ECE344 Fall07

HOMEWORK 2

Energy Band Theory and Semiconductor Fundamentals

1 Energy Band Theory (60pts)

We consider an infinite chain of atoms (going from $-\infty$ to ∞) where l is the distance between the atoms. For a given (isolated) atom n, only one energy state $v_n(x)$ is available. We write the total wave function of the chain of atoms as a linear combination of basis functions $v_n(x)$:

$$\Psi(x) = \sum_{n=-\infty}^{\infty} c_n \, v_n(x)$$

where we introduce the coefficients c_n. In addition, we will consider the following condition:

$$\int_{-\infty}^{+\infty} v_n(x) v_p(x) = \delta_{n,p}.$$

We would like to solve the Schrödinger equation $H\Psi = E\Psi$ for this system (H is a given operator Hamiltonian).

1. Show that c_n satisfies the following equation:

   $$E_0 c_n - A c_{n+1} - A c_{n-1} = E c_n,$$

   where you will give the expression of E_0 (on site energy) and A (coupling term) in function of H. Hint: You can first replace the expression of $\Psi(x)$ in the Schrodinger equation then pre-multiply by $v_m(x)$, and integrate over all the real space. Also, you will consider for the atoms only the interactions between the first neighbors.

2. We consider solutions of this form: $c_n = \exp(iknl)$, where k belongs to the first Brillouin zone. Find and plot the dispersion relation. Comment

3. From the graph, comment on what would happen if the tunneling effect between atoms increases.

4. Considering that the state v_n can be obtained by translation nl of the state v_0 (i.e. $v_n(x) = v_0(x - ql)$), demonstrate the first form of the Bloch theorem:

   $$\Psi_k(x + l) = \exp(ikl)\Psi_k(x)$$

5. In the atom chain, where is the electron associated with the state Ψ_k ?

6. We consider a finite chain L with N number of atoms such as N is very large. Using Born-Von Karman boundary conditions (periodic B.C.), the possible values for k are $k_n = n2\pi/L$. How many k states are available in the first brillouin zone (give the result in fonction of N, also we will not consider the spin factor). How can we approximate this expression if the number of atoms is very large ($N >> 1$).

7. Calculate and plot the group velocity of the electrons which is given by

   $$V_G = \frac{1}{\hbar}\left(\frac{dE(k)}{dk}\right).$$

   What is happening if the energy of the electron goes to $E_0 + 2A$?

2 Carrier densities (40pts)

1. Using the effective mass approximation, derive the expression of the density of state (DOS) $g(E)$ for a 2D and 1D electron gas. We will use the fact that E_1 is the minimum energy for the electrons ($E_1 > E_c$ due to quantization effects in systems with low-dimensionalities).

2. Calculate the number of states per unit of energy in a 3D $100nm$ by $100nm$ by $10nm$ piece of Silicon ($m^* = 1.08m_0$, m_0: mass of the electron) $100meV$ above the conduction band edge. Write the result in units of eV^{-1}. Do the same for a $100nm$ by $100nm$ 2D silicon sheet and $100nm$ 1D silicon wire (we consider $E_1 = 40meV$). Comment on all these results.

3. For non-degenerate semiconductors, derive analytically the expressions of the effective density of states for a 2D and 1D system (N_c^{2D} and N_c^{1D}).

4. In the general case (Fermi-Dirac distribution), derive analytically the expression of electron density for a 2D electron gas (you will give the expression in function of N_c^{2D}).