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May 10th, 2017
SS 2017

Exercise 1: Sommerfeld expansion for the free electron gas

At $T = 0$, free electrons occupy all states up to a Fermi energy ε_F, i.e. the probability of finding an electron with momentum k and spin σ is,

$$\begin{aligned} f_{\boldsymbol{k}\sigma} &= 1, \quad \varepsilon(\boldsymbol{k}) \leq \varepsilon_F, \\ f_{\boldsymbol{k}\sigma} &= 0, \quad \varepsilon(\boldsymbol{k}) > \varepsilon_F. \end{aligned} \tag{1}$$

At $T \neq 0$, the Fermi-Dirac distribution,

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

describes the small deviations around the chemical potential, μ, which is related to the Fermi energy as $\lim_{T\to 0} = \varepsilon_F$. In this exercise, we are interested in studying the effect of these thermal fluctuations on a key quantitity to describe metals, i.e. the specific heat,

$$c_v = \left(\frac{\partial u}{\partial T}\right)_V, \tag{3}$$

where $u = U/V$ is the density of internal energy, $U = 2\sum_{\boldsymbol{k}} \varepsilon(\boldsymbol{k}) f(\varepsilon(\boldsymbol{k}))$. The Sommerfeld expansions accounts to assume that the main contributions of the thermal fluctuations are originated near the Fermi surface, and thus we can expand around the chemical potential. This exercise will lead you step-by-step through this expansion.

a) Write the energy density, u, and the density of electrons, n, as an integral in energy making use of the Fermi-Dirac distribution (2) and the density of states (DOS), $g(\varepsilon)$,

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon), \tag{4}$$

how is $H(\varepsilon)$ defined in either case? Which are the limits $H(\varepsilon \to \pm\infty)$ in either case?

b) Define $K(\varepsilon) = \int_{-\infty}^{\varepsilon} d\varepsilon' H(\varepsilon')$, such that, $H(\varepsilon) = dK(\varepsilon)/d\varepsilon$. Integrate by parts Equation (4), arriving to

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\infty} K(\varepsilon) \left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon. \tag{5}$$

c) Taylor expand $K(\varepsilon)$ around $\varepsilon = \mu$ and plug it in Eq. (5), arriving to

$$\int_{-\infty}^{\infty} d\varepsilon H(\varepsilon) f(\varepsilon) = \int_{-\infty}^{\mu} d\varepsilon H(\varepsilon) + \sum_{n=1}^{\infty} a_n (k_BT)^{2n} \frac{d^{2n-1}}{d\varepsilon^{2n-1}} H(\varepsilon)\Big|_{\varepsilon=\mu}, \tag{6}$$

where

$$a_n = \int_{-\infty}^{\infty} dx \frac{x^{2n}}{(2n)!}\left(-\frac{d}{dx}\frac{1}{e^x+1}\right). \tag{7}$$

Why are there only even terms in n?

d) Rewrite Eq. (7) in terms of the Riemann zeta function,

$$\zeta(2n) = 2^{2n-1}\frac{\pi^{2n}}{(2n)!}B_n, \tag{8}$$

where B_n are the Bernoulli numbers, to get the final result,

$$\int_{-\infty}^{\infty} H(\varepsilon)d\varepsilon = \int_{-\infty}^{\mu} H(\varepsilon)d\varepsilon + \frac{\pi^2}{6}(k_BT)^2H'(\mu) + \frac{7\pi^4}{360}(k_BT)^4H'''(\mu) + \mathcal{O}\left(\frac{k_BT}{\mu}\right)^6. \tag{9}$$

e) Apply the Sommerfeld expansion to the energy density u and the density n (task a), up to $\mathcal{O}(T^4)$. Inspect the form of the density to convince yourself that μ differs from ε_F by terms of order T^2, and thus we can replace,

$$\int_0^{\mu} H(\varepsilon)d\varepsilon = \int_0^{\varepsilon_F} H(\varepsilon)d\varepsilon + (\mu-\varepsilon_F)H(\varepsilon_F). \tag{10}$$

f) Since we are computing the specific heat at constant density, n is independent of temperature. Show that

$$\mu = \varepsilon_F\left[1 - \frac{1}{3}\left(\frac{\pi k_BT}{2\varepsilon_F}\right)^2\right]. \tag{11}$$

g) Finally, show that

$$c_v = \left(\frac{\partial u}{\partial T}\right)_n = \frac{\pi^2}{3}k_B^2Tg(\varepsilon_F). \tag{12}$$