CBE 310
Molecular Concepts and Applications

Particle in a Box, well, double well

09 08 2014

For Today: 1) Talk about some formal math relating to how we will be dealing with quantum mechanical equations

2) Start talking about our first quantum mechanical model, a particle confined to a 1D region of space

3) Talk about more complicated versions of this problem

4) Quantum Tunneling

Reading: Finish Chapter 2 and start Chapter 3 of Quantum Chemistry Book,
HW #2 due Wednesday September 10th

What you should take home from the first 3 lectures

For the experiments that we talked about leading up to the development of Quantum Mechanics, that is for Rayleigh's and Plank's laws about blackbody radiation, Einstein's formula for the heat capacity of solids, Eisnstins explanation of the photoelectric effect and the experiments concerning the wave-particle duality of light and matter. You should

(1) Be able to describe the experiments / phenomena.

(2) Be able to describe the quantum mechanical principle that each of these experiments involves.

(3) be familiar with the derivations that we went over, not to the point that you could reproduce them but in general terms the logic that was followed.

(4) Be able to use the final equations to do calculations.

(5) Be able to answer questions about the meaning of terms in the equation and how the results change with changes in the terms.

What you should take home from the last 1.5 lectures

The last lecture and a half, from the derivation of the equations describing wave motion in a string to the derivation of Schrödinger's equation, is the basis for quantum mechanics. For these topics and the things that we will be discussing in the next few lectures the derivations are important.

You should be very comfortable with the idea of waves and the math that describes them.

You should understand de Broglie's relation and be able to use it to calculate the wavelength of anything. This relation basically says that every particle is described by a wavefunction having a wavelength related to its momentum.

Understand the idea that a wave function itself does not have physical meaning but the square of the wave function is a probability density for finding a particle.

You should be familiar with the logic of the derivation of Schrödinger's equation and understand the significance of the terms that make up the Hamiltonian.

You should be familiar with the rules defining operators, and acceptable wavefunctions