

Sommerfeld expansion

In the course of calculating physical properties of electronic systems one frequently needs to evaluate integrals of the type

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon) d\epsilon$$

where

$$f(\epsilon) = \frac{1}{1 + \exp\left(\frac{\epsilon - \mu}{k_B T}\right)}$$

is Fermi's function and μ the chemical potential to be fixed by the requirement

$$n = \frac{N}{V} = 2 \int_{-\infty}^{\infty} \mathcal{N}(\epsilon) f(\epsilon) d\epsilon .$$

The quantity $\mathcal{N}(\epsilon)$ is the density of states. Modern computers allow to do this efficiently numerically, but in order to obtain an idea about temperature and parameter dependencies simple approximations are often still helpful.

In normal metals we are typically interested in temperatures much smaller than the Fermi energy E_F , i.e. the Fermi function varies appreciably only over a small window $O(k_B T)$ around E_F respectively μ . If furthermore $H(\epsilon)$ does not vary too strongly in this energy region, we may expand the function about $\epsilon = \mu$ as

$$H(\epsilon) = \sum_{i=0}^{\infty} \frac{d^i}{d\epsilon^i} H(\epsilon) \Big|_{\epsilon=\mu} \frac{(\epsilon - \mu)^i}{i!} .$$

For the integral we are interested in this means

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon) d\epsilon = \int_{-\infty}^{\mu} H(\epsilon) d\epsilon + \sum_{i=1}^{\infty} a_i (k_B T)^{2i} \frac{d^{2i-1}}{d\epsilon^{2i-1}} H(\epsilon) \Big|_{\epsilon=\mu}$$

$$a_i = 2 (1 - 2^{1-2i}) \Gamma(2i) \cdot \zeta(2i)$$

with the Gamma function $\Gamma(x)$ and Riemann's Zeta function $\zeta(x)$. The most important coefficient is the one for $i = 1$, which evaluates to $a_1 = \pi^2/6$. The next coefficient is $a_2 = 7\pi^4/360$.

Density of states

Determine the density of states for a Fermi gas with dispersion $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ in dimensions $d = 1, 2$.

Bulk modulus of the Fermi gas

(a) Calculate the pressure P of the Fermi gas at $T = 0$ from

$$P = - \left(\frac{\partial U}{\partial V} \right)_N ,$$

with

$$U = \frac{3}{5} N E_F$$

the internal energy.

(b) Calculate the bulk modulus

$$B_0 = -V \left(\frac{\partial P}{\partial V} \right)_T$$

c) Using the Sommerfeld expansion and $n(T) = \text{const.}$ calculate the energy density $\frac{1}{V}U(T)$ and the specific heat at constant volume

$$c_V = \frac{1}{V} \frac{\partial U(T)}{\partial T}$$

to lowest order in T .