Fermi gas in a metal

Occupation number $\langle n_j \rangle_{F.D} = \dfrac{1}{e^{\beta(\epsilon_j - \mu)} + 1} = F(\epsilon_j)$ "Fermi-function"

This gives $N = \sum_j \langle n_j \rangle_{F.D.} = \sum_j F(\epsilon_j)$ ——— (1)

& $E = \sum_j \epsilon_j \langle n_j \rangle_{F.D.} = \sum_j \epsilon_j F(\epsilon_j)$ ——— (2)

Develop a notion of density of states :

No. of modes in range $[k, k+dk] = \rho_k(k)\, dk = \dfrac{4\pi k^2\, dk}{(2\pi/L)^3}$

$$= \frac{k^2 V}{2\pi^2} dk$$

If $\epsilon_j = \dfrac{\hbar^2 k^2}{2m}$, then $k = \dfrac{\pi}{L}(n_x \hat{i} + n_y \hat{j} + n_z \hat{k})$

$\therefore$ j is defined as a triplet (n_x, n_y, n_z)

Now $\rho(\epsilon)\, d\epsilon = \underbrace{2}_{\text{degeneracy of Fermions}} \rho_k(k)\, dk$ $\cancel{= 2 \rho_k(k) \frac{dk}{d\epsilon} d\epsilon}$

$$= \frac{(2m)^{3/2}}{2\pi^2} \frac{V}{\hbar^3} \epsilon^{1/2} d\epsilon$$ .... prove this!

$\therefore$ $\rho(\epsilon) = \dfrac{(2m)^{3/2}}{2\pi^2} \dfrac{V}{\hbar^3} \epsilon^{1/2}$ ——— (3)

For tightly packed modes ($L \to \infty$)

$$N = \int_0^\infty d\epsilon \, g(\epsilon) F(\epsilon) \quad \text{--- (4)}$$

"Summation is now changed to integral"

$$\& \quad E = \int_0^\infty d\epsilon \, g(\epsilon) F(\epsilon) \epsilon \quad \text{--- (5)}$$

R.H.S of (4) & (5) are like

$$\int_0^\infty F(\epsilon) \, \phi(\epsilon) \, d\epsilon$$

$\phi(\epsilon)$ is a smoothly varying f^n of ϵ. Take $\phi(\epsilon) = \frac{d\psi(\epsilon)}{d\epsilon}$

Now $$\int_0^\infty F(\epsilon) \phi(\epsilon) d\epsilon = \Big[F(\epsilon)\psi(\epsilon)\Big]_0^\infty - \int_0^\infty F'(\epsilon)\psi(\epsilon)\, d\epsilon.$$

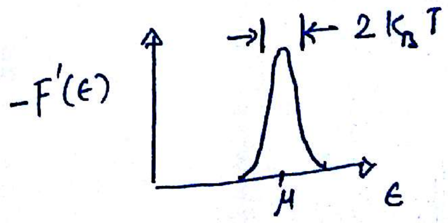
$$= -\int_0^\infty F'(\epsilon)\psi(\epsilon)\, d\epsilon \quad \text{--- (6)}$$

$\because \psi(\infty) F(\infty) = 0$

& $\psi(0) = 0$

$\because \psi(\epsilon) = \int_0^\epsilon \phi(\epsilon') d\epsilon'$

Now at low T ($k_B T \ll \mu$), $F'(\epsilon)$ is non-zero sharply around $\epsilon = \mu$. Everywhere else $F'(\epsilon)$ is zero. Also $\psi(\epsilon)$ is smooth,



$\therefore$ Expanding $\psi(\epsilon)$ around $\epsilon = \mu$:

$$\psi(\epsilon) = \sum_{m=0}^{\infty} \frac{1}{m!} \left.\frac{d^m \psi}{d\epsilon^m}\right|_{\epsilon=\mu} (\epsilon - \mu)^m \quad \text{--- (7)}$$

Plugging (7) in (6) :

$$\int_0^{\infty} F(\epsilon)\,\phi(\epsilon)\,d\epsilon = -\sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m\psi}{d\epsilon^m}\Bigg|_{\epsilon=\mu} \int_0^{\infty} F'(\epsilon)\,(\epsilon-\mu)^m\,d\epsilon$$

... Plugging $F(\epsilon) = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$ ...

$$= \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m\psi}{d\epsilon^m}\Bigg|_{\epsilon=\mu} \int_0^{\infty} \frac{e^{\beta(\epsilon-\mu)}}{\left(e^{\beta(\epsilon-\mu)}+1\right)^2}\,\beta.\,(\epsilon-\mu)^m\,d\epsilon$$

... substituting $\beta(\epsilon-\mu) = x$ ...

$$= \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m\psi}{d\epsilon^m}\Bigg|_{\epsilon=\mu} \beta^{-m} \int_{-\beta\mu}^{\infty} \frac{e^x\,x^m}{(e^x+1)^2}\,dx$$

As we are at low T ($k_BT \ll \mu$), therefore

we can write for lower limit $-\beta\mu$ as $-\infty$.

It also helps that integrand has a sharp

maximum at $x = 0$

$$\therefore \int_0^{\infty} F(\epsilon)\,\phi(\epsilon)\,d\epsilon = \sum_{m=0}^{\infty} \frac{1}{m!} \frac{d^m\psi}{d\epsilon^m}\Bigg|_{\epsilon=\mu} \beta^{-m} \int_{-\infty}^{+\infty} \frac{e^x\,x^m}{(e^x+1)^2}\,dx$$

$$= \sum_{m=0}^{\infty} \frac{\beta^{-m}}{m!} \frac{d^m \psi}{d\epsilon^m}\bigg|_{\epsilon=\mu} I_m \qquad \text{—(8)}$$

where $$I_m = \int_{-\infty}^{+\infty} \frac{e^x x^m \, dx}{(e^x+1)^2}$$

Above integrand is symmetric in x for even 'm', since $\frac{e^x}{(e^x+1)^2}$ is already symmetric in x.

$$\therefore \quad I_{m=0} = \int_{-\infty}^{\infty} \frac{e^x}{(e^x+1)^2} dx = 1$$

Also $$I_2 = \int_{-\infty}^{+\infty} \frac{e^x x^2}{(e^x+1)^2} dx = \frac{\pi^2}{3}$$ "Prove this!" —(9)

$$\therefore \int_0^{\infty} F(\epsilon)\,\phi(\epsilon)\, d\epsilon = \int_0^{\mu} \phi(\epsilon)\, d\epsilon + \frac{\pi^2}{6} (k_B T)^2 \frac{d\phi}{d\epsilon}\bigg|_{\epsilon=\mu} + O[(k_B T)^4]$$

$$\because \frac{d^2\psi}{d\epsilon^2} = \frac{d\phi}{d\epsilon}$$

Now using eq (9) & (4)

$$N = \int_0^{\mu} g(\epsilon)\, d\epsilon + \frac{\pi^2}{6} (k_B T)^2 \frac{dg}{d\epsilon}\bigg|_{\epsilon=\mu} + O[(k_B T)^4]$$

Using the values of $g(\epsilon) = \frac{(2m)^{3/2}}{2\pi^2} \frac{V}{\hbar^2} \epsilon^{1/2}$ from eq^n (3)

$$N \simeq \frac{V}{3\pi^2} \frac{(2m)^{3/2}}{\hbar^3} \mu^{3/2} + \frac{V}{24} \frac{(2m)^{3/2}}{\hbar^3} (k_B T)^2 \mu^{-1/2} \qquad \text{——— (10)}$$

To lowest order i.e $T = 0$

$$\mu_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$$ "Fermi - energy"

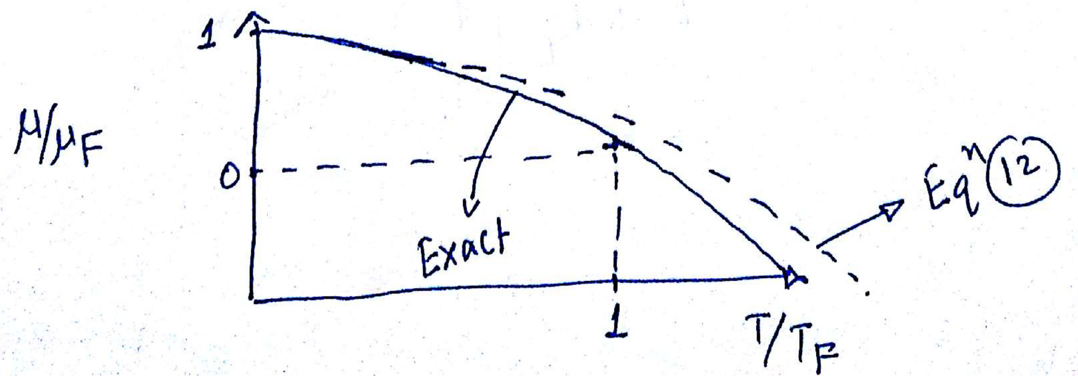
Plugging this in eq^n (10) . . .

$$\mu_F^{3/2} \simeq \mu^{3/2} + \frac{\pi^2}{8} (k_B T)^2 \mu^{-1/2} \qquad \text{——— (11)}$$

Re-arranging . . . $$\mu \simeq \mu_F \left[1 + \frac{\pi^2}{8} \left(\frac{k_B T}{\mu} \right)^2 \right]^{-2/3}$$

$$\simeq \mu_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\mu_F} \right)^2 \right] \qquad \because k_B T << \mu_F$$

——— (12)



Eq^n (4) & Eq^n (5) reveal

$$E = \int_0^{\mu} \epsilon\, g(\epsilon)\, d\epsilon + \frac{\pi^2}{6}(k_B T)^2 \frac{d}{d\epsilon}(g\epsilon)\Big|_{\epsilon=\mu} + O\left[(k_B T)^4\right]$$

Plugging values of $g(\epsilon)$ from eq^n (3), we get

$$E \simeq \frac{3}{5} N \mu_F \left[\left(\frac{\mu}{\mu_F}\right)^{5/2} + \frac{5\pi^2}{24}\left(\frac{k_B T}{\mu_F}\right)^2 \left(\frac{\mu}{\mu_F}\right)^{1/2}\right]$$

... making use of Eq^n (12) ...

$$E \simeq \frac{3}{5} N \mu_F + \frac{\pi^2}{4} N \mu_F \left(\frac{k_B T}{\mu_F}\right)^2$$

$$\simeq (3/5) N \mu_F + (\pi^2/4) N k_B T \,(T/T_F) \quad \text{... show this!}$$

$$\therefore\ C_V^{(electronic)} = \frac{dE}{dT} = \frac{\pi^2}{2} N k_B \frac{k_B T}{\mu_F}$$

$$= \frac{\pi^2}{2} N k_B \left(\frac{T}{T_F}\right)$$