Physics 880.06: Problem Set 5

Due Friday, November 1, 2002

1. **Kronig-Penney model** In this problem you will work out a slightly different version of the Kronig-Penney model from that treated in class. Consider an electron moving in a one-dimensional crystal which has potential
$$U(x) = U_0 \sum_{n=-\infty}^{\infty} \delta(x - na), \tag{1}$$
where $\delta(x)$ is the usual Dirac delta function, and a is the lattice constant. The total Hamiltonian is
$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x). \tag{2}$$

   (a). What is the Bloch condition on the eigenstates $\psi(x)$?

   (b). What are the continuity (or discontinuity) conditions on ψ and $d\psi/dx$ at $x = a$?

   (c). What is the general form of the wave function for (i) $0 < x < a$; and (ii) $a < x < 2a$?

   (d). Using the above results, obtain a transcendental equation whose solutions give the eigenvalues $E_n(k)$ as a function of the Bloch vector k.

2. Consider a two-dimensional crystal which has a square Bravais lattice with lattice constant a. Suppose that one of the electronic bands in this crystal is described by the following relation between the energy E and the Bloch vector $\mathbf{k} = (k_x, k_y)$:
$$E(\mathbf{k}) = -t_0[\cos(k_x a) + \cos(k_y a)]. \tag{3}$$
Here t_0 is a positive real constant.

(a). Show that $E(\mathbf{k})$ is periodic in k-space, as stated in class - that is, show that $E(\mathbf{k}) = E(\mathbf{k} + \mathbf{K})$, where $\mathbf{K}$ is any reciprocal lattice vector of the square lattice. What are these reciprocal lattice vectors?

(b). Show that $E(\mathbf{k})$ has a minimum at $\mathbf{k} = 0$. Show that near the minimum, $E\mathbf{k} \sim E_0 + \hbar^2 k^2/(2m^*)$, and find the constants E_0 and m^*, in terms of t_0, a, and $\hbar$.

(c). Where is the band maximum? Hint: there may appear to be more than one in the first Brillouin zone, but they are all equivalent. Why is this? Are there any saddle points (where the electron group velocity is zero, but which are neither band minima nor band maxima)?

(d). Suppose that the Fermi energy of the crystal is $E_F = 0$. Find the shape of the Fermi surface in the first Brillouin zone. Hint: in a two-dimensional crystal, the Fermi "surface" is actually a Fermi curve, not a surface. Explain why, for this Fermi energy, the band contains exactly one electron per primitive cell.