

ECE609 Spring06
HOMWORK 2 - SOLUTIONS
 Energy Band Theory and Semiconductor Fundamentals

1 Energy band theory using the LCAO method

1.

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

2. We replace the expression of $\Psi(x)$ in the Schrödinger equation then we multiply by $v_m(x)$ and integrate over all the real space (projection). We get:

$$\sum_n c_n \left(\int v_m(x) H v_n(x) dx \right) = E \sum_n c_n \left(\int v_m(x) v_n(x) dx \right),$$

where the second term is equal to zero but for $m = n$. Since we consider only the coupling between first neighbors, in the first term, the sum over n is different of zero only for $n = m, m + 1, m - 1$.

$$c_m \left(\int v_m(x) H v_m(x) dx \right) + c_{m+1} \left(\int v_m(x) H v_{m+1}(x) dx \right) + c_{m-1} \left(\int v_m(x) H v_{m-1}(x) dx \right) = E c_m,$$

or ($m \equiv n$):

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

with

$$E_0 = \int v_n(x) H v_n(x) dx$$

and

$$A = - \int v_n(x) H v_{n+1}(x) dx = \int v_n(x) H v_{n-1}(x) dx.$$

3.

$$E = E(k) = E_0 - 2A \cos(kl),$$

we can plot this relation on the first brillouin zone $-\pi/l \leq k < \pi/l$. We obtain a permitted energy band between the energy $E_0 - 2A$ and $E_0 + 2A$. The width of the band is equal to $4A$ depending on the strength of the coupling term A (i.e. tunneling effect between atoms). So if the tunneling effect increases the energy band becomes larger.

4.

$$\Psi_k(x) = \sum_{n=-\infty}^{\infty} \exp(iknl) v_0(x - nl)$$

it comes for $\Psi(x + l)$:

$$\Psi_k(x+l) = \sum_{n=-\infty}^{\infty} \exp(iknl) v_0(x - (n-1)l) = \exp(ikl) \sum_{n=-\infty}^{\infty} \exp(ik(n-1)l) v_0(x - (n-1)l) = \exp(ikl) \Psi_k(x)$$

5. we can easily show that $u_k(x) = u_k(x + l)$, and we get the second form of the Bloch theorem.

6. $|\Psi_k(x + nl)|^2 = |\Psi_k(x)|^2 \quad \forall n$, so the probability to find an electron on a given atom is periodic and it is the same on each atom site. We say that the electron is delocalized.
7. we get $\exp(ikl) = 1$ so $k_n = n2\pi/L$. The length of the Brillouin zone is equal to $2\pi/l$. So, the number of states available is $(2\pi/l)/(2\pi/L) = N - 1$. One can also use the definition of the density of state in the k-space $g(k)dk$ (then integration) to show this result. If $N \gg 1$, then $N - 1 \simeq N$.
- 8.

$$V_G = \frac{2Al}{\hbar} \sin(kl)$$

If the energy goes to $E_0 + 2A$, k goes to $+\pi/l$ or $-\pi/l$ (extremities of the first Brillouin zone - see figure of the dispersion relation becomes zero). This means that the electron cannot move in the crystal if its energy is too close to the maximum $E_0 + 2A$. Just for information: this situation is similar with what is happening in optic with the Bragg reflection.

2 Carrier densities

1. For 1D or 2D, we have

$$E = \frac{\hbar^2 k^2}{2m^*} + E_1.$$

- For 2D, we have in k-space:

$$g(k)dk = 2 * \frac{S}{(2\pi)^2} 2\pi k dk$$

and in energy space

$$g(E) = \frac{S}{\pi} k \left(\frac{dE}{dk} \right)^{-1} = \frac{Sm^*}{\pi\hbar^2}$$

the DOS does not depend on the energy E .

- For 1D (per unit of volume), we have in k-space:

$$g(k)dk = 2 * \frac{L}{(2\pi)} 2dk$$

and in energy space

$$g(E) = \frac{2L}{\pi} \left(\frac{dE}{dk} \right)^{-1} = \frac{2L}{\pi\hbar} \left(\frac{m}{2(E - E_1)} \right)^{1/2}$$

the DOS does not depend on the energy E .

- 2.

$$\frac{3D \quad 2.41 * 10^5 eV^{-1}}{\frac{2D}{1D}}$$

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}).

$$N_c^{2D} = \frac{m^*}{\beta\pi\hbar^2}$$

$$N_c^{1D} = \left(\frac{2m^*}{\beta\pi\hbar^2} \right)^{1/2}$$

4.

$$n = N_c^{2D} \ln(1 + \exp(\beta(E_F - E_1)))$$

3 Electrons and holes

We note that

$$J_{VB} = \frac{1}{V} \sum_{\text{filled sates}} (-q)v_i = \frac{1}{V} \left(\sum_{\text{all sates}} (-q)v_i \right) - \sum_{\text{empty sates}} (-q)v_i.$$

The sum over all the states in the lower band has to equal zero since electrons in a completely filled band do not contribute to current, while the remaining term can be written as:

$$J_{VB} = \frac{1}{V} \sum_{\text{empty sates}} (+q)v_i,$$

which states that the current is due to positively charged particles associated with the empty states in the almost-filled band (these are holes). Holes are moving in the same direction than the electric field. Holes therefore “move upper hill” in the valence band