Department of Electrical and Computer Engineering, Cornell University

ECE 4070: Physics of Semiconductors and Nanostructures

Spring 2014

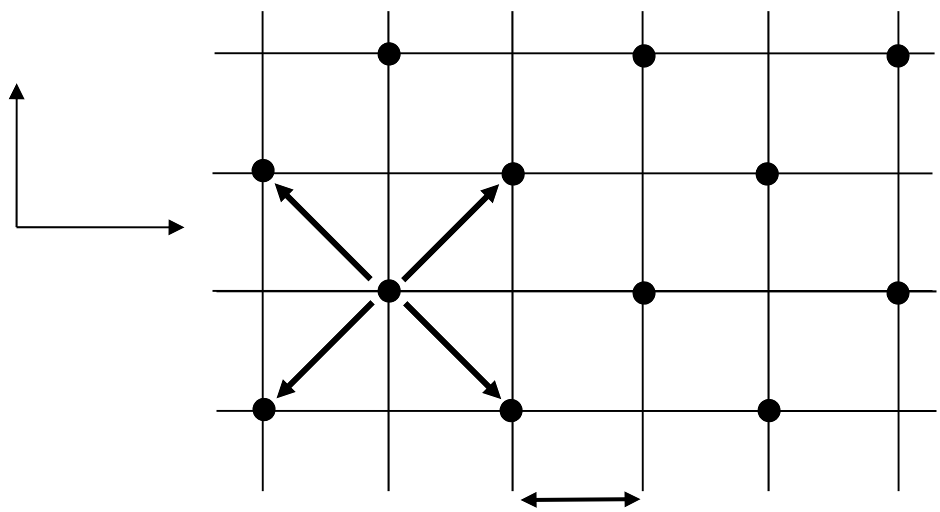
Homework 8 **Due on April 29, 2014 at 5:00 PM**

Suggested Readings:

a) Lecture notes

Problem 8.1 (Phonons of a 2D lattice)

Consider the following 2D crystal:



Each atom has a mass ***M***. The crystal has a bond-stretching force constant of α.

The dynamical equation can be written as:

$$\overline{\overline{D}}(\vec{q})\begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix} = \omega^2\, M \begin{bmatrix} u_x(\vec{q}) \\ u_y(\vec{q}) \end{bmatrix}$$

a) Find all four components of the dynamical matrix $\overline{\overline{\boldsymbol{D}}}$.

b) Using results from part (a), find analytical expressions for the frequency dispersions, $\omega_{LA}(\vec{q})$ and $\omega_{TA}(\vec{q})$, of the LA and TA phonon modes propagating in the $\hat{x}$ and also in the $(\hat{x}+\hat{y})/2$ directions near the zone center (i.e. find the frequencies as a function of the magnitude of the wavevector, q , for $q \approx 0$) and also find the corresponding phonon mode eigenvectors for each case.

c) Using results from part (a), find analytical expressions for the frequency dispersions, $\omega_{LO}(\vec{q})$ and $\omega_{TO}(\vec{q})$, of the LO and TO phonon modes at the zone center (i.e. find the frequencies for $q = 0$) and also find the corresponding phonon mode eigenvectors for each case.

Problem 8.2: (Time-dependent effective mass equation)

Sometimes, for example when the external potential is time-dependent, time-dependent solutions are sought. Suppose the external potential is time-dependent and is $U(\vec{r},t)$. We want to solve the time-dependent Schrodinger equation,

$$\left[\hat{H} + U(\vec{r},t)\right]\psi(\vec{r},t) = i\hbar \frac{\partial \psi(\vec{r},t)}{\partial t}$$

Suppose we assume a solution for electron state near wavevector $\vec{k}_o$ based on a time-dependent envelope function,

$$\psi(\vec{r},t) = \phi(\vec{r},t)\,\psi_{n,\vec{k}_o}(\vec{r})$$

The underlying assumption for the above form of the solution is that the applied potential is slowly varying both in space and time so that the electron does not transition to another band. Then, following exactly the same steps as in the lecture notes, the envelope function can be shown to satisfy the time-dependent effective mass equation,

$$\left[E_n\left(\vec{k}_o - i\nabla\right) + U(\vec{r},t)\right]\phi(\vec{r},t) = i\hbar \frac{\partial \phi(\vec{r},t)}{\partial t}$$

a) Consider the case when a uniform DC electric field is applied so that,

$$U(\vec{r}) = e\,\vec{E}.\,\vec{r}$$

Although the potential is time-independent we seek a time-dependent solution by solving the time-dependent effective mass equation. Find $\phi(\vec{r},t)$ that satisfies,

$$\left[E_n\left(\vec{k}_o - i\nabla\right) + e\vec{E}.\,\vec{r}\right]\phi(\vec{r},t) = i\hbar \frac{\partial \phi(\vec{r},t)}{\partial t}$$

subject to the initial condition,

$$\psi(\vec{r},t=0) = \psi_{n,\vec{k}_o}(\vec{r}) \qquad \text{or} \qquad \phi(\vec{r},t=0) = 1$$

And show that your solution indeed satisfies the time-dependent effective mass equation.
Hint: look back at your earlier handout on electron dynamics in an applied uniform DC electric field.

b) The time-dependent solution found in part (a) has a time-dependent energy $E(t)$. What is it?

Problem 8.3: (Effective mass equation and probability current)

Consider a material with the conduction band dispersion given by,

$$E_c\left(\vec{k}\right) = E_c + \frac{\hbar^2 (k_x - k_{ox})^2}{2m_x} + \frac{\hbar^2 \left(k_y - k_{oy}\right)^2}{2m_y} + \frac{\hbar^2 (k_z - k_{oz})^2}{2m_z}$$

a) Show that the plane wave envelope function,

$$\phi(\vec{r}) = e^{i\,(q_x x + q_y y + q_z z)} \qquad\qquad \psi(\vec{r}) = \phi(\vec{r})\,\psi_{c,\vec{k}_o}(\vec{r})$$

is a solution of the effective mass equation with $U(\vec{r}) = 0$,

$$\left[\hat{E}_c\left(\vec{k}_o - i\nabla\right) + U(\vec{r})\right]\phi(\vec{r}) = E\,\phi(\vec{r})$$

b) Show that with $U(\vec{r}) = 0$, the complete solution $\psi(\vec{r})$ is a Bloch function (i.e. satisfies the Bloch's theorem) and has a crystal momentum equal to $\vec{k} = \vec{q} + \vec{k}_o$. Note that in the absence of any external potential the solution must necessarily satisfy Bloch's theorem and must be a Bloch state.

c) Find the probability current vector associated with the plane wave envelope function of part (a). Note that the probability current is given by a vector with x,y, and z components.

Problem 8.4: (Semiconductor quantum well problem)

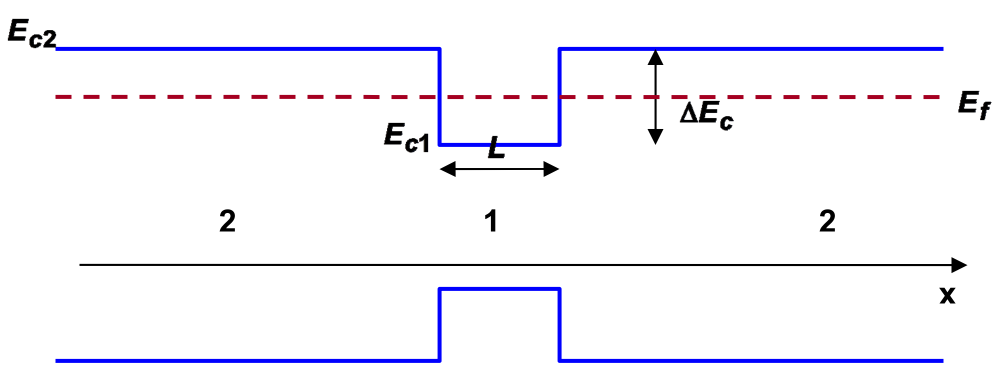
Consider a 80 Angstroms thick quantum well (i.e. $L = 80A$), as shown below. Suppose that $\Delta E_c = 150\text{ meV}$. The conduction band dispersion relations are as follows:

Well: $E_{c1}(\vec{k}) = E_{c1} + \frac{\hbar^2 k_x^2}{2m_{x1}} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z}$

Barrier: $E_{c2}(\vec{k}) = E_{c2} + \frac{\hbar^2 k_x^2}{2m_{x2}} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z}$

where:

$m_z = 0.10\ m_o$
$m_y = 0.045\ m_o$
$m_{x1} = 0.067\ m_o$
$m_{x2} = 0.20\ m_o$



a) How many conduction band bounds states are there in the quantum well? Analysis done in the lecture notes will not apply directly since the masses in the x-direction are different in the well and barrier materials.

b) Find the quantized energies relative to the conduction band edge E_{c1} of all the bound states in meV units? You will have to numerically or graphically solve this part.

c) Suppose the position of the Fermi level E_f is known. Using your results from parts (a) and (b), write an expression that relates the total electron density n (units: #/m^2) in the quantum well to the Fermi level. There should be no unevaluated integrals in your answer. **Hint:** The following integral might prove helpful:

$$\int_{E_a}^{\infty} dE \frac{1}{1+e^{(E-E_f)/KT}} = KT\log\left[1+e^{(E_f-E_a)/KT}\right]$$

d) Suppose somebody tells you that the total electron density in the quantum well is 10^{16} 1/m^2. Find the position of the Fermi level with respect to the conduction band edge (i.e. find $E_f - E_{c1}$) in meV units. Assume room temperature. You might have to solve this part numerically.