Physics 560A Lecture 16

Sommerfeld Expansion

For fermionic systems, we often need to compute averages of the form:

$$\langle A \rangle = \int_{-\infty}^{\infty} d\varepsilon \; A(\varepsilon) f(\varepsilon),$$

where $f(\varepsilon) = \dfrac{1}{e^{\beta(\varepsilon-\mu)}+1}$.

Assuming $A(-\infty)=0$, one can integrate by parts:

$$\langle A \rangle = \int_{-\infty}^{\infty} d\varepsilon \left[\int_{-\infty}^{\varepsilon} d\varepsilon' \, A(\varepsilon') \right] \left(-\frac{\partial f}{\partial \varepsilon} \right)$$

$-\frac{\partial f}{\partial \varepsilon}$ is sharply peaked about $\varepsilon = \mu$ and has unit integral.

Thus we can expand

$$\int_{-\infty}^{\varepsilon} d\varepsilon' A(\varepsilon') = \int_{-\infty}^{\mu} d\varepsilon' A(\varepsilon') + \int_{\mu}^{\varepsilon} d\varepsilon' A(\varepsilon')$$

Using $A(\varepsilon') = A(\mu) + A'(\mu)(\varepsilon' - \mu) + \cdots$

$$= \sum_{n=0}^{\infty} \left.\frac{d^n A}{d\varepsilon^n}\right|_{\mu} \frac{(\varepsilon' - \mu)^n}{n!}$$

$$\int_{\mu}^{\varepsilon} d\varepsilon' A(\varepsilon') = A(\mu)(\varepsilon - \mu) + A'(\mu)\frac{(\varepsilon - \mu)^2}{2} + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{d^n A(\mu)}{d\mu^n} \frac{(\varepsilon - \mu)^{n+1}}{(n+1)!}$$

$-\frac{\partial f}{\partial \varepsilon}$ is an even function of $\varepsilon - \mu$, so only the even powers in the series contribute to $\langle A \rangle$.

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon\, A(\varepsilon) + \sum_{n=1}^{\infty} \frac{d^{2n-1} A(\mu)}{d\mu^{2n-1}} \frac{1}{(2n)!}$$

$$\times \int_{-\infty}^{\infty} d\varepsilon\, (\varepsilon - \mu)^{2n} \left(-\frac{\partial f}{\partial \varepsilon} \right)$$

let $x = \beta(\varepsilon - \mu)$

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon\, A(\varepsilon) + \sum_{n=1}^{\infty} a_n (k_B T)^{2n} \frac{d^{2n-1} A(\mu)}{d\mu^{2n-1}}$$

where

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

$$a_1 = \frac{\pi^2}{6} \quad , \quad a_2 = \frac{7\pi^4}{360} \quad , \quad \text{etc.}$$

So

$$\langle A \rangle = \int_{-\infty}^{\mu} d\varepsilon \, A(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 A'(\mu) + \frac{7\pi^4}{360} (k_B T)^4 A'''(\mu) + \cdots$$

Example: Specific heat of a Fermi gas (revisited).

$$E = \int_{-\infty}^{\infty} d\varepsilon \ \varepsilon D(\varepsilon) f(\varepsilon)$$

$$A(\varepsilon) = \varepsilon D(\varepsilon)$$

$$E = \int_{-\infty}^{\mu} d\varepsilon \ \varepsilon D(\varepsilon) + \frac{\pi^2}{6}(k_B T)^2 \frac{d}{d\mu}(\mu D(\mu))$$

$$+ \mathcal{O}((k_B T)^4)$$

How does μ depend on temperature?

$$\left.\frac{\partial \mu}{\partial T}\right|_{N,V} = - \frac{\left.\frac{\partial N}{\partial T}\right|_{\mu,V}}{\left.\frac{\partial N}{\partial \mu}\right|_{T,V}}$$

$$N = \int_{-\infty}^{\infty} d\varepsilon\, f(\varepsilon)\, D(\varepsilon)$$

$$= \int_{0}^{\mu} d\varepsilon\, D(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 D'(\mu)$$

$$\Rightarrow \left.\frac{\partial \mu}{\partial T}\right|_{N,V} = -\frac{\pi^2}{3} k_B^2 T \frac{D'(\mu)}{D(\mu)}$$

$$+ \mathcal{O}(k_B T)^3$$

$$\mu = \varepsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)}$$

$$D(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2}\right)^{3/2} \varepsilon^{1/2} \quad \text{in 3D}$$

$$\frac{D'(\varepsilon_F)}{D(\varepsilon_F)} = \frac{1}{2\varepsilon_F}$$

$$\mu \simeq \varepsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\varepsilon_F}$$

$$E = \int_0^{\varepsilon_F} d\varepsilon \, \varepsilon D(\varepsilon) + \frac{\pi^2}{6} (k_B T)^2 D(\varepsilon_F)$$

$$+ \varepsilon_F \underbrace{\left\{ (\mu - \varepsilon_F) D(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 D'(\varepsilon_F) \right\}}_{\to 0}$$

$$\Rightarrow C_V = \frac{\pi^2}{3} k_B^2 T \, D(\varepsilon_F)$$