Fermi - Dirac Distribution : Derivation

start with probability weighting factors using the canonical ensemble

$$P_N(E) = \frac{e^{-E/k_BT}}{\sum e^{-E_\alpha^N/k_BT}}$$

E_α^N is a stationary state of the system

$$\sum e^{-E_\alpha^N/k_BT} = \text{partition function}$$

related to Helmholtz free energy

$$F = U - TS$$

U = internal energy ; S = entropy

$$\sum e^{-E_\alpha^N/k_BT} = e^{-F_N/k_BT}$$

$$\Rightarrow P_N(E) = e^{-(E-F_N)/k_BT}$$

define $f_i^N = \sum P_N(E_\alpha^N)$

From the above and after a short derivation, it is straightforward to show that:

$$f_i = \frac{1}{e^{(\varepsilon_i - \mu)/k_B T} + 1}$$

f_i is the mean number of electrons in the 1-electron level i

total number of electrons $N = \sum_i f_i$

$$\Rightarrow \quad N = \sum_i \frac{1}{e^{(\varepsilon_i - \mu)/k_B T} + 1}$$

From now, we will call f the <u>Fermi function</u>

$$f(\varepsilon) = \frac{1}{e^{(\varepsilon - \mu)/k_B T} + 1}$$

Note that $f(\varepsilon)$ gives the ground state distribution at $T = 0$

$$\left.\begin{aligned} \lim_{T \to 0} f_{ks} &= 1 \quad \varepsilon(\vec{k}) < \mu \\ &= 0 \quad \varepsilon(\vec{k}) > \mu \end{aligned}\right\} \text{Consistent with ground state}$$

$$\Rightarrow \quad \lim_{T \to 0} \mu = \varepsilon_F$$

Towards thermal properties of metals using Fermi function $f(\varepsilon)$

constant-volume specific heat

$$u = \frac{U}{V} = \frac{F + TS}{V}$$

$$c_v = \left(\frac{\partial u}{\partial T}\right)_V = \left(\frac{\partial u}{\partial S}\right)_V \left(\frac{\partial S}{\partial T}\right)_V =$$

$$c_v = \left(\frac{\partial u}{\partial T}\right)_V = \frac{T}{V}\left(\frac{\partial S}{\partial T}\right)_V$$

$$U = 2 \sum_k \varepsilon(\vec{k})\, f(\varepsilon(\vec{k}))$$

$$\rightarrow \quad u = \frac{U}{V} = \frac{2}{V} \sum \varepsilon(\vec{k})\, f(\varepsilon(\vec{k}))$$

$$u = \int \frac{d\vec{k}}{4\pi^3}\, \varepsilon(\vec{k})\, f(\varepsilon(\vec{k}))$$

recall that

$$\Delta \vec{k} = \frac{8\pi^3}{V}$$

$$\frac{1}{\Delta \vec{k}} = \frac{V}{8\pi^3}$$

similarly

$$n = \int \frac{d\vec{k}}{4\pi^3}\, f(\varepsilon(\vec{k}))$$

General function $F(\vec{k})$

$$\int \frac{d\vec{k}}{4\pi^3} F(\varepsilon(\vec{k})) = \int_{-\infty}^{\infty} d\varepsilon \, g(\varepsilon) F(\varepsilon)$$

$$\left.\begin{aligned} g(\varepsilon) &= \frac{m}{\hbar^2 \pi^2} \sqrt{\frac{2m\varepsilon}{\hbar^2}}, \quad \varepsilon > 0 \\ g(\varepsilon) &= 0, \quad \varepsilon < 0 \end{aligned}\right\} \text{density of levels}$$

which can also be written as:

$$g(\varepsilon) = \frac{3}{2} \frac{n}{\varepsilon_F} \left(\frac{\varepsilon}{\varepsilon_F}\right)^{1/2} \qquad \varepsilon > 0$$

$$g(\varepsilon) = 0 \qquad \varepsilon < 0$$

Then, at the Fermi level,

$$g(\varepsilon_F) = \frac{m k_F}{\hbar^2 \pi^2}$$

or

$$g(\varepsilon_F) = \frac{3}{2} \frac{n}{\varepsilon_F}$$

Using the density of levels $g(\varepsilon)$,

$$\left.\begin{aligned} u &= \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\, \varepsilon\, f(\varepsilon) \\ &\text{and} \\ n &= \int_{-\infty}^{\infty} d\varepsilon\, g(\varepsilon)\, f(\varepsilon) \end{aligned}\right\} \begin{array}{c} \text{energy density} \\ \text{and} \\ \text{number density} \\ \text{in} \\ \text{terms of} \\ \varepsilon,\ g(\varepsilon),\ f(\varepsilon) \end{array}$$

Evaluating above equations is not simple

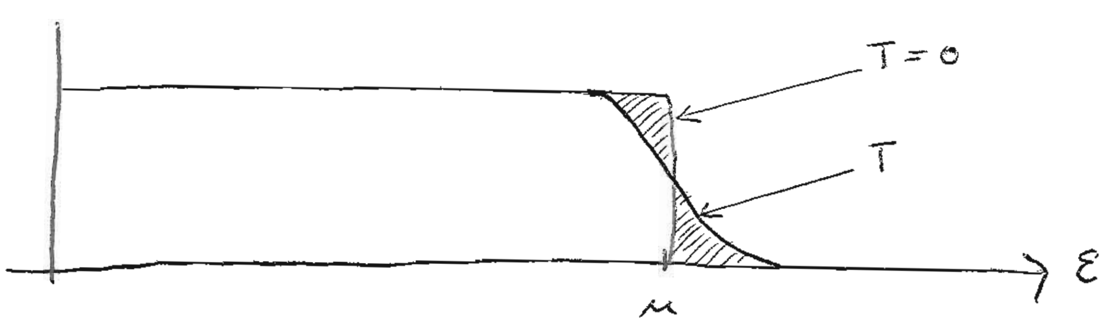
But fortunately, there exists a systematic expansion which can be applied for most temperatures of interest

- makes use of fact that $k_B T \ll k_B T_F$

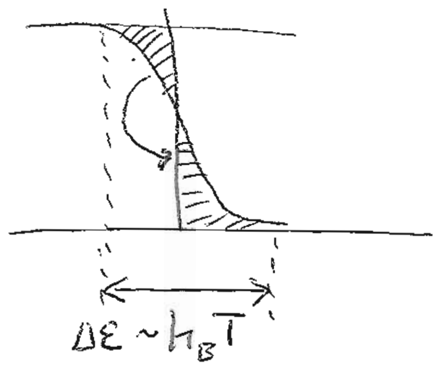
at room temperature,

$$\frac{k_B T}{k_B T_F} \sim \frac{3 \times 10^2\ K}{3 \times 10^4\ K} = \underline{.01}$$

→ means that



First, though, consider how much thermal energy density is excited when going from $T = 0$ to $T = T$



number density of excited electrons is:

$$n_{ex} \simeq k_B T \, g(\varepsilon_F)$$

excitation energy / electron is

$$\varepsilon_{ex} \simeq k_B T$$

$$\Rightarrow \quad \Delta u \simeq n_{ex}\,\varepsilon_{ex} = g(\varepsilon_F)(k_B T)^2$$

$$c_v = \left(\frac{\partial u}{\partial T}\right)_n = \left[2\, g(\varepsilon_F)\, k_B^2\right] T$$

if we had another factor of $\frac{\pi^2}{6} \sim \frac{3}{2}$ we would already get the correct result

$$c_v = \left[\frac{\pi^2}{3}\, g(\varepsilon_F)\, k_B^2\right] T$$

But $g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F}$

$$\Rightarrow \quad C_v = \frac{\pi^2}{2}\frac{n}{\varepsilon_F} k_B^2 T$$

$$C_v = \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B$$

compare to classical

$$C_v^{class} = \left[\frac{3}{2}\right] n k_B$$

$$\Rightarrow \quad C_v = A \, C_v^{class}$$

$$A = \frac{\pi^2}{3}\left(\frac{k_B T}{\varepsilon_F}\right)$$

$$A \sim .01 = 10^{-2}$$

$\Rightarrow$ C_v smaller than classical one by 10^{-2}

Note: this is part of what Drude theory missed