ECE-606 Homework No. 2 Assigned: Aug. 28 Due: Sept. 4

Q1. In the last homework, you worked out the nearest, second nearest neighbours and their coordinate positions for a simple cubic lattice. Repeat the same exercise for a **bcc** and **fcc** lattice.

Work out the following related sub-parts

Silicon (Si) is widely used in the semiconductor industry. It has an indirect band gap of 1.13 eV at 300 K.

a. What type of lattice is the silicon crystal?

b. How many silicon atoms we have in each unit cell?

c. What are the fractional coordinates for each silicon atom in the unit cell?

Q2. The wave-function of an electron in a hydrogen-like atom is given by

$\Psi = A\exp(-Zr/a)$; Z = charge on nucleus and $a = h/(2\pi me^2)$.

Using the above information, work out the following sub-parts

a. Compute the constant A such that the wave function is normalized to unity.

b. At what distance from the origin, the probability of finding the electron is a maximum?

Q3. Define the terms in bold

a. **Quantum well**. How many directions are confined in this structure?

   Provide one example of a current commercially available electronic gadget that uses this structure

b. **Bravais Lattice**: How many Bravais lattices exist in the two dimensional case?

c. **Quantum Mechanical Tunneling**. Give one example of a real electronic device that utilizes this principle.

Q4. This exercise uses the Periodic Potential Lab on nanoHub. You can launch the tool by following the link given below.

(http://nanohub.org/resources/3847).

Follow the steps outlined and supply answer to the questions presented.

i. Choose the potential type as “step” (potential type tab)

ii. Set the maximum barrier height (U) to 2eV, the minimum to zero and energy of particle over barrier as 0 eV (energy details tab)

iii. Set the width of single periodic cell to 12A (well geometry tab)

iv. Use “a” equal to 8A (well geometry tab)

v. Set the effective mass to unity.

   a. Launch the tool for U = 2eV. Estimate the band-gap between the first and second energy bands. You should choose the “Allowed Bands” option from the drop down menu to answer this question.

   b. Repeat part a) with U = 4eV. Did the band gap between the first and second bands

   c. Did the bands themselves become wider (bandwidth) or narrower than in part a)?

   d. Use the drop down menu to look at the effective mass, you might notice certain values are negative; provide a physical interpretation of the change in sign of the effective mass

Q5. Consider a particle of mass ***m*** moving freely between x = 0 and x = a inside an infinite square well-potential. Calculate the expectation value for position and momentum operator.

Q6. Construct the Wigner-Seitz cell for all the two-dimensional Bravais lattices.