

Electronic Structure - Fudan - 2010 - Homework 2 - Solutions

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.

Solution: The expression for the dispersion in the lecture 5 is wrong: k_x and k_y should be interchanged. (The correct version is in later versions of the book.)

One way to see that x and y must be interchanged is to note that two neighbors are at $(\pm a/2, a/2\sqrt{3})$. The sum for these two neighbors gives a factor $\cos(k_x a/2)$. This is sufficient to show that the expression for H_{12} contains the factor $\cos(k_x a/2)^2$, the opposite of the expression in the lecture.

The expressions can be derived in detail by many choices that are equivalent. Here I choose the cell to be atoms at $(0, 0)$ and $\tau(0, 1)$ as shown in the lecture. Then one can over neighbors for each atom. One neighbor is in the same cell and two are in neighboring cells. This can be written

$$H_{12}(\mathbf{k}) = t \sum_i \exp(i\mathbf{k} \cdot \mathbf{T}_i) = t[1 + \exp(i\mathbf{k} \cdot \mathbf{a}_2) + \exp(i\mathbf{k} \cdot (\mathbf{a}_2 - \mathbf{a}_1))].$$

From this $\pm|H_{12}(\mathbf{k})|$ gives the dispersion given in the lecture, except that x and y are interchanged. An alternative form that is more convenient to me is to treat all the neighbors equivalently; this is to define the matrix elements as $t \exp(i\mathbf{k} \cdot \mathbf{R}_i)$ where $\mathbf{R}_i$ is the actual position $\mathbf{R}_1 = \tau(0, 1)$, $\mathbf{R}_2 = -\mathbf{a}_2 + \tau(0, 1)$, and $\mathbf{R}_3 = -\mathbf{a}_2 + \mathbf{a}_1 + \tau(0, 1)$. This is just a complex factor that does not affect the results, but the expression is more symmetrical. This leads to the form in the lecture, except with x and y interchanged. The bands touch at the points where $H_{12} = 0$ which are the 6 points: $(4\pi/3a, 0)$ and the other 5 points found by rotations of $\pm 60^\circ$, $\pm 120^\circ$ and 180° degrees.

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 .

Solution: the results are 4 times the number of neighbors: $4t$, $8t$, $12t$.

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.

The bands are given by $\epsilon(k) = \pm t(\cos(k_x a))$, $\epsilon(k) = \pm t(\cos(k_x a) + \cos(k_y a))$, and $\epsilon(k) = \pm t(\cos(k_x a) + \cos(k_y a) + \cos(k_z a))$. For half filling it is a square in 2 d, using the relation $\epsilon = \cos(\pi - k_x a) + \cos(k_x a) = 0$ for $k_y = \pi - k_x$. But the requirement that $\epsilon = 0$ does NOT lead to cube in three dimensions. For example, at the center of a face of the BZ, where $k + z = k_y = 0$, $k_x = \pi/a$, the energy is t and is not zero. Also you can realize that the generalization of the square in 2d is a cube in 3d that has 1/4 the volume of the Brillouin zone, not one half.
Extra credit for the right answer - subtract only a point if you make a good try but did not get the correct answer.

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.

Solution: This is a 2x2 determinant equation with diagonal terms ϵ_A and ϵ_B and off-diagonal the same as for the one atom per cell case. This leads to

$$\epsilon(k) = \frac{\epsilon_A + \epsilon_B}{2} \pm \sqrt{\left(\frac{\epsilon_A - \epsilon_B}{2}\right)^2 + 4t^2 \cos^2(ka)}$$

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

Solution: There are two electrons per cell that fills the lower band. Thus it is an insulator.

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

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

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

$$H(k)u_k(x) = \epsilon_k u_k(x). \quad (2)$$

Give the expression for $H(k)$.

Solution: This follows from straightforward differentiation, with the result

$$H\psi = \left[-\frac{\hbar^2}{2m}(\nabla + ik)^2 + V(x)\right]\psi_k(x) = \epsilon_k\psi_k(x), \quad (3)$$

where the potential term is not modified.

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).

Solution: The states are degenerate for $V_0 = 0$ and solution of the perturbation equations with only these bands gives $\epsilon = \pm V_0$.

1. Does the energy gap depend upon the sign of V_0 ? If so, what is the difference?
No
 2. Does the wavefunction of the lowest band depend upon the sign of V_0 ?
If so, what is the difference?
Yes - changes the positions of the maxima and minima in the wavefunction.
 3. Does the density of the lowest band depend upon the sign of V_0 ?
Yes - changes the positions of the maxima and minima in the density. (FULL CREDIT if you understood this to mean the average density which of course does not change.)
 4. What is the change in energy of the lowest state at $k = 0$ to lowest order in V_0 ? (No points subtracted if you interpreted this to mean the lower state at the band edge.)
In this case the lowest order is quadratic and is given by second-order perturbation theory. The state is shifted down by $\Delta\epsilon = V_0^2/E_1$, where $E_1 = (\hbar^2/2m)(2\pi/a)^2$.
- 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?
The lattice constant is $2a'$
 2. What is the Brillouin zone?
 $-\pi/2a' < k < \pi/2a'$.
 3. To first order in V_0 and V_1 , what is the energy gap? Solution: To first order V_0 has no effect; it is only the matrix element between $\exp(ikx)$ and $\exp(-ikx)$ for $k = \pi/2a'$ that has an effect to first order, and the gap is $\epsilon = \pm V_1$.