You are allowed and encouraged to work together as a group, but make sure the solution you turn in is your own and not simply copied from each other. Any unauthorized assistance (including, but not limited to, past course solutions and solution manuals) will be deemed as a violation of the honor code and handed over to the honor committee. If in doubt, check with me.

Please remember to pledge the homework as below:

On my honor as a student, I have neither given nor received unauthorized assistance on this homework.

(sign name above)
1. The Kronig-Penny model solution presented in class can be solved numerically using the provided code, or graphically as in many textbooks. Instead of going through the mathematical details, let’s try to get a feel for the solutions by playing with the numerics.

(a) Plot the eigenvalues and eigenvectors for well depth $E_{\text{well}} = 10$ and 40, without changing the kinetic energy terms. Compare the results and rationalize it. Explain the change you see as you increase the well depth. (10)

(b) Building off these results, describe what would happen if you make the barriers narrower while keeping the well widths the same. (10)

2. A certain hypothetical material with cubic crystal symmetry is characterized by the E-k diagram shown below. Which set of holes, band A or band B holes will exhibit greater [100]-direction effective mass? (5)

3. The E-k relationship about the GaAs conduction-band minimum becomes non-parabolic at energies only slightly removed from the $E_c$ and is more accurately described by

$$E - E_c = ak^2 - bk^4 \ (a > 0, b > 0)$$

What effect will the cited fact have on the effective mass of electrons in the GaAs conduction band? Substantiate your conclusion. Is your answer here in agreement with the note that $m_e^*$ increases at energies slightly removed from $E_c$? (10)

4. 1-D tight binding electrons have a dispersion $E = E_c + 2t[1-\cos(ka)]$.

(a) What is its effective mass $m^*$ at the bottom of the conduction band? (10)
(b) How much is the band-width? (5)
(c) If we increase the coupling t between neighboring atoms, what happens to the band-width? Does this agree with your observations from problem 1? (5)
5. (5 + 5 + 5 + 10 pts)

Log into the ABACUS online simulation tool on the nanohub and try out the following simulation.

Select "Periodic Potential Lab" from the ABACUS tool’s drop-down menu. Once the tool loads, you will be presented with three input options. For the type of periodic potential, select "step well", this will simulate a Kronig-Penny type crystal potential.

![Figure 1: input screen](image)

The following parameters are to be used as input for the well geometry: Width of single periodic cell = 8Å, a = 2Å, effective mass = 1. As for the energy details, use the following parameters: set the maximum barrier height to 13.6eV, the minimum barrier to 0eV, and the energy of the particle over the barrier to 1eV. Your periodic potential well should look like this:

![Figure 2: periodic potential well](image)
Now you are ready to simulate a particle in a periodic potential well. Take some time to examine the results. Your Energy functional should look like the analytical result from Pierret:

![Energy functional graph](image)

**Figure 3: Energy functional**

Try to answer the following questions:

1) How would one find the allowed bands from the Energy functional?
2) What is the band-gap of the material? How does it compare to real materials such as Silicon or Germanium?
3) Plot your results for the reduced dispersion relation. Is this a direct band-gap material or not?
4) Select "Reduced E-K compared to eff mass E-K" from the results menu. Can you justify the relationship between the curvatures of the energy bands and the effective masses of the different bands? The effective masses can be found by clicking on "effective mass information" section of the results.