From Last Time…

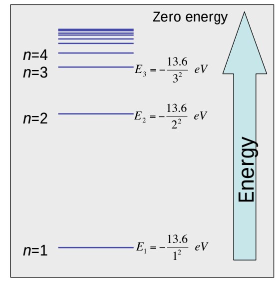
- Observation of atoms indicated quantized energy states.
  - Atom only emitted certain wavelengths of light
  - Structure of the allowed wavelengths indicated the what the energy structure was
- Quantum mechanics and the wave nature of the electron allowed us to understand these energy levels.

Today

- The quantum wave function
- The atom in 3 dimensions
- Uncertainty principle again

Hydrogen atom energies

- Electrons orbit the atom in quantized energy states
- Energy states are resonant states where the electron wave constructively interferes with itself. n whole wavelengths around
- Wavelength gets longer in higher *n* states and the kinetic energy goes down proportions to $1/n^2$
- Potential energy goes up as with gravity also as $1/n^2$



$$E_n = -\frac{13.6}{n^2} eV$$

Hydrogen atom question

Here is Peter Flanary's sculpture 'Wave' outside Chamberlin Hall. What quantum state of the hydrogen atom could this represent?

A. n=2
B. n=3
C. n=4

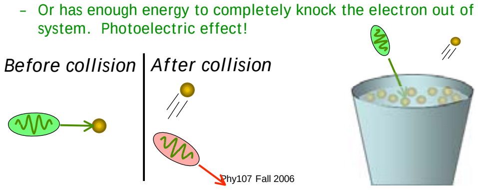
Another question

Here is Donald Lipski's sculpture 'Nail's Tail' outside Camp Randall Stadium.
What could it represent?

A. A pile of footballs
B. "I hear its made of plastic. For 200 grand, I'd think we'd get granite"
- Tim Stapleton (Stadium Barbers)
C. "I'm just glad it's not my money"
- Ken Kopp (New Orlean's Take-Out)
D. Amazingly physicists make better sculptures!

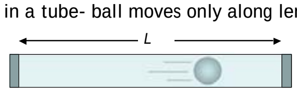
Compton scattering and Photoelectric effect

- Collision of photon and electron
- Photon loses energy and momentum, transfers it to electron
- Either:
  - Loses enough energy/momentum to bump it up one level
  - Electron later decays back to ground state releasing a photon
  - See reflected and emitted photons when looking at an object
  - Or has enough energy to completely knock the electron out of the system. Photoelectric effect!



Simple Example: 'Particle in a box'

Particle confined to a fixed region of space
e.g. ball in a tube- ball moves only along length *L*



- **Classically**, ball bounces back and forth in tube.
  - No friction, so ball continues to bounce back and forth, retaining its initial speed.
  - This is a 'classical state' of the ball. A different classical state would be ball bouncing back and forth with different speed.
  - Could label each state with a speed, **momentum**=(mass)x(speed), or kinetic energy.
  - Any momentum, energy is possible. Can increase momentum in arbitrarily small increments.

Quantum Particle in a Box

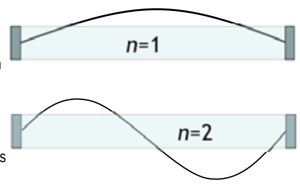
- In Quantum Mechanics, ball represented by wave
  - Wave reflects back and forth from the walls.
  - Reflections cancel unless wavelength meets the standing wave condition:
    integer number of half-wavelengths fit in the tube.

$\lambda = 2L$
One half-wavelength

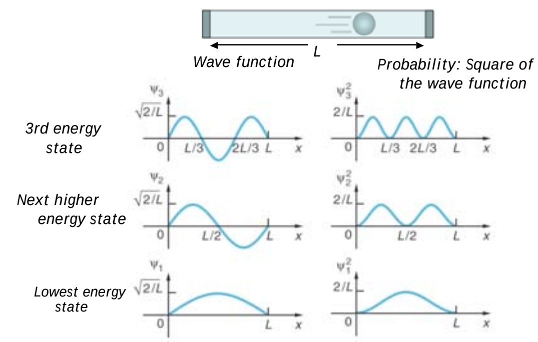
momentum
$p = \frac{h}{\lambda} = \frac{h}{2L} \equiv p_o$

$\lambda = L$
Two half-wavelengths

momentum
$p = \frac{h}{\lambda} = \frac{h}{L} = 2p_o$



Particle in a box



Particle in box question

A particle in a box has a mass m.
It's energy is all energy of motion = $p^2/2m$.
We just saw that it's momentum in state n is np_o.
It's energy levels

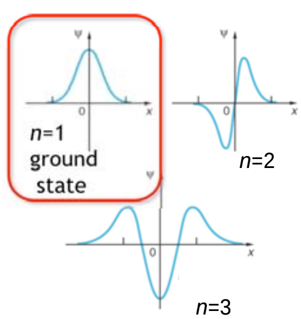
A. are equally spaced everywhere
B. get farther apart at higher energy
C. get closer together at higher energy.

General aspects of Quantum Systems

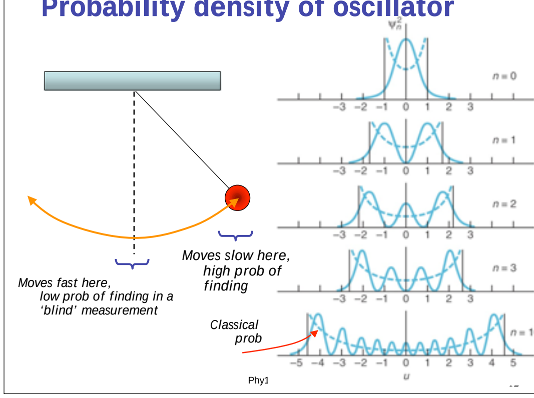
- System has set of quantum states, labeled by an integer (n=1, n=2, n=3, etc)
- Each quantum state has a particular frequency and energy associated with it.
- These are the only energies that the system can have: the energy is quantized
- Analogy with classical system:
  - System has set of vibrational modes, labeled by integer fundamental (n=1), 1st harmonic (n=2), 2nd harmonic (n=3), *etc*
  - Each vibrational mode has a particular frequency and energy.
  - These are the only frequencies at which the system resonates.

Wavefunction of pendulum

Here are quantum wavefunctions of a pendulum. Which has the lowest energy?



Probability density of oscillator



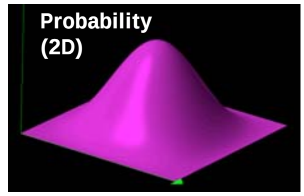
Wavefunctions in two dimensions

- Physical objects often can move in more than one direction (not just one-dimensional)
- Could be moving at one speed in *x*-direction, another speed in *y*-direction.
- From deBroglie relation, wavelength related to momentum in that direction

$$\lambda = \frac{h}{p}$$

- So wavefunction could have different wavelengths in different directions.

Two-dimensional (2D) particle in box

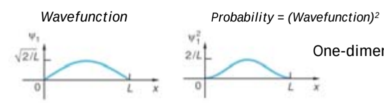


Ground state: same wavelength (longest) in both *x* and *y*

Need two quantum #'s, one for *x*-motion, one for *y*-motion

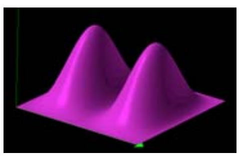
Use a pair (n_x, n_y)

Ground state: (1,1)

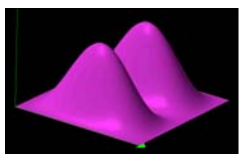


One-dimensional (1D) case

2D excited states



(n_x, n_y) = (2,1)



(n_x, n_y) = (1,2)

These have exactly the same energy, but the probabilities look different.

The different states correspond to ball bouncing in *x* or in *y* direction.

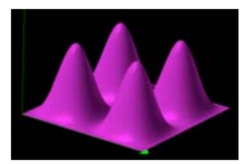
Particle in a box

What quantum state could this be?

$\boxed{\text{A. } n_x=2,\ n_y=2}$

B. $n_x=3$, $n_y=2$

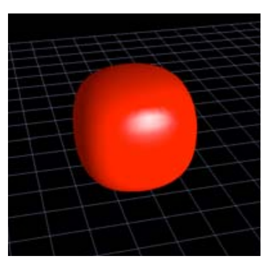
C. $n_x=1$, $n_y=2$



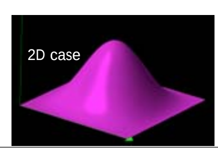
Three dimensions

- Object can have different velocity (hence wavelength) in *x*, *y*, or *z* directions.
  - Need three quantum numbers to label state
- (n_x, n_y , n_z) labels each quantum state (a triplet of integers)
- Each point in three-dimensional space has a probability associated with it.
- Not enough dimensions to plot probability
- But can plot a surface of constant probability.

3D particle in box



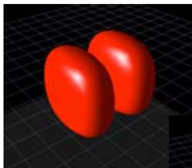
- Ground state surface of constant probability
- (n_x, n_y, n_z)=(1,1,1)
- Like the 2D case - highest probability in the center and less further out

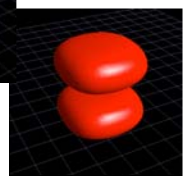


(121)

(112)

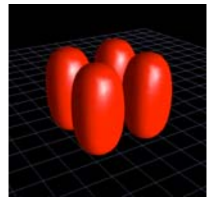
(211)





All these states have the same energy, but different probabilities

(222)



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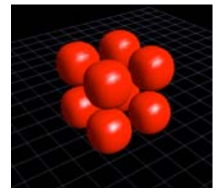


Hydrogen atom

- Hydrogen a little different, in that it has spherical symmetry
- Not square like particle in a box.
- Still need three quantum numbers, but they represent 'spherical' things like
  - Radial distance from nucleus
  - Azimuthal angle around nucleus
  - Polar angle around nucleus
- Quantum numbers are integers (n, l, m_l)

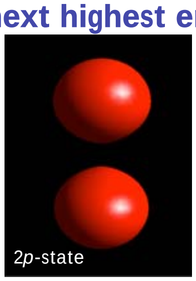
Hydrogen atom: Lowest energy (ground) state

$n=1,\ \ell=0,\ m_\ell=0$

- Lowest energy state is same in all directions.
- Surface of constant probability is surface of a sphere.

n=2: next highest energy

$n=2,\ \ell=0,\ m_\ell=0$



$n=2,\ \ell=1,\ m_\ell=0$

$n=2,\ \ell=1,\ m_\ell=\pm 1$

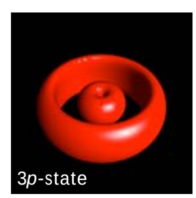
Same energy, but different probabilities

Found by solving for when the wave equation leads to constructive interference. But more complicated in 3D!

n=3: two *s*-states, six *p*-states and…

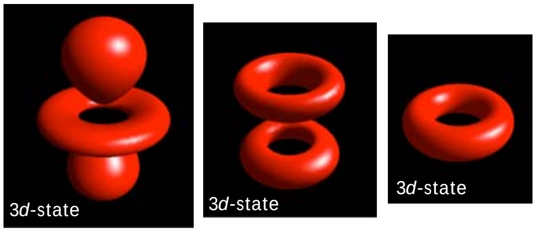
$n=3,\ \ell=0,\ m_\ell=0$

$n=3,\ \ell=1,\ m_\ell=0$



$n=3,\ \ell=1,\ m_\ell=\pm 1$

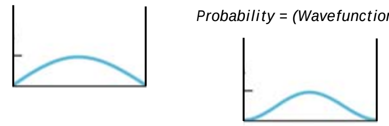
...ten *d*-states



$n=3,\ \ell=2,\ m_\ell=0$ $\quad$ $n=3,\ \ell=2,\ m_\ell=\pm1$ $\quad$ $n=3,\ \ell=2,\ m_\ell=\pm2$

Back to the particle in a box

Wavefunction $\quad$ *Probability = (Wavefunction)^2*



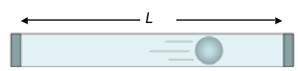
- Here is the probability of finding the particle along the length of the box.
- Can we answer the question:
  Where is the particle?

Where is the particle?

- Can say that the particle is inside the box, (since the probability is zero outside the box), but that's about it.
- The wavefunction extends throughout the box, so particle can be found anywhere inside.
- Can't say exactly where the particle *is*, but I can tell you how likely you are to find at a particular location.

How fast is it moving?

- Box is stationary, so average speed is zero.
- But remember the classical version

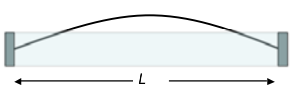


- Particle bounces back and forth.
  - On average, velocity is zero.
  - But not instantaneously
  - Sometimes velocity is to left, sometimes to right

Quantum momentum

- Quantum version is similar. Both contributions

$\lambda = 2L$
One half-wavelength

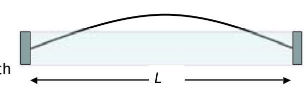


momentum
$|p| = \frac{h}{\lambda} = \frac{h}{2L}$

- Ground state is a standing wave, made equally of
  - Wave traveling right (positive momentum $+h/\lambda$)
  - Wave traveling left (negative momentum $-h/\lambda$)

Particle in a box

$\lambda = 2L$
One half-wavelength



momentum
$|p| = \frac{h}{\lambda} = \frac{h}{2L}$

What is the uncertainty of the momentum in the ground state?

A. Zero
B. *h* / 2L
C. *h* / L

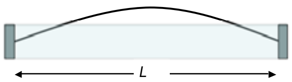
Uncertainty in Quantum Mechanics

Position uncertainty = L

(Since λ=2L)

Momentum ranges from $-\frac{h}{\lambda}$ to $+\frac{h}{\lambda}$: range $= 2\frac{h}{\lambda} = \frac{h}{L}$

$\lambda = 2L$
One half-wavelength



Reducing the box size reduces position uncertainty, but the momentum uncertainty goes up!

The product is constant:
(position uncertainty)x(momentum uncertainty) ~ h

Heisenberg Uncertainty Principle

- Using
  - Δx = position uncertainty
  - Δp = momentum uncertainty
- Heisenberg showed that the product

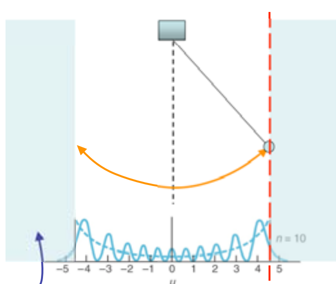
Planck's constant

(Δx) • (Δp) is always greater than (h / 4π)

In this case we found:
(position uncertainty)x(momentum uncertainty) ~ h

Unusual wave effects

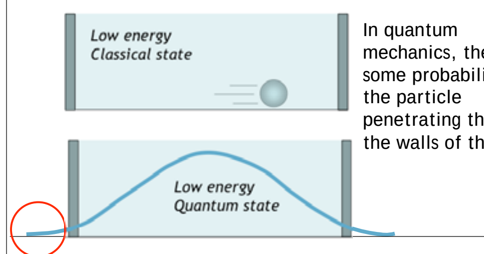
- Classically, pendulum with particular energy never swings beyond maximum point.
- This region is 'classically forbidden'
- Quantum wave function extends into classically forbidden region.



Classically forbidden region

End of swing

Quantum mechanics says something different!

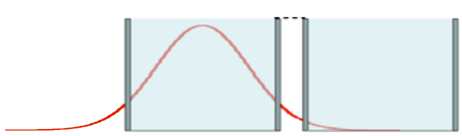


In quantum mechanics, there is some probability of the particle penetrating through the walls of the box.

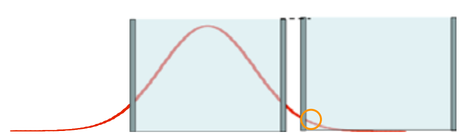
Nonzero probability of being outside the box!

Two neighboring boxes

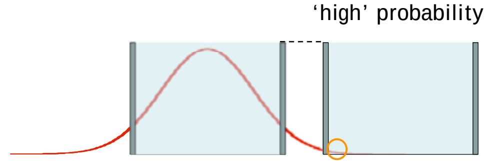
- When another box is brought nearby, the electron may disappear from one well, and appear in the other!
- The reverse then happens, and the electron oscillates back an forth, without 'traversing' the intervening distance.



The tunneling distance

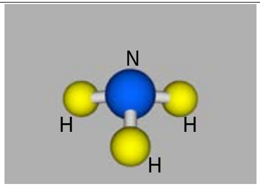


'high' probability



Low probability

Example: Ammonia molecule



- NH_3
- Nitrogen (N) has two equivalent ‘stable’ positions.
- It quantum-mechanically tunnels between 2.4×10^{11} times per second (24 GHz)
- Was basis of first ‘atomic’ clock (1949)

Atomic clock question

Suppose we changed the ammonia molecule so that the distance between the two stable positions of the nitrogen atom INCREASED. The clock would

A. slow down.
B. speed up.
C. stay the same.