The Sommerfeld expansion and properties of electrons in metals

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The Sommerfeld expansion is applied to integrals of the form

$$\mathcal{I} = \int_{-\infty}^{\infty} d\epsilon H(\epsilon) f(\epsilon), \tag{1}$$

where

$$f(\epsilon) = \frac{1}{e^{(\epsilon-\mu)/k_BT}+1} \tag{2}$$

is the Fermi-Dirac distribution, and $H(\epsilon)$ vanishes as $\epsilon \to -\infty$ and diverges no more rapidly than some power of ϵ as $\epsilon \to \infty$. If one defines

$$K(\epsilon) = \int_{-\infty}^{\epsilon} H(\epsilon')d\epsilon' \tag{3}$$

so that $H(\epsilon) = dK(\epsilon)/d\epsilon$. Then Eq. (1) is

$$\mathcal{I} = K(\epsilon)f(\epsilon)|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} d\epsilon K(\epsilon) f'(\epsilon). \tag{4}$$

The first term vanishes, because $K(\epsilon)$ increases slowly and $f(\epsilon)$ vanishes exponentially at high ϵ $(K(\infty)f(\infty) \to 0)$ and we suppose $K(-\infty) = 0$. The ϵ-derivative is appreciable only within a few k_BT around μ. Next, we expand $K(\epsilon)$ in a Taylor series about $\epsilon = \mu$, with the expectation that only the first few terms will be of importance. We have

$$\mathcal{I} \simeq -\int_{-\infty}^{\infty} d\epsilon \Big\{ K(\mu) + K'(\mu)(\epsilon-\mu) + \frac{1}{2}K''(\mu)(\epsilon-\mu)^2 \Big\} f'(\epsilon). \tag{5}$$

$\int_{-\infty}^{\infty} d\epsilon f'(\epsilon) = -1$ and $f'(\epsilon)$ is an even function, thus the middle term vanishes being an integral of an odd function and we have

$$\mathcal{I} \simeq \int_{-\infty}^{\mu} d\epsilon H(\epsilon) - \frac{H'(\mu)}{2} \int_{-\infty}^{\infty} d\epsilon \epsilon^2 \frac{d}{d\epsilon}(\frac{1}{1+e^{\beta\epsilon}}). \tag{6}$$

By changing the variable in the second term to $x = \beta\epsilon$ and knowing that $\int_{-\infty}^{\infty} dx \frac{x^2 e^x}{(1+e^x)^2} = \frac{\pi^2}{3}$, we have

$$\mathcal{I} \simeq \int_{-\infty}^{\mu} d\epsilon H(\epsilon) + \frac{\pi^2}{6}(k_BT)^2 H'(\epsilon_f). \tag{7}$$

Here we have set $H'(\mu) \simeq H'(\epsilon_F)$ in the correction term.

A. Example

Now we consider $H(\epsilon) = n(\epsilon)$, where $n(\epsilon)$ is density of states. This means we want to calculate the number of particles in the Fermi sea $N = \int_{-\infty}^{\infty} d\epsilon n(\epsilon) f(\epsilon)$ and from there we will have the lowest order correction in T for the chemical potential μ. Based on Eq. (7) we have

$$N = \int_{-\infty}^{\mu} d\epsilon n(\epsilon) + \frac{\pi^2}{6}(k_BT)^2 n'(\epsilon_F). \tag{8}$$

Assuming the correction of μ with respect to ϵ_F is small, the first term is

$$\int_{-\infty}^{\mu} d\epsilon n(\epsilon) \simeq \int_{-\infty}^{\epsilon_F} d\epsilon n(\epsilon) + (\mu - \epsilon_F) n(\epsilon_F), \tag{9}$$

where $\int_{-\infty}^{\epsilon_F} d\epsilon n(\epsilon) = N(T=0)$ is the number of particles at $T = 0$. Then we have

$$N(T) = N(T=0) + (\mu - \epsilon_F)n(\epsilon_F) + \frac{\pi^2}{6}(k_B T)^2 n'(\epsilon_F). \tag{10}$$

Since the number of particles does not change with temperature, $N(T) = N(T=0)$, we need to request

$$(\mu - \epsilon_F)n(\epsilon_F) + \frac{\pi^2}{6}(k_B T)^2 n'(\epsilon_F) = 0, \tag{11}$$

i.e.

$$\mu = \epsilon_F - \frac{\pi^2}{6}\frac{n'(\epsilon_F)}{n(\epsilon_F)}(k_B T)^2. \tag{12}$$

Because $n(\epsilon) \propto \sqrt{\epsilon}$, $\frac{n'(\epsilon_F)}{n(\epsilon_F)} = 1/(2\epsilon)$, thus we find the promised lowest order correction as

$$\mu = \epsilon_F[1 - \frac{\pi^2}{12}(\frac{k_B T}{\epsilon_F})]^2. \tag{13}$$

In Problem E, you apply the technique with $H(\epsilon) = \epsilon n(\epsilon)$ meaning you will calculate the internal energy and from there the heat capacity.