CBE 310 Molecular Concepts and Applications

Particle in a Half Well, Double Well and two and three Dimensional Boxes

2014 09 10

For Today:

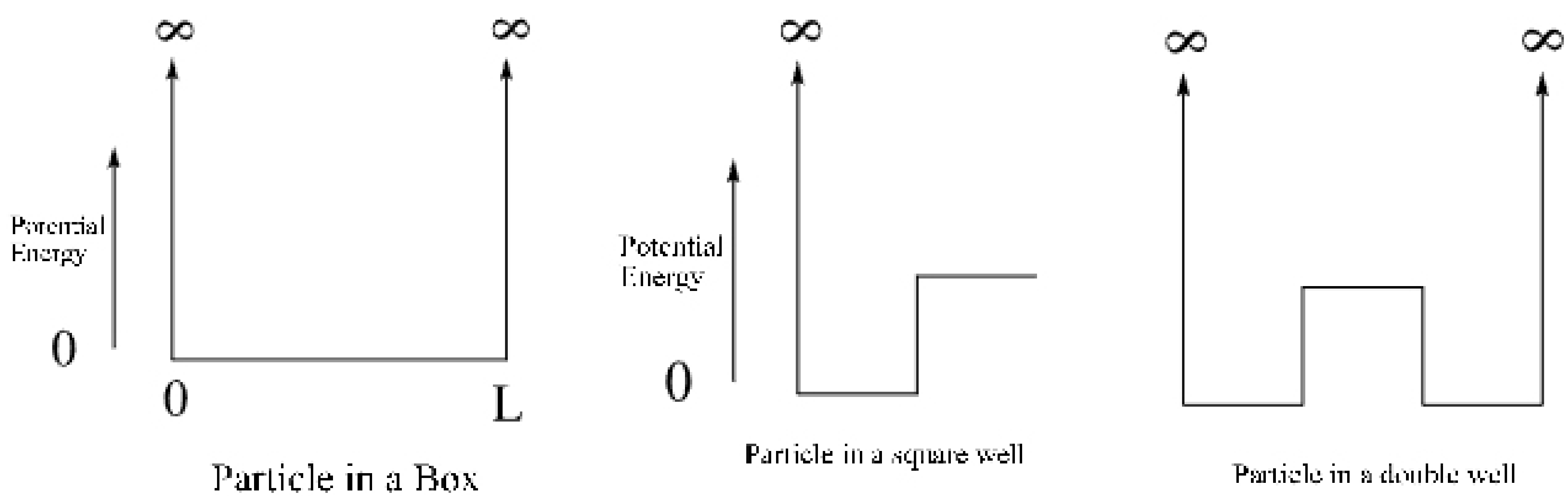
1) Continue talking about our first quantum mechanical model, a particle confined to a 1D regions of space
3) Quantum Tunneling
4) Expanded versions of this problem

Reading: Finish Chapter 2 and start Chapter 3 of Quantum Chemistry Book,
HW #3 is due by Monday 9/15 (Short HW)
HW will be back by Monday

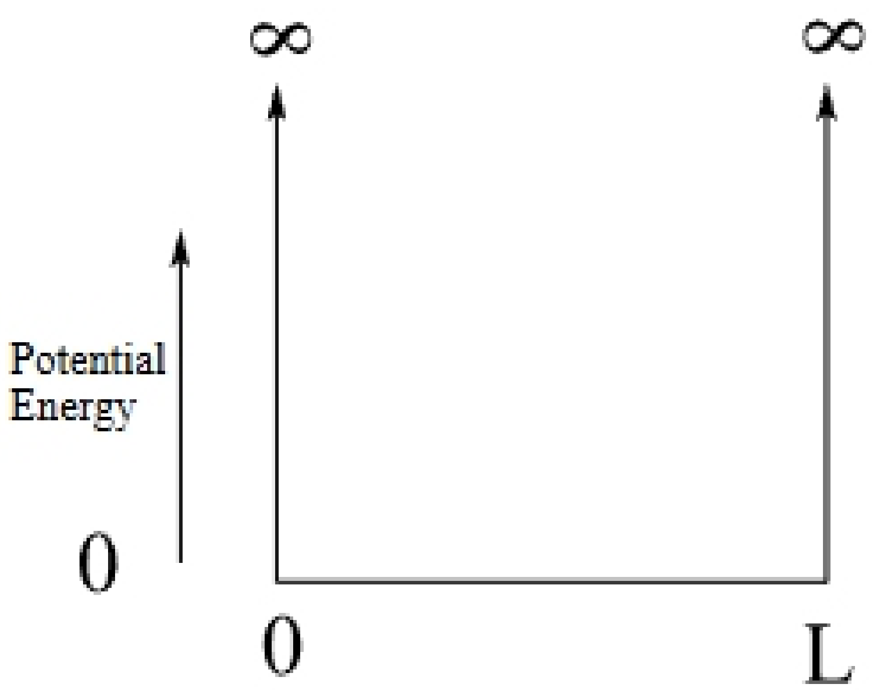
Quiz #1 will be next Wednesday 9/17

Schrödinger's Equation and Solutions to Basic Problems

$$\left[\left(\frac{-h^2}{8\pi^2 m}\right)\nabla^2 + V(x,y,z)\right]\psi(x,y,z) = E(x,y,z)\psi(x,y,z)$$



Particle in a Box (c1)



- This is a good model for a electron in a pi system
- This is also a good model for an atom constrained in a small area

- We want to understand how a particle behaves in this system. We can easily measure the energy but we want to know where the particle is and what it is doing.

We can describe three regions in this physical set up, inside the box, outside the box and at the boundary. 1) Inside the box:

$$\left[\left(\frac{-h^2}{8\pi^2 m}\right)\nabla^2 + V(x,y,z)\right]\psi(x,y,z) = E(x,y,z)\psi(x,y,z) \longrightarrow \left[\left(\frac{-h^2}{8\pi^2 m}\right)\frac{d^2}{dx^2} + 0\right]\psi(x) = E\psi(x)$$

2. Outside the box the potential is infinite, the particle can never have infinite energy so it must never be able to get outside the box so $\psi(x)$ outside the box must be 0.

3. The boundary: the conditions inside and outside the box must vary continuously, so $\psi(x)$ at the boundary must also be 0.