PROBLEM SET #2

"Thermodynamics of Fermi gas"

due on 4/19/2021

Physics–172 / Applied Physics–272

Introduction to Solid State Physics

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Comment. *Note that since these lecture notes are part of a manuscript, much of the language used here follows that of a book, with reference to chapters, sections, etc. In addition, some material in the notes may be more advanced, or will not directly be related to discussions in class. Please view these parts as stimulating extensions, where you are welcome to contact me about questions and relevant references.*

Problem 2.1 (Two electrons— **2 points**). Consider the simplest multi-electron problem, namely the two electron problem. Let us introduce notations

$$|\mathbf{k};\mathbf{q}\rangle \equiv \frac{1}{\sqrt{2}}\left[|\mathbf{k}\uparrow\rangle_1\,|\mathbf{q}\downarrow\rangle_2 - |\mathbf{q}\downarrow\rangle_1\,|\mathbf{k}\uparrow\rangle_2\right].$$

$$|\pm\rangle \equiv \frac{1}{\sqrt{2}}\left[|\mathbf{k};\mathbf{q}\rangle \pm |\mathbf{q};\mathbf{k}\rangle\right].$$

1. What is the total spin of $|\mathbf{k};\mathbf{k}\rangle$?

2. What is the total spin of $|+\rangle$ and $|-\rangle$?

Problem 2.2 (Entropy — **2 points**). Derive the following expression for the entropy of the free electron system.

$$S = -\int \frac{V d^3\mathbf{k}}{4\pi^3}\left[n_F \ln n_F + (1-n_F)\ln(1-n_F)\right],$$

where $n_F = n_F(\varepsilon_{\mathbf{k}} - \mu)$ is the Fermi function, and μ is the chemical potential. You may use expression for the Grand canonical ensemble free energy $\Omega = \Omega(\mu, V, T)$ as your starting point.

$$\Omega = -T\int \frac{V d^3\mathbf{k}}{4\pi^3}\ln\left[1+\exp\frac{\mu-\varepsilon_{\mathbf{k}}}{T}\right], \quad \varepsilon_{\mathbf{k}} \equiv \frac{\hbar^2\mathbf{k}^2}{2m}.$$

Problem 2.3 (Equation of state — **3 points**). In that problem P is the pressure defined through the Grand canonical ensemble free energy $\Omega = \Omega(\mu, V, T)$ as

$$P = -\left(\frac{\partial\Omega}{\partial V}\right)_{\mu,T}.$$

1. (**1 point**) Show that $P(\mu, T)$ is a homogeneous function of degree 5/2 in its variables μ, T. In other words, show that the following relation holds.

$$P(\lambda\mu, \lambda T) = \lambda^{5/2} P(\mu, T).$$

2. (**1 point**) Show that

$$\left(\frac{\partial P}{\partial \mu}\right)_T = n \qquad \text{and} \qquad \left(\frac{\partial P}{\partial T}\right)_\mu = s.$$

3. (**1 point**) Derive equation of state of a free electron gas

$$P = \frac{2}{3}u,$$

where $u = E/V$ is the internal energy per volume.

Remark. Heat capacity of real metals behaves (see Figure 1) at low temperatures as $C \sim \gamma T + \alpha T^3$, where linear–in–$T$ contribution comes from electrons and cubic term appears due to energy of lattice vibrations — energy of phonons. Naturally, phonon contributions becomes dominant in insulators and semiconductors, so it is important to include it into consideration. In the next problems we will calculate cubic contribution from electrons, derive an expression for phonon heat capacity within Debye model and compare them.

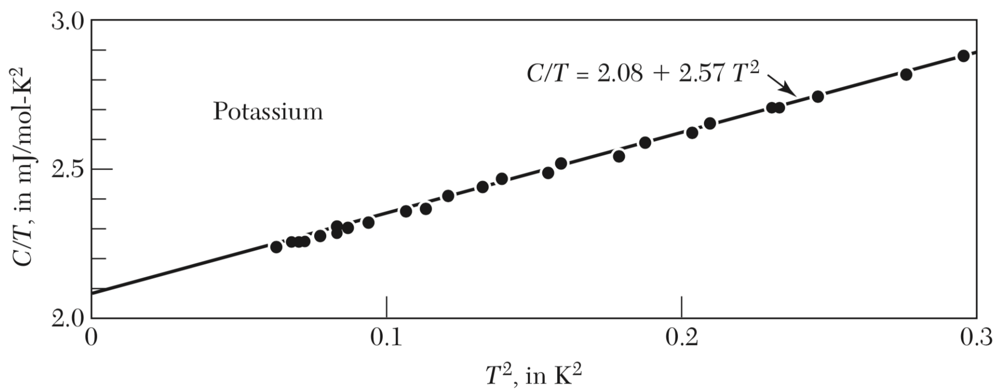

Figure 1: (Borrowed from Kittel) Experimental heat capacity values for potassium, plotted as C/T versus T^2. After W. H. Lien and N. E. Phillips.

Problem 2.4 (Correction to the specific heat of electron gas — **4 points**). Compute the T^3 contribution to the specific heat for a free electron gas. In fact, show that

$$\Delta c_V = A n k_B \left(\frac{k_B T}{\epsilon_F}\right)^3$$

and, calculate the prefactor A.

Problem 2.5 (Phonon heat capacity — **3 points**). Phonons have linear energy–momentum relation $\varepsilon_{\mathbf{k}} \equiv \hbar\omega_{\mathbf{k}} = c|\mathbf{k}|$, where c is the speed of sound (we only consider acoustic phonons and disregard optical phonons). While real phonons have linear dispersion only at the center of the

Brillouin zone, Debye model assumes that such relation holds for all momenta such that $|\mathbf{k}| < k_D$, where k_D is Debye wavevector, which is determined from the following normalization condition. One acoustic branch can host as many phonons as there are primitive cells (phonons are bosons — each one occupies its own slot in momenta space).

$$N_c = \int_{|\mathbf{k}|<k_D} \frac{V d^3\mathbf{k}}{(2\pi)^3}.$$

Here N_c is the number of crystal's primitive cells. Number of phonons, however, is not fixed (not conserved), hence chemical potential $\mu = 0$.

There are three acoustic modes in three–dimensional solid, as many as there are displacement directions. Hence total energy is

$$E = 3\int_{|\mathbf{k}|<k_D} \frac{V d^3\mathbf{k}}{(2\pi)^3}\,\varepsilon_{\mathbf{k}} n_B(\varepsilon_{\mathbf{k}}), \qquad n_B(\varepsilon) \equiv \left(e^{\varepsilon} - 1\right)^{-1}.$$

1. (**1 point**) Find expression for the Debye wavevector and corresponding energy scale — Debye temperature $\Theta = ck_D$.

2. (**1 point**) Write down an expression for the heat capacity in the following form

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V = N_c k_B \times F\left(\frac{\Theta}{T}\right),$$

   where F is some dimensionless function. Find asympotic expression for the C_V at high temperatures $T \gg \Theta$ (leading term only). Does your answer make sense from the point of view of equipartition theorem?

3. (**1 point**) Find asympotic expression for the C_V at low temperatures $T \ll \Theta$, i.e. show that

$$C_V \propto N k_B \left(\frac{T}{\Theta}\right)^3, \quad T \ll \Theta$$

   and calculate the prefactor. Find characteristic values for Debye and Fermi temperatures of metals online and compare phonon heat capacity to cubic–in–T contribution from electrons.

BONUS PROBLEM

Problem 2.6 (Specific heat at constant pressure — **0 points**)**.** We emphasized many times in class that in the lab we always measure the specific heat at constant pressure (c_P), while in most of our calculations we stop at calculating the specific heat at constant volume (c_V). Rationalize this process by showing that for electronic Fermi gas

$$\frac{c_P}{c_V} = 1 + \frac{\pi^2}{3}\left(\frac{k_B T}{\epsilon_F}\right)^2 + \mathcal{O}\left(\frac{k_B T}{\epsilon_F}\right)^4.$$