Electronic Structure - Fudan - 2010 - Homework 2

Posted Wednesday April 21, 2010
Due Wednesday April 28, 2010
There may be mistakes! Let me know if you find an error in the statement of a problem!

1. Calculate the bands for graphene.

   Consider only the π states and assume the tight-binding form with matrix element t between nearest neighbors. The problem is described in detail in lecture 5, but you must work it out yourself. There is a mistake (inconsistent definitions of x and y axes) in one edition of the book and you must work it out yourself to be sure you have the right solution. See notes in Lecture 5.

   Use the coordinate system defined in Lecture 5, and give explicitly the points in (k_x, k_y) where the bands touch.

2. Consider a line, square and simple cubic lattices with one state per site and matrix elements t between states on nearest neighbor sites.

   A. In each of the three cases (line, square cube) give the band width W, which is the difference between the highest and lowest energy states. Give the answer in units of t.

   B. If the band is half filled (one electron per site, with equal numbers of up and down spins) show that the Fermi surface is a square in two dimensions (the orientation of the square surface is shown in lecture 5) and a cube in three dimensions.

3. Consider an infinite line of atoms A–B–A–B– with energies on each atom of ϵ_A and ϵ_B, and nearest neighbor matrix element t.

   A. Calculate the bands as a function of k in the Brillouin zone.

   B. If the is one electron per atom, is this an insulator or a metal?

4. Show that if the Bloch state $\psi_k(x) = exp(ikx)u_k(x)$ is an eigenstate of the Hamiltonian,

$$H\psi = [-\frac{\hbar}{2m}\nabla^2 + V(x)]\psi_k(x) = \epsilon_k\psi_k(x), \tag{1}$$

   then $u_k(x)$ is an eigenstate of a k-dependent Hamiltonian, $H(k)$ with the same eigenvalue ϵ_k,

$$H(k)u_k(x) = \epsilon_k u_k(x). \tag{2}$$

   Give the expression for $H(k)$.

5. For a 1 dimensional crystal of length L the eigenstates of kinetic energy are plane waves $\frac{1}{\sqrt{L}}e^{ikx}$. A small potential periodic $V(x) = V_0 cos(2\pi x/a)$ can be considered a perturbation, and the eigenvalues can be expanded in powers of V_0.

   A. Find the energy gap between the lowest band and the second band *to first order in V_0. (Do not try to evaluate the gap exactly).* 1. Does the energy gap depend upon the sign of V_0? If so, what is the difference? 2. Does the wavefunction of the lowest

band depend upon the sign of V_0? If so, what is the difference? 3. Does the density of the lowest band depend upon the sign of V_0? 4. What is the change in energy of the lowest state at $k = 0$ to lowest order in V_0?

B. Suppose the potential is $V(x) = V_0 cos(2\pi x/a') + V_1 cos(\pi x/a')$ in 1 dimension: 1. What is the lattice constant for this periodic crystal? 2. What is the Brillouin zone? 3. To first order in V_0 and V_1, what is the energy gap?