Homework H4 Solution

1. Turn in: Go to the 1-D quantum app that I ran in lecture … Select "Setup: Well array (Coulomb)" and reduce the "Well Count" to just two wells, using the slider. Make the simulation speed pretty slow. The app now calculates the wavefunction for a negatively charged particle (like an electron) near two protons (that attract the electron into the two Coulomb wells).

a. You will see that the wavefunction has two peaks, one near each proton. Is there some wavefunction of the negative particle being between the two protons, thus binding them together?

Solution:
No, there is no wavefunction between the two protons, so the particle spends no time there. This is because the particle is initially set to be very heavy (more classical –like), and it cannot pass through the Coulomb potential wells of the protons due to the energy barrier in between. Thus, wavefunction is peaked near the protons.

b. Electrons are very light particles. Slide the slider "Particle Mass" all the way to the left to make the particle as light as an electron. Now is there some probability of finding the electron between the two protons? This wavefunction, with two peaks, but not zero between the two protons, is called a "sigma bonding orbital." The electron spends time between the two nuclei, thus binding them into a molecule.

Solution:

Now, for the lighter "quantum-like" particle, the electron, there is a finite probability of finding it in the region between the two protons. The Δx of the wavefunction gets wider the smaller/lighter the particle is, which allows the formation of a sigma bonding orbital, which is a lower energy quantum state than if the wavefunction was peaked at the two protons only. Thus quantum mechanics leads to the formation of the ever-present "chemical bond" ! [Note: As the wavefunction becomes wider, uncertainty Δx in position increases; as a result, the momentum of the particle, shown by the bottom wavefunction plotted in the graph, has a smaller Δp, and becomes more "certain".]