Problems for Solid State Physics
(3rd Year Course BVI)
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"Everything should be made as simple as possible, but no simpler."

— Frequently attributed to Albert Einstein

Actual quote:

"It can scarcely be denied that the supreme goal of all theory is to make the irreducible basic elements as simple and as few as possible without having to surrender the adequate representation of a single datum of experience"

— Albert Einstein, lecture delivered at Oxford 10 June 1933

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‡ Denotes crucial problems that you need to be able to do in your sleep.
* Denotes problems that are slightly harder.

Problem Set 1

Einstein, Debye, Drude, and Free Electron Models

1.1. **Einstein Solid**

(a) **Classical Einstein Solid (or "Boltzmann" Solid):**
Consider a single harmonic oscillator in three dimensions with Hamiltonian

$$H = \frac{\mathbf{p}^2}{2m} + \frac{k}{2}\mathbf{x}^2$$

▷ Calculate the classical partition function

$$Z = \int \frac{\mathbf{dp}}{(2\pi\hbar)^3} \int \mathbf{dx}\, e^{-\beta H(\mathbf{p},\mathbf{x})}$$

Note: in this problem $\mathbf{p}$ and $\mathbf{x}$ are three dimensional vectors (they should appear bold to indicate this unless your printer is defective).

▷ Using the partition function, calculate the heat capacity $3k_B$.

▷ Conclude that if you can consider a solid to consist of N atoms all in harmonic wells, then the heat capacity should be $3Nk_B = 3R$, in agreement with the law of Dulong and Petit.

(b) **Quantum Einstein Solid:** Now consider the same Hamiltonian quantum mechanically.

▷ Calculate the quantum partition function

$$Z = \sum_j e^{-\beta E_j}$$

where the sum over j is a sum over all Eigenstates.

▷ Explain the relationship with Bose statistics.

▷ Find an expression for the heat capacity.

▷ Show that the high temperature limit agrees with the law of Dulong of Petit.

▷ Sketch the heat capacity as a function of temperature.

1.2. **Debye Theory:**

(a)‡ State the assumptions of the Debye model of heat capacity of a solid.

▷ Derive the Debye heat capacity as a function of temperature (you will have to leave the final result in terms of an integral that cannot be done analytically).

▷ From the final result, obtain the high and low temperature limits of the heat capacity analytically.

You may find the following integral to be useful
$\int_0^\infty dx \frac{x^3}{e^x-1} = \sum_{n=1}^\infty \int_0^\infty x^3 e^{-nx} = 6\sum_{n=1}^\infty \frac{1}{n^4} = \frac{\pi^4}{15}$
By integrating by parts this can also be written as $\int_0^\infty dx \frac{x^4 e^x}{(e^x-1)^2} = \frac{4\pi^4}{15}$

(b) The following table gives the heat capacity C for potassium iodide (KI) as a function of temperature.

T(K)	0.1	1.0	5	8	10	15	20
C (J K $^{-1}$ mol $^{-1}$)	8.5×10^{-7}	8.6×10^{-4}	1.2×10^{-1}	5.9×10^{-1}	1.1	2.8	6.3

$\triangleright$ Discuss, with reference to the Debye theory, and make an estimate of the Debye temperature.

1.3. **Drude Theory of Transport in Metals**

(a) Assume a scattering time τ and use Drude theory to derive an expression for the conductivity of a metal.

(b) Define the resistivity matrix $\underset{\sim}{\rho}$ as $\vec{E} = \underset{\sim}{\rho}\vec{j}$.

$\triangleright$ Use Drude theory to derive an expression for the matrix $\underset{\sim}{\rho}$ for a metal in a magnetic field. (You might find it convenient to assume $\vec{B}$ parallel to the $\hat{z}$ axis. The under-tilde notation means that the quantity $\underset{\sim}{\rho}$ is a matrix.)

$\triangleright$ Invert this matrix to obtain an expression for the conductivity matrix $\underset{\sim}{\sigma}$.

(c) Define the Hall coefficient.

$\triangleright$ Estimate the magnitude of the Hall voltage for a specimen of sodium in the form of a rod of rectangular cross section 5mm by 5mm carrying a current of 1A in a magnetic field of 1T orthogonal to the direction of the current. The density of sodium atoms is roughly 1 gram/cm^3, and sodium has atomic mass of roughly 23. You may assume that there is one free electron per sodium atom (Sodium has *valence* one).

$\triangleright$ What practical difficulties would there be in measuring the Hall voltage and resistivity of such a specimen (and how might these difficulties be addressed).

(d) What properties of metals does Drude theory not explain well?

(e)* Consider now an applied AC field $\vec{E} \sim e^{i\omega t}$ which induces an AC current $\vec{j} \sim e^{i\omega t}$. Modify the above calculation (in the presence of a magnetic field) to obtain an expression for the complex AC conductivity matrix $\underset{\sim}{\sigma}(\omega)$. For simplicity in this case you may assume that the metal is very clean, meaning that $\tau \to \infty$, and you may assume that $\vec{E} \perp \vec{B}$. You might again find it convenient to assume $\vec{B}$ parallel to the $\hat{z}$ axis. (This problem might look hard, but if you think about it for a bit, it isn't really much harder than what you did above!)

$\triangleright$ At what frequency is there a divergence in the conductivity?

$\triangleright$ What does this divergence mean? (When τ is finite, the divergence is cut off).

$\triangleright$ Explain how could one use this divergence (known as the cyclotron resonance) to measure the mass of the electron. (In fact, in real metals, the measured mass of the electron is generally not equal to the well known value $m_e = 9.1095 \times 10^{-31}$ kg. This is a result of *band structure* in metals, which we will explain later in the course.)

1.4. **Fermi Surface in the Free Electron (Sommerfeld) Theory of Metals**

(a)‡ Explain what is meant by the Fermi energy, Fermi temperature and the Fermi surface of a metal.

(b)‡ Obtain an expression for the Fermi wavevector and the Fermi energy for a gas of electrons (in 3D).

▷ Show that the density of states at the Fermi surface, dN/dE_F can be written as $3N/2E_F$.

(c) Estimate the value of E_F for sodium [As above, the density of sodium atoms is roughly 1 gram/cm^3, and sodium has atomic mass of roughly 23. You may assume that there is one free electron per sodium atom (Sodium has *valence* one)]

(d) Now consider a two dimensional Fermi gas. Obtain an expression for the density of states at the Fermi surface.

1.5. **Velocities in the Free Electron Theory**

(a) Assuming that the free electron theory is applicable: show that the speed v_F of an electron at the Fermi surface of a metal is $v_F = \frac{\hbar}{m}(3\pi^2 n)^{1/3}$ where n is the density of electrons.

(b) Show that the mean drift speed v_d of an electron in an applied electric field E is $v_d = |\sigma E/(ne)|$, where σ is the electrical conductivity, and show that σ is given in terms of the mean free path λ of the electrons by $\sigma = ne^2\lambda/(mv_F)$.

(c) Assuming that the free electron theory is applicable to copper:

(i) calculate the values of both v_d and v_F for copper at 300K in an electric field of 1 V m^{-1} and comment on their relative magnitudes.

(ii) estimate λ for copper at 300K and comment upon its value compared to the mean spacing between the copper atoms.

Copper is monovalent, meaning there is one free electron per atom. The density of atoms in copper is $n = 8.45 \times 10^{28}$ m^{-3}. The conductivity of copper is $\sigma = 5.9 \times 10^7 \Omega^{-1}\text{m}^{-1}$ at 300K.

1.6. **Physical Properties of the Free Electron Gas**

In both (a) and (b) you may always assume that the temperature is much less than the Fermi temperature.

(a)‡ Give a simple but approximate derivation of the Fermi gas prediction for heat capacity of the conduction electron in metals

(b)‡ Give a simple (not approximate) derivation of the Fermi gas prediction for magnetic susceptibility of the conduction electron in metals. Here susceptibility is $\chi = dM/dH = \mu_0 dM/dB$ at small H and is meant to consider the magnetization of the electron spins only.

(c) How are the results of (a) and (b) different from that of a classical gas of electrons?

▷ What other properties of metals may be different from the classical prediction?

(d) The experimental heat capacity of potassium metal at low temperatures has the form:

$$C = (\gamma T + \alpha T^3)$$

where $\gamma = 2.08\text{mJ mol}^{-1}\,\text{K}^{-2}$ and $\alpha = 2.6\text{mJ mol}^{-1}\,\text{K}^{-4}$.

▷ Explain the origin of each of the two terms in this expression.

▷ Make an estimate of the Fermi energy for potassium metal.