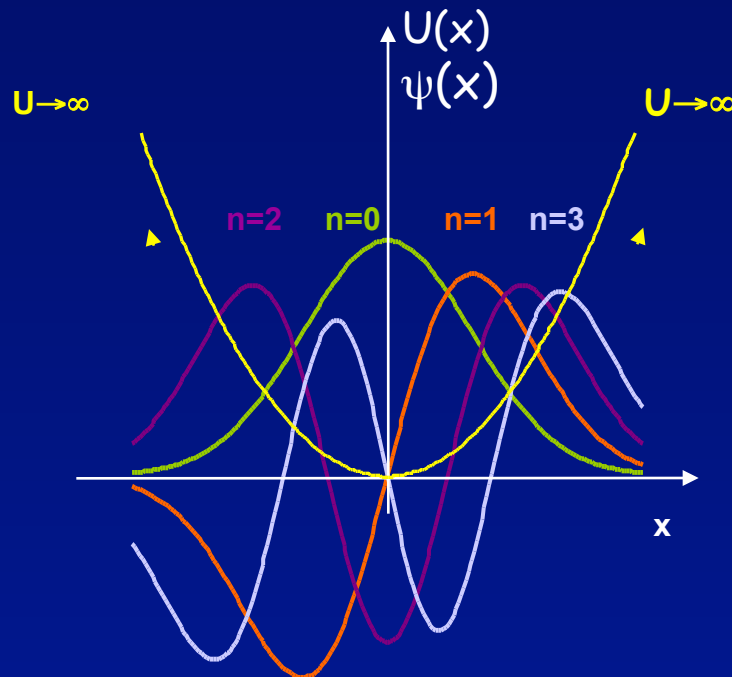


# Lecture 12:

## Particle in 1D boxes, Simple Harmonic Oscillators



# This week and last week are critical for the course:

Week 3, Lectures 7-9:

Light as Particles

Particles as waves

Probability

Uncertainty Principle

Week 4, Lectures 10-12:

Schrödinger Equation

Particles in infinite wells, finite wells

## Midterm Exam Monday, week 5

It will cover lectures 1-11 and some aspects of lecture 12 (not SHOs).

Practice exams: Old exams are linked from the course web page.

Review: Sunday before Midterm

Office hours: Sunday and Monday

Next week:

Homework 4 covers material in lecture 10 – due on Thur. after midterm.

We strongly encourage you to look at the homework before the midterm!

Discussion: Covers material in lectures 10-12. There will be a quiz.

# Properties of Bound States

Several trends exhibited by the particle-in-box states are generic to bound state wave functions in any 1D potential (even complicated ones).

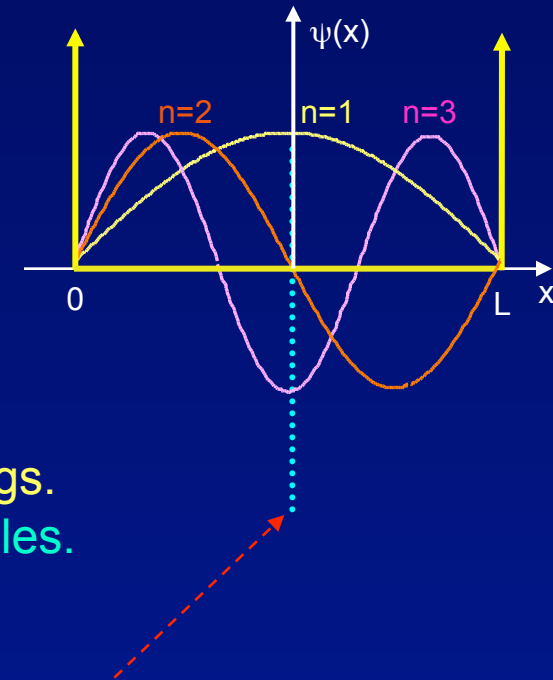
- 1: The overall curvature of the wave function increases with increasing kinetic energy.

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} = \frac{p^2}{2m} \text{ for a sine wave}$$

- 2: The lowest energy bound state always has finite kinetic energy -- called “zero-point” energy. Even the lowest energy bound state requires some wave function curvature (kinetic energy) to satisfy boundary conditions.

- 3: The  $n^{\text{th}}$  wave function (eigenstate) has  $(n-1)$  zero-crossings. Larger  $n$  means larger  $E$  (and  $p$ ), which means more wiggles.

- 4: If the potential  $U(x)$  has a center of symmetry (such as the center of the well above), the eigenstates will be, alternately, even and odd functions about that center of symmetry.



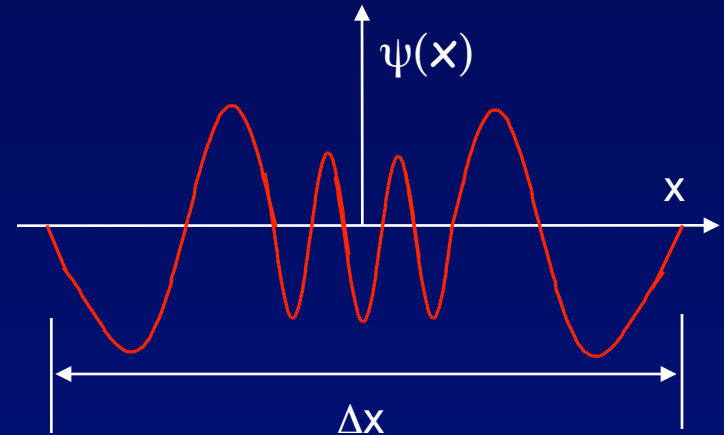
# Act 1

The wave function below describes a quantum particle in a range  $\Delta x$ :

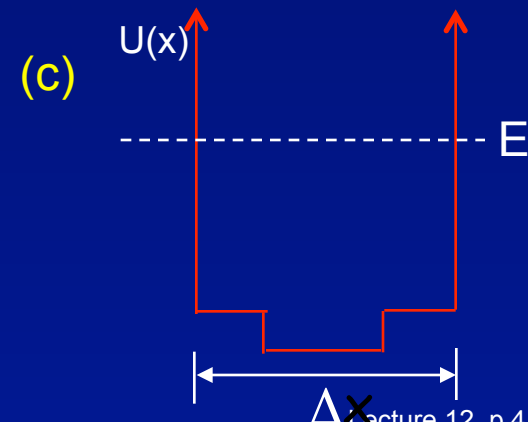
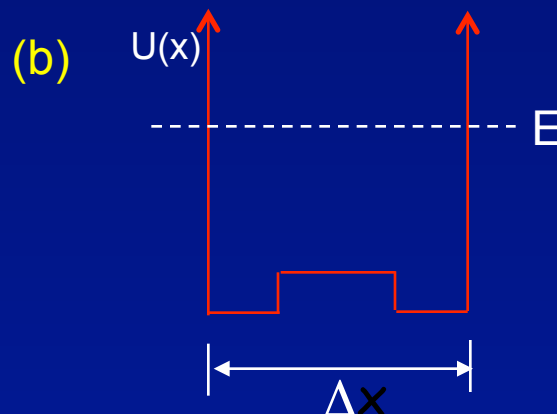
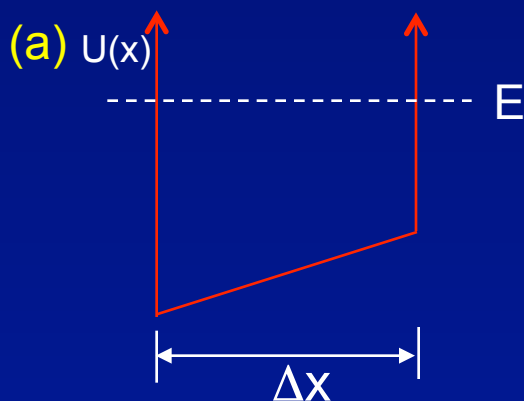
1. In what energy level is the particle?

$n =$

(a) 7    (b) 8    (c) 9



2. What is the approximate shape of the potential  $U(x)$  in which this particle is confined?



# Solution

The wave function below describes a quantum particle in a range  $\Delta x$ :

1. In what energy level is the particle?

$n =$

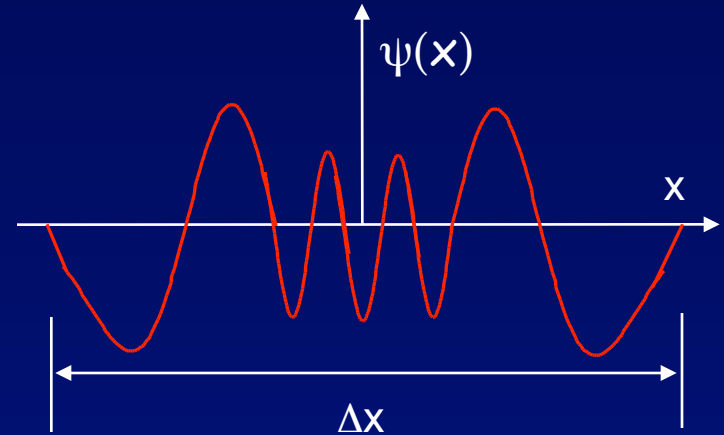
(a) 7

(b) 8

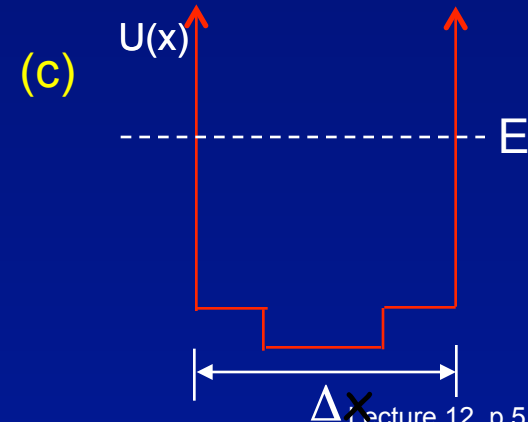
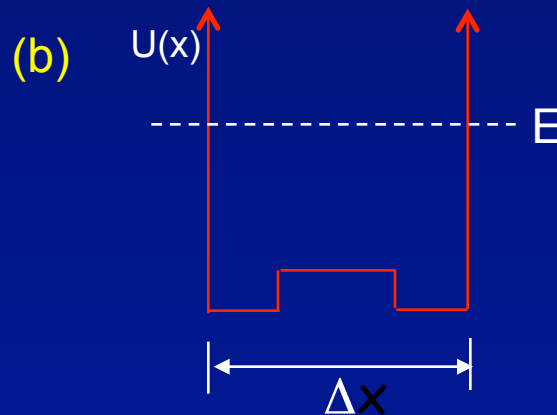
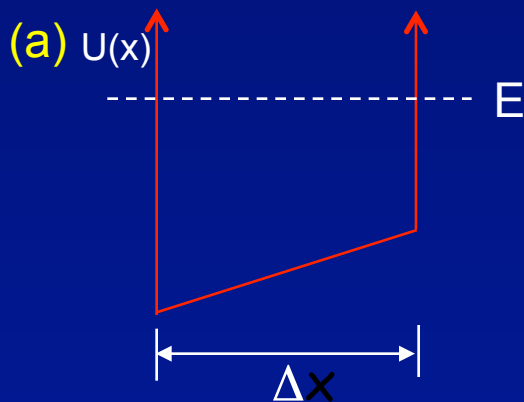
(c) 9

Eight nodes.

Don't count the boundary conditions.



2. What is the approximate shape of the potential  $U(x)$  in which this particle is confined?



# Solution

The wave function below describes a quantum particle in a range  $\Delta x$ :

1. In what energy level is the particle?

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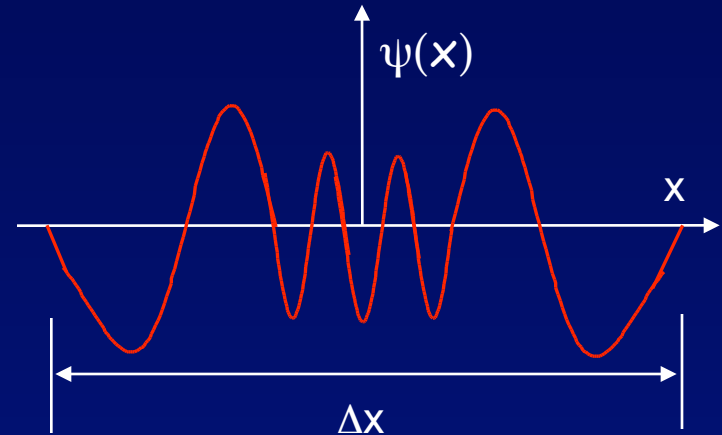
(a) 7

(b) 8

(c) 9

Eight nodes.

Don't count the boundary conditions.

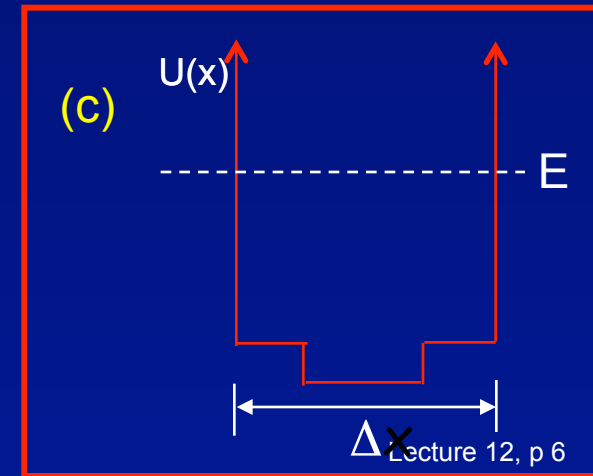
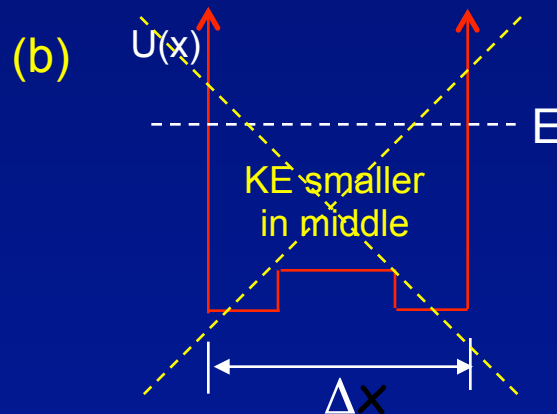
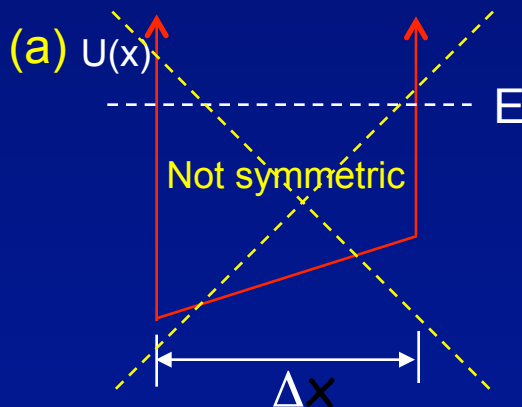


2. What is the approximate shape of the potential

$U(x)$  in which this particle is confined?

Wave function is symmetric.

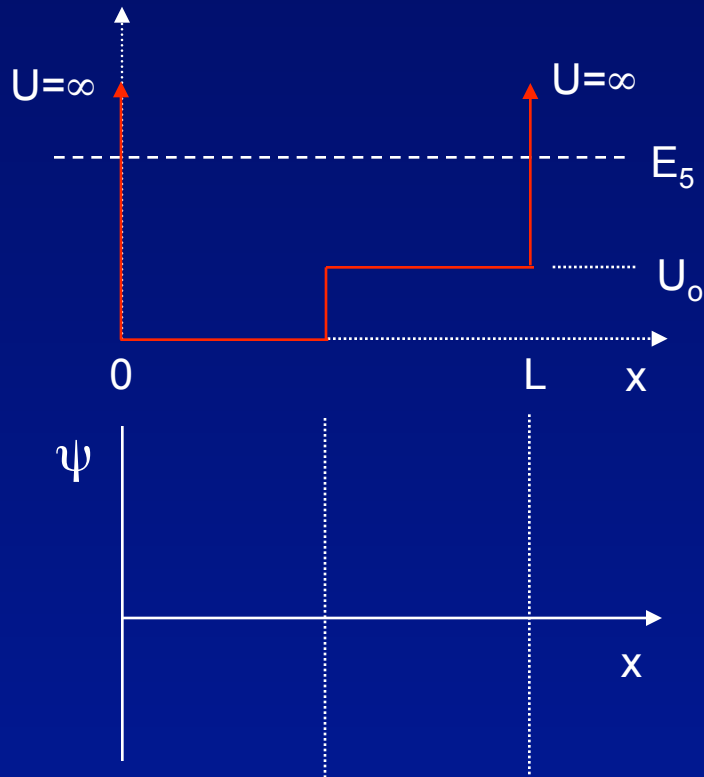
Wavelength is shorter in the middle.



# Bound State Properties: Example

Let's reinforce your intuition about the properties of bound state wave functions with this example:

Through nano-engineering, one can create a step in the potential seen by an electron trapped in a 1D structure, as shown below. You'd like to estimate the wave function for an electron in the 5th energy level of this potential, without solving the SEQ. The actual wavefunction depends strongly on the parameters  $U_0$  and  $L$ . Qualitatively sketch a possible 5th wave function:



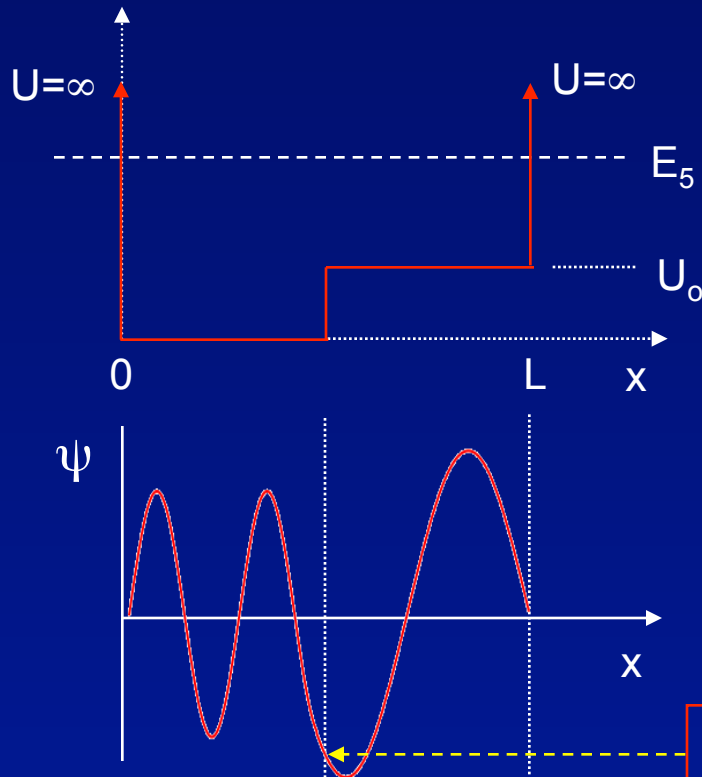
Consider these features of  $\psi$ :

- 1: 5th wave function has \_\_ zero-crossings.
- 2: Wave function must go to zero at \_\_\_\_ and \_\_\_\_.
- 3: Kinetic energy is \_\_\_\_ on right side of well, so the curvature of  $\psi$  is \_\_\_\_ there.

# Bound State Properties: Solution

Let's reinforce your intuition about the properties of bound state wave functions with this example:

Through nano-engineering, one can create a step in the potential seen by an electron trapped in a 1D structure, as shown below. You'd like to estimate the wave function for an electron in the 5th energy level of this potential, without solving the SEQ. The actual wavefunction depends strongly on the parameters  $U_0$  and  $L$ . Qualitatively sketch a possible 5th wave function:



Consider these features of  $\psi$ :

- 1: 5th wave function has 4 zero-crossings.
- 2: Wave function must go to zero at  $x = 0$  and  $x = L$ .
- 3: Kinetic energy is lower on right side of well, so the curvature of  $\psi$  is smaller there.

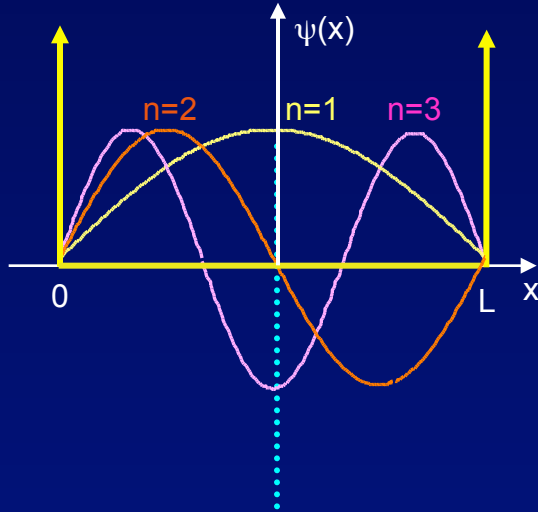
The wavelength is longer.

$\psi$  and  $d\psi/dx$  must be continuous here.



# Particle in Infinite Square Well Potential

$$\psi_n(x) \propto \sin(k_n x) = \sin\left(\frac{2\pi}{\lambda_n} x\right) = \sin\left(\frac{n\pi}{L} x\right) \quad \text{for } 0 \leq x \leq L$$



$$n\lambda_n = 2L$$

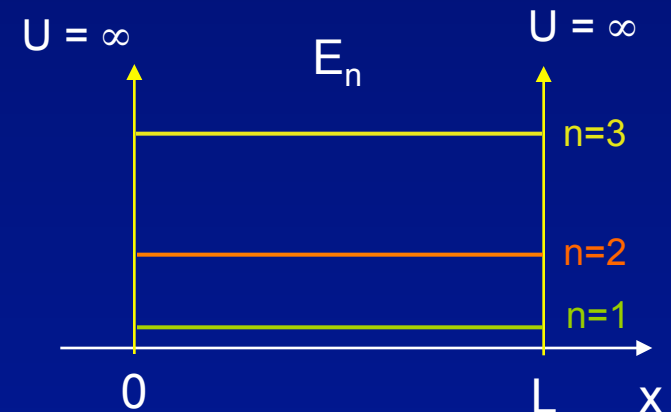
$$-\frac{\hbar^2}{2m} \frac{d^2 \psi_n(x)}{dx^2} + U(x) \psi_n(x) = E_n \psi_n(x)$$

The discrete  $E_n$  are known as “energy eigenvalues”:

$$E_n = \frac{p^2}{2m} = \frac{h^2}{2m\lambda_n^2} = \frac{1.505 \text{ eV} \cdot \text{nm}^2}{\lambda_n^2}$$

electron

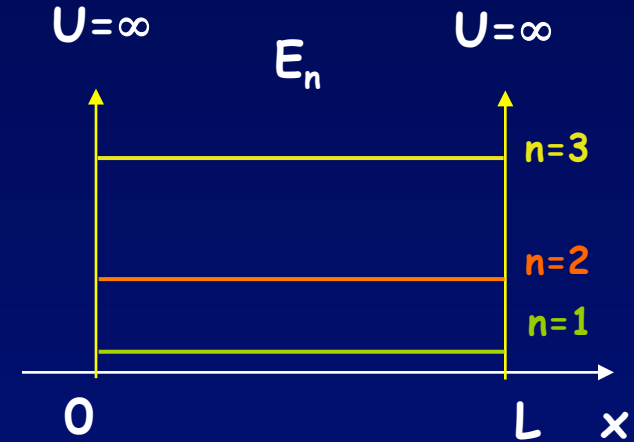
$$E_n = E_1 n^2 \quad \text{where} \quad E_1 \equiv \frac{h^2}{8mL^2}$$



# Act 2

1. An electron is in a quantum “dot”. If we decrease the size of the dot, the ground state energy of the electron will

- a) decrease
- b) increase
- c) stay the same



2. If we decrease the size of the dot, the difference between two energy levels (e.g., between  $n = 7$  and  $2$ ) will

- a) decrease
- b) increase
- c) stay the same

# Solution

1. An electron is in a quantum “dot”. If we decrease the size of the dot, the ground state energy of the electron will

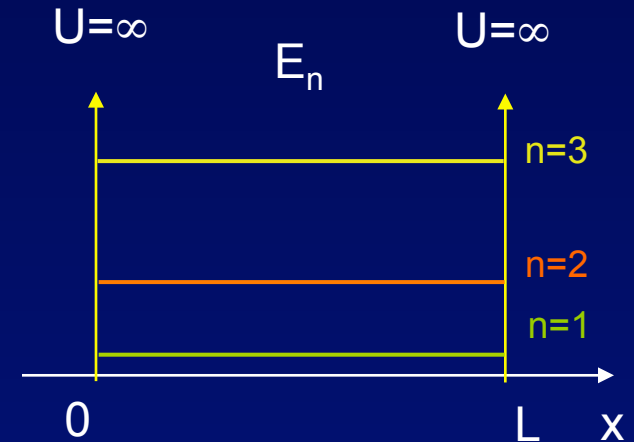
a) decrease

b) increase

c) stay the same

$$E_1 = \frac{h^2}{8mL^2}$$

The uncertainty principle, once again!



2. If we decrease the size of the dot, the difference between two energy levels (e.g., between  $n = 7$  and  $2$ ) will

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# Solution

1. An electron is in a quantum “dot”. If we decrease the size of the dot, the ground state energy of the electron will

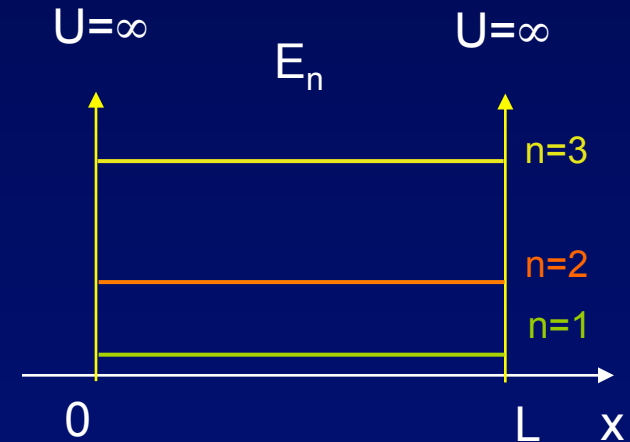
a) decrease

b) increase

c) stay the same

$$E_1 = \frac{h^2}{8mL^2}$$

The uncertainty principle, once again!



2. If we decrease the size of the dot, the difference between two energy levels (e.g., between  $n = 7$  and 2) will

a) decrease

b) increase

c) stay the same

$$E_n = n^2 E_1$$

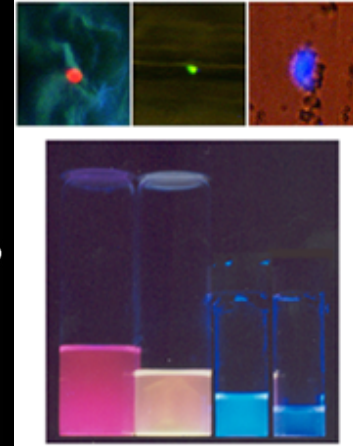
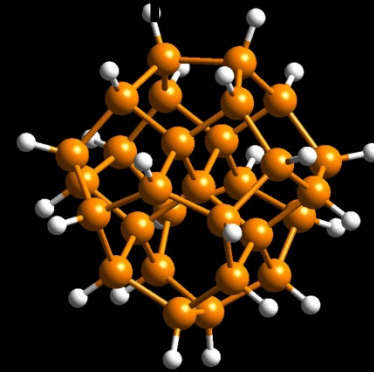
$$E_7 - E_2 = (49 - 4)E_1 = 45E_1$$

Since  $E_1$  increases, so does  $\Delta E$ .

# “Quantum Confinement” – size of material affects “intrinsic” properties

## M. Nayfeh (UIUC) : Discrete uniform Si nanoparticles

- 
- 
- nanoparticles
- No magic sizes > 20 atoms for non-hydrogenated clusters
- Small clusters *glow*: color depends on size →
- Used to create Si nanoparticle microscopic laser:



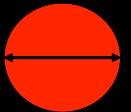
1 nm  
Blue



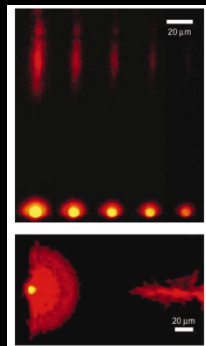
1.67 nm  
Green



2.15 nm  
Yellow



2.9 nm  
Red

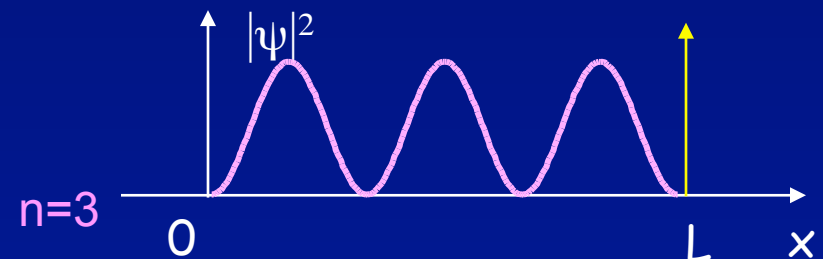
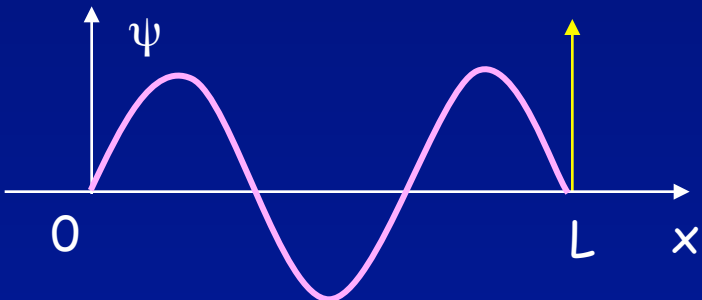
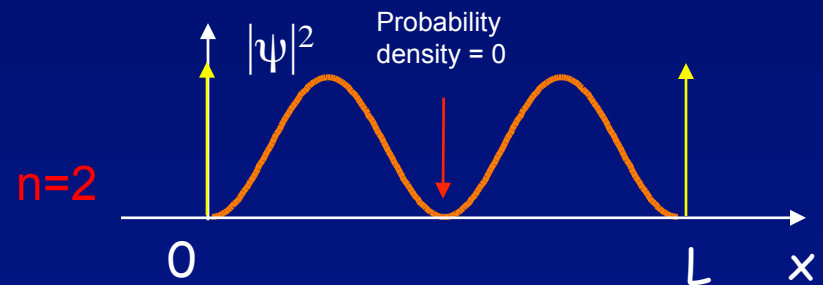
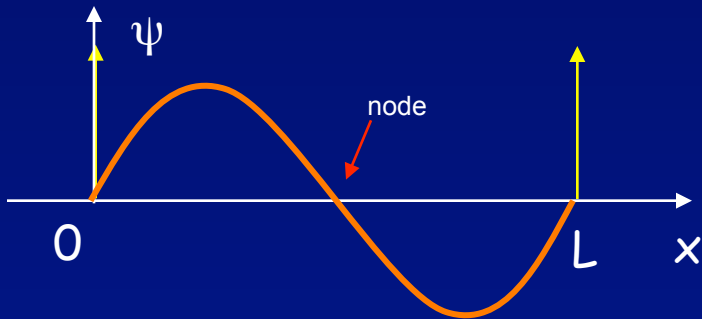
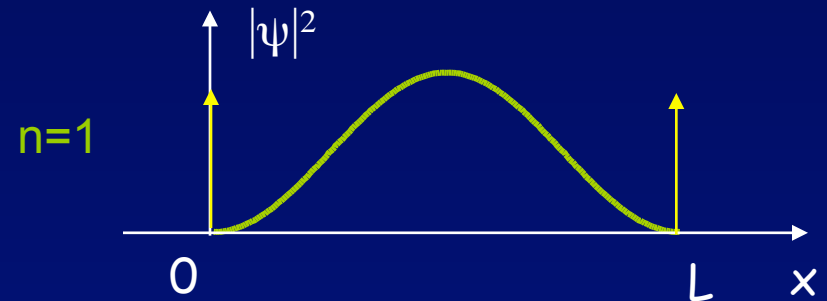
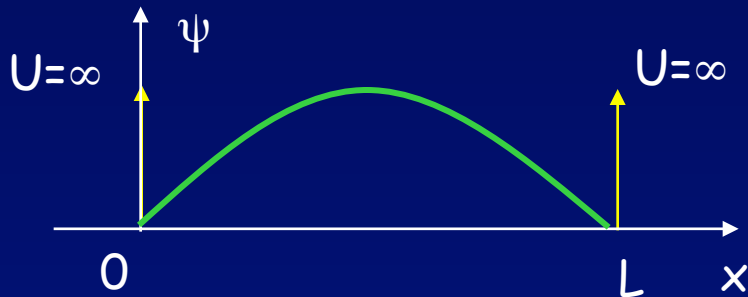


# Probabilities

Often what we measure in an experiment is the probability density,  $|\psi(x)|^2$ .

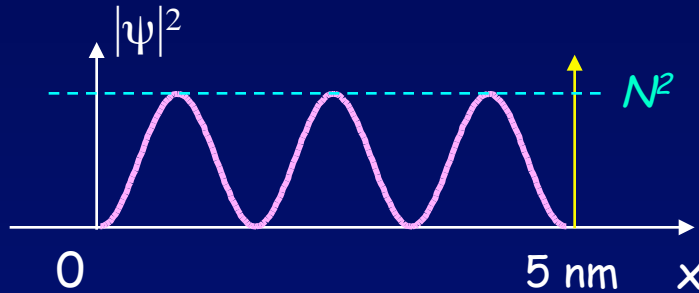
$$\psi_n(x) = N \sin\left(\frac{n\pi}{L}x\right) \quad \begin{array}{l} \text{Wavefunction =} \\ \text{Probability amplitude} \end{array}$$

$$|\psi_n(x)|^2 = N^2 \sin^2\left(\frac{n\pi}{L}x\right) \quad \begin{array}{l} \text{Probability per} \\ \text{unit length} \\ \text{(in 1-dimension)} \end{array}$$



# Probability Example

Consider an electron trapped in a 1D well with  $L = 5 \text{ nm}$ . Suppose the electron is in the following state:

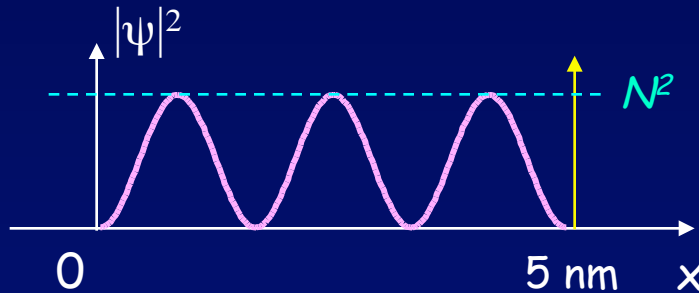


$$|\psi_n(x)|^2 = N^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

- a) What is the energy of the electron in this state (in eV)?
- b) What is the value of the normalization factor squared  $N^2$ ?
- c) Estimate the probability of finding the electron within  $\pm 0.1 \text{ nm}$  of the center of the well? (No integral required. Do it graphically.)

# Solution

Consider an electron trapped in a 1D well with  $L = 5 \text{ nm}$ . Suppose the electron is in the following state:



$$|\psi_n(x)|^2 = N^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

a) What is the energy of the electron in this state (in eV)?

$$n = 3, \quad E_n = E_1 n^2 = \frac{1.505 \text{ eV} \cdot \text{nm}^2}{4(5 \text{ nm})^2} 3^2 = 0.135 \text{ eV}$$

b) What is the value of the normalization factor squared  $N^2$ ?

$$P_{\text{tot}} = 1 = N^2 \frac{L}{2} \Rightarrow N^2 = \frac{2}{L} = 0.4 \text{ nm}^{-1}$$

c) Estimate the probability of finding the electron within  $\pm 0.1 \text{ nm}$  of the center of the well? (No integral required. Do it graphically.)

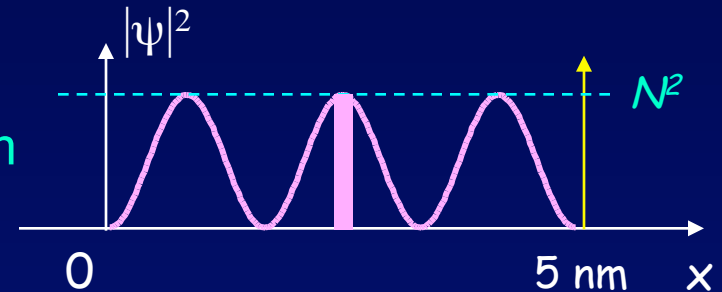
$$\text{Probability} = (\Delta x) \psi_{\text{middle}}^2 \approx (0.2 \text{ nm}) N^2 = 0.08 \quad [(\sin(3\pi x/L))^2 \approx 1 \text{ for } x \approx L/2]$$

This works because the entire interval is very close to the middle peak.



# Act 3

In the previous exercise, we found that the probability to find the electron within  $\pm 0.1$  nm of the center of the well was  $\sim 8\%$ .

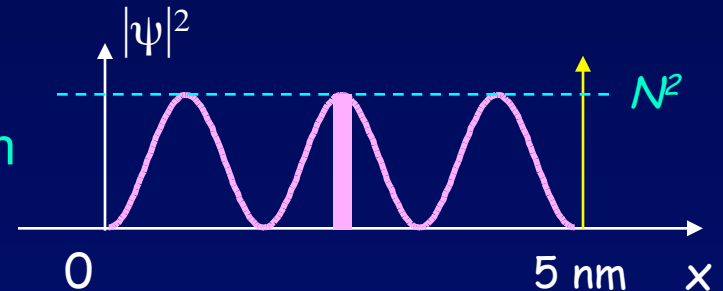


If the original energy of the particle was 0.135 eV, what is the likely new energy after we make the measurement (and find the particle in the center)?

- a)  $< 0.135$  eV
- b) 0.135 eV
- c)  $> 0.135$  eV

# Solution

In the previous exercise, we found that the probability to find the electron within  $\pm 0.1$  nm of the center of the well was  $\sim 8\%$ .



If the original energy of the particle was 0.135 eV, what is the likely new energy after we make the measurement (and find the particle in the center)?

a)  $< 0.135$  eV

b) 0.135 eV

c)  $> 0.135$  eV

We've greatly reduced the uncertainty in the location of the particle, and therefore greatly increased its momentum uncertainty, and hence, its likely energy.

# Harmonic Oscillator Potential

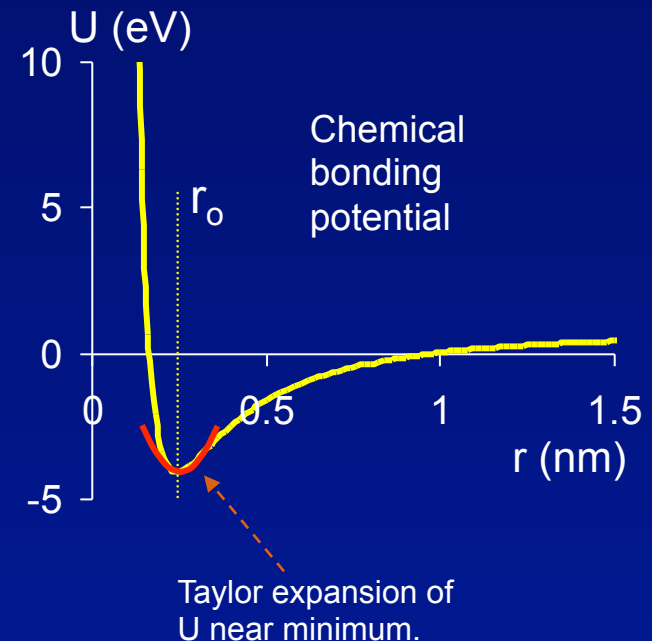
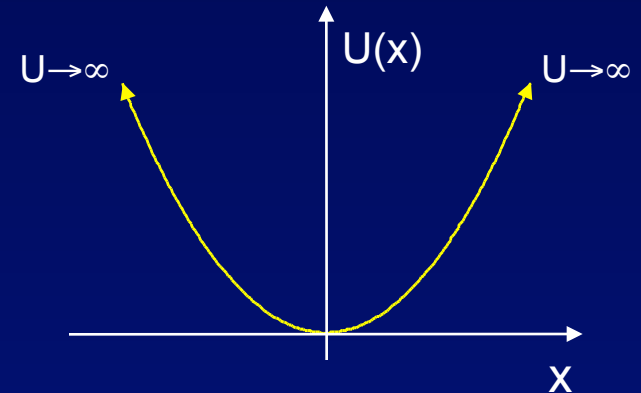
Another very important potential is the harmonic oscillator:

$$U(x) = \frac{1}{2} \kappa x^2 \quad \omega = (\kappa/m)^{1/2}$$

Why is this potential so important?

- It accurately describes the potential for many systems. *E.g.*, sound waves.
- It approximates the potential in almost every system for small departures from equilibrium. *E.g.*, chemical bonds.

To a good approximation, everything is a harmonic oscillator.



# Harmonic Oscillator (2)

The differential equation that describes the HO is too difficult for us to solve here. Here are the important features of the solution.

The most important feature is that the energy levels are equally spaced:  $E_n = (n+1/2)\hbar\omega$ .

The ground state ( $n = 0$ ) does not have  $E = 0$ . Another example of the uncertainty principle.

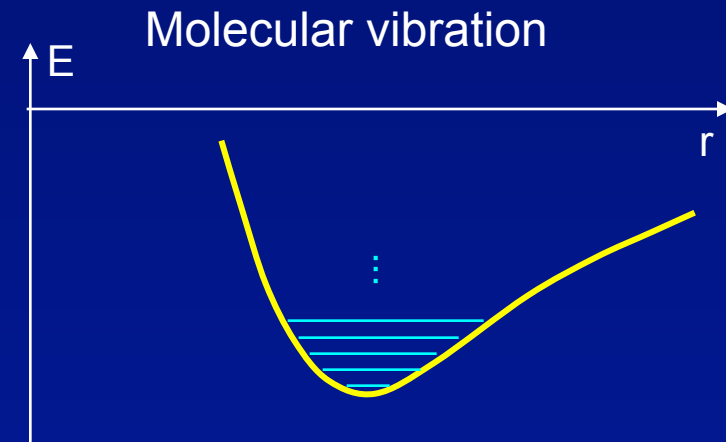
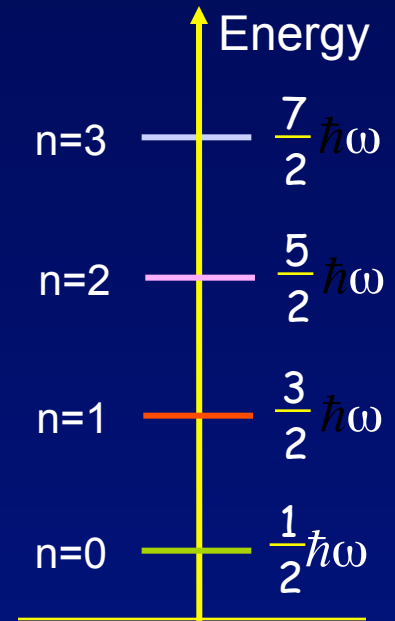
**Beware!!** The numbering convention is not the same as for the square well.

Spacing between vibrational levels of molecules in atmospheric  $\text{CO}_2$  and  $\text{H}_2\text{O}$  are in the infrared frequency range.

$$\Delta E = \hbar\omega = hf \sim 0.01 \text{ eV}$$

This is why they are important greenhouse gases.

$\omega$  is the classical oscillation frequency



# Harmonic Oscillator Wave Functions

To obtain the exact eigenstates and associated allowed energies for a particle in the HO potential, we would need to solve this SEQ:

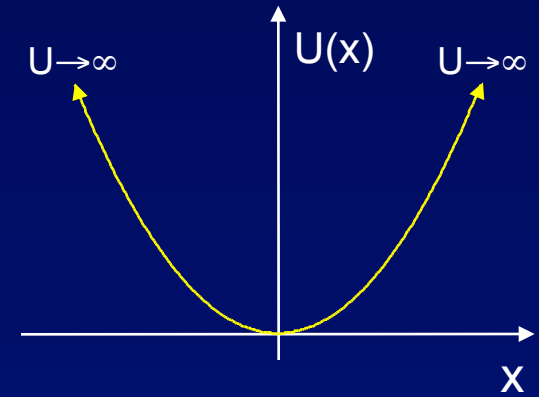
$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + \frac{1}{2} \kappa x^2 \psi(x) = E \psi(x)$$

This is solvable, but not here, not now ...

However, we can get a good idea of what  $\psi_n(x)$  looks like by applying our general rules.

The important features of the HO potential are:

- It's symmetrical about  $x = 0$ .
- It does not have a hard wall (doesn't go to  $\infty$  at finite  $x$ ).

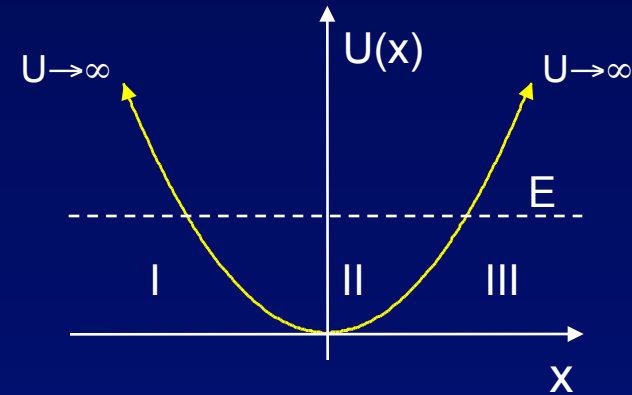


# HO Wave Functions (2)

Consider the state with energy  $E$ . There are two forbidden regions and one allowed region.

Applying our general rules, we can then say:

- $\psi(x)$  curves toward zero in region II and away from zero in regions I and III.
- $\psi(x)$  is either an even or odd function of  $x$ .

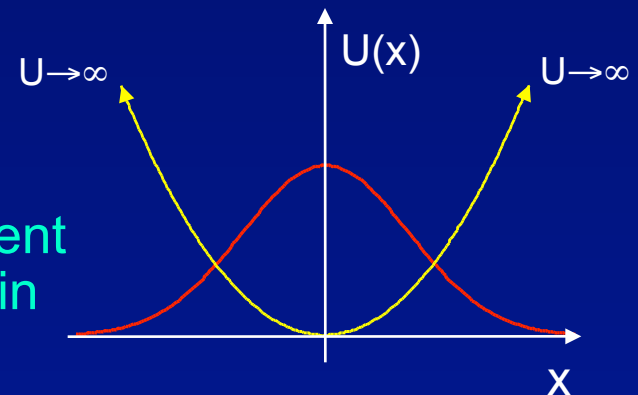


Let's consider the ground state:

- $\psi(x)$  has no nodes.
- $\psi(x)$  is an even function of  $x$ .

This wave function resembles the square well ground state. The exact functional form is different—a 'Gaussian'—but we won't need to know it in this course:

$$\psi_{n=0}(x) \propto e^{-x^2 / 2a^2} \quad a^2 = \frac{\hbar}{\sqrt{m\kappa}}$$

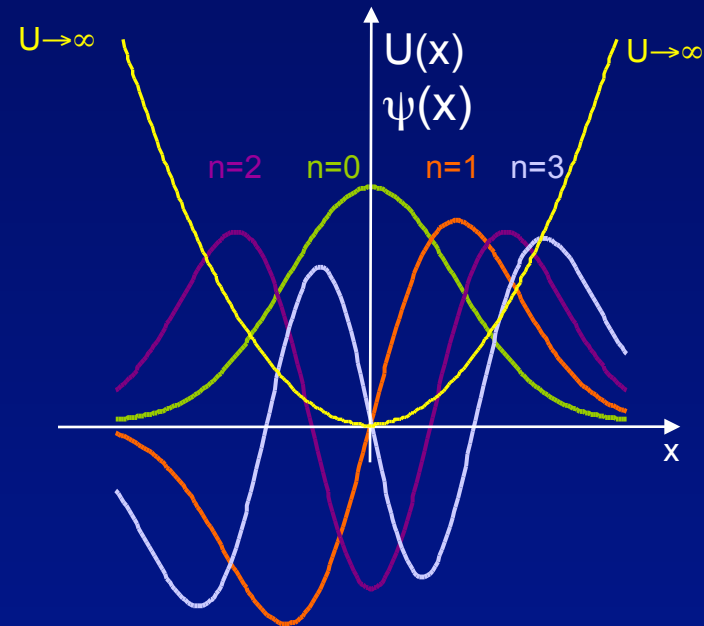


# HO Wave Functions (3)

For the excited states, use these rules:

- Each successive excited state has one more node.
- The wave functions alternate symmetry.

Unlike the square well, the allowed region gets wider as the energy increases, so the higher energy wave functions oscillate over a larger  $x$  range. (but that's a detail...)



# Harmonic Oscillator Exercise

A particular laser emits at a wavelength  $\lambda = 2.7 \mu\text{m}$ . It operates by exciting hydrogen fluoride (HF) molecules between their **ground** and **1<sup>st</sup> excited** vibrational levels. Estimate the ground state energy of the HF molecular vibrations.



# Solution

A particular laser emits at a wavelength  $\lambda = 2.7 \mu\text{m}$ . It operates by exciting hydrogen fluoride (HF) molecules between their **ground** and **1<sup>st</sup> excited** vibrational levels. Estimate the ground state energy of the HF molecular vibrations.

Recall:

$$E_{\text{photon}} = hc/\lambda = (1240 \text{ eV}\cdot\text{nm})/2.7\mu\text{m} = 0.46 \text{ eV}$$

and: (by energy conservation)

$$E_{\text{photon}} = \Delta E = E_1 - E_0 = \hbar\omega = 2E_0$$

Therefore,

$$E_0 = \frac{1}{2} \hbar\omega = 0.23 \text{ eV}$$

