Sommerfeld Expansion

to expand integrals of the type

$$\int_{-\infty}^{\infty} F(\epsilon) f(\epsilon)\, d\epsilon \quad \text{at small } T.$$

$$f(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)}+1} \qquad \beta = \frac{1}{k_B T}$$

$F(\epsilon)$ = "well-behaved" function

We want to use the fact that $-\dfrac{df(\epsilon)}{d\epsilon}$

is substantial only in a small region

around $\epsilon \sim \mu$ of width $\sim k_B T$

Let $G(\epsilon) = \displaystyle\int_{-\infty}^{\epsilon} F(\epsilon')\, d\epsilon'$

Then $F(\epsilon) = \dfrac{dG(\epsilon)}{d\epsilon}$

$$\int_{-\infty}^{\infty} d\epsilon\, F(\epsilon) f(\epsilon) = \int d\epsilon \left[\frac{d}{d\epsilon} G(\epsilon)\right] f(\epsilon)$$

$$= -\int d\epsilon\, G(\epsilon) \frac{df(\epsilon)}{d\epsilon}$$

[Integrating by parts (integrand vanishes at $\pm\infty$)]

Expand $G(\epsilon)$ in power series about

$\epsilon = \mu$

$$G(\epsilon) = G(\mu) + (\epsilon - \mu)\, G'(\mu) + \frac{1}{2}(\epsilon-\mu)^2 G''(\mu) + \cdots$$

Then (using definition of $G(\epsilon)$)

$$\int d\epsilon\, F(\epsilon)\, f(\epsilon)$$

$$= \int_{-\infty}^{\mu} F(\epsilon)\, d\epsilon - \int_{-\infty}^{\infty} d\epsilon\, \frac{1}{2}(\epsilon-\mu)^2 F'(\mu)\, \frac{d f(\epsilon)}{d\epsilon} + \cdots$$

$\left[\int d\epsilon\, (\epsilon - \mu) \frac{d f}{d\epsilon} = 0 \text{ , because } \frac{df}{d\epsilon} \right.$ is an even function of $\left. (\epsilon-\mu) \right]$

The second term can be evaluated analytically using

$$\int_{-\infty}^{\infty} x^2 \frac{d}{dx} \frac{1}{e^x+1}\, dx = \frac{\pi^2}{3}$$

One obtains

$$\int_{-\infty}^{\infty} d\epsilon\, F(\epsilon)\, f(\epsilon) \simeq \int_{-\infty}^{\mu} F(\epsilon)\, d\epsilon + \frac{(\pi k_B T)^2}{6} F'(\mu) + \cdots$$