ECE-606 Homework No. 3 Assigned: Sept. 4 Due: Sept. 11

1) We consider a one-dimensional wire with the following energy dispersion

$$E = U + \frac{\hbar^2 k^2}{2m}$$

a) By finite difference scheme, show that the Schrodinger equation can be written in the following form,

$$E\Psi_j = (U + 2t)\Psi_j - t\Psi_{j-1} - t\Psi_{j+1}$$

Where $t = \hbar^2 / 2ma^2$ and $\boldsymbol{a}$ is the lattice constant.

b) Show that the numerical dispersion for the plane wave $\Psi(x) = \exp(ikx)$ described by the Schrödinger equation of 1a) is given by

$$E = U + 2t[1 - \cos(ka)]$$

Show that when the lattice constant $\boldsymbol{a}$ is sufficiently small, it gives the parabolic dispersion.

c) 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.

d) If an electric field is applied along the x direction, state the motion of the particle (i.e. velocity and acceleration) when **ka** = 0, π/2 and π.

2) Problem 3.6 in ASF

3) Problem 3.9 in ASF

4) In HW1, we introduced a material called graphene; we shall probe it further here.

a) Recall that it has two unit lattice vectors given by,

$$\vec{a}_1 = \begin{pmatrix} 1.5 \\ -\sqrt{3}/2 \\ 0 \end{pmatrix} L \qquad \vec{a}_2 = \begin{pmatrix} 1.5 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} L$$

Work out its reciprocal lattice vectors using the following formula

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \qquad \text{and} \qquad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \qquad \text{where } \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

b) Using the Wigner-Seitz algorithm, draw the first 2D Brillouin zone and indicate the position vectors of all the corners. Indicate also the Γ point.

c) Using the following energy dispersion for graphene,

$$E = \pm t\sqrt{1 + 4\cos\left(\frac{3L}{2}k_x\right)\cos\left(\frac{\sqrt{3}L}{2}k_y\right) + 4\cos^2\left(\frac{\sqrt{3}L}{2}k_y\right)}$$

Plot the energy dispersion from Γ point to one of the corner where t=3eV. What is the effective mass and velocity **v** in the vicinity of the corner at E=0? Verify that it is a good estimate to write the energy dispersion at the corner (valley) as
$E = \hbar vk$
What is the valley degeneracy for graphene?

d) Derive the density of states and zero temperature electron density as function of energy for only a single valley for the following materials:

(i) Graphene: $E = \hbar vk$

(ii) Parabolic band semiconductor: $E = \frac{\hbar^2}{2m}k^2$

Comment on their differences. Do you think the electron density is temperature dependent, invoke the Fermi Dirac function in your argument.
Note: there is a spin degeneracy factor of 2.

5) Use the Band structure Lab, follow the steps outlined and answer the following questions

Simulate bulk material under the geometry option
Choose material as GaAs
Click on Electronic Structure tab to move to the next screen
Set the Tight Binding model to sp3s*d5 and check the Spin-Orbit coupling box
Note that some of the options given here would be preset as default, you need to leave them unchanged.
Now press the Analysis button to go forward.
Leave all preset options unchanged. Press the Advanced User option to take you to the next menu options.
Click simulate on this screen to launch the tool.

- 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
- 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 three bands below the 0eV mark, what are these bands called and how are they classified.

- You will notice a split in the bands you identified in the previous part, how is it commonly know ? How much is the split measured on the plot?

- From the effective mass table information, write down the effective masses at the gamma and L point. What quantitative difference do you see?

- Perform a search on the web to find how this difference in effective masses gives rise to an exotic phenomenon known as Negative Differential Resistance. Write your answer in not more than 5 sentences

- Which device commercially uses the above phenomenon?