You will be using the CUPS software package entitled "Quantum Mechanics Simulations", specifically the program "Electron States in a 1-Dimensional Lattice". The program allows you to explore some interesting features of the square well potential as well as a periodic array of such potentials. Notice that the program deals only with the bound state solutions, namely those with energies lower than the top of the well, and is limited to one-dimensional potentials.

To run the simulation, double-click the MS_DOS “LatceId” icon on the desktop.

**Note:** Under the current (2009) configuration of the computers, a DOS window will open. Type “temp” at the prompt to proceed.

Here are some basic instructions.

**THE SINGLE WELL:**

1. From the menu "Wells", choose a single well, square, width 0.075 nm, depth 300 eV. This is the problem we formulated in class, and found the bound state eigenenergies.

   **Note:** With the computers currently in use (2008), the program will crash if you attempt to change the width or depth of the well. Proceed with the experiment using the default parameters.

2. From the Spectrum menu, choose Find Eigenvalues. The program searches for the eigenvalues and they appear in no particular order. Confirm that the values agree with the results we found in class.

3. From the Spectrum menu, choose See Wave Functions. Type in the number of the level you wish to see. Is the ground state even or odd? What about the other two? Do higher energy states have more nodes or fewer nodes? Why do you think this is so? Look also at the probability distributions under See Wfs and Probs.

4. You can find the eigenvalues for yourself rather than having the program find them. Use the Method menu to enter a value for the energy close to one of the eigenvalues, and see what the solution to the Schrödinger equation looks like. Notice what happens at the boundaries as you choose energies further away from the eigenvalue, and closer to the eigenvalue. What is special about the wave function when you have the eigenvalue exactly correct?

**TWO SQUARE WELLS:**

1. Set up two square wells with the same parameters as above. Discuss with a fellow student what you think the eigenenergies of this potential are. Then choose Find Eigenvalues from the Spectrum menu and test your prediction.

2. How many bound states are there, and how do their energies compare with the energies of the single well?
3. Look at the shapes of the wave functions of the closely spaced levels. How are they different? How the same? Look at the probability functions, too. Are they more similar than they are different? How far apart are the closely spaced levels?

4. Make each well narrower - say 0.06 nm. How does the energy spacing change? Does this seem to agree with what you’d observe if you spaced the wells further and further apart? Think back to your chemistry lessons and what you know about the hydrogen molecule. Can you draw an analogy between 2 hydrogen atoms and the hydrogen molecule on the one hand and 2 square wells infinitely far apart and the double well system on the other?

**LATTICE OF WELLS:**

1. Now choose 3 wells, then 4 and so on up to 12, (with same parameters as your original single well) observing at each step what happens to the energy level structure.

2. If you have \( N \) wells, how many energy levels cluster together? What would you expect to happen if the number of wells became very large, \( 10^{23} \) for example?

3. For the 12-well case, measure the band edge energies and compare with the single well results.

4. Now look carefully at the wave functions in the different bands for the 12-well and see if you can determine any patterns. What do you notice about the wave function within individual cells, and what about an overall modulation?

5. What happens when you change the form of the well (for example - square to parabolic)? What changes and what features remain similar?

**DENSITY OF STATES**

An important concept is that of the "density of states". This simply tells you how closely energy eigenstates are packed in a particular energy interval. If there are many energy eigenstates in a particular energy interval in the vicinity of, say, \( E_0 \), we say "The density of states is large at \( E_0 \)."

For the problems above decide in which regions the density of states is largest and smallest. You are probably familiar with the term “band gap” applied to solids. How would you describe it in terms of density of states?

**LATTICE OF WELLS WITH IRREGULARITIES**

1. Set up a lattice of 12 wells, and again note the energy bands. Now choose “Irregular lattice”, and make one of the wells narrower than the others. What do you notice about the energy levels? Look at the wave function associated with the special level, and state how it is different from the wave functions associated with the other states. Think about the implications for a semiconductor system.

2. Try making the singular well wider, shorter or deeper than the others. Is the phenomenon similar?

3. Try an “irregular lattice” with random spacing as a model of an amorphous lattice. What features are similar and what features are different from the regular lattice?