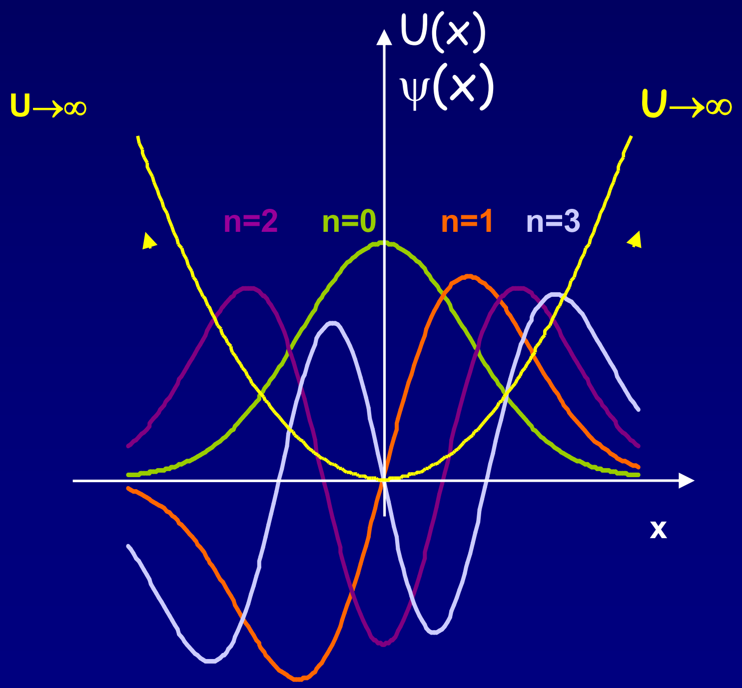
Lecture 12:
Particle in 1D boxes, Simple Harmonic Oscillators



This week and last week are critical for the course:

Week 3, Lectures 7-9:	Week 4, Lectures 10-12:
Light as Particles	Schrödinger Equation
Particles as waves	Particles in infinite wells, finite wells
Probability	
Uncertainty Principle	

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.

Lab: Go to 257 Loomis (a computer room).

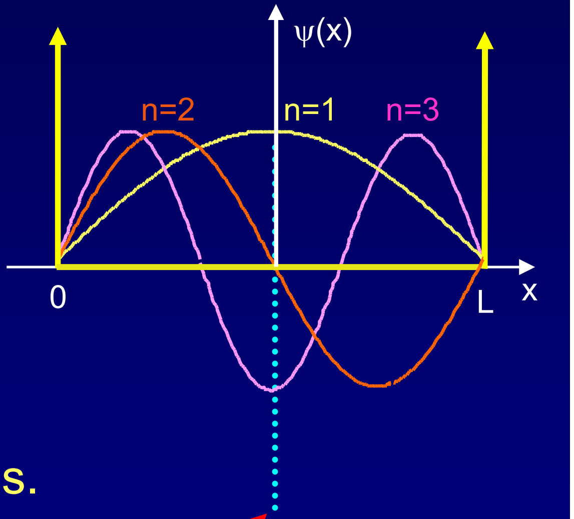
You can save a lot of time by reading the lab ahead of time –
It's a tutorial on how to draw wave functions.

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.

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



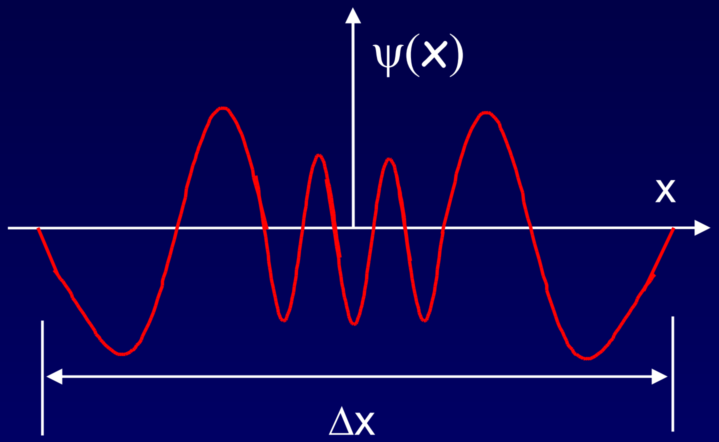
2: The lowest energy bound state always has finite kinetic energy -- called "zero-point" energy. Even the lowest energy bound state requires some wave function curvature (kinetic energy) to satisfy boundary conditions.

3: The n^{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

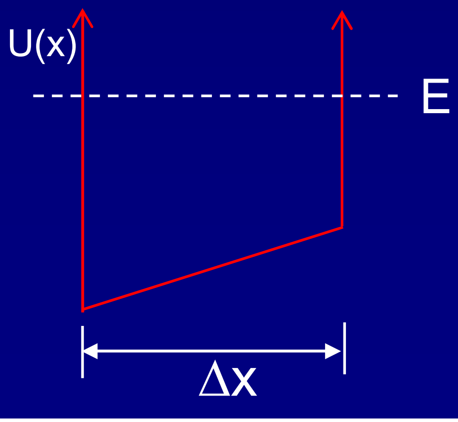
The wave function below describes a quantum particle in a range Δx:

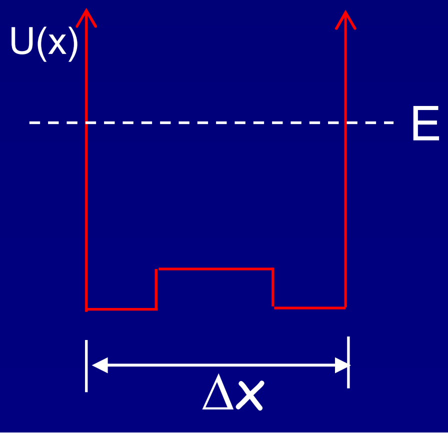


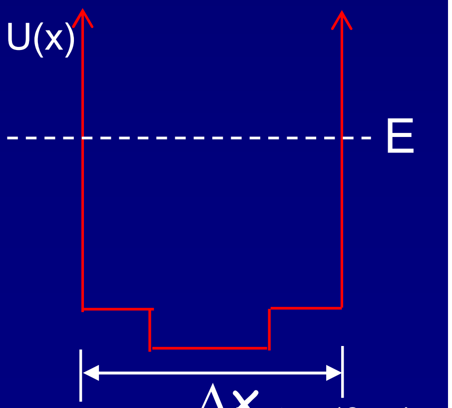
1. In what energy level is the particle?
   n =

(a) 7 (b) 8 (c) 9

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

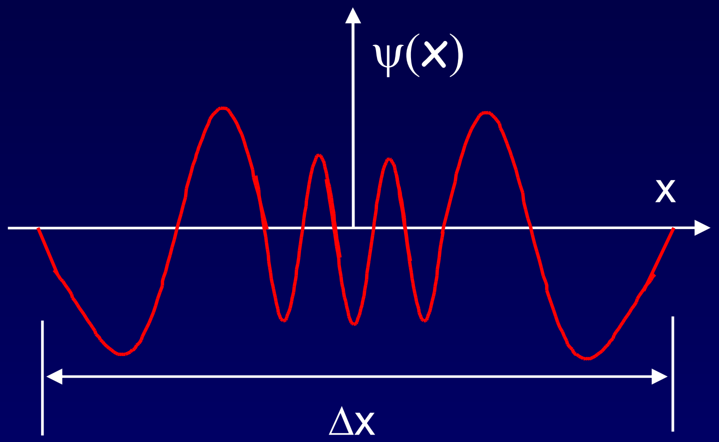
(a)


(b)


(c)


Solution

The wave function below describes a quantum particle in a range Δx:



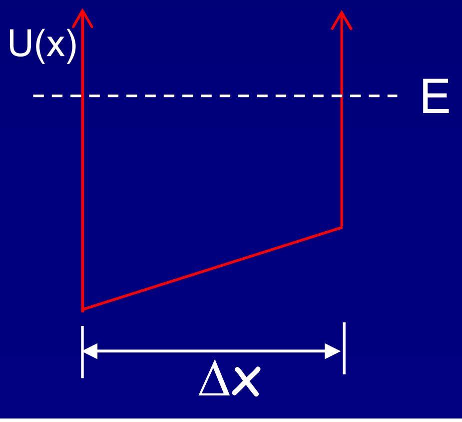
1. In what energy level is the particle?
   n =

(a) 7 (b) 8 (c) 9

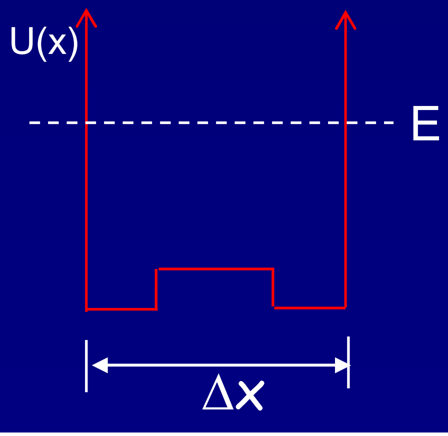
Eight nodes.
Don't count the boundary conditions.

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

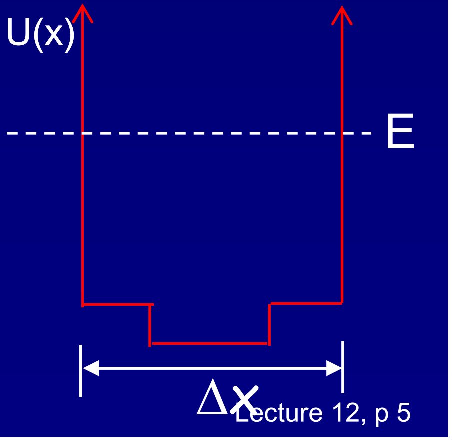
(a)



(b)



(c)



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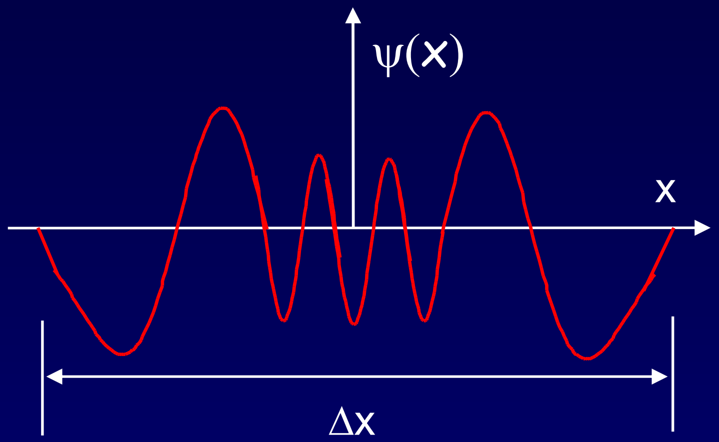


1. In what energy level is the particle?
n =

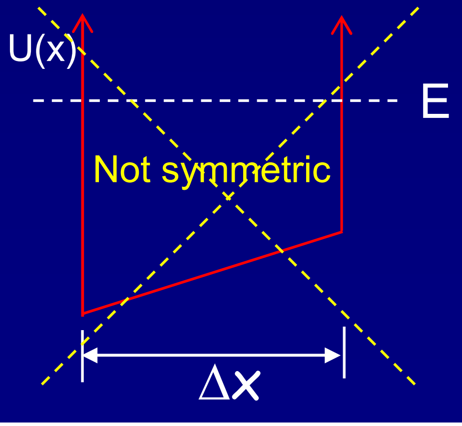
(a) 7 (b) 8 (c) 9

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?

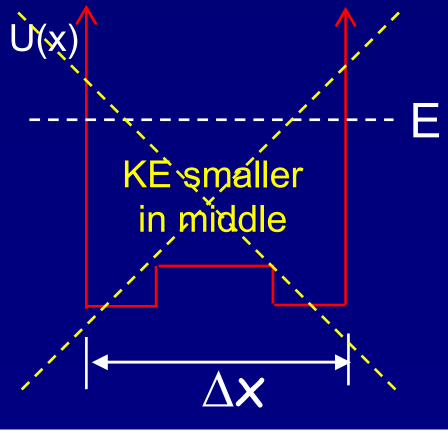
Wave function is symmetric.
Wavelength is shorter in the middle.

(a)



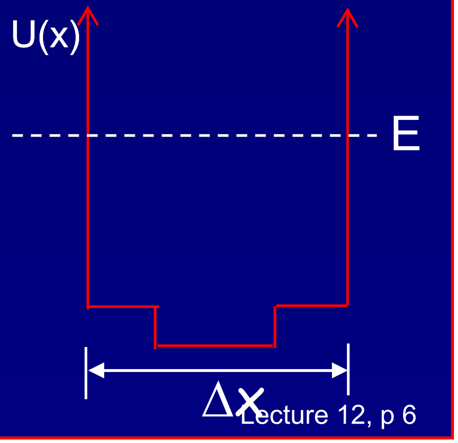
Not symmetric

(b)



KE smaller
in middle

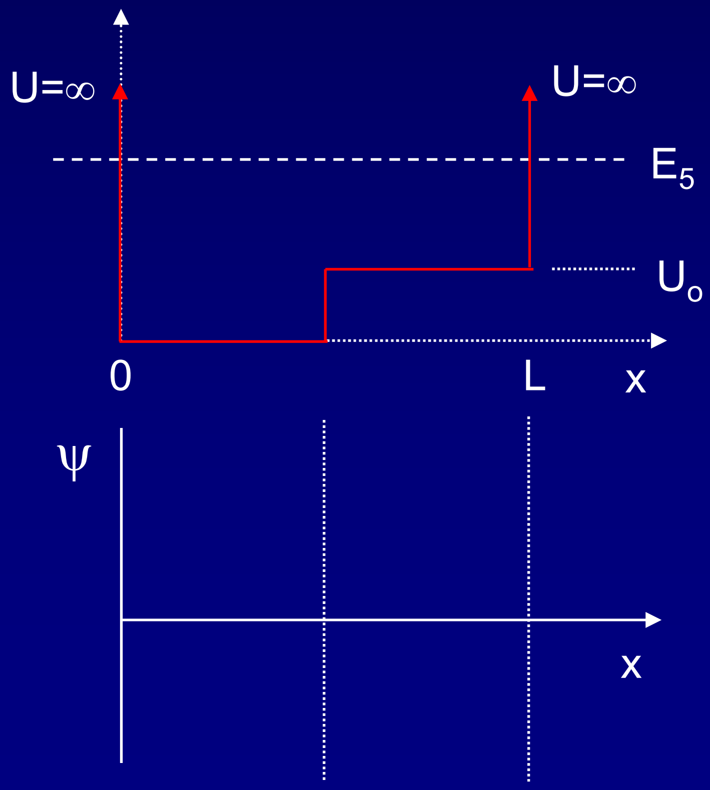
(c)



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_o and L. Qualitatively sketch a possible 5th wave function:



Consider these features of ψ:

1: 5th wave function has __ zero-crossings.

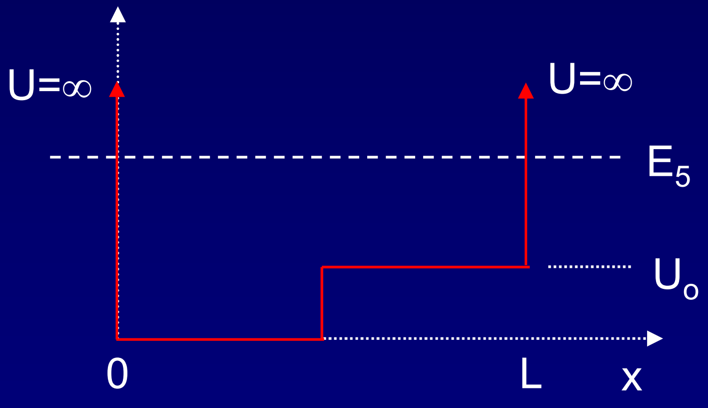
2: Wave function must go to zero at ____ and ____.

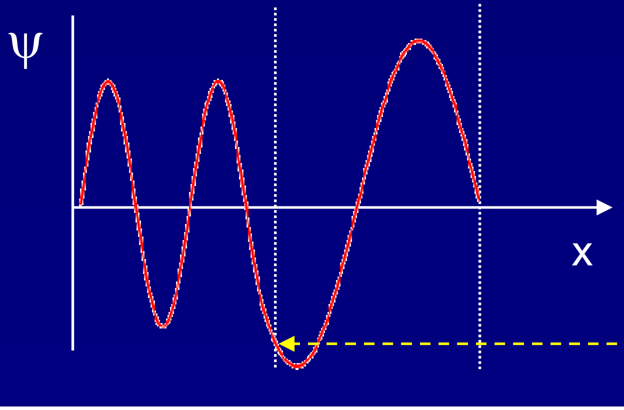
3: Kinetic energy is _____ on right side of well, so the curvature of ψ is ______ there.

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_o and L. Qualitatively sketch a possible 5th wave function:





ψ and dψ/dx must be continuous here.

Consider these features of ψ:

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 ψ is smaller there.

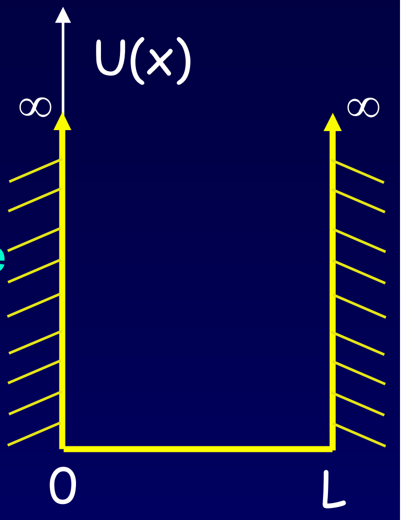
The wavelength is longer.

Particle in a Box

As a specific important example, consider a quantum particle confined to a region, $0 < x < L$, by *infinite* potential walls. We call this a “one-dimensional (1D) box”.

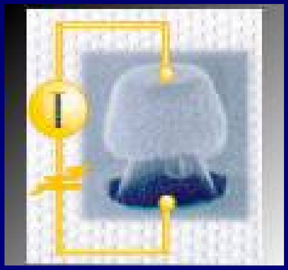
$U = 0$ for $0 < x < L$

$U = \infty$ everywhere else



This is a basic problem in “Nano-science”. It’s a simplified (1D) model of an electron confined in a quantum structure (e.g., “quantum dot”), which scientists/engineers make, *e.g.*, at the UIUC Microelectronics Laboratory.

Quantum dots



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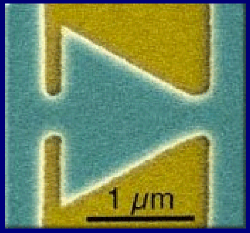
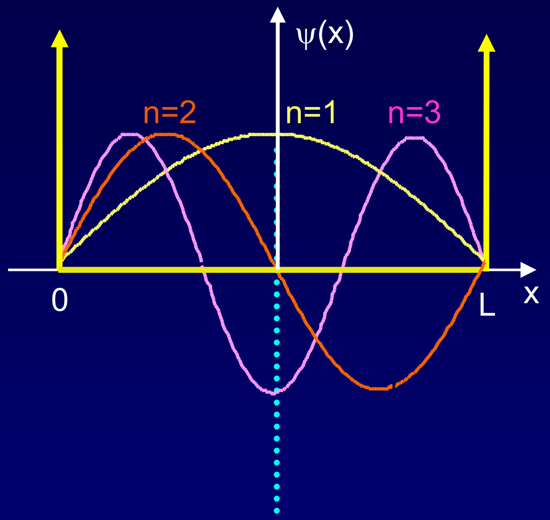


newt.phys.unsw.edu.au

We already know the form of ψ when $U = 0$: sin(kx) or cos(kx).
However, we can constrain ψ more than this…

Particle in Infinite Square Well Potential

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



$$n\lambda_n = 2L$$

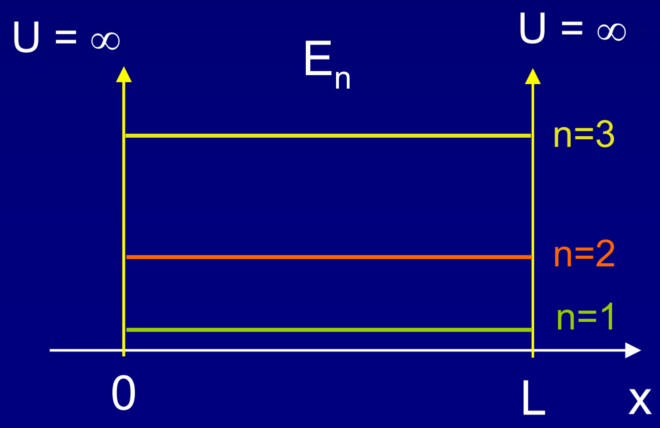
$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \cancel{U(x)\psi_n(x)} = E_n\psi_n(x)$$

The discrete E_n are known as “energy eigenvalues”:

electron

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

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



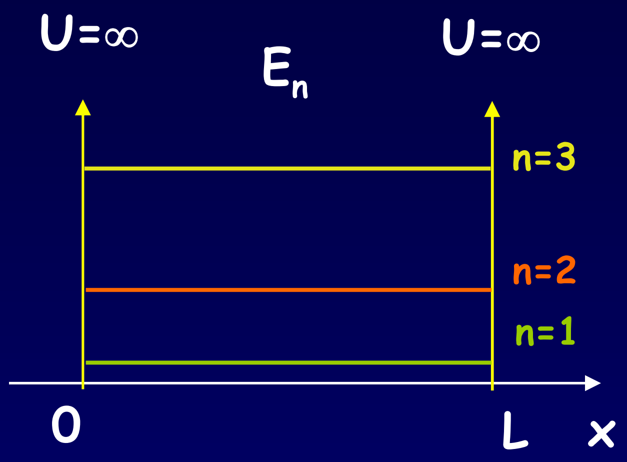
Act 2

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

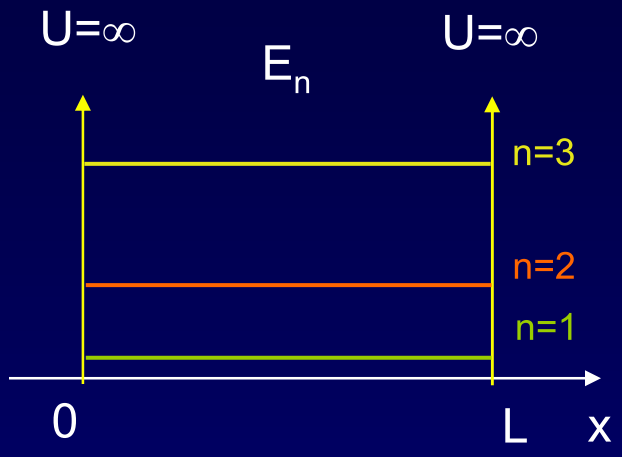
a) decrease

[✓ b) increase]

c) stay the same

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

The uncertainty principle, once again!



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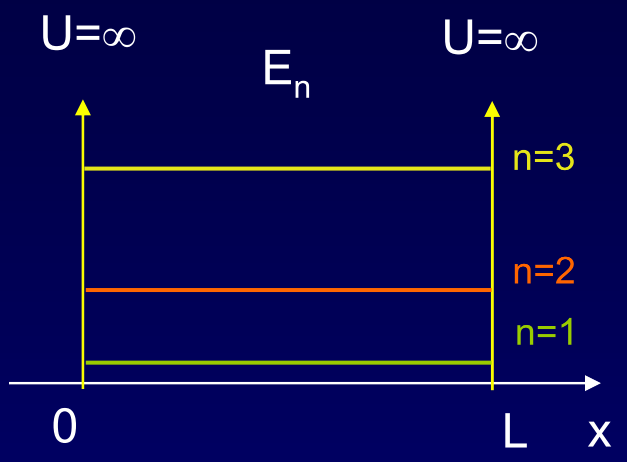

a) decrease

b) increase

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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

$E_n = n^2 E_1$

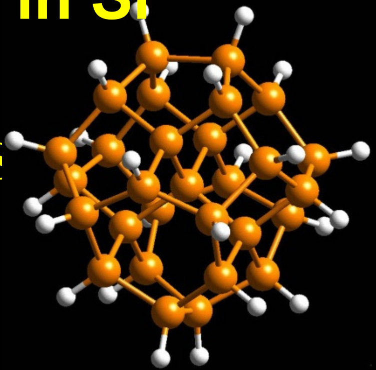
$E_7 - E_2 = (49 - 4)E_1 = 45E_1$

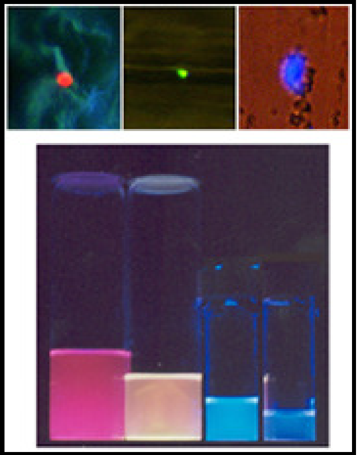
Since E_1 increases, so does ΔE.

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

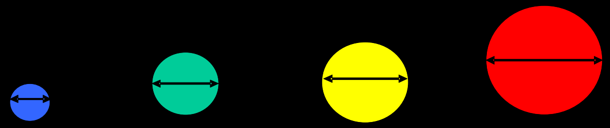
M. Nayfeh (UIUC) : Discrete uniform Si nanoparticles

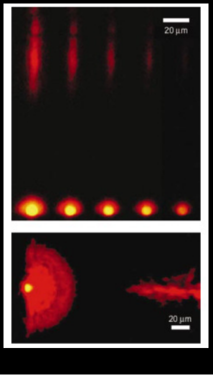
- Transition from bulk to molecule-like in Si





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



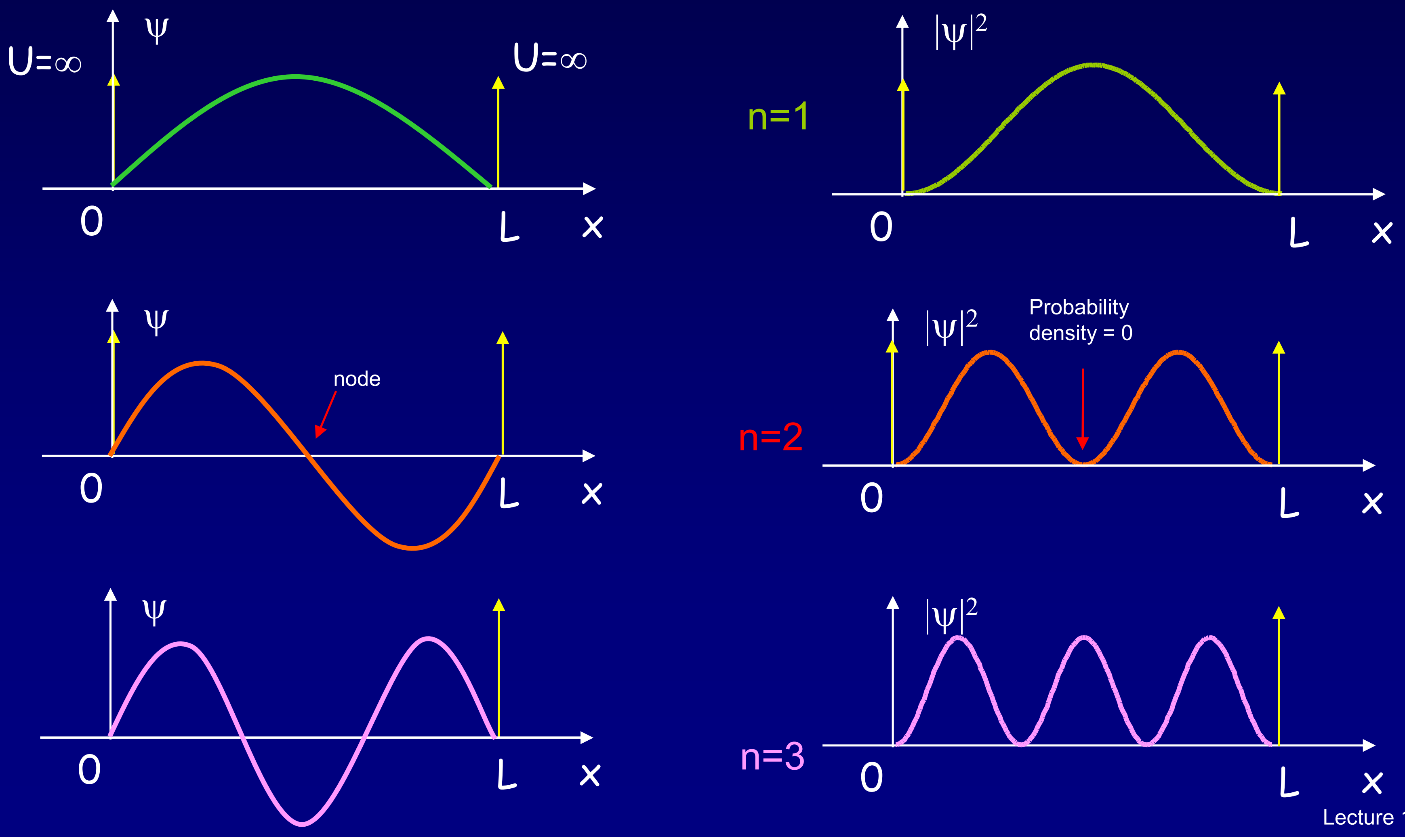


Probabilities

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

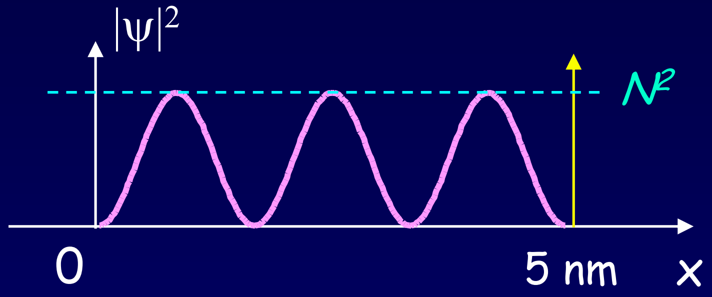
$\psi_n(x) = N\sin\left(\frac{n\pi}{L}x\right)$ Wavefunction = Probability amplitude

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



Probability Example

Consider an electron trapped in a 1D well with L = 5 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 ±0.1 nm of the center of the well? (No integral required. Do it graphically.)

Solution

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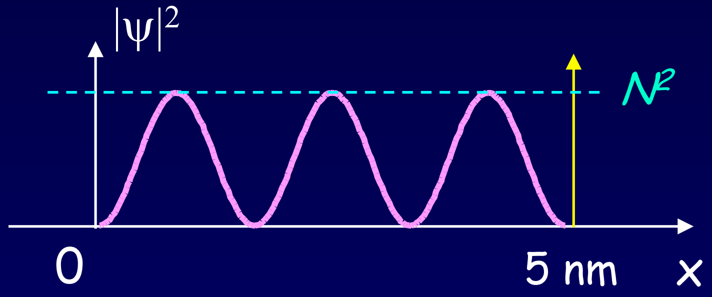


$$|\psi_n(x)|^2 = N^2 \sin^2\left(\frac{n\pi}{L}x\right)$$

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

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

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

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

c) Estimate the probability of finding the electron within ±0.1 nm of the center of the well? (No integral required. Do it graphically.)

$$\text{Probability} = (\Delta x)\psi^2_{\text{middle}} \approx (0.2\text{ nm})N^2 = 0.08$$

$[(\sin(3\pi x/L))^2 \approx 1$ for $x \approx L/2]$

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

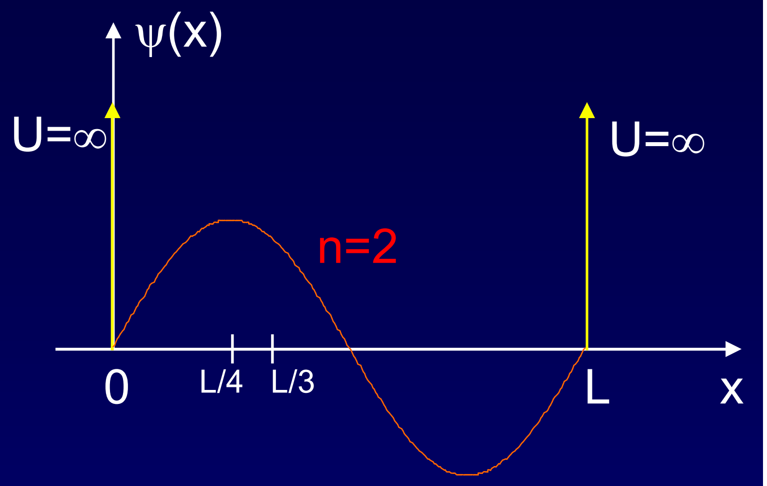
Probability Example

Consider a particle in the n = 2 state of a box.

a) Where is it most likely to be found?

b) Where is it least likely to be found?

c) What is the ratio of probabilities for the particle to be near x = L/3 and x = L/4?



Solution

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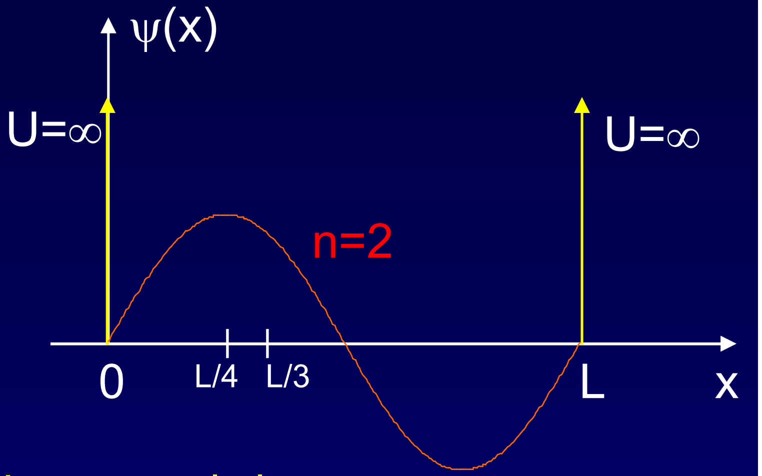


Solution:

a) x = L/4 and x = 3L/4. Maximum probability is at max |ψ|.

b) x = 0, x = L/2, and x = L. Minimum probability is at the nodes.

The sine wave must have nodes at x = 0, x = L, and, because n = 2, at x = L/2 as well.

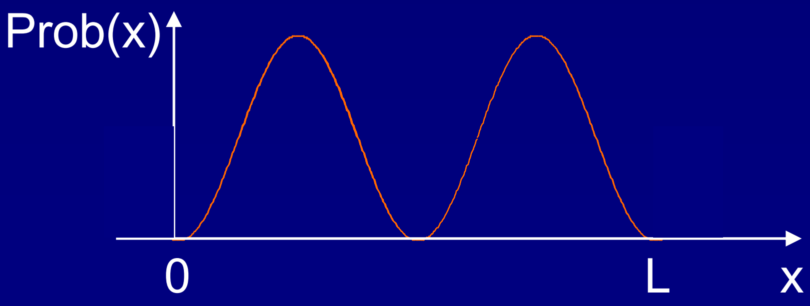
c) $\psi(x) = N\sin(2\pi x/L)$

Prob(L/3) / Prob(L/4)

$= |\psi(L/3)|^2 / |\psi(L/4)|^2$

$= \sin^2(2\pi/3) / \sin^2(\pi/2)$

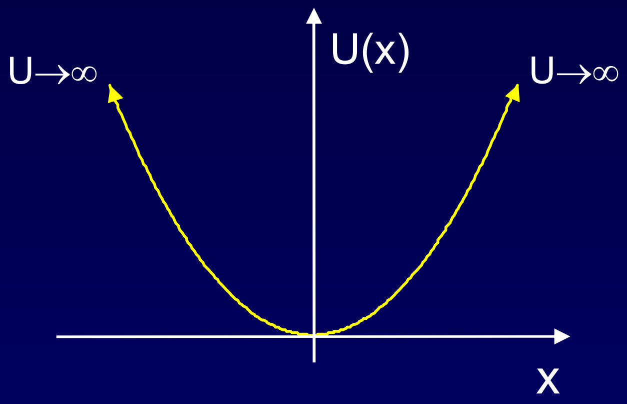
$= 0.866^2 = 0.75$



Harmonic Oscillator Potential

Another very important potential is the harmonic oscillator:

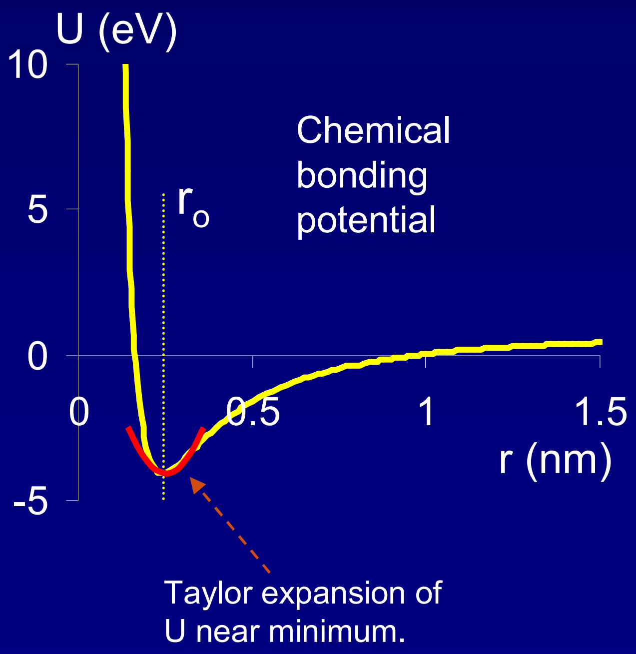
$U(x) = \frac{1}{2} \kappa x^2$ $\omega = (\kappa/m)^{1/2}$



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)

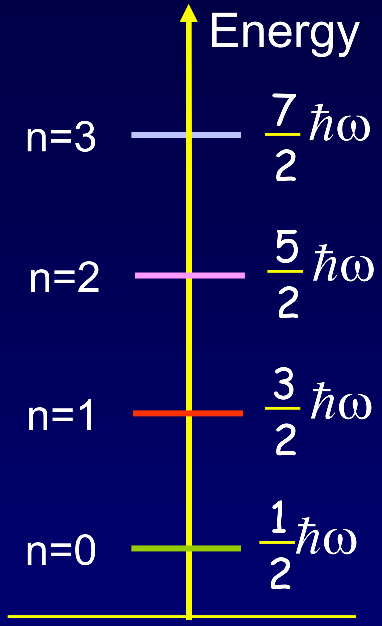
The differential equation that describes the HO is too difficult for us to solve here. Here are the important features of the solution.

ω is the classical oscillation frequency

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.

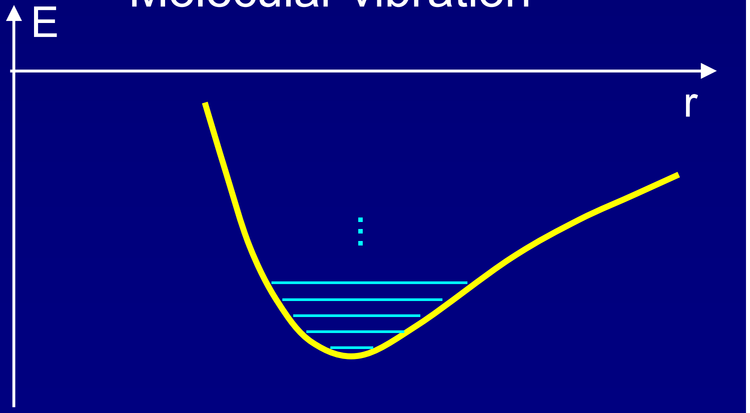


Spacing between vibrational levels of molecules in atmospheric CO_2 and H_2O are in the infrared frequency range.

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

This is why they are important greenhouse gases.

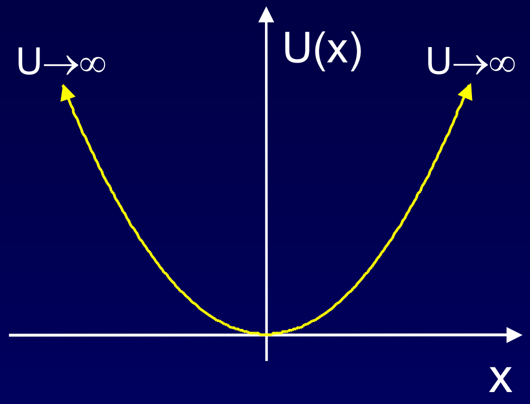
Molecular vibration



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:

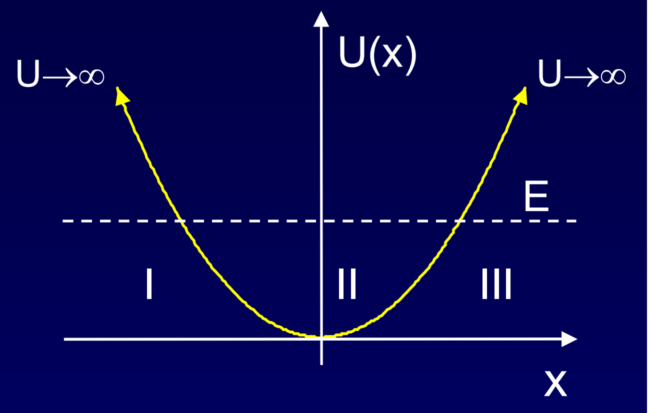
- It's symmetrical about x = 0.
- It does not have a hard wall (doesn't go to ∞ at finite x).

HO Wave Functions (2)

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

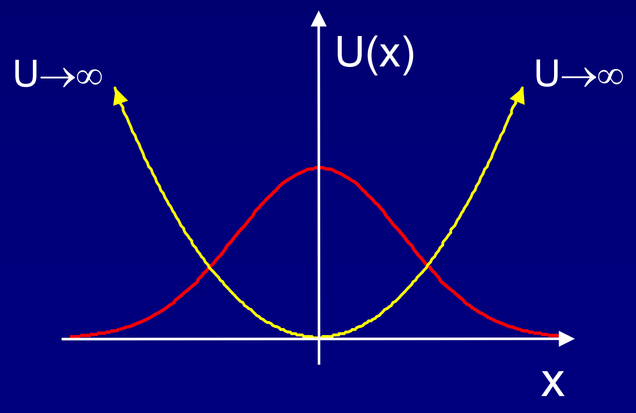
Applying our general rules, we can then say:

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



Let's consider the ground state:

- ψ(x) has no nodes.
- ψ(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:

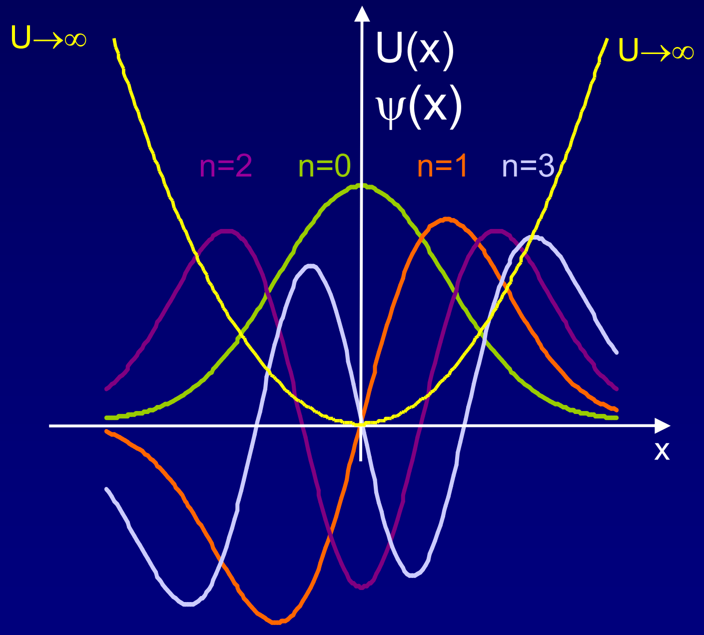
$$\psi_{n=0}(x) \propto e^{-x^2/2a^2} \qquad a^2 = \frac{\hbar}{\sqrt{m\kappa}}$$

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 1st excited vibrational levels. Estimate the ground state energy of the HF molecular vibrations.

Solution

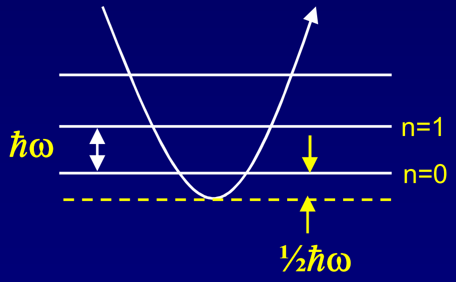
A particular laser emits at a wavelength $\lambda = 2.7\ \mu m$. It operates by exciting hydrogen fluoride (HF) molecules between their ground and 1st excited vibrational levels. Estimate the ground state energy of the HF molecular vibrations.

Recall:

$E_{photon} = hc/\lambda = (1240\ eV\text{-}nm)/2.7mm = 0.46\ eV$

and: (by energy conservation)

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



Therefore,

$$\boxed{E_0 = \tfrac{1}{2}\hbar\omega = 0.23\ eV}$$