Sommerfeld Expansion

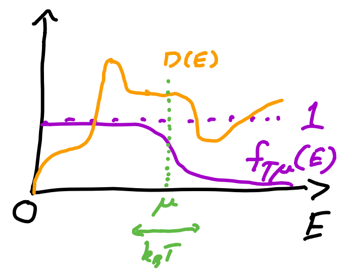
Recall: Fermi-Dirac occupation $f_{T\mu}(E) = \left(e^{\beta(E-\mu)}+1\right)^{-1}$

$$\left.\begin{aligned} N &= \int_0^\infty dE\; D(E) f_{T\mu}(E) \\ U &= \int_0^\infty dE\; E\, D(E) f_{T\mu}(E) \end{aligned}\right\} \text{both of form } I \equiv \int_0^\infty dE\; \underbrace{\phi(E)}_{\text{smooth}} f_{T\mu}(E)$$

Recall: $\frac{1}{x+1} + \frac{1}{1/x+1} = 1 \Rightarrow \left(e^{\beta(E-\mu)}+1\right)^{-1} = 1 - \left(e^{-\beta(E-\mu)}+1\right)^{-1}$ ★

note: $f_{T\mu}(E) \to \begin{cases} 1 & (E<\mu) \\ 0 & (\mu<E) \end{cases}$ as $T \to 0$

break $\int_0^\infty dE = \int_0^\mu dE + \int_\mu^\infty dE$ (apply ★ for $E<\mu$)



$$I = \int_0^\mu dE\; \phi(E)\left\{1 - \left(e^{-\beta(E-\mu)}+1\right)^{-1}\right\} + \int_\mu^\infty dE\; \phi(E)\left(e^{\beta(E-\mu)}+1\right)^{-1}$$

$$= \int_0^\mu dE\, \phi(E) - \frac{1}{\beta}\int_0^{\beta\mu \to \infty \text{ low error}} dz\; \phi(\mu - z/\beta)(e^z+1)^{-1} + \frac{1}{\beta}\int_0^\infty dz\; \phi(\mu + z/\beta)(e^z+1)^{-1}$$

$z = -\beta(E-\mu)$ $\qquad$ $z = \beta(E-\mu)$

$$= \int_0^\mu dE\, \phi(E) + k_BT\int_0^\infty dz \left\{\phi(\mu + k_BTz) - \phi(\mu - k_BTz)\right\}$$

even terms cancel

Taylor expansion: $\phi(\mu \pm k_BTz) = \sum_{j=0}^\infty \frac{(\pm 1)^j}{j!}\phi^{(j)}(\mu)(k_BTz)^j$

$$I = \int_0^\mu dE\, \phi(E) + 2\sum_{j\,\text{odd}} \frac{1}{j!}\phi^{(j)}(\mu)(k_BT)^{j+1} \underbrace{\int_0^\infty dz\; z^j (e^z+1)^{-1}}_{j!\,(1-2^{-j})\,\zeta(j+1)}$$

$\zeta(2) = \frac{\pi^2}{6}$

$\zeta(4) = \frac{\pi^4}{90}$

$$\therefore\; I = \int_0^\mu dE\, \phi(E) + \frac{\pi^2}{6}\phi'(\mu)(k_BT)^2 + \frac{7\pi^4}{360}\phi'''(\mu)(k_BT)^4$$