Department of Electrical and Computer Engineering, Cornell University

ECE 4070: Physics of Semiconductor and Nanostructures

Spring 2014

Homework 5 **Due on March 25, 2014 at 5:00 PM**

Suggested Readings:

a) Lecture notes

Problem 5.1 (1D lattice energy bands outside the FBZ – periodicity of energy bands)

In a previous homework (problem 3.4), you found the exact solution for an electron in a periodic 1D lattice. You will consider the same problem again here. Consider a 1D lattice of lattice constant a equal to 5 Angstroms. Suppose the potential has the form:

$$V(x) = 2V_1 \cos\left(\frac{2\pi}{a}x\right) + 2V_2 \cos\left(\frac{4\pi}{a}x\right)$$

Where V_1 equals 0.3 eV and V_2 also equals 0.3 eV. The exact solution for any wavevector k in the FBZ can be written as a superposition of plane waves in the form:

$$|\psi_k\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m)\,|\phi_{k+G_m}\rangle = \sum_{m=-\infty}^{\infty} c_k(G_m)\sqrt{\frac{1}{L}}\,e^{i(k+G_m)x}$$

where:

$$G_m = m\frac{2\pi}{a}$$

A good approximation to the exact solution can be obtained by terminating the series above at both ends, as follows:

$$|\psi_k\rangle = \sum_{m=-N}^{N} c_k(G_m)\,|\phi_{k+G_m}\rangle$$

Where N is some large number, say 10. The way you hopefully solved the problem in homework 4 was to first choose a value of the wavevector k in the FBZ, then setup a matrix, and then find its three smallest eigenvalues. The question is what if one chooses a value of the wavevector k that is not in the FBZ? Would one end up with some new energy eigenvalues and new energy eigenfunctions? The goal of the problem is to explore this point.

If you are not confident of your answer in homework 4, you can download a matlab routine from the course website that will plot the first three energy bands in the FBZ

a) Choose values of the wavevector k between $-3\pi/a$ and $+3\pi/a$, and for each chosen value of wavevector k find the smallest three energy eigenvalues by repeating the same procedure as you followed in problem 4.3 – the only difference being that now your range of wavevector values include higher order BZs. What do you find? How do the energy bands look like outside the first BZ? Hand in your plots.

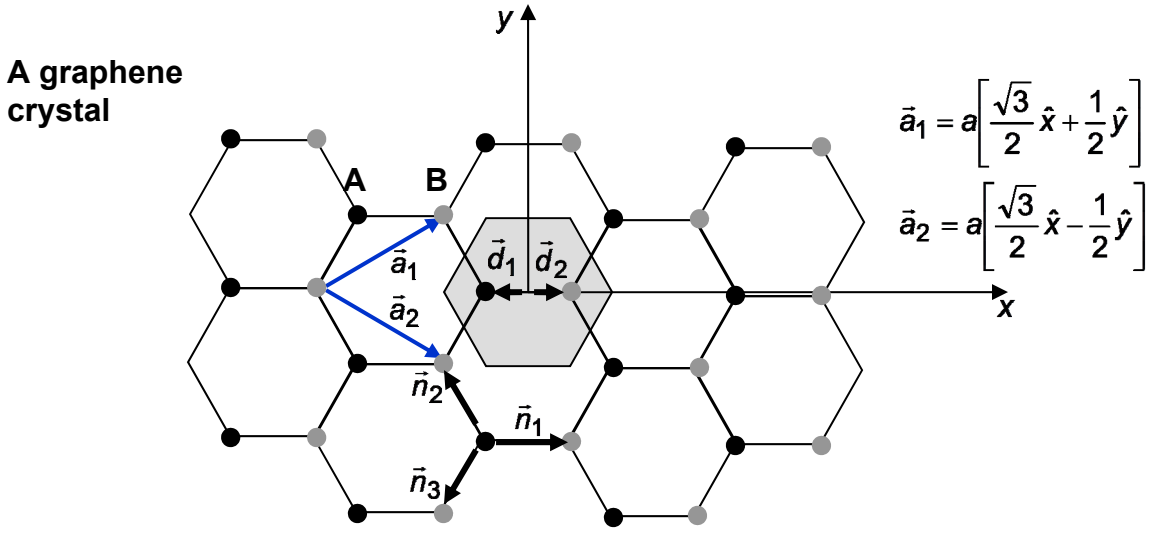
IMPORTANT NOTE ADDED: Recall that by convention the wavevector $\vec{k}$ is restricted to the first BZ. The previous part of this problem tells us that no NEW energy levels (or wavefunctions) are obtained if, say inadvertently, one were to use a value of $\vec{k}$ outside the FBZ in calculations of the bandstructure. Sometimes this mathematical property is expressed by saying that the energy bands are periodic in k-space with the periodicity of the reciprocal lattice, i.e.,

$E_n\left(\vec{k}+\vec{G}\right)=E_n\left(\vec{k}\right)$

where $\vec{k}$ is in the FBZ and $\vec{G}$ is any reciprocal lattice vector.

Problem 5.2 (Graphene σ-bands ala tight binding)

Consider the graphene crystal. In this problem you will perform tight binding calculations for the σ-bands that come from the s, px, and py orbitals of each carbon atom (ignoring the sp2 hybridization picture). The energies of these orbitals are: E_s, E_p, and E_p, respectively.



The trial tight binding solution can be written as:

$$|\psi(\vec{r})\rangle = \sum_m \frac{e^{i\,\vec{k}\,.\,(\vec{R}_m+\vec{d}_1)}}{\sqrt{N}}\left[c_1\; e|\phi_s(\vec{r}-\vec{R}_m-\vec{d}_1)\rangle + c_2\,|\phi_{px}(\vec{r}-\vec{R}_m-\vec{d}_1)\rangle + c_3\,|\phi_{py}(\vec{r}-\vec{R}_m-\vec{d}_1)\rangle\right]$$
$$+\sum_m \frac{e^{i\,\vec{k}\,.\,(\vec{R}_m+\vec{d}_2)}}{\sqrt{N}}\left[c_4\; e|\phi_s(\vec{r}-\vec{R}_m-\vec{d}_2)\rangle + c_5\,|\phi_{px}(\vec{r}-\vec{R}_m-\vec{d}_2)\rangle + c_6\,|\phi_{py}(\vec{r}-\vec{R}_m-\vec{d}_2)\rangle\right]$$

The resulting 6x6 matrix can be written as:

$$\begin{bmatrix} H_{11} & H_{12} & H_{13} & H_{14} & H_{15} & H_{16} \\ H_{21} & H_{22} & H_{23} & H_{24} & H_{25} & H_{26} \\ H_{31} & H_{32} & H_{33} & H_{34} & H_{35} & H_{36} \\ H_{41} & H_{42} & H_{43} & H_{44} & H_{45} & H_{46} \\ H_{51} & H_{52} & H_{53} & H_{54} & H_{55} & H_{56} \\ H_{61} & H_{62} & H_{63} & H_4 & H_{65} & H_{66} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{bmatrix} = E(\vec{k}) \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \end{bmatrix}$$

In answers to questions below, use the standard expressions for the matrix elements (i.e. $V_{ss\sigma}$, $V_{pp\sigma}$, etc).

a) Find the 6 diagonal elements of the matrix: $H_{11,}\, H_{22}$, H_{33} , H_{44}, H_{55}, H_{66}

b) Find the matrix elements: H_{14} , H_{15} , H_{16}

c) Find the matrix elements: H_{24} , H_{34}

d) Find the matrix elements: H_{25} , H_{36}

e) Describe how many bands will result from the above calculation and how many will be completely filled with electrons and how many will be partially filled with electrons at zero temperature

Problem 5.3 (Energy bands in GaAs)

a) In lecture handout, the matrix *H,* which results from the tight binding solution for GaAs, is given. Calculate the following elements of the matrix and verify your results by comparing them with the expressions given in the handout:

H_{15}
H_{16}
H_{25}
H_{26}
H_{27}

b) Using the following parameters values, calculate all 8 energy bands of GaAs along Γ-X $(2\pi/a,0,0)$ and Γ-L $(\pi/a,\pi/a,\pi/a)$ directions and plot them.

$a = 5.65325$ Angstroms

$E_{SG} = -11.37$ eV

$E_{PG} = -4.90$ eV

$E_{SA} = -17.33$ eV

$E_{PA} = -7.91$ eV

$V_{ss\sigma} = 1.70$ eV

$V_{sp\sigma} = 2.15$ eV

$V_{pp\sigma} = 3.44$ eV

$V_{pp\pi} = 0.89$ eV

You will need to setup the matrix for each value of the wavevector, and then solve for its eigenvalues. Save your code for future. You will need it later in the course.