Chapter 11

- Using the form of the *Schrödinger Equation* we can learn some qualitative properties of energy eigenfunctions. General Goals for this chapter
  - ➤
  - ➤
  - ➤
  - ➤

- Let's start with the shapes of the energy eigenfunctions. First recall the *Schrödinger Equation* and let's write it in the following form $\dfrac{d^2\psi_E(x)}{dx^2} = -\dfrac{2m}{\hbar^2}[E - V(x)]\psi_E(x)$

- If the second derivative (left-hand side) is negative, the function is concave **down**. If the second derivative is positive the function is concave **up.**

- **Classically Allowed Region (E − V(x)>0)**
  - ➤ If $\Psi_E(x) > 0$,
  - ➤ If $\Psi_E(x)<0$,
  - ➤ **The wave function in the classically allow region always** _____

_____

Shape of Ψ_E

- **Classically Forbidden Region: (E – V < 0)**
  - ➢ If $\Psi_E(x) > 0$,

  - ➢ If $\Psi_E(x) < 0$,

  - ➢ **The wave function in the classically forbidden region always** _____

- These features lead to the general statements that we observed before
  - ➢ In the classically allowed region the eigenfunction is

  _____
  - ➢ In the classically forbidden region the eigenfunction is

  _____

- In addition, from the form of the *Schrödinger Equation* we can also see that:
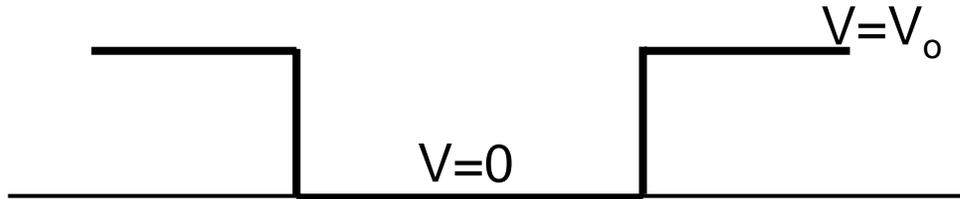 - ➢ **Classical Allowed Region:**
    - ❑ The larger E – V , the larger the curvature which implies a shorter wavelength (higher momentum)
  - ➢ **Classically Forbidden Region:**
    - ❑ The large E – V, the shorter (steeper) exponential tails…less probing into forbidden region.

Simple Case

- Consider the very simple case of a square well with finite sides:

$$V=V_o$$

$$V=0$$

- In the allowed region, the simple sine function satisfies the *Schrödinger Equation.* Let's see how:

- Now, this is a solution if the term in the brackets is zero so

- Notice that we got an expression for b, but not for E or ϕ.
  - ➢ We know this Ψ_E works but we need to bring some other information into the problem to determine E and ϕ. Let's consider the solution in the classically forbidden region.

Square Well

- In the classically forbidden region we believe the solution is exponential-like. For starts let's choose an exponential and see if that works.

$$\psi_E(x) = Be^{\beta x} + Ce^{-\beta x}$$

$$\frac{d\psi_E}{dx} = \beta Be^{\beta x} - \beta Ce^{-\beta x}$$

$$\frac{d^2\psi_E}{dx^2} = \beta^2 Be^{\beta x} + \beta^2 Ce^{-\beta x}$$

$$\frac{\hbar^2}{2m}\left(\beta^2 Be^{\beta x} + \beta^2 Ce^{-\beta x}\right) + \left[E - V_0\right]\left(Be^{\beta x} + Ce^{-\beta x}\right) = 0$$

$$\left[\frac{\hbar^2\beta^2}{2m} + E - V_0\right]\left(Be^{\beta x} + Ce^{-\beta x}\right) = 0$$

- We see that we satisfy the *Schrödinger Equation* if the following condition is meet:

- Again we determined the parameter β but we still have no more insight into E, C, or B (or ϕ). How do we get these?
  - ➤ "Boundary" conditions: We know that at the walls of the well where the wave function makes the transition from the sine-wave solution to the exponential solution that the wave-function must be **smooth** and **continuous.**
    - ❏ This gives us 4 more equations, plus 1 more for norm
   - ❏ This is an exercise for the student.

Discrete Energy Levels

- Moore makes an argument that the *Schrödinger Equation* demands that the energy levels are discrete for a bound system. (Section 11.2).

- If once again we consider the square well just discussed, we can think about the lowest energy level state, which has something like ½ wavelength in the classically allowed region it would look something like

$$V=V_o$$

- Assuming that this is valid for an energy, E_1, imagine making the energy slight higher. That would say that the quantity $E – V$ was slightly larger and so the curvature in the classical region is slightly larger.

- If we think about starting at the far left and mapping out our function, the higher curvature will make the function strike the right forbidden region at a lower level.

  - Once inside the right forbidden region, the curvature up will not be quite as fast as the E_1 case (see previous example)

  - However, since it hit the forbidden region at a lower level, the function will not be able to "pull" up completely before hitting the x-axis.

  - When it cross the x-axis, the S.E. will demand it curve away from the x-axis and will go to negative infinity.

Bumps

- As we saw in the previous discussion the valid energy levels will be isolated (discrete) because of this curvature "problem".
  - ➤ A similar argument can be made for the energy being slight too small…the curvature does not work out for the other problem that the function will never make it down to the x-axis…it will curve away and head to + infinity.
- However, we can think about what this tells us about the next valid energy level.
  - ➤ When the curvature gets large enough to add a "new" bump, we will get a new valid energy level.
  - ➤ So the lowest energy solution will have a single bump (peak or valley) in the classically allowed region.
  - ➤ The next energy solution will have a curvature such that there are two bumps in the classically allowed region.
  - ➤ This is a general feature for bound states:
    - ❑ 1-D is very straight forward
    - ❑ 3-D…as we saw for hydrogen is more complicated
      - o 1 radial bump was somehow equal to 2 angular bumps.

E_1

E_2

E_3
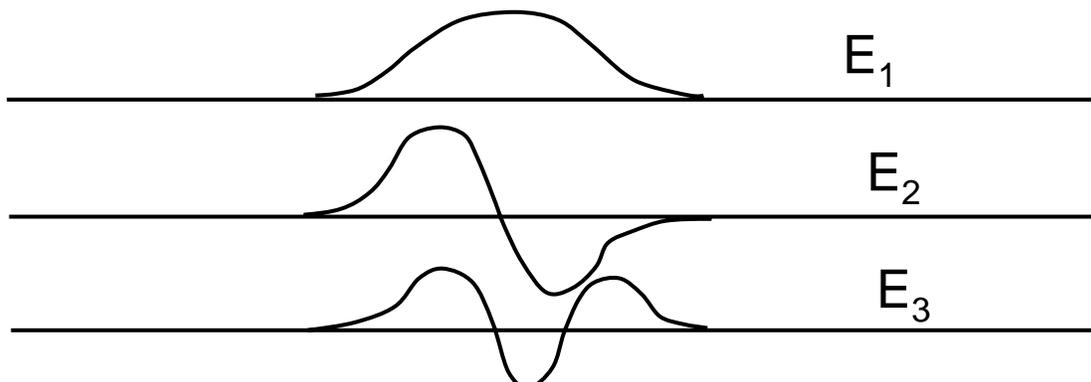
Quantum Tunneling

- One of the more interesting features of quantum mechanics is the concept of **quantum tunneling.**
  - ➢ Quantum Tunneling is when a quanta passes through a barrier which it should be classically forbidden from passing through.

- Consider the following 1-D potential

$V=V_o$

Wave function has not gone all the way to 0.
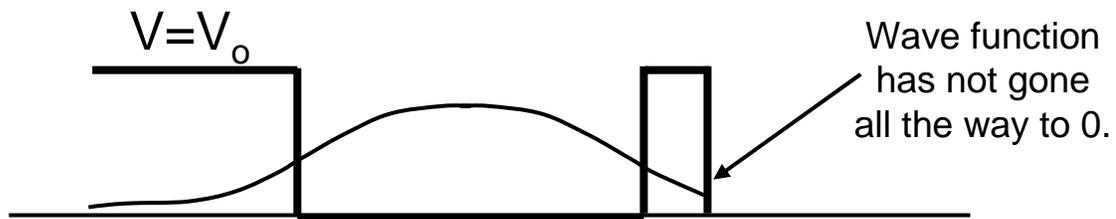
- If we draw what we think are the solutions to this potential, we see that if the "wall" is thin enough, the wave function has not gone all the way to zero by the time it reaches the other side.
  - ➢ Interestingly, on the other side of the wall is another classically **allowed** region.
  - ➢ If we solve the *Schrödinger Equation* we will find that there are "free particle" sine waves in this other classically allowed region to the right.

  - ➢ If we initially "drop" the particle into the box, as it settles into an energy eigenfunction, there will be a nonzero prob. that we find it **outside** the well…it got there by "tunneling" through the wall…**not** by going "over" the wall.

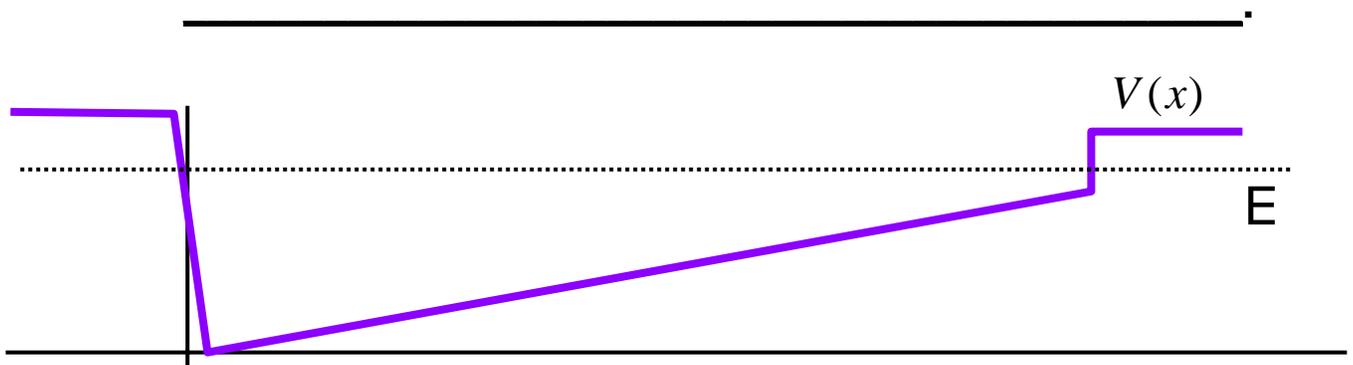# Sketching Energy Eigenfunctions

- There is a nice discussion in the text with regard to quantum tunneling and how it applies to a "scanning-tunneling microscope" (Read Section 11.3).

- Now we want to learn about sketching energy eigenfunctions. We have done this already many times and we have stated some of the rules as we have gone along, however, now let's list these rules in detail so that we can remember them all.

- Before we actually list the rules there is one more that we need to explicitly think about. Consider once again our slanted potential well.
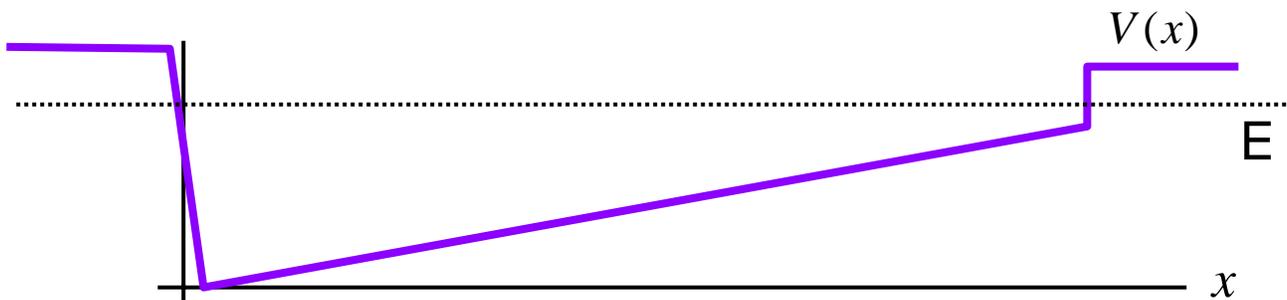
- We already stated that the local wavelength had to be small in the region where the particle had a large momentum. But what about the **amplitude** of the wave function?
  - ➢ Again, let's turn to some classical ideas to try to answer this question.

Sketching Energy Eigenfunctions

- As a particle moves around in this potential:
  - ➢

  - ➢

- If we think about making a measurement of exactly where the particle is located, we are more likely to find it in a "slow moving" region…simply because it spends more time there.
  - ➢ The probability that we find the particle in a particular location is proportional to the square of the wave function.
  - ➢ Therefore, we would expect that **the amplitude of the wave function in slow moving regions should**

    _____**.**

$V(x)$

E

Energy Eigenvector Sketching Rules

- (1) Solutions to the *Schrödinger Equation* curve *toward* the x axis in classically allowed regions and *away* from the x axis in classically forbidden regions:
    - ➢ Implications: Solutions are wave-like in allowed regions and exponential-like in the forbidden regions.

- (2) The curvature of solutions increases with $|E - V(x)|$. Note that $|E - V(x)|$ corresponds to the distance between the energy line and the potential energy curve on a potential energy graph.
    - ➢ In classically allowed regions, the *local wavelength* of the wave-like part of the solution gets shorter as $|E - V(x)|$ increases.
    - ➢ In classically forbidden regions, the *length* of any exponential-like tail get shorter as $|E - V(x)|$ increases.

- (3) The local amplitude of the wave-like part of the solution *decreases* as the value of $|E - V(x)|$ increases.

- (4) Solutions area always *continuous* and *smooth* as long as any discontinuous jumps in V(x) are finite.

- (5) Physically reasonable wave functions remain finite as $|x| \to \infty$.
    - ➢ The exponential-like parts of physically reasonable solutions for bound quantons must actually decrease to *zero* as $|x| \to \infty$ in the classically forbidden regions that flank the central allowed region.
    - ➢ Only certain quantized energy values E_n give rise to physically reasonable solutions for bound quantons.

- (6) Energy eigenfunctions for bound quantons have an integer number of bumps in the central classically allowed region: the more bumps, the greater the corresponding energy. The energy eigenfunction corresponding to the quanton's lowest possible energy, E_1, has one bump in its wave-like part, the eigenfunction corresponding to the quanton's second-lowest energy, E_2, has two bumps, etc.

Example

- Consider the potential shown below. Draw the energy eigenvectors for the second and third lowest states.
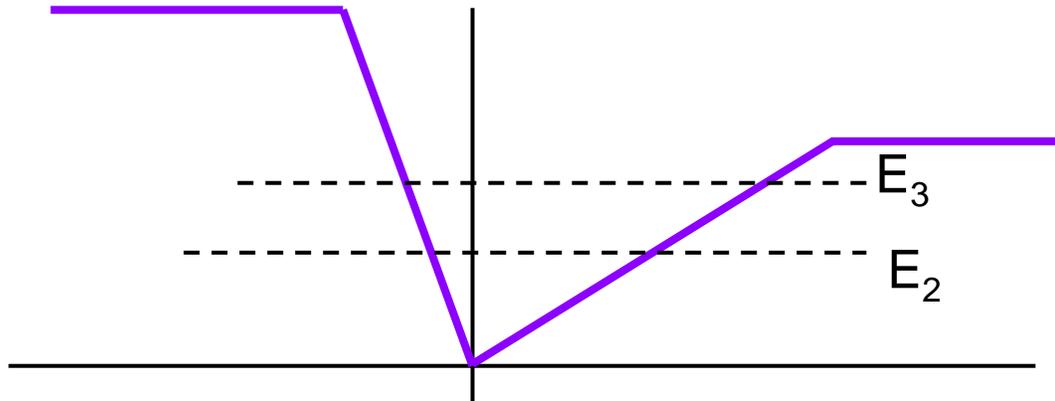
- First the second lowest energy state
  - ➢ Expect something with two "bumps"
  - ➢ Shorter wavelength and smaller amplitude around x at bottom of well.
  - ➢ The exponential-like decay on the left should be faster than on the right.
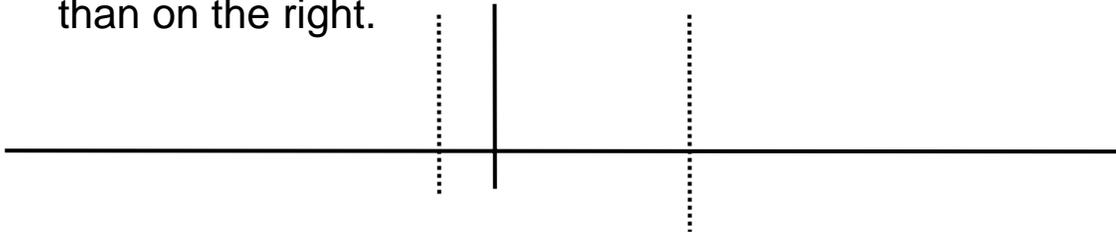
- Now the third lowest energy state
  - ➢ Expect three bumps; same trend with wavelength as above; the exponential tails should be longer than the case above:
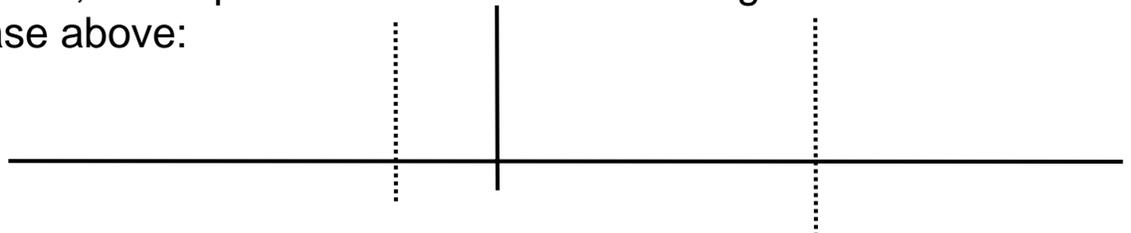
"Particles act like Waves"

- This is the extent of the material that we will cover in Unit Q.
- We have seen that when we look at the behavior of small particles that they do not behave Newtonian Mechanics…instead they seem to have their own set of rules, which are outlined by quantum mechanics.
- A couple of key points:
  - Particles are not localized…unless we go looking for them
  - Particles don't necessarily have a definite position, spin, etc.
  - Their behavior can be explained by thinking of them as having wave functions which encode the probability of measuring certain observables:
    - Position, Momentum, Spin Projection, Energy, Orbital angular momentum, etc.
- Quantum Mechanics had some very bizarre behaviors:
  - The 2-slit experiment with electrons or photons
    - Knowledge of the location around the slit impacted the diffraction pattern.
  - The measurement of spin projection.
    - First measure S_z then measure S_x then measure S_z.
  - "Collapse Rule"
    - Recall the 2 - photons light years a part.
- **There are many other strange and interesting features of quantum mechanics to be explored…but that will have to wait for another class!**