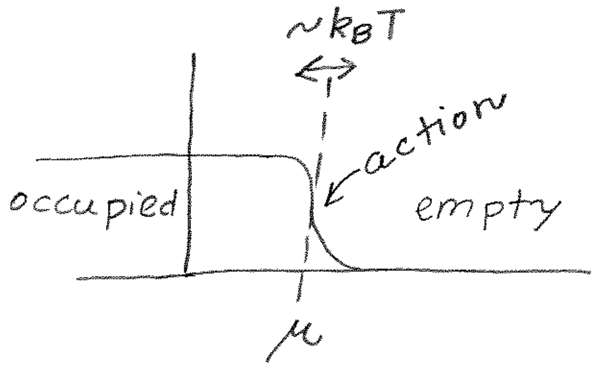
Chapter 2 Sommerfeld Theory of Metals

Fermi-Dirac distribution $f(E) = \dfrac{1}{1+e^{\beta(E-\mu)}}$



Periodic boundary conditions:

$$\psi(r) = \frac{e^{ik\cdot r}}{\sqrt{Vol}}$$

$$\psi(x+L, y, z) = \psi(x, y, z) \rightarrow e^{ik_x L} = 1$$

same for y & z directions

$$\rightarrow k_x = \frac{2\pi n_x}{L}, \ \Delta k = \frac{2\pi}{L}$$

$$\frac{1}{Vol}\sum_k = \frac{1}{Vol}\sum_{n_x, n_y, n_z} = \frac{1}{Vol.}\left(\frac{L}{2\pi}\right)^3 \sum_k (\Delta k)^3$$

$$\boxed{\frac{1}{Vol.}\sum_k = \int \frac{d^3k}{(2\pi)^3}}$$

Physical quanities:

$$\langle \vec{p} \rangle = \langle \frac{\hbar}{i}\vec{\nabla} \rangle = \hbar \vec{k}$$

$$\vec{v} = \hbar \vec{k}/m$$

$$\mathcal{E} = \frac{\hbar^2 k^2}{2m}$$

Orders of magnitude:

$T = 0$ or $T \ll \varepsilon_F$

$$n = \underset{\substack{\uparrow \\ \text{spin}}}{2} \int_{k<k_F} \frac{d^3k}{(2\pi)^3} = 2 \frac{1}{(2\pi)^3} \frac{4\pi}{3} k_F^3 = \frac{k_F^3}{3\pi^2}$$

Table 2.1: $k_F \sim 10^8 \text{cm}^{-1} = 1/\text{Å}$

$$v_F = \frac{\hbar k_F}{m} \sim 1 \text{ to } 2 \times 10^8 \frac{\text{cm}}{\text{s}} \sim \frac{1}{100} c$$

$$E_F = \frac{\hbar^2 k_F^2}{2m} \sim 1 \text{ to } 10 \text{ eV}$$

$$T_F = E_F/k_B \sim 10^4 \text{ to } 10^5 \text{K}$$

$\gg$ room temp. $\left(\frac{1 \text{eV}}{k_B} \sim 10^4 \text{K}\right)$

Total energy:

$$\frac{E}{\text{Vol.}} = 2 \int_{k<k_F} \frac{d^3k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} = \frac{1}{\pi^2} \frac{\hbar^2 k_F^5}{10m}$$

$$\frac{E}{N} = \frac{\frac{1}{\pi^2} \frac{\hbar^2 k_F^5}{10m}}{\frac{k_F^3}{3\pi^2}} = \boxed{\frac{3}{5} \varepsilon_F = \frac{E}{N}}$$

Free electron Bulk modulus

$$\left.\begin{aligned} P &= \text{pressure} = -\left(\frac{\partial E}{\partial V}\right)_N \\ E &= \frac{3}{5} N \varepsilon_F \\ \varepsilon_F &\propto k_F^2 \propto n^{2/3} = \left(\frac{N}{V}\right)^{2/3} \end{aligned}\right\} P = \frac{2}{3}\frac{E}{V}$$

$$B = \text{bulk modulus} = \frac{1}{K} = -V\frac{\partial P}{\partial V} \quad \left(\text{like } \frac{\Delta P}{\Delta V/V}\right)$$

compressibility

$$E \propto V^{-2/3}, \quad P \propto V^{-5/3} \rightarrow B = \frac{5}{3}P = \frac{5}{3}\cdot\frac{2}{3}\frac{E}{V}\frac{N}{N}$$

$$= \frac{5}{3}\cdot\frac{2}{3}\cdot\frac{3}{5}\cdot n\,\varepsilon_F$$

$$\boxed{B = \frac{2}{3} n\,\varepsilon_F}$$

Table 2.2 correct order of magnitude.

Density of states:

$$2\int\frac{d^3k}{(2\pi)^3}\,F(\varepsilon_k) = \int d\varepsilon\, F(\varepsilon)\,\underbrace{2\int\frac{d^3k}{(2\pi)^3}\,\delta(\varepsilon-\varepsilon_k)}_{\text{density of states} \,\equiv\, g(\varepsilon)}$$

$$g(\varepsilon) = \frac{2}{(2\pi)^3}\,4\pi\int k^2 dk\,\delta\left(\varepsilon - \frac{\hbar^2 k^2}{2m}\right),$$

$$= \frac{2}{(2\pi)^3}\,4\pi\,\frac{k^2}{\hbar^2 k/m} = \frac{1}{\hbar^2\pi^2}\,mk, \text{ where } \frac{\hbar^2k^2}{2m} = \varepsilon$$

or $k = \sqrt{\dfrac{2m\varepsilon}{\hbar^2}}$

$$\rightarrow \boxed{g(\varepsilon) = \frac{m}{\hbar^2\pi^2}\,k = \frac{m}{\hbar^2\pi^2}\sqrt{\frac{2m\varepsilon}{\hbar^2}}}$$

note $\sqrt{\varepsilon}$ in 3D

$$g(\varepsilon_F) = \frac{mk_F}{\hbar^2\pi^2} = \frac{3}{2}\frac{n}{\varepsilon_F}$$

Specific heat & temperature dependence:

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

$$u = \frac{U}{Vol} = 2\int\frac{d^3k}{(2\pi)^3}\,\varepsilon_k\, f(\varepsilon_k)$$ ← Fermi fnt.

$$n = 2\int\frac{d^3k}{(2\pi)^3}\,f(\varepsilon_k)$$ held fixed (μ varies w/ temperature)

$$u = \int d\varepsilon\, g(\varepsilon)\,\varepsilon\, f(\varepsilon)$$

$$n = \int d\varepsilon\, g(\varepsilon)\, f(\varepsilon)$$

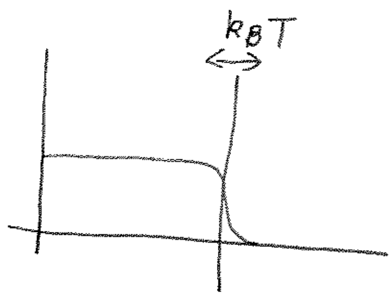
Specific heat comparison:

$$C_V = \frac{\pi^2}{3} k_B^2 T\, g(\varepsilon_F) \quad , \; g(\varepsilon_F) = \frac{3}{2}\frac{n}{\varepsilon_F} \propto m$$

$$= \frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) n k_B \qquad \text{vs. classical } \frac{3}{2} n k_B$$

$$\frac{k_B T}{\varepsilon_F} \sim \frac{100}{10^4} \sim 10^{-2}$$

Simple argument:



Fraction of els. $k_B T/\varepsilon_F$ moved $k_B T$

$$u \sim \frac{n (k_B T)^2}{\varepsilon_F}$$

$$C_V \sim n k_B \frac{k_B T}{\varepsilon_F}$$

Sizes:

$$\gamma \equiv \frac{C_V}{T} \sim \text{few} \times 10^{-4}\ \text{cal/mole/K}^2$$

$\gamma_{meas.}/\gamma_{\substack{free\\elec.}} \sim$ few w/exceptions (Table 2.3)

Commonly plotted as

$$C_V = \gamma T + A T^3 \longrightarrow \frac{C_V}{T} = \gamma + A T^2$$

$$C_V/T \text{ vs } T^2$$

Sommerfeld model = Drude + Fermi-Dirac statistics

$\frac{k_B T}{m} \ll v_F^2$ by $\frac{k_B T}{\varepsilon_F}$

$\ell = v_F \tau$ larger smaller

$$K = \frac{1}{3} v_F^2 \tau c_V$$

$$\sigma = \frac{n e^2 \tau}{m}$$

$$\frac{K}{\sigma T} = \frac{1}{3} \underbrace{m v_F^2}_{\cancel{2}\cancel{\varepsilon_F}} e^{-2} \underbrace{\frac{c_V}{n}}_{\frac{\pi^2}{\cancel{2}}\left(\frac{k_B T}{\cancel{\varepsilon_F}}\right) k_B}$$

$$= \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2 \sim 2.44 \times 10^{-8}\ \mathrm{W\Omega/K^2}$$

(Drude: $\frac{K}{\sigma T} = \frac{3}{2}\left(\frac{k_B}{e}\right)^2 \sim 1.11 \times 10^{-8}\ \mathrm{W\Omega/K^2}$)

Thermopower:

$$Q = -\frac{c_V}{3ne} = -\frac{1}{3e}\frac{\pi^2}{2}\left(\frac{k_B T}{\varepsilon_F}\right) k_B$$

$$= -\frac{\pi^2}{6}\frac{k_B}{e}\left(\frac{k_B T}{\varepsilon_F}\right) \quad \text{vs.} \quad \underbrace{-\frac{k_B}{2e}}_{\text{Drude}}$$

Big puzzles: (Chpt. 3)

Why are some elements not metals?

How can the electrons be treated as free or weakly interacting?