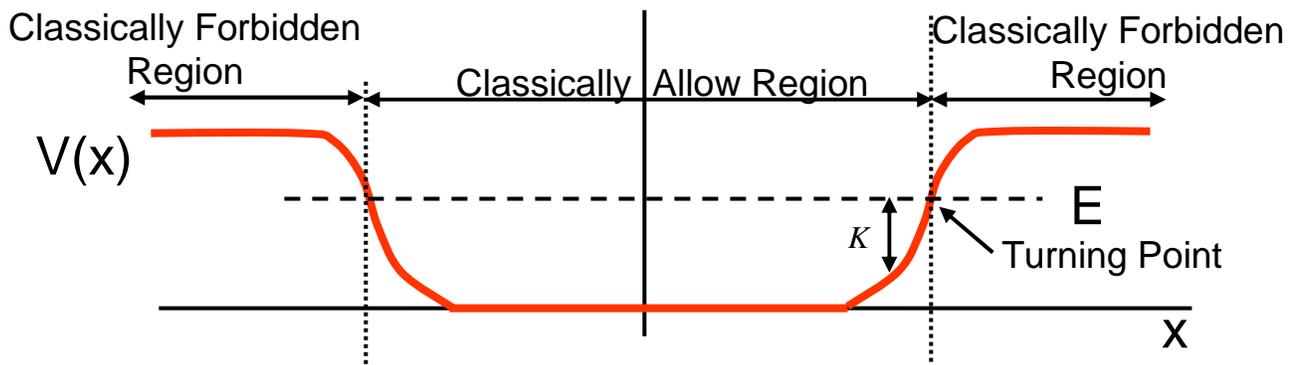# Chapter 7

- In chapter 6 we learned about a set of rules for quantum mechanics. Now we want to apply them to various cases and see what they predict for the behavior of quanta under different conditions.
  - Free Particle: We already looked at a special case of this for the 2-slit experiment where the free particle was in an eigenstate of momentum…it had a well defined momentum and therefore wavelength.
  - Bound Particle: Many particles in nature are not free but bound in a system.
    - Electron in an atom.
    - Proton in a nucleus
    - Atom in a lattice.
- Bound Systems are perhaps the most interesting cases for us to consider. We see much of the interesting features of quantum mechanics.
  - However, bound systems can be very complicated (even for advanced physics courses!)
    - Uranium Atom…no way of solving that in an exact way…in fact you get much beyond helium and it gets very hard.
  - We will make a number of simplifying assumptions (approximations). Although these are approximations do not significantly alter our results…all the interesting features of quantum mechanics will still be there.

Bound System

- Typically if a particle is bound it is because there is a force from other near by particles.
    - e.g. electron bound to a proton in the hydrogen atom.
    - In many cases one of the particles (electron) is much less massive that the particles that are holding it near by (proton.)
        - In this case, the motion of the less massive particle does not significantly effect the motion of the more massive particle(s).
        - We can think of the less massive particle as being in a potential energy field ("well") of the more massive particles…and forget about the more massive particles.

$$V(r) = -\frac{ke^2}{r}$$

r
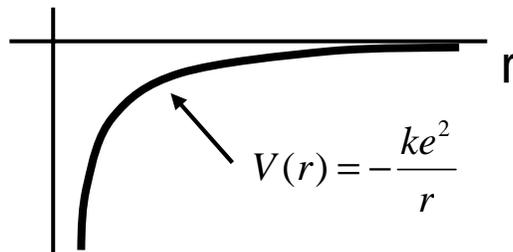
- We will start with examples that are simpler than the hydrogen atom (we'll get back to that later).
    - Start with one-dimensional potential

Classically Forbidden Region

Classically Allow Region

Classically Forbidden Region

V(x)

E

K

Turning Point

x

Energy Eigenfunctions

- When we discuss bound system it is very useful to discuss them in terms of energy eigenfunctions.
  - ➢ By definition these state functions have a well defined energy.
  - ➢ Its important to realize that not all wave functions are energy eigenfunctions and therefore don't have a definite energy…rather a probability of being a range of energies.
- There are four reasons why energy eigenfunctions play such a central role:
  - ➢ (1) Since energy eigenfunctions have a definite energy we can unambiguously tell whether the particle is bound.
    - ❑ Is the Energy, E < V (barrier height).
  - ➢ (2) Energy is a very important quantity. In QM this is one of the quantities of interest…much more so than say position.
  - ➢ (3) The time-evolution rule in QM says that energy eigenfunctions are somehow special since they are used to describe the time evolution of a quantum state.
  - ➢ (4) In many practical cases a wave function that is not in an energy eigenfunction will quickly evolve to one.
    - ❑ Energy eigenfunctions are "stationary"…their shape does not change with time:

$$\left|\psi_E(r,t)\right|^2 = \left|\psi_E(r,0)e^{-iEt/\hbar}\right|^2 = \left|\psi_E(r,0)\right|^2 \left|e^{-iEt/\hbar}\right|^2 = \left|\psi_E(r,0)\right|^2 \cdot 1$$

  - ❑ A charged quanton in a state that is not an energy eigenfunction will "wiggle" and radiate photons until it falls into an energy eigenfunction. (t ~ 10^{-8} sec).

Quanton in a Box

- Perhaps the simplest example of a bound system is a particle in a 1-dimensional "box". The potential looks like the following:

$$x = 0 \qquad\qquad x = L$$

$$V(x) = \infty \qquad V(x) = 0 \qquad V(x) = \infty$$
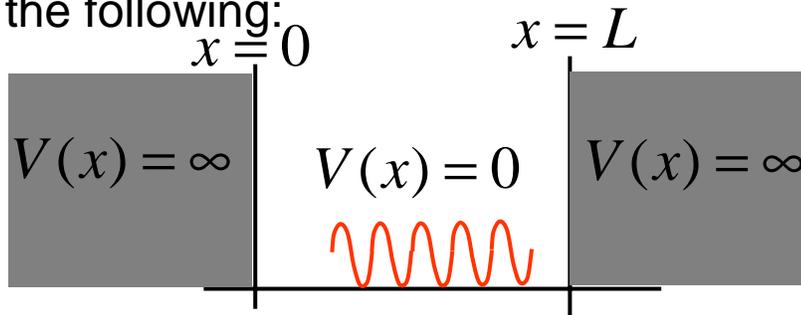
- When the particle is not at the boundaries it feels no potential (V=0) so it acts like a free particle. We saw that the free particles had a definite wavelength, λ.

- In addition, at the boundaries it is impossible for the particle to enter the forbidden region, therefore the wave function must go to zero at x=0 and x=L.

- These last two conditions describe something like a string with fixed ends and a standing wave.

$$\psi = A\sin(kx) \qquad k = \frac{2\pi}{\lambda}$$

- Just as a standing wave on a string there are only certain wavelengths that will satisfy the boundary conditions.

$$L = n\frac{\lambda_n}{2} \Rightarrow \lambda_n = \frac{2L}{n} \qquad k_n = \frac{2\pi}{\lambda_n} = \frac{n\pi}{L} \qquad n = 1,2,3,...$$

Quanton in a box

- Using the de Broglie wavelength we can convert the condition on the wavelength into a condition on the energy of the particle. The energy of the particle is given by:

- So the *energy eigenfunctions* for a quanton in a box is given by:

- Perhaps **the most important conclusion** from this example is that only **certain energies** are allowed.
  - .
  - .
  - .

Examples of Wave Functions

- Let's look at the first few examples of energy eigenfunctions:

_____   n=1

_____   n=2

_____   n=3
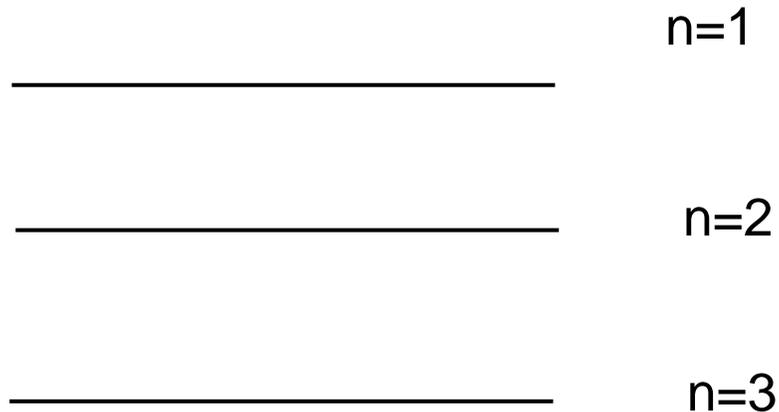
- It is important to emphasis that a particles does not have to be in one of these states.
  - However, also remember that any state can be described by a linear combination of energy eigenfunctions.
- Example:
  Consider a particle which is a combination of the first and second eigenfunctions.

1-D Harmonic Oscillator

- Another example is that of a simple harmonic oscillator. For this case the potential takes the form
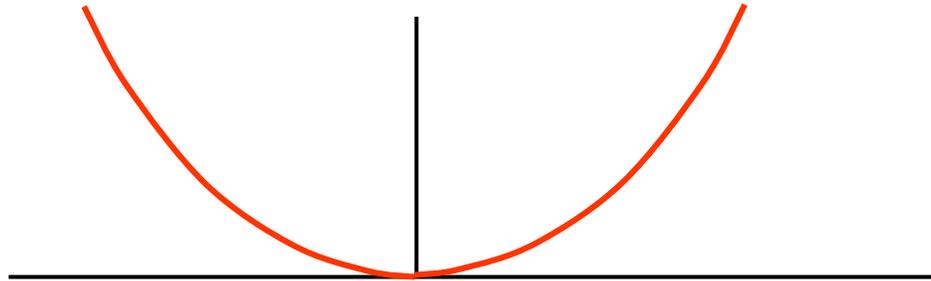
$$V(x) = \tfrac{1}{2}k_s x^2 = \tfrac{1}{2}m\frac{k_s}{m}x^2 = \tfrac{1}{2}m\omega^2 x^2 \quad \omega = \sqrt{\tfrac{k}{m}}$$

- This is a much more complicated result than the particle in a box. Nonetheless, it does share some similarities. However, some interesting differences as well.
  - ➤ .
  - ➤ .
  - ➤ .
- We have not yet developed the techniques to solve for the wave functions for this type of potential (we will later). For now let's look at the solution and some of its qualitative properties

Harmonic Oscillator

- Energy States
  - ➢ Quantized just as the case of the particle in the box.
  - ➢ Lowest energy state is **not** zero.

- Wave functions: The three lowest energy states are shown below:
  - ➢ Notice that each has approximately the same number of half wave lengths as the three lowest energy states of the particle in a box.
  - ➢ Notice the wave function does **not** go to zero at the classical "turning point".
    - ❑ Implies there is a small probability of finding the particle in the classically forbidden region.
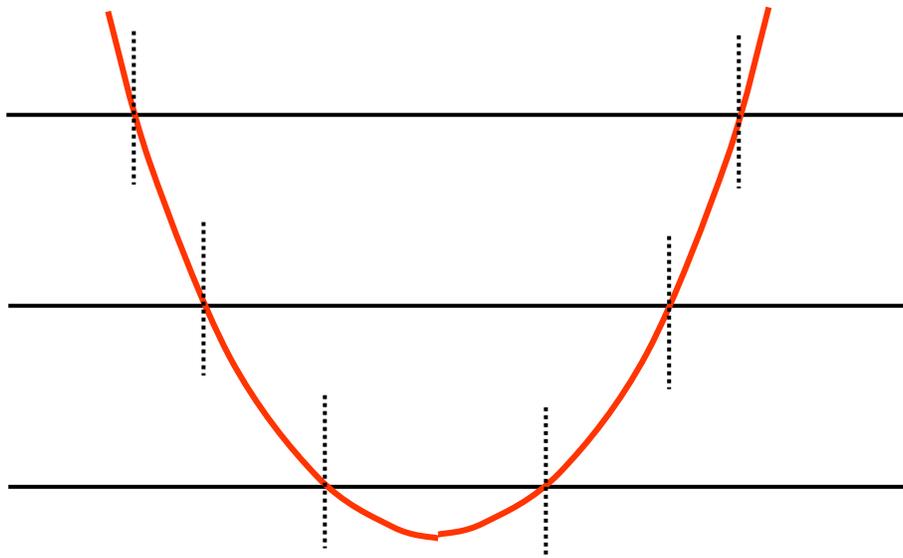
Bohr's Model of Hydrogen

- Before the theory of quantum mechanics was fully developed Niels Bohr developed a model for the simplest atom, Hydrogen.
  - ➢ The model attempted to solve the problem that the electron, which was thought to orbit the proton, should radiate (EM waves) it's energy away and fall into the proton.
  - ➢ This model is a very simplified view of the hydrogen atom that cannot possibly be correct but it is amazingly accurate in the determinations of the energy levels of the electron in hydrogen.
  - ➢ Efforts to extend this model to other atoms failed…the fully theory of quantum mechanics came along shortly after and more fully explained the hydrogen atom.
  - ➢ Nonetheless, let's look at Bohr's model.
- Assumptions made by Bohr:
  - ➢ Electron is confined to a plane
  - ➢ Electron is confined to a circle.
  - ➢ The electron has a definite momentum, p and therefore definite wavelength, λ.
  - ➢ The de Broglie wavelength of the electron must fit into the circular orbit so that there is no discontinuity/boundary.
- Other than the the introduction of the de Broglie wavelength, Bohr's treatment of the H atom was more or less *classical.*

Hydrogen Atom

- The last condition leads to the following mathematical constraint:

- Now treat the classical orbit.

- This last line are the radii of the possible orbits of the electron around the proton. For the case n=1, we give it a special name, *Bohr Radius, a_o*.

Bohr's Energy Levels

- With the radii of the orbits determined, we can then determine the energy levels. Again we take the classical approach which gives the energy by

- Using the circular orbit equation from above we find

- The lowest energy state (n=1) gives the following energy:

- Notice that the energy is negative. However, as n increases, the energy becomes less negative. Also, when n gets large the energy goes to zero…this corresponds to an electron at a radius of infinity.

- Although Bohr's model is clearly very classically based, it did remarkably well at predicting the energy levels of hydrogen…which is one reason it still appears in textbooks.