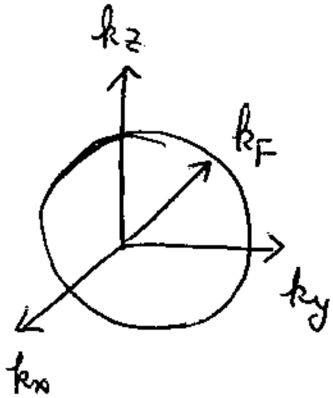
Lect 2: Sommerfeld theory — quantum

§ free Fermi gas



periodical boundary condition

$$\Delta k_{x,y,z} = \frac{2\pi}{L}$$

DOS in the momentum space 1 state per $\left(\frac{2\pi}{L}\right)^3$

density of space

$$\sum_k \rightarrow \frac{V}{(2\pi)^3}\int d^3k \qquad V = L^3$$

$$\frac{4\pi}{3}k_F^3 \cdot \frac{V}{(2\pi)^3} = N \Rightarrow n = \frac{k_F^3}{6\pi^2} \quad \text{for a single component fermion.}$$

k_F: fermi wavevector $\qquad n = \frac{k_F^3}{3\pi^2}$ for electrons $\uparrow, \downarrow$

$v_F = k_F/m$

$$k_F = (3\pi^2 n)^{\frac{1}{3}} = \left(3\pi^2 \cdot \frac{3}{4\pi r_s^3}\right)^{1/3} = \frac{(9\pi/4)^{1/3}}{r_s} = \frac{1.92}{r_s}$$

$$= \frac{3.63}{r_s/a_0}\ \mathring{A}^{-1}$$

$$v_F = \left(\frac{\hbar}{m}\right)k_F = \frac{4.2}{r_s/a_0} \times 10^8\ \text{cm/S}$$

$$a_0 = \frac{\hbar^2}{me^2}$$

$$\varepsilon_F = \frac{\hbar^2 k^2}{2m} = \left(\frac{e^2}{2a_0}\right)(k_F a_0)^2 = R_y (k_F a_0)^2 = \frac{50.1\,\text{eV}}{(r_s/a_0)^2}$$

$$\boxed{\varepsilon_F \sim 1.5 \sim 15\,\text{eV}}$$

internal energy

$$\frac{E}{V} = \frac{2}{(2\pi)^3}\int_0^{k_F} d^3k \, \frac{\hbar^2 k^2}{2m} = \frac{8\pi}{8\pi^3}\frac{\hbar^2}{2m} \int_0^{k_f} k^4 \, dk = \frac{1}{10\pi^2}\frac{\hbar^2 k_f^2}{m}$$

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2}$$

$$\Rightarrow \boxed{\frac{E}{N} = \frac{3}{10}\frac{\hbar^2 k_F^2}{m} = \frac{3}{5}\varepsilon_F} \rightarrow T_F = \frac{\varepsilon_F}{k_B} = \frac{58.2}{(r_s/a_0)^2} \times 10^4 \, K$$

$$P = -\left(\frac{\partial E}{\partial V}\right)_{N,S} \leftarrow dE = -p\,dV + T\,dS + \mu\,dN$$

since every k-state energy $\propto \left(\frac{1}{L}\right)^2 \propto V^{-\frac{2}{3}} \Rightarrow E \propto V^{-\frac{2}{3}}$

$$\frac{\partial E}{\partial V} = -\frac{2}{3}\frac{E}{V} \Rightarrow \boxed{P = \frac{2}{3}\frac{E}{V}}$$

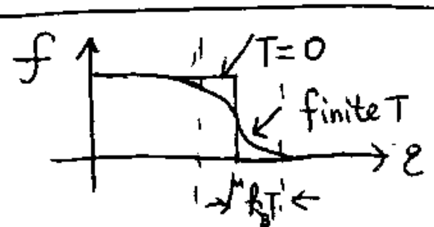
Compressibility $K = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)$, or $B = \frac{1}{K} = -V\left(\frac{\partial P}{\partial V}\right)$

$$P \propto V^{-\frac{5}{3}} \qquad \frac{\partial P}{\partial V} = -\frac{5}{3}\frac{P}{V} \Rightarrow \boxed{B = \frac{5}{3}P = \frac{10}{9}\frac{E}{V} = \frac{2}{3}n\varepsilon_F}$$

§ Fermi distribution

$$f_k = \frac{1}{e^{(\varepsilon_k - \mu)/k_BT} + 1}$$ μ is the chemical potential

$$\boxed{N = \sum_k f_k = \frac{V}{(2\pi)^3}\cdot 2\int d^3k \, \frac{1}{e^{(\varepsilon_k - \mu)/k_BT} + 1}} \leftarrow$$ determine $\mu(n, T)$



Density of states (DOS)

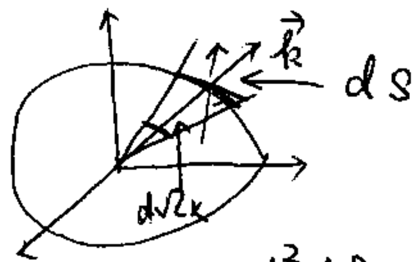
$$\int_0^{\varepsilon} d\varepsilon' \, g(\varepsilon) = 2\int \frac{d^3k}{(2\pi)^3}\, \theta(\varepsilon - \varepsilon(\vec{k})) \leftarrow \text{take derivative on } \varepsilon$$

$$g(\varepsilon) = 2\int \frac{d^3\vec{k}}{(2\pi)^3}\, \delta(\varepsilon - \varepsilon(\vec{k})) .$$

For the general case, the solution of $\varepsilon - \varepsilon(\vec{k})$ span a surface in 3D space, which is not necessary to be sphere.

$$\int k^2 dk\, d\Omega_k \, \delta(\varepsilon - \varepsilon(k,\Omega_k)) = \int d\Omega_k \int k^2 dk \, \frac{\delta(k - k(\Omega_k))}{\left|\frac{\partial \varepsilon(k,\Omega_k)}{\partial k}\right|}$$

$$= \int d\Omega_k \frac{k^2(\Omega_k)}{\left|\frac{\partial \varepsilon(k,\Omega_k)}{\partial k}\right|} = \oiint \frac{dS}{|\nabla_k \varepsilon(\vec{k})|}$$



$$dS = \frac{k^2 d\Omega_k}{|\cos\theta|}$$

θ is the angle between k and $\nabla_k \varepsilon(k)$

$$\cos\theta = \frac{\hat{k}\cdot \nabla_k \varepsilon(k)}{|\nabla_k \varepsilon(k)|} = \frac{\partial_k \varepsilon(k,\Omega_k)}{|\nabla_k \varepsilon(k)|}$$

$$\Rightarrow g(\varepsilon) = \frac{1}{4\pi^3} \oiint \frac{dS}{|\nabla_k \varepsilon(k)|} \leftarrow \text{Fermi velocity}$$

For free fermi gas

$$g(\epsilon_F) = \frac{1}{4\pi^3} \frac{4\pi k_f^2}{\frac{\hbar^2 k_f}{m}} = \frac{m k_f}{\hbar^2 \pi^2} = \frac{3}{2}\frac{n}{\varepsilon_F}$$

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

Sommerfield expansion: for a smooth function $H(\varepsilon)$

$$H(\epsilon) = \sum_{n=0}^{\infty} \frac{d^n}{d\epsilon^n} H(\epsilon)\Big|_{\epsilon=\mu} \frac{(\epsilon-\mu)^n}{n!}$$

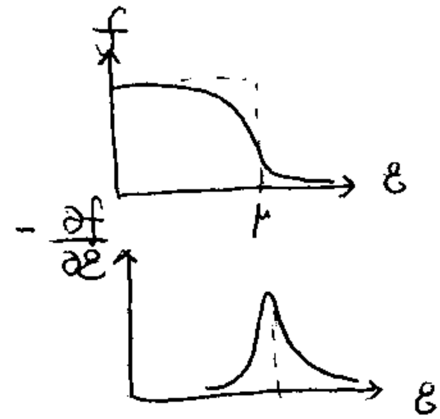
Calculate $\int_{-\infty}^{+\infty} H(\epsilon) f(\epsilon) d\epsilon$ where $f(\epsilon) = \dfrac{1}{e^{(\epsilon-\mu)/k_BT}+1}$ at $T \to 0$

derivative of $f(\epsilon)$ is very sharp $\to \delta(\epsilon-\mu)$ at $T\to 0$

define $K(\epsilon) = \int_{-\infty}^{\epsilon} H(\epsilon') d\epsilon'$

$$\Rightarrow \int_{-\infty}^{+\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_{-\infty}^{+\infty} f(\epsilon)\, dK(\epsilon) = \underbrace{f(\epsilon) K(\epsilon)\Big|_{-\infty}^{+\infty}}_{=0} - \int_{-\infty}^{+\infty} K(\epsilon) \frac{\partial f}{\partial \epsilon} d\epsilon$$

$$K(\epsilon) = K(\mu) + \sum_{n=1}^{\infty} \left[\frac{(\epsilon-\mu)^n}{n!}\right]\left[\frac{d^n}{d^n} K(\epsilon)\right]\Bigg|_{\epsilon=\mu}$$



$$\Rightarrow \int_{-\infty}^{+\infty} H(\epsilon) f(\epsilon) d\epsilon = \left[-\int_{-\infty}^{+\infty} \frac{\partial f}{\partial \epsilon} d\epsilon\right] K(\mu)$$

$$+ \sum_{n=1}^{\infty} \int_{-\infty}^{+\infty} \frac{(\epsilon-\mu)^n}{n!} \frac{d^n}{d^n} K(\epsilon)\Big|_{\epsilon=\mu} \left(-\frac{\partial f}{\partial \epsilon}\right) d\epsilon$$

$$= K(\mu) + \sum_{n=1}^{\infty} \frac{d^{n-1}}{d^{n-1}} H(\epsilon)\Big|_{\epsilon=\mu} \int_{-\infty}^{+\infty} \frac{(\epsilon-\mu)^n}{n!} \left(-\frac{\partial f}{\partial \epsilon}\right) d\epsilon$$

$$-\frac{\partial f}{\partial \epsilon} = \frac{+e^{(\epsilon-\mu)/k_BT}}{(e^{(\epsilon-\mu)/k_BT}+1)^2} \frac{1}{k_BT} = \left[\frac{1}{e^{(\epsilon-\mu)/k_BT}+1} \frac{1}{e^{-(\epsilon-\mu)/k_BT}+1}\right] \frac{1}{k_BT} \Rightarrow$$ which is even respect to $\varepsilon - \mu$

$\Rightarrow$ only even n has no zero contribution

$$\int_{-\infty}^{+\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_{-\infty}^{\mu} H(\epsilon') f(\epsilon') d\epsilon' + \sum_{n=1}^{\infty} \frac{d^{2n-1}}{d^{2n-1}} H(\epsilon)\Big|_{\epsilon=\mu} \underbrace{\int_{-\infty}^{+\infty} \frac{x^{2n}}{(2n)!} \frac{dx}{(e^x+1)(e^{-x}+1)}}_{(k_BT)^{2n}}$$

$$= \int_{-\infty}^{\mu} H(\epsilon) f(\epsilon) d\epsilon + \sum_{n=1}^{\infty} (k_BT)^{2n} a_n \frac{d^{2n-1}}{d^{2n-1}} H(\epsilon)\Big|_{\epsilon=\mu},$$ where

$$\boxed{a_n = \frac{1}{(2n)!} \int_{-\infty}^{+\infty} dx \frac{e^x}{(e^x+1)^2}}$$

$$a_{2n} = -\int_{-\infty}^{+\infty} \frac{x^{2n}}{(2n)!}\left[\frac{d}{dx}\frac{1}{e^{x}+1}\right]dx = \left(2 - \frac{1}{2^{2(n-1)}}\right)\zeta(2n)$$

← zeta function

$$\int_{-\infty}^{+\infty} H(\epsilon)\, f(\epsilon)\, d\epsilon = \int_{-\infty}^{\mu} H(\epsilon)\, d\epsilon + \frac{\pi^2}{6}(k_BT)^2 H'(\mu) + \frac{7\pi^4}{360}(k_BT)^4 H'''(\mu) + \cdots$$

f(epsilon)

$$u = \int_{-\infty}^{+\infty} d\epsilon\, g(\epsilon)\, \epsilon \approx \int^{\mu} \epsilon\, g(\epsilon)\, d\epsilon + \frac{\pi^2}{6}(k_BT)^2 \left[\mu g'(\mu) + g(\mu)\right] \qquad (1)$$

f(epsilon)

$$n = \int_{-\infty}^{+\infty} d\epsilon\, g(\epsilon) \approx \int_{0}^{\mu} g(\epsilon)\, d\epsilon + \frac{\pi^2}{6}(k_BT)^2 g'(\mu) \qquad (2)$$

eq 2 implies that $\mu - \epsilon_F \propto O(k_BT)^2$, at this order

$$\int_0^{\mu} H(\epsilon)\, d\epsilon = \int_0^{\epsilon_F} H(\epsilon)\, d\epsilon + (\mu - \epsilon_F)\, H(\epsilon_F)$$

$$\Rightarrow \quad n \approx \int_0^{\epsilon_F} g(\epsilon)\, d\epsilon + (\mu - \epsilon_F)\, g(\epsilon_F) + \frac{\pi^2}{6}(k_BT)^2 g'(\epsilon_F)$$

$\mu = \epsilon_F\left(1 - \frac{1}{3}\left(\frac{\pi k_BT}{2\epsilon_F}\right)^2\right)$ free EG.

$$\Rightarrow \quad 0 = (\mu - \epsilon_F)\, g(\epsilon_F) + \frac{\pi^2}{6}(k_BT)^2 g'(\epsilon_F) \Rightarrow \boxed{\mu = \epsilon_F - \frac{\pi^2}{6}(k_BT)^2 \frac{g'(\epsilon_F)}{g(\epsilon_F)}}$$

$$u = \int_0^{\epsilon_F} \epsilon\, g(\epsilon)\, d\epsilon + \epsilon_F\left\{(\mu - \epsilon_F)\, g(\epsilon_F) + \frac{\pi^2}{6}(k_BT)^2 g'(\epsilon_F)\right\} + \frac{\pi^2}{6}(k_BT)^2 g(\epsilon_F)$$

$$= \int_0^{\epsilon_F} \epsilon\, g(\epsilon)\, d\epsilon + \frac{\pi^2}{6}(k_BT)^2 g(\epsilon_F)$$

$$\Rightarrow \quad \boxed{C_v = \frac{\partial u}{\partial T} = \frac{\pi^2}{3} k_B^2\, g(\epsilon_F)\, T} \leftarrow \frac{\pi^2}{2}\left(\frac{k_BT}{\epsilon_F}\right) n k_B \quad \text{free EG}$$

Compare $C_{classic} = \frac{3}{2} k_B\, n$

$$\Rightarrow \quad \frac{C_v}{C_{classic}} = \frac{2\pi^2}{9n}(k_BT)\, g(\epsilon_F) \sim \frac{\pi^2}{3}\frac{k_BT}{\epsilon_F} \quad \text{for free electron}$$

§ Drude conductivity

$$\chi = \frac{1}{3} v^2 \tau C_v$$

plug in

$$C_v = \frac{\pi^2}{2}\left(\frac{k_B T}{\epsilon_F}\right) n k_B \qquad v^2 \to v_F^2 = \frac{2\epsilon_F}{m}$$

$$= \frac{2}{3}\frac{\pi^2}{2} n k_B \frac{k_B T}{m} \tau$$

$$\frac{\chi}{\sigma T} = \frac{\frac{\pi^2}{3} n k_B^2 \frac{\tau}{m}}{\frac{n e^2 \tau}{m}} = \frac{\pi^2}{3}\left(\frac{k_B}{e}\right)^2$$

at the same order of classic value

$$Q = -\frac{1}{3e}\frac{d}{dT}\frac{mv^2}{2} = -\frac{C_v}{3ne} = -\frac{\pi^2}{6}\frac{k_B}{e}\left(\frac{k_B T}{\epsilon_F}\right)$$

which is much smaller than Drude formula.

Fermi distribution is not very sensitive to temperate.