1 Electrons I (FEG)

(a)

For a system at temperature T the free energy is given by $G(p,T) = E + pV - TS$ and for $T = 0$ this reduces to

$$G(p,T) = E + pV \tag{1}$$

where E is the energy of the system, p is the pressure and V the volume.
The energy of a system of fermions can be computed as

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

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

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

and indicates the average number of fermions in a single-particle state.
In the limit of zero temperature one gets

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

The 3D density of state function

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

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

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

and 3 reduces to

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

In the last integral the extrema are $E_{min} = 0$ and $E_{max} = E_f$, that is the Fermi energy which is the energy of the last occupied state. Hence

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

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

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

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 $T = 0$

$$\epsilon_f = \mu \tag{7}$$

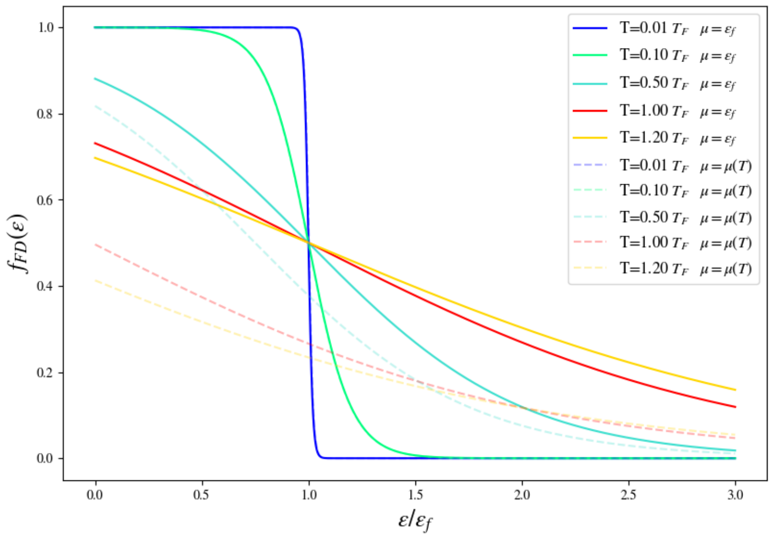

Figure 1

(b)

(c)

The number of orbitals whose energy is less than or equal to ϵ is given by

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

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

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

but on the other side

$$n =$$

(d)

(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 easilly 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

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

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

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