HOMEWORK 2 - SOLUTIONS
Energy Band Theory and Semiconductor Fundamentals

1   Energy Band Theory

- (ii) to (i): $\Psi_k(r+R) = e^{ikR}e^{ikr}u_k(r+R) = e^{ikR}e^{ikr}u_k(r) = e^{ikR}\Psi_k(r)$

  (i) to (ii): we set $u_k(r) = e^{-ikr}\Psi_k(r)$, then $u_k(r+R) = e^{-ikr}e^{-ikR}\Psi_k(r+R) = u_k(r)$, since $e^{-ikR}\Psi_k(r+R) = \Psi_k(r)$.

-
$$\nabla(e^{ikr}u_k(r)) = ike^{ikr}u_k(r) + e^{ikr}\nabla u_k(r)$$
$$\Delta(e^{ikr}u_k(r)) = -k^2 e^{ikr}u_k(r) + ike^{ikr}u_k(r) + ike^{ikr}u_k(r) + e^{ikr}\Delta u_k(r) = e^{ikr}(-k^2 + 2ik\nabla + \Delta)u_k(r)$$

  Finally, we obtain the expression we saw in class.

2   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 $N >> 1$, 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.

3 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.

$$\frac{\begin{array}{ll} 3D & 2.41 * 10^5 eV^{-1} \\ 2D & 4.5 * 10^4 \end{array}}{\begin{array}{ll} 1D & 6.93 * 10^2 \end{array}}$$

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.

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