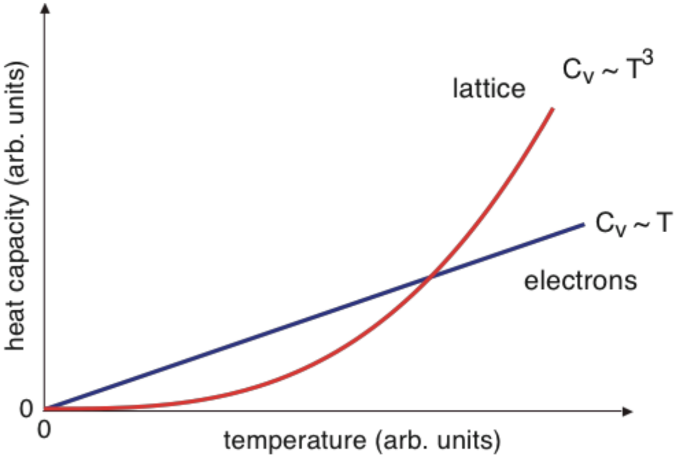

Figure 8: two contributions: lattice and electrons. Electrons unimportant at high T but dominating and sufficiently low T