Problem Set 6 due March 22

1. *Periodic Potentials in One Dimension*

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):

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

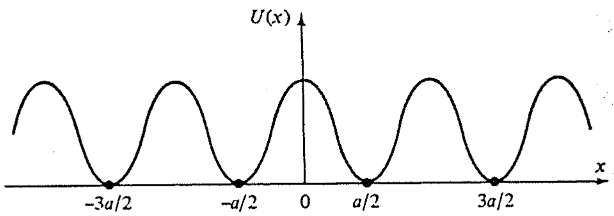

Figure 8.4
A one-dimensional periodic potential $U(x)$. Note that the ions occupy the positions of a Bravais lattice of lattice constant a. It is convenient to take these points as having coordinates $(n + \frac{1}{2})a$, and to choose the zero of potential to occur at the position of the ion.

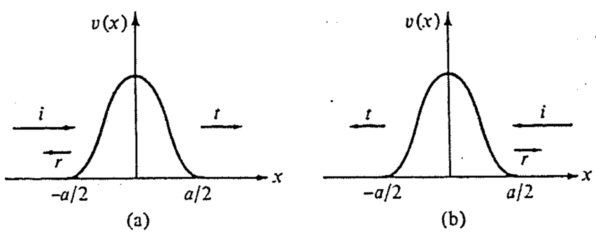

Figure 8.5
Illustrating particles incident from the left (a) and right (b) on a single one of the barriers separating neighboring ions in the periodic potential of Figure 8.4. The incident, transmitted, and reflected waves are indicated by arrows along the direction of propagation, proportional to the 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 energy[33] $\mathcal{E} = \hbar^2 K^2/2m$. Since $v(x) = 0$ when $|x| \geqslant a/2$, in these regions the wave function $\psi_l(x)$ will have the form

$$\psi_l(x) = e^{iKx} + re^{-iKx}, \qquad x \leqslant -\frac{a}{2},$$
$$= te^{iKx}, \qquad x \geqslant \frac{a}{2}. \tag{8.65}$$

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 v. 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 $\mathcal{E}$. From (8.65) it follows that $\psi_r(x)$ has the form

$$\psi_r(x) = te^{-iKx}, \qquad x \leqslant -\frac{a}{2},$$
$$= e^{-iKx} + re^{iKx}, \qquad x \geqslant \frac{a}{2}. \tag{8.66}$$

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 combination[34] 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 $-a/2 \leqslant x \leqslant a/2$, any solution to the crystal Schrödinger equation with energy $\mathcal{E}$ must be a linear combination of ψ_l and ψ_r in that region:

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

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

$$\psi(x + a) = e^{ika}\psi(x), \tag{8.68}$$

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

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

(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:

$$\cos ka = \frac{t^2 - r^2}{2t} e^{iKa} + \frac{1}{2t} e^{-iKa}, \qquad \mathcal{E} = \frac{\hbar^2 K^2}{2m}. \tag{8.70}$$

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

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[33] *Note:* in this problem K is a continuous variable and has nothing to do with the reciprocal lattice.
[34] A special case of the general theorem that there are n independent solutions to an nth-order linear differential equation.

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:

$$t = |t|\, e^{i\delta}. \tag{8.71}$$

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:

$$1 = |t|^2 + |r|^2. \tag{8.72}$$

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:

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

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

$$w(\phi_1, \phi_2) = \phi_1'(x)\phi_2(x) - \phi_1(x)\phi_2'(x). \tag{8.74}$$

(b) Prove that w is independent of x by deducing from (8.73) that its derivative vanishes.

(c) Prove (8.72) by evaluating $w(\psi_l, \psi_l^*)$ for $x \leqslant -a/2$ and $x \geqslant a/2$, noting that because $v(x)$ is real ψ_l^* will be a solution to the same Schrödinger equation as ψ_l.

(d) By evaluating $w(\psi_l, \psi_r^*)$ prove that rt^* is pure imaginary, so r must have the form

$$r = \pm i\,|r|\, e^{i\delta}, \tag{8.75}$$

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

$$\boxed{\frac{\cos(Ka + \delta)}{|t|} = \cos ka, \qquad \mathcal{E} = \frac{\hbar^2 K^2}{2m}.} \tag{8.76}$$

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 $\mathcal{E}(k) = \hbar^2 K^2/2m$) 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

$$Ka + \delta = n\pi \tag{8.77}$$

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

$$\mathcal{E}_{gap} \approx 2\pi n \frac{\hbar^2}{ma^2}|r|. \tag{8.78}$$

(g) Suppose the barrier is very strong, so that $|t| \approx 0$, $|r| \approx 1$. Show that the allowed bands of energies are then very narrow, with widths

$$\mathcal{E}_{max} - \mathcal{E}_{min} = O(|t|). \tag{8.79}$$

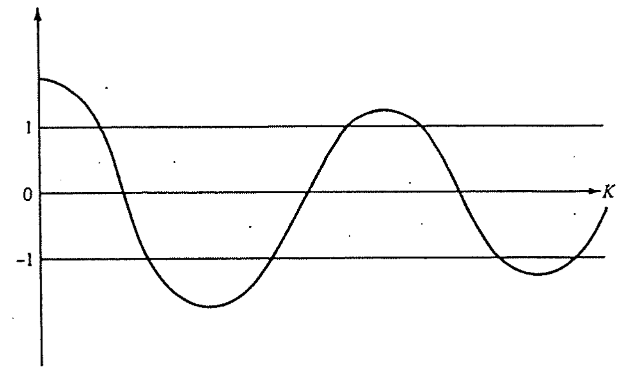

Figure 8.6
Characteristic form of the function $\cos(Ka + \delta)/|t|$. Because $|t(K)|$ is always less than unity the function will exceed unity in magnitude in the neighborhood of solutions to $Ka + \delta(K) = n\pi$. Equation (8.76) can be satisfied for real k if and only if the function is less than unity in magnitude. Consequently there will be allowed (unshaded) and forbidden (shaded) regions of K (and therefore of $\mathcal{E} = \hbar^2K^2/2m$). 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.

(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

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

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.