Sommerfeld Expansion

$$\int_0^\infty f(\varepsilon)\langle n(\varepsilon)\rangle\, d\varepsilon$$

for an arbitrary function $f(\varepsilon)$, where $f(0)=0$ and $\lim_{\varepsilon\to\infty} f(\varepsilon)$ diverges slower than exponential (typically some power of ε)

$$\langle n(\varepsilon)\rangle = \frac{1}{e^{\beta(\varepsilon-\mu)}+1}$$

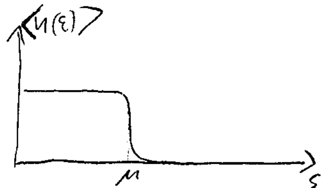
Fermi-Dirac distribution

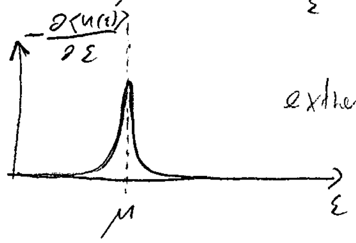
$$\int_0^\infty f(\varepsilon)\langle n(\varepsilon)\rangle\, d\varepsilon = \text{integrating by parts} = \underbrace{h(\varepsilon)\langle n(\varepsilon)\rangle\Big|_0^\infty}_{=0} - \int_0^\infty h(\varepsilon)\frac{\partial\langle n(\varepsilon)\rangle}{\partial\varepsilon}\, d\varepsilon$$

where $h(\varepsilon) \equiv \int_0^\varepsilon f(\varepsilon')\, d\varepsilon'$

$=0$ because of the properties of $f(\varepsilon)$ and $\langle n(\varepsilon)\rangle$

$$= -\int_0^\infty h(\varepsilon)\frac{\partial\langle n(\varepsilon)\rangle}{\partial\varepsilon}\, d\varepsilon$$





extremely **narrow** function with width $\sim kT \ll \mu$ (almost like a "δ" function)

$\frac{\partial\langle n(\varepsilon)\rangle}{\partial\varepsilon}$ is a <u>symmetric</u> function about μ, and rapidly decays for $\varepsilon > \mu$ and $\varepsilon < \mu$

Thus, if $h(\varepsilon)$ is non-singular function of ε in the neighborhood of μ, we can use its Taylor series about μ:

$$h(\varepsilon) = h(\mu) + \sum_{n=1}^{\infty} \frac{1}{n!} \left.\frac{\partial^n h}{\partial \varepsilon^n}\right|_{\varepsilon=\mu} (\varepsilon-\mu)^n$$

$$\int_0^{\infty} h(\varepsilon)\left[-\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}\right] d\varepsilon = h(\mu)\int_0^{\infty}\left[-\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}\right] d\varepsilon \; +$$

$$+ \sum_{n=1}^{\infty} \frac{1}{n!} \left.\frac{\partial^n h}{\partial \varepsilon^n}\right|_{\varepsilon=\mu} \int_0^{\infty} (\varepsilon-\mu)^n \left[-\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}\right] d\varepsilon$$

(i) Since the integrals are dominated by the narrow region $|\varepsilon-\mu| \ll kT$ we can write $\int_0^{\infty} d\varepsilon \to \int_{-\infty}^{+\infty}$. What we add is asymptotically $\emptyset$.

$$\int_{-\infty}^{+\infty} -\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon} d\varepsilon = -\langle n(\varepsilon)\rangle\Big|_{-\infty}^{+\infty} = 1$$

(ii) $-\dfrac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}$ is an even function about μ, thus only even powers of $(\varepsilon-\mu)^n$ will not vanish.

Thus,
$$\int_0^{\infty} f(\varepsilon)\langle n(\varepsilon)\rangle d\varepsilon \simeq h(\mu) + \sum_{n=1}^{\infty} \frac{1}{(2n)!} \left.\frac{\partial^{2n} h}{\partial \varepsilon^{2n}}\right|_{\varepsilon=\mu} \int_{-\infty}^{+\infty} (\varepsilon-\mu)^{2n}\left[-\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}\right] d\varepsilon$$

$$= \int_0^{\mu} f(\varepsilon)d\varepsilon + \sum_{n=1}^{\infty} \frac{1}{(2n)!} \left.\frac{\partial^{2n-1} f}{\partial \varepsilon^{2n-1}}\right|_{\varepsilon=\mu} \int_{-\infty}^{+\infty} (\varepsilon-\mu)^{2n}\left[-\frac{\partial\langle n(\varepsilon)\rangle}{\partial \varepsilon}\right] d\varepsilon$$

since $h(\varepsilon) = \int_0^{\varepsilon} f(\varepsilon')d\varepsilon'$ and $\dfrac{\partial h(\varepsilon)}{\partial \varepsilon} = f(\varepsilon)$

using the substitution : $\frac{\varepsilon-\mu}{kT} \equiv x \qquad d\varepsilon = kT\,dx$

$$-\frac{\partial}{\partial\varepsilon}\langle u(\varepsilon)\rangle = -\frac{1}{kT}\frac{\partial}{\partial x}\frac{1}{e^x+1}$$

$$I \equiv \int_0^\infty f(\varepsilon)\langle u(\varepsilon)\rangle d\varepsilon \simeq \int_0^\mu f(\varepsilon)d\varepsilon + \sum_{n=1}^{\infty}\frac{1}{(2n)!}\frac{\partial^{2n-1} f}{\partial\varepsilon^{2n-1}}\bigg|_{\varepsilon=\mu}(kT)^{2n}\int_{-\infty}^{+\infty} x^{2n}\left(-\frac{\partial}{\partial x}\frac{1}{e^x+1}\right)dx$$

$$= \int_0^\mu f(\varepsilon)d\varepsilon + \sum_{n=1}^{\infty}\frac{(kT)^{2n}}{(2n)!}\frac{\partial^{2n-1} f}{\partial\varepsilon^{2n-1}}\bigg|_{\varepsilon=\mu}\cdot\int_{-\infty}^{+\infty} x^{2n}\left(-\frac{\partial}{\partial x}\frac{1}{e^x+1}\right)dx$$

- $\int_{-\infty}^{+\infty} x^{2n}\left(-\frac{\partial}{\partial x}\frac{1}{e^x+1}\right)dx$ = integrating by parts (and exploiting that the integrand is an even funct. of x, thus $\int_{-\infty}^{+\infty}\ldots \to 2\int_0^{\infty}\ldots$) $= 2n\int_{-\infty}^{\infty} x^{2n-1}\frac{dx}{e^x+1}$

$$= 2\cdot(2n)\int_0^\infty x^{2n-1}\frac{dx}{e^x+1} = 2\underbrace{(2n)\,\Gamma(2n)}_{(2n)!}\sum_{l=1}^{\infty}(-1)^{l-1}\frac{1}{l^{2n}}$$

(~~using same manipulations as in~~ HW3/problem 3)

$$\boxed{I = \int_0^\mu f(\varepsilon)d\varepsilon + \sum_{n=1}^{\infty} a_n (kT)^{2n}\frac{\partial^{2n-1} f}{\partial\varepsilon^{2n-1}}\bigg|_{\varepsilon=\mu}}$$

where $a_n = 2\sum_{l=1}^{\infty}(-1)^{l-1}\frac{1}{l^{2n}} = 2\left(1-\frac{1}{2^{2n}}+\frac{1}{3^{2n}}-\frac{1}{4^{2n}}\pm\ldots\right)$

$$= 2\left[\left(1+\frac{1}{2^{2n}}+\frac{1}{3^{2n}}+\ldots\right) - 2\cdot\frac{1}{2^{2n}}\left(1+\frac{1}{2^{2n}}+\frac{1}{3^{2n}}+\ldots\right)\right]$$

$$= 2\left[\zeta(2n) - \frac{1}{2^{2n-1}}\zeta(2n)\right] = \left(2-\frac{1}{2^{2(n-1)}}\right)\zeta(2n)$$

$\zeta(\nu) = \sum_{l=1}^{\infty}\frac{1}{l^\nu}$ the Riemann zeta function

One can obtain from tables:

$$\zeta(2) = \frac{\pi^2}{6} \quad , \quad \zeta(4) = \frac{\pi^4}{90} \quad , \quad \ldots$$

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

Finally, upto the first two corrections terms:

$$\boxed{\int_0^\infty f(\varepsilon) \langle n(\varepsilon) \rangle \, d\varepsilon \simeq \int_0^\mu f(\varepsilon) \, d\varepsilon + \frac{\pi^2}{6}(kT)^2 \left.\frac{\partial f}{\partial \varepsilon}\right|_{\varepsilon=\mu} + \frac{7\pi^4}{360}(kT)^4 \left.\frac{\partial^3 f}{\partial \varepsilon^3}\right|_{\varepsilon=\mu} + \ldots}$$