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Keble College - Hillary 2010

B2: Condensed Matter Physics and Photonics
Tutorial 5 - Free and Nearly Free Electrons

Please leave your work in my Keble pigeon hole by 5pm on Wednesday of 1st week.
Suggested reading: Hook & Hall 3, 4; Kittel 6, 7; Ashcroft/Mermin 2, 3, 8, 9.

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1 The Free Electron Model

1. What is meant by the terms *Fermi energy* and *Fermi temperature*? Obtain an expression for the Fermi energy, at absolute zero, of a free electron gas in 1, 2 and 3 dimensions.

   Consider a 2-dimensional crystal with a simple cubic structure and a monoatomic basis. Using the free electron model, draw pictures in **k**-space showing the first Brillouin zone and the Fermi surface when the atoms are

   (a) monovalent
   (b) divalent

2. Show that the electronic contribution to the heat capacity of a metal is of the form:

   $$C = ANk^2T/E_F$$

   where E_F is the Fermi energy, N is the number of conduction electrons, T is the temperature and A is a constant which need not be evaluated. What other contribution to the heat capacity would you expect? What is its behaviour at low T?

   Using this result and simple kinetic theory arguments obtain the Wiedemann-Franz law which relates the electrical conductivity σ of a metal to its thermal conductivity K. (The constant A can be taken as $\pi^2/2$.)

   Which assumption in our derivation of the Wiedemann-Franz law is most likely to break down? Sketch the change to the Fermi surface due to the application of i) an electric field and ii) a heat gradient.

   Inelastic scattering from phonons causing a small change in wavevector is effective at reducing which type of current? Discuss whether it is important at $T = 0$, $T < T_{Debye}$, $T > T_{Debye}$. Hence explain at which temperatures you expect the Wiedemann-Franz law to hold. *Please note, I think the discussion in Hook and Hall is very unsatisfactory here - try and think through the problem yourself, and then decide on which you think is the better explanation.*

3. Please attempt question A4 and from Prof Robin Nicholas's problem set.

4. Please attempt question A5 and from Prof Robin Nicholas's problem set.

2 An Introduction to Band Theory

Band theory is, in simple terms, how we understand the differences between metals, semiconductors and insulators. First, we will approximately solve a system with a periodic potential consisting of one component. We will then go on to discuss the more general case.

5. Consider an electron in a 1-dimensional system with periodic potential $V(x)$. Argue that the potential can be written as:

$$V(x) = \sum_K V_K \exp(iKx). \tag{1}$$

Which values of K are summed over? We will consider the effect of one component of the periodic potential. Assuming $V(x)$ is real and symmetric, show that $V_K = V_{-K} = V_K^*$. Thus our perturbation becomes $V(x) = V_K(\exp(iKx) + \exp(-iKx))$.

We can write the Schrödinger equation in matrix from as

$$\langle\Psi|H_0|\Psi\rangle + \langle\Psi|V(x)|\Psi\rangle = E \tag{2}$$

Our unperturbed eigenstates are plane waves, $|\Psi_k(x)\rangle$. Argue that

$$\langle\Psi_k|V(x)|\Psi'_k\rangle = V_K\delta_{k-k',\pm K} \tag{3}$$

The Hamiltonian only acts to connect states with $k - k' = \pm K$. Unfortunately, this is still an infinite number of states. Ideally, we would like to restrict ourselves to pairs of states with $|k| \approx |k'| \approx |K|/2$, as this makes the problem easy to solve. Why might this be a reasonable assumption? Think about the second order term in perturbation theory: is it large if the unperturbed states have very different energies?

Hence show that a state given by $|\Psi(x)\rangle = a|\Psi_k(x)\rangle + b|\Psi_{k-K}(x)\rangle$ obeys the Schrödinger equation:

$$\begin{pmatrix} \frac{\hbar^2k^2}{2m} & V_K \\ V_K & \frac{\hbar^2(k-K)^2}{2m} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix} \tag{4}$$

Solve for the eigenvalues, expanding to quadratic order in $\delta = k - K/2$. What are the eigenvectors if k lies on the Brillouin zone boundary at $K/2$? What sort of waves are these?

6. Consider an electron moving in a box of volume Ω with periodic boundaries and subject to a periodic crystal potential, $V(r)$. Prove Bloch's theorem for the eigenstates of the Hamiltonian:

$$\psi(r + R) = \mathrm{e}^{ik.R}\psi(r),$$

where R is any lattice vector. Show that an equivalent form for Bloch's theorem is

$$\psi(r) = \mathrm{e}^{ik.r}u_k(r),$$

where the Bloch function $u_k(r)$ has the periodicity of the lattice.

The wavevector k which appears in Bloch's theorem is not unique. What is the indeterminacy? Sketch the dispersion relation of the nearly free electron model in 1d using the reduced zone scheme, referring to the previous question.

In more than 1 dimension, the picture is more interesting. Show how the Fermi surfaces from question 1 are modified when the crystal potential is taken into account. With reference to band structure, explain briefly why:

(a) Sodium (BCC crystal with trivial basis) is a metal.

(b) Calcium (FCC crystal with trivial basis) is a metal.

(c) Diamond (FCC lattice with 2 atom basis) is an insulator whereas silicon and germanium, which have similar structures, are semiconductors.