

Physics of Electronics

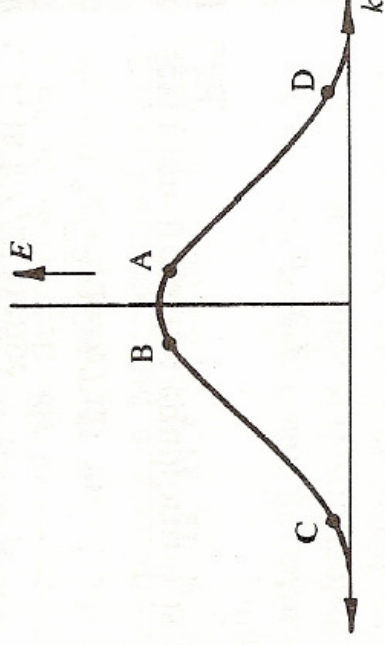
Problem Set 2:
Chapters 05 to 06

July – December 2008

Electrons in Solids

1.

1. The E - k diagram for an energy band in a particular material is as shown. If



an electric field is applied to the material in the negative k direction (force in the positive direction), find (a) the polarity of the effective masses of the four wavepackets made up of groups of states near A, B, C and D, (b) the direction of the velocity of each of the four wavepackets and (c) the direction of the acceleration of each. What are the physical consequences of these results?

Electrons in Solids

2.

Kronig-Penney model. (a) For the delta-function potential and with $P \ll 1$, find at $k = 0$ the energy of the lowest energy band. (b) For the same problem find the band gap at $k = \pi/a$.

3.

2. The conductivity of a metal having n free electrons per unit volume is given by Eq.(4.37) and the Fermi energy by Eq.(4.22). Consider a metal with a simple-cubic lattice structure of side 0.2 nm and one free conduction electron per atom. Assuming that the mean free path for electron collisions with the lattice is 100 lattice constants, find the relaxation time for an electron with the Fermi energy.

$$E_{F0} = \frac{h^2}{8m} \left(\frac{3n}{\pi} \right)^{2/3} = 3.65 \times 10^{-19} n^{2/3} \text{ eV} \quad (4.22)$$

$$\sigma = \frac{ne^2\tau_F}{m} = \frac{ne^2\bar{l}_F}{mv_F} \quad (4.37)$$

Electrons in Solids

4.

Generalization of the Kronig-Penney Model

The general analysis of electronic levels in a periodic potential, independent of the detailed features of that potential, can be carried considerably further in one dimension. Although the one-dimensional case is in many respects atypical (there is no need for a concept of a Fermi surface) or misleading (the possibility—indeed, in two and three dimensions the likelihood—of band overlap disappears), it is nevertheless reassuring to see some of the features of three-dimensional band structure we shall describe through approximate calculations, in Chapters 9, 10, and 11, emerging from an exact treatment in one dimension.

Consider, then, a one-dimensional periodic potential $U(x)$ (Figure 8.4). It is convenient to view the ions as residing at the minima of U , which we take to define the zero of energy. We choose to view the periodic potential as a superposition of potential barriers $v(x)$ of width a , centered at the points $x = \pm na$ (Figure 8.5):

$$U(x) = \sum_{n=-\infty}^{\infty} v(x - na). \quad (8.64)$$

Figure 8.4

A one-dimensional periodic potential $U(x)$. Note that the ions occupy the positions of a Bravais lattice of lattice constant a . It is convenient to take these points as having coordinates $(n + \frac{1}{2})a$, and to choose the zero of potential to occur at the position of the ion.

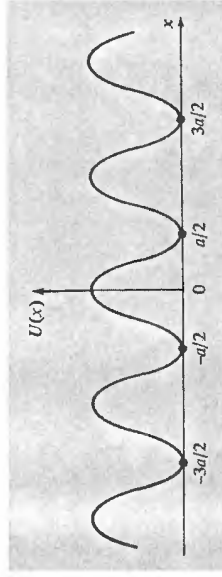
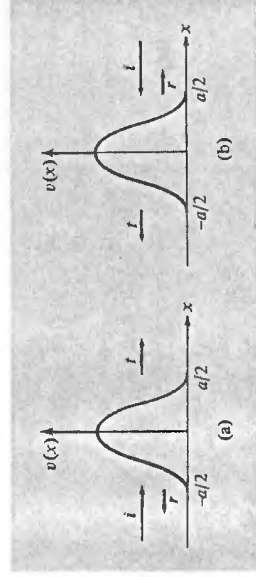


Figure 8.5

Illustrating particles incident from the left (a) and right (b) on a single one of the barriers separating neighboring ions in the periodic potential of Figure 8.4. The incident, transmitted, and reflected waves are indicated by arrows along the direction of propagation, proportional to the corresponding amplitudes.



The term $v(x - na)$ represents the potential barrier against an electron tunneling between the ions on opposite sides of the point na . For simplicity we assume that $v(x) = v(-x)$ (the one-dimensional analogue of the inversion symmetry we assumed above), but we make no other assumptions about v , so the form of the periodic potential U is quite general.

The band structure of the one-dimensional solid can be expressed quite simply in terms of the properties of an electron in the presence of a single-barrier potential $v(x)$. Consider therefore an electron incident from the left on the potential barrier $v(x)$ with energy³³ $\varepsilon = \hbar^2 K^2/2m$. Since $v(x) = 0$ when $|x| \geq a/2$, in these regions the wave function $\psi(x)$ will have the form

$$\begin{aligned} \psi_l(x) &= e^{iKx} + r e^{-iKx}, & x &\leq -\frac{a}{2}, \\ &= t e^{iKx}, & x &\geq \frac{a}{2}. \end{aligned} \quad (8.65)$$

This is illustrated schematically in Figure 8.5a.

The transmission and reflection coefficients t and r give the probability amplitude that the electron will tunnel through or be reflected from the barrier; they depend on the incident wave vector K in a manner determined by the detailed features of the barrier potential U . However, one can deduce many properties of the band structure of the periodic potential U by appealing only to very general properties of t and r . Because v is even, $\psi_r(x) = \psi_l(-x)$ is also a solution to the Schrödinger equation with energy ε . From (8.65) it follows that $\psi_r(x)$ has the form

$$\begin{aligned} \psi_r(x) &= t e^{-iKx}, & x &\leq -\frac{a}{2}, \\ &= e^{-iKx} + r e^{iKx}, & x &\geq \frac{a}{2}. \end{aligned} \quad (8.66)$$

Evidently this describes a particle incident on the barrier from the right, as depicted in Figure 8.5b.

Since ψ_l and ψ_r are two independent solutions to the single-barrier Schrödinger equation with the same energy, any other solution with that energy will be a linear combination³⁴ of these two: $\psi = A\psi_l + B\psi_r$. In particular, since the crystal Hamiltonian is identical to that for a single ion in the region $-a/2 \leq x \leq a/2$, any solution to the crystal Schrödinger equation with energy ε must be a linear combination of ψ_l and ψ_r in that region:

$$\psi(x) = A\psi_l(x) + B\psi_r(x), \quad -\frac{a}{2} \leq x \leq \frac{a}{2}. \quad (8.67)$$

Now Bloch's theorem asserts that ψ can be chosen to satisfy

$$\psi(x + a) = e^{ik_a} \psi(x), \quad (8.68)$$

for suitable k . Differentiating (8.68) we also find that $\psi' = d\psi/dx$ satisfies

$$\psi'(x + a) = e^{ik_a} \psi'(x). \quad (8.69)$$

(a) By imposing the conditions (8.68) and (8.69) at $x = -a/2$, and using (8.65) to (8.67), show that the energy of the Bloch electron is related to its wave vector k by:

$$\cos ka = \frac{t^2 - r^2}{2t} e^{ik_a} + \frac{1}{2t} e^{-iK_a}, \quad \varepsilon = \frac{\hbar^2 K^2}{2m}. \quad (8.70)$$

Verify that this gives the right answer in the free electron case ($v \equiv 0$).

Electrons in Solids

(cont.)

Equation (8.70) is more informative when one supplies a little more information about the transmission and reflection coefficients. We write the complex number t in terms of its magnitude and phase:

$$t = |t| e^{i\delta}. \quad (8.71)$$

The real number δ is known as the phase shift, since it specifies the change in phase of the transmitted wave relative to the incident one. Electron conservation requires that the probability of transmission plus the probability of reflection be unity:

$$1 = |t|^2 + |r|^2. \quad (8.72)$$

This, and some other useful information, can be proved as follows. Let ϕ_1 and ϕ_2 be any two solutions to the one-barrier Schrödinger equation with the same energy:

$$-\frac{\hbar^2}{2m} \phi_i'' + v \phi_i = \frac{\hbar^2 K^2}{2m} \phi_i, \quad i = 1, 2. \quad (8.73)$$

Define $w(\phi_1, \phi_2)$ (the "Wronskian") by

$$w(\phi_1, \phi_2) = \phi_1'(x)\phi_2(x) - \phi_1(x)\phi_2'(x). \quad (8.74)$$

- (b) Prove that w is independent of x by deducing from (8.73) that its derivative vanishes.
 (c) Prove (8.72) by evaluating $w(\psi_i, \psi_r^*)$ for $x \leq -a/2$ and $x \geq a/2$, noting that because $v(x)$ is real ψ_r^* will be a solution to the same Schrödinger equation as ψ_i .
 (d) By evaluating $w(\psi_i, \psi_r^*)$ prove that rt^* is pure imaginary, so r must have the form

$$r = \pm i |r| e^{i\delta}, \quad (8.75)$$

where δ is the same as in (8.71).

- (e) Show as a consequence of (8.70), (8.72), and (8.75) that the energy and wave vector of the Bloch electron are related by

$$\frac{\cos(Ka + \delta)}{|t|} = \cos ka, \quad \varepsilon = \frac{\hbar^2 K^2}{2m}. \quad (8.76)$$

Since $|t|$ is always less than one, but approaches unity for large K (the barrier becomes increasingly less effective as the incident energy grows), the left side of (8.76) plotted against K has the structure depicted in Figure 8.6. For a given k , the allowed values of K (and hence the allowed energies $\varepsilon(k) = \hbar^2 K^2/2m$) are given by the intersection of the curve in Figure 8.6 with the horizontal line of height $\cos(ka)$. Note that values of K in the neighborhood of those satisfying

$$Ka + \delta = n\pi \quad (8.77)$$

give $|\cos(Ka + \delta)|/|t| > 1$, and are therefore not allowed for any k . The corresponding regions of energy are the energy gaps. If δ is a bounded function of K (as is generally the case), then there will be infinitely many regions of forbidden energy, and also infinitely many regions of allowed energies for each value of k .

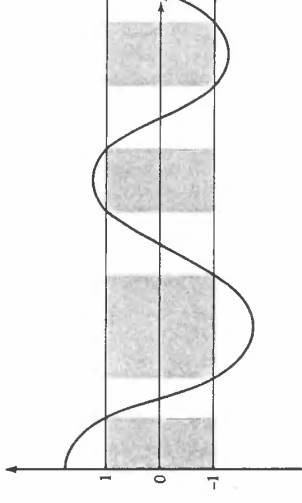
- (f) Suppose the barrier is very weak (so that $|t| \approx 1$, $|r| \approx 0$, $\delta \approx 0$). Show that the energy gaps are then very narrow, the width of the gap containing $K = n\pi/a$ being

$$\varepsilon_{\text{gap}} \approx 2\pi\hbar \frac{\hbar^2}{m\alpha^2} |r|. \quad (8.78)$$

- (g) Suppose the barrier is very strong, so that $|t| \approx 0$, $|r| \approx 1$. Show that the allowed bands

Figure 8.6

Characteristic form of the function $\cos(Ka + \delta)/|t|$. Because $|t(K)|$ is always less than unity the function will exceed unity in magnitude in the neighborhood of solutions to $Ka + \delta(K) = n\pi$. Equation (8.76) can be satisfied for real k if and only if the function is less than unity in magnitude. Consequently there will be allowed (unshaded) and forbidden (shaded) regions of K (and therefore of $\varepsilon = \hbar^2 K^2/2m$). Note that when $|t|$ is very near unity (weak potential) the forbidden regions will be narrow, but if $|t|$ is very small (strong potential) the allowed regions will be narrow.



of energies are then very narrow, with widths

$$\varepsilon_{\text{max}} - \varepsilon_{\text{min}} = O(|t|). \quad (8.79)$$

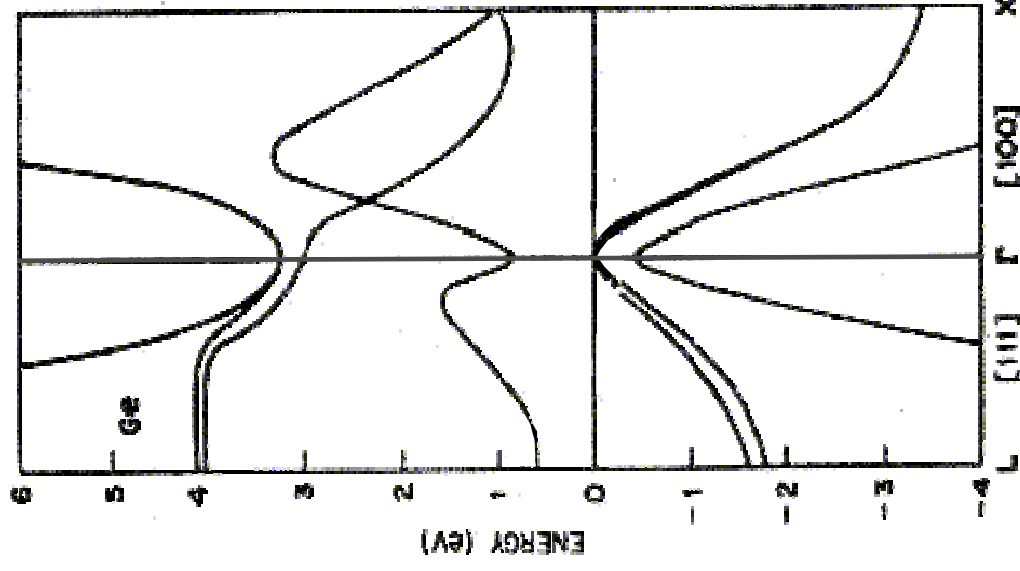
- (h) As a concrete example, one often considers the case in which $v(x) = g\delta(x)$, where $\delta(x)$ is the Dirac delta function (a special case of the "Kronig-Penney model"). Show that in this case

$$\cot \delta = -\frac{\hbar^2 K}{mg}, \quad |t| = \cos \delta. \quad (8.80)$$

This model is a common textbook example of a one-dimensional periodic potential. Note, however, that most of the structure we have established is, to a considerable degree, independent of the particular functional dependence of $|t|$ and δ on K .

Semiconductors

5. Given the following band structure for Ge: a) Find the value of the band gap and determine the type of gap. b) Sketch the effective mass for the different bands



Semiconductors

6.

6. Show that the minimum conductivity attainable by a particular semiconductor at a given temperature is of the form

$$\sigma_{\min} = C(\mu_e \mu_h)^{1/2}$$

where μ_e and μ_h are the carrier mobilities and C is a constant to be determined. Why does the conductivity not possess its minimum value when the semiconductor is intrinsic? How might the minimum conductivity be realized in practice?

7.

7. An unknown semiconductor has $E_g = 1.1 \text{ eV}$ and $N_c = N_v$. It is doped with 10^{15} cm^{-3} donors where the donor level is 0.2 eV below E_C . Given that E_F is 0.25 eV below E_C , calculate n_i and the concentration of electrons and holes in the semiconductor at 300 K .

8.

8. **Ionization of donors.** In a particular semiconductor there are $10^{13} \text{ donors/cm}^3$ with an ionization energy E_d of 1 meV and an effective mass $0.01 m$. (a) Estimate the concentration of conduction electrons at 4 K . (b) What is the value of the Hall coefficient? Assume no acceptor atoms are present and that $E_g \gg k_B T$.

Semiconductors

9.

A rod of p-type germanium, 6 mm long, 1 mm wide and 0.5 mm thick, has an electrical resistance of 120Ω . What is the impurity concentration? Assume $\mu_h = 0.19 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$, $\mu_e = 0.39 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$ and $n_i = 2.5 \times 10^{19} \text{ m}^{-3}$. What proportion of the conductivity is due to electrons in the conduction band?

10.

When a particular intrinsic semiconductor is doped n-type, its resistance at 20°C drops to 1 per cent of its original value. Assuming a gap energy of 1.1 eV and carrier mobilities of 0.13 and $0.05 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$, estimate the movement of the Fermi energy, as a proportion of the gap energy, when the intrinsic material is doped.

11.

A bar of n-type germanium $10 \text{ mm} \times 1 \text{ mm} \times 1 \text{ mm}$ is mounted in a magnetic field of 0.2 T. The electron density in the bar is $7 \times 10^{21} \text{ m}^{-3}$. If 1 mV is applied across the long ends of the bar, determine the current through the bar, the Hall coefficient and the voltage between Hall electrodes placed across the short dimensions of the bar. Assume $\mu_e = 0.39 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$.