

Assignment 2

EE 698N, Advanced Semiconductor Physics

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1 Bloch-Function Solutions

By writing the crystal potential as the Fourier series $V(\vec{r}) = \sum_{\vec{G}} V_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$, and electron wavefunction in the Bloch form $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u(\vec{r})$, where the crystal-periodic term is also written in its Fourier series $u(\vec{r}) = \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}}$, show the following.

- a) The Schrödinger equation (a differential equation) in real space is converted to the following (algebraic equation) in the k-space:

$$\left[E - \frac{\hbar(\vec{k} + \vec{G})^2}{2m} \right] C_{\vec{G}} = \sum_{\vec{G}'} V_{\vec{G}'} C_{\vec{G} - \vec{G}'} \quad (1)$$

- b) Show that the way to calculate the Fourier coefficients is

$$V_{\vec{G}} = \frac{1}{v_0} \int_{u.c.} d^3r e^{-i\vec{G}\cdot\vec{r}} V(\vec{r}), \quad (2)$$

where v_0 is the volume of the unit cell.

2 2-D Bandstructure

In the k-space of a 2D square lattice (lattice constant: a), denote the points $\Gamma : (k_x, k_y) = (0,0)$, $X : (\pi/a, 0)$, and $W : (\pi/a, \pi/a)$. I have drawn this in Figure 1. In class, we considered the bandstructure for the case ($V(x, y) = 0$) in the $\Gamma - X$ direction in the 1st Brillouin Zone (BZ). The bandstructure, of course, exhibited no gaps, since there was no crystal potential.

- a) Draw the free-electron bandstructure from the BZ center in the $\Gamma - W$ direction up to the BZ edge. Identify the magnitude of k at the BZ edge, and express the energy in terms of $F = \hbar^2 \pi^2 / ma^2$. Include reciprocal lattice vectors smaller than $2 \times 2\pi/a$.
- b) Label each band with the reciprocal lattice vector it is associated with. Clearly point out the degeneracies of each band, similar to the diagram shown in class.

We also saw that for the 1-D case, turning on a crystal potential led to the appearance of energy gaps at the BZ edge. In this problem, you do the same for the 2-D case. Consider a 2-D potential

$$V(x, y) = -4V_0 \cos\left(\frac{2\pi x}{a}\right) \cos\left(\frac{2\pi y}{a}\right) \quad (3)$$

- c) Find the bandgap at the W point. Be judicious in choosing the basis set. Hint: It is sufficient to include only those states in the basis that have similar energies as the plane wave state at the W -point.

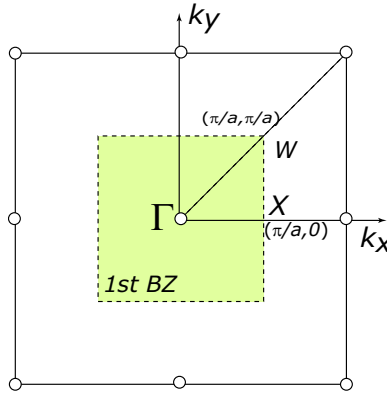


Figure 1: 2D reciprocal lattice.

- d) (For the more adventurous, not compulsory) Draw the 2-D bandstructure in the 1st BZ for the lowest three bands. This is drawn as a 2-D plot of energy as a function of every point in the (k_x, k_y) plane.

3 Real Semiconductor: Nearly Free Electron Model

Calculate the bandstructure of the general FCC crystal, and plot it the same way as in Cardona & Yu, Fig 2.9.

- Start by considering the real space FCC primitive lattice vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$, finding the primitive reciprocal lattice vectors $\vec{b}_1, \vec{b}_2, \vec{b}_3$, and proving that the reciprocal space lattice is BCC.
- Write the energy as a function of the wavevector for each reciprocal lattice vector \vec{G} . Draw up a table. Plot the bandstructure in the $\Gamma - L$ and $\Gamma - X$ directions in the same figure. Indicate each section of the bands with the corresponding \vec{G} it comes from. Indicate the degeneracies for each band.

4 Matrix elements

Problem 2.9, Cardona & Yu. What are the dimensions of the matrix element squared? Explain the result intuitively, drawing upon your knowledge of bandstructure.