Electronic Structure - Fudan - 2010 - Homework 1

Posted Thursday April 15, 2010
Due Thursday April 22, 2010
There may be mistakes! Let me know if you find an error in the statement of a problem!

1. Crystals

   Give the Bravais lattice and the basis for:

   (a) A line of atoms spaced by a, $X--X--X--X--$

   (b) If the above crystal is dimerized, this is alternating short and long bonds $X-X---X-X--$. Give two ways to choose the basis.

   (c) A line of atoms spaced by equal distance a with alternating A and B atoms $A--B--A--B--$. Give two ways to choose the basis.

   (d) If there is the combination of both alternating A and B atoms and alternating short and long bonds. Give two ways to choose the basis.

   (e) A two dimensional graphene crystal with the distance between atoms denoted by D.

   (f) A NaCl crystal with the side of conventional cell having length a.

   (g) A Si crystal with the side of conventional cell having length a.

2. Reciprocal lattice

   (a) Show explicitly that fcc and bcc lattices are reciprocal to one another.

   (b) For the two-dimensional graphene lattice, show that the reciprocal space lattice is hexagonal and that it is rotated with respect to the real space lattice. What is the angle of rotation?

3. Density of electrons

   The local density approximation is best for high densities of electrons. The density can be characterized by r_s, the radius of a sphere that has the average volume per electrons: $(4\pi/3)r_s^3 = 1/n$ where n is the density. Note that n is the density counting both up and down spin electrons. Typical values in solids are $\approx 2-4$ in units of the bohr radius a_0. For $r_s > \approx 5$, the electrons may become highly correlated.

   (a) Consider an fcc crystal with a denoting the length of the side of the conventional cube, show that $r_s = \frac{a}{2}(\frac{3}{2\pi Z})^{1/3}$ where Z is the number of electrons per cell.

   (b) For the valence electrons in diamond carbon, show that your result in the previous exercise gives $r_s \approx 2.0$ in units of the bohr radius a_0.

4. Special points

   Special points are designed to evaluate the integral over periodic functions $f(k)$ as the sum over only a few points. We can use the fact that all the properties of bands

are periodic in k with periodic volume equal to the Brillouin zone (BZ). Examples: The average of eigenvalues ϵ_k is needed for the total energy per cell; the total density $n(r)$ normalized to one electron per band in the cell (2 electrons counting spin) is the integral of the density of the eigenfunction at wavevector k, $|\psi_k(r)|^2$. We can find the average of $f(k)$ by summing over a fine grid, but we can do this much more efficiently for smooth periodic functions. Since bands functions are smooth they can always be represented by a Fourier series $f(k) = A_0 + A_1\cos(ka) + A_2\cos(2ka) + A_3\cos(3ka) + \ldots$. Often $f(k)$ can be represented by a very small number of Fourier components with $A_i = 0$ for all $i > n_{max}$. However, we do not know the values of $A_0, A_1, \ldots$ in advance; we need to find the average A_0 by calculating $f(k)$ at points k in the BZ. Special points are chosen so that the average of each cosine function is zero for $0 < i, n$,so that the average of $f(k)$ gives the desired value A_0.

a. For a one-dimensional crystal with cell length a, show that the average of f(k) over the Brillouin zone (BZ) is given correctly by $\frac{1}{2}(f(\frac{1}{4}\frac{\pi}{a}) + f(\frac{3}{4}\frac{\pi}{a}))$, if f is given by the Fourier components $f(k) = A_0 + A_1\cos(ka) + A_2\cos(2ka) + A_3\cos(3ka)$ and all higher Fourier components are zero.

b. However, there is an error if higher Fourier components are not negligible. What is the error due to a term $A_4\cos(4ka)$?

c. Extend the arguments to a two dimensional square lattice with side a where we consider a function $f(k_x, k_y) = A_{00} + A_{10}\cos(k_x a) + A_{01}\cos(k_y a) + A_{1,1}\cos(k_x a + k_y a) + \ldots$. Consider the three points (1/4,1/4), (3/4,3/4) and (1/4,3/4), where (1/4,3/4) is weighted by a factor of 2 since it actually represents two equivalent points (1/4,3/4) and (1/4,1/4). Show that this is sufficient correctly give the average A_{00} for all Fourier components up through $(3, 3)$. where a is the square edge.

ASK PROF. MARTIN IF IT IS NOT CLEAR WHAT YOU NEED TO DO IN THIS EXERCISE.

5. "Force Theorem" ("Helmann-Feynman theorem")

In his undergraduate thesis, Feynman showed that the force on any nucleus in simply the charge of the nucleus times the electric field at the site of the nucleus due to the electron density $n(r)$ and the other nuclei. This is obvious if the electron density does not change as one nucleus is given an infinitesimal displacement. But in fact the electrons respond, the wavefunction changes, etc.

The object of this problem is to show that if the electrons are in their ground state, these complicated changes in the electron state do not affect the force. This can be done in extremely difficult ways or by a very easy argument. DO NOT SPEND A LONG TIME ON THIS - ASK PROF. MARTIN IF THIS SEEMS DIFFICULT.

Hint: All changes in the electrons are described by the changes in their ground state wavefunction as the atoms is displaced. However, we know something about ground state wavefunction; it is the function that gives the lowest energy. This is sufficient to find the desired result.