Chem 442: Homework for lecture 4

(due at start of first lecture following week)

Note on running applets: some browsers have strong restrictions on running Java applets or HTML5 applets. If you have no luck with your computer, a library computer (chem library) may do better, or do it with a friend from class.

In lecture 4, we discussed a work sheet showing Coulomb potentials, and we filled it in with classical particles, or wavefunctions of quantum particles, to discuss qualitatively how classical mechanics fails to describe molecules.

1. Turn in: Go to the 1-D quantum app that I ran in lecture to show the falling particle (Listed under "play with" homework for lecture 4). 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?

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 tow nuclei, thus binding them into a molecule.

In lecture, we saw that a classical particle would just emit energy and fall onto the proton. And even if that did not happen, we saw that a classical particle can never be between the two protons because there is an energy barrier preventing it from getting there. The barrier is also there for the quantum particle, but because wavefunctions always have a width, its wavefunction can stick into the middle between the nuclei and thus make a bond.