FÍSICA DA MATÉRIA CONDENSADA

Problemas – 4ª Série*

1 **‡Nearly Free Electron Model**

Consider an electron in a weak periodic potential in one dimension $V(x) = V(x+a)$. Write the periodic potential as

$$V(x) = \sum_G e^{iGx} V_G$$

where the sum is over the reciprocal lattice $G = 2\pi n/a$, and $V_G^* = V_{-G}$ assures that the potential $V(x)$ is real.

(a) Explain why for k near to a Brillouin zone boundary (such as k near π/a) the electron wavefunction should be taken to be

$$\psi = Ae^{ikx} + Be^{i(k+G)x} \qquad (15.1)$$

where G is a reciprocal lattice vector such that $|k|$ is close to $|k+G|$.

(b) For an electron of mass m with k exactly at a zone boundary, use the above form of the wavefunction to show that the eigenenergies at this wavevector are

$$E = \frac{\hbar^2 k^2}{2m} + V_0 \pm |V_G|$$

where G is chosen so $|k| = |k+G|$.

▷ Give a qualitative explanation of why these two states are separated in energy by $2|V_G|$.

▷ Give a sketch (don't do a full calculation) of the energy as a function of k in both the extended and the reduced zone schemes.

(c) *Now consider k close to, but not exactly at, the zone boundary. Give an expression for the energy $E(k)$ correct to order $(\delta k)^2$ where δk is the wavevector difference from k to the zone boundary wavevector.

▷ Calculate the effective mass of an electron at this wavevector.

2 ***Nearly Free Electrons in Two Dimensions** Consider the nearly free electron model for a square lattice with lattice constant a. Suppose the periodic potential is given by

$$\begin{aligned} V(x,y) &= 2V_{10}[\cos(2\pi x/a) + \cos(2\pi y/a)] \\ &+ 4V_{11}[\cos(2\pi x/a)\cos(2\pi y/a)] \end{aligned}$$

(a) Use the nearly free electron model to find the energies of states at wavevector $\mathbf{G} = (\pi/a, 0)$.

(b) Calculate the energies of the states at wavevector $\mathbf{G} = (\pi/a, \pi/a)$. (Hint: You should write down a 4 by 4 secular determinant, which looks difficult, but actually factors nicely. Make use of adding together rows or columns of the determinant before trying to evaluate it!)

3 **Decaying Waves**

As we saw in this chapter, in one dimension, a periodic potential opens a band gap such that there are no plane-wave eigenstates between energies $\epsilon_0(G/2) - |V_G|$ and $\epsilon_0(G/2) + |V_G|$ with G a reciprocal lattice vector. However, at these forbidden energies, decaying (evanescent) waves still exist. Assume the form

$$\psi(x) = e^{ikx - \kappa x}$$

with $0 < \kappa \ll k$ and κ real. Find κ as a function of energy for $k = G/2$. For what range of V_G and E is your result valid?

4 **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.

You will need the following information: 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 $\sigma = 5.9 \times 10^7 \Omega^{-1}$m^{-1} at 300K.

5 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 specific heat of potassium metal at low temperatures has the form:

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

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

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

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

6 Another Review of Free Electron Theory

▷ What is the *free electron model* of a metal.

▷ Define *Fermi energy* and *Fermi temperature*.

▷ Why do metals held at room temperature feel cold to the touch even though their Fermi temperatures are much higher than room temperature?

(a) A d-dimensional sample with volume L^d contains N electrons and can be described as a free electron model. Show that the Fermi energy is given by

$$E_F = \frac{\hbar^2}{2mL^2}(N a_d)^{2/d}$$

Find the numerical values of a_d for $d = 1, 2$, and 3.

(b) Show also that the density of states at the Fermi energy is given by

$$g(E_F) = \frac{Nd}{2L^d E_F}$$

▷ Assuming the free electron model is applicable, estimate the Fermi energy and Fermi temperature of a one-dimensional organic conductor which has unit cell of length 0.8 nm, where each unit cell contributes one mobile electron.

(c) Consider relativistic electrons where $E = c|\mathbf{p}|$. Calculate the Fermi energy as a function of the density for electrons in $d = 1, 2, 3$ and calculate the density of states at the Fermi energy in each case.

7 Chemical Potential at $T = 0$

Consider a system of N non-interacting electrons. At $T = 0$ the N lowest-energy eigenstates will be filled and all the higher energy eigenstates will be empty. Show that at $T = 0$ the energy of the chemical potential is precisely half way between the highest energy filled eigenstate and the lowest-energy unfilled eigenstate.

8 Heat Capacity of a Free Electron Gas*

In Exercise 4.3.a we approximated the heat capacity of a free electron gas

(a*) Calculate an exact expression for the heat capacity of a 2d metal at low temperature.

(b**) Calculate an exact expression for the heat capacity of a 3d metal at low temperature.

The following integral may be useful for these calculations:

$$\int_{-\infty}^{\infty} dx \frac{x^2 e^x}{(e^x+1)^2} = \frac{\pi^2}{3} = \zeta(2)/2$$

Note that for the 3d case you have to worry about the fact that the chemical potential will shift as a function of temperature. Why does this not happen (at least for low T) in the 2d case?