ECE 606 Homework Week 4
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1) Consider a one-dimensional wire with the following energy dispersion:

\[ E(k) = U_0 + \frac{\hbar^2 k^2}{2m} \]

1a) Use the finite difference scheme, and show that the Schrödinger equation can be written in the following form:

\[ E\psi_j = (U_0 + 2t)\psi_j - t\psi_{j-1} - t\psi_{j+1} \]

where \( t = \frac{\hbar^2}{2m^* a^2} \) and \( a \) is the lattice constant.

1b) Show that a plane wave of the form \( \psi(x) = \exp(ikx) \) must satisfy the following “numerical dispersion”:

\[ E(k) = U_0 + 2t\left[1 - \cos(ka)\right] \]

1c) Show that when the lattice constant, \( a \), is sufficiently small, the numerical dispersion reduces to the parabolic dispersion:

\[ E(k) = U_0 + \frac{\hbar^2 k^2}{2m} \]

1d) Derive the group velocity and effective mass using the numerical dispersion and compare them with the parabolic one. Also, sketch by hand the energy dispersion, group velocity and effective mass as function of \( k \). Comment if they agree well with the continuum Schrödinger case.

1e) If an electric field is applied along the +x-direction, describe the motion of the particle (i.e. velocity and acceleration) when \( ka = 0, \pi/2 \) and \( \pi \).

2) Use the BandStructure Lab tool on nanoHUB.org to explore the bandstructure of GaAs. Follow the steps outlined below, and then answer the questions.

a) Choose a bulk material from the “Geometry” option.

b) Specify the “Material” as GaAs

c) Click on the “2 Electronic Structure” tab to move to the next screen

d) Set the Tight Binding model to sp3s*d5 and check the Spin-Orbit coupling box
(Note that some of the options given here are preset as defaults; you need to leave them unchanged.)

e) Press the “3 Analysis” button to proceed.
f) Leave all preset options unchanged. Press the “4 Advanced User” option to take you to the next menu options.
g) Press “Simulate” on the bottom of this screen to start the simulation.

You should be able to answer the following questions.

• What is the crystal structure of GaAs?
• How many atoms are there in the unit cell of GaAs?
• Use the “Bulk Central” band plot to locate the Gamma, L, and X point. (You will want to re-scale the vertical axis to see these points clearly.)
• What are the corresponding energies at these points?
• Obtain the band gap information from the plot you used for the previous sub-parts.
• On the same plot you will notice bands below the 0 eV mark. What are these bands called and how are they classified?
• You will notice an energy split in the bands below 0 eV at the Gamma point. You will notice the so-called “split-off” band. How much is the energy split on the plot?
• From the effective mass table information, write down the effective masses at the gamma and L point conduction bands. What quantitative difference do you see between these masses?

3) Derive an expression for the density-of-states in energy for a 1D semiconductor for states near the center of the band at $k_x = 0$. Assume a valley degeneracy of $g_v$.

3a) Assume a parabolic dispersion near $k_x = 0$.

$$E(k_x) = E_C + \frac{\hbar^2 k_x^2}{2m^*}$$

3b) Assume a linear dispersion near $k_x = 0$.

$$E(k_x) = E_C + \hbar v_F |k_x|$$
4) Assume a nonparabolic, 1D energy bandstructure described by the so-called Kane dispersion as:

\[ E(k_x)[1 + \alpha E(k_x)] = \frac{\hbar^2 k_x^2}{2m^*(0)}. \]

where

\[ \frac{1}{m^*(0)} = \frac{1}{\hbar^2} \left. \frac{d^2 E(k_x)}{dk_x^2} \right|_{k_x=0}. \]

4a) Sketch (or produce a Matlab plot) of \( E(k) \) vs. \( k \) for two cases: i) \( \alpha = 0 \) and ii) \( \alpha > 0 \). If you are producing a Matlab plot, the energy range should be from 0 to 1 eV, and you can assume \( \alpha = 0.5 \) eV.

4b) For this bandstructure, derive an expression for the velocity, \( v_x(E) \) as a function of energy, \( E \).

5) For parabolic energy bands, the 2D density of states is

\[ D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \Theta\left( E - E_C \right). \]

Assume a non-parabolic band described by the so-called Kane dispersion,

\[ E(k)[1 + \alpha E(k)] = \frac{\hbar^2 k^2}{2m^*(0)}, \]

and derive the corresponding density of states.

6) Consider a Si quantum well (like the inversion layer of a MOSFET) with the confining potential in the \( z \)-direction. Recall that the constant energy surfaces for the parabolic conduction band are described by ellipsoids of revolution with the long axis described by the longitudinal effective masses and the two transverse axes by the transverse effective mass. That is, for the two ellipsoids oriented along the \( z \)-axis, we have:

\[ E - E_C = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m^*_i} + \frac{\hbar^2 k_z^2}{2m^*_i}. \]
The confining potential in the \( z \)-direction will lead to a set of quantized energy levels that are determined by the shape of the well (approximately triangular) and by the effective mass in the direction of confinement. Answer the following questions.

6a) For the ellipsoids with their long axes in the \( z \)-direction, what is \( E(k) \) in the plane of the channel (the \( k_x,k_y \) plane)? What is the valley degeneracy (i.e. how many ellipsoids respond to the confining potential with the longitudinal effective mass? 

6b) For the ellipsoids with their long axes perpendicular to the \( z \)-direction, what is \( E(k) \) in the plane of the channel (the \( k_x,k_y \) plane)? What is the valley degeneracy (i.e. how many ellipsoids respond to the confining potential with the transverse effective mass? 

6c) The first set of subbands (the quantum confined states of 6a), are known as the unprimed subbands. What is the 2D density of states for electrons in these subbands? What is the DOS effective mass for these subbands? 

6d) The second set of subbands (the quantum confined states of 6b), are known as the primed subbands. What is the 2D density of states for electrons in these subbands? What is the DOS effective mass for these subbands? 

6e) Which subband do you expect to be lowest in energy? Is the \( n = 1 \) unprimed subband lower or higher in energy than the \( n = 1 \) primed subband? Explain why.