

Introduction to Quantum Mechanics (Prelude to Nuclear Shell Model)

Heisenberg Uncertainty Principle

In the microscopic world,

$$\Delta x \times \Delta p \geq \hbar \qquad \hbar = \frac{h}{2\pi}$$

- If you try to specify/measure the exact position of a particle you cannot simultaneously know its momentum exactly.
- If you try to specify/measure the exact momentum of a particle, you cannot simultaneously know its position exactly.

Notice that this is very different from the macroscopic world (like throwing a football around). In the latter case, you CAN specify both the position and the momentum very well. We call the position as a function of time the **TRAJECTORY**

Introduction to Quantum Mechanics

A series of experiments at the beginning of the 20th century taught us that light can behave both as particle (photoelectric effect) and wave (two slit diffraction)

Louis deBroglie postulated that any particle of mass m travelling with velocity v (i.e. momentum $p = m.v$) would have a wavelength given by:

$$\lambda = \frac{h}{p} \quad \text{deBroglie wavelength}$$

deBroglie was shown to be correct by the Davisson Germer experiment which showed that a beam of electrons were diffracted (wave behavior) through a nickel crystal.

Schrodinger's equation

In 1926, Erwin Schrodinger describes how particles behave on a microscopic scale (Quantum Mechanics)

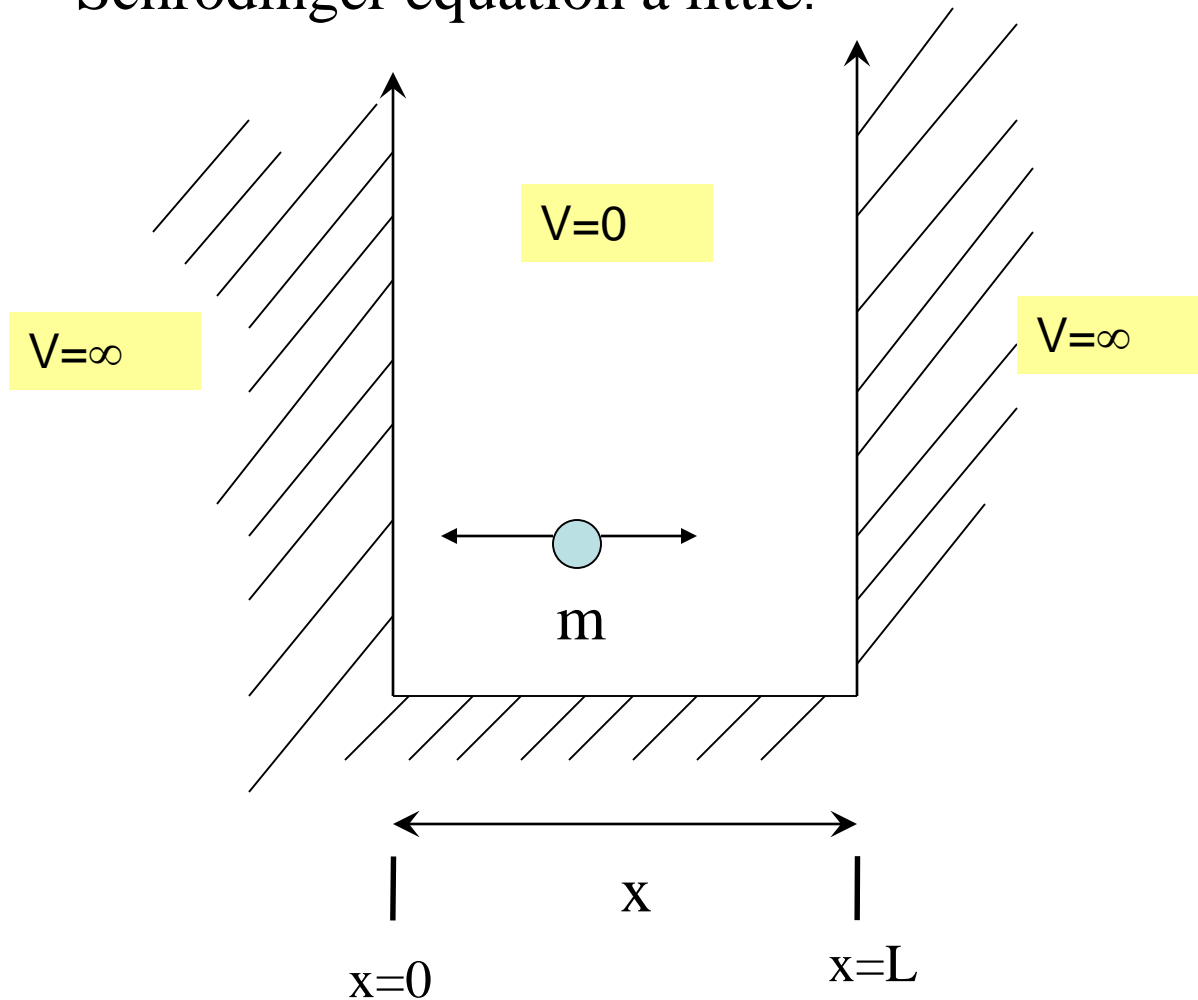
$$\hat{H}\Psi = E\Psi$$

The diagram shows the Schrodinger equation $\hat{H}\Psi = E\Psi$ with four labels and arrows pointing to the terms: 'Hamiltonian operator' points to \hat{H} , 'wavefunction' (bottom) points to Ψ on the left, 'energy' points to E , and 'wavefunction' (right) points to Ψ on the right.

One particular case (result) in Quantum Mechanics is the behavior of the electron in the hydrogen atom.

Particle (electron) in a box (one dimensional)

This is NOT the problem of the Hydrogen atom or the nucleus but will allow us to UNDERSTAND Quantum Mechanics and the Schrodinger equation a little.



1. Electron is forced to be inside box. It cannot be outside (Thick repulsive walls).
2. The particle experiences no force acting on it inside the box (until it reaches a wall).
3. Can the electron simply move around the box (Follow a trajectory)?
NO! Why not?

$$\hat{H}\Psi = E\Psi$$

$$(\hat{T} + \hat{V})\Psi = E\Psi$$

T and V are the kinetic energy operator and the potential energy operator respectively.

However, inside the box $V(x) = 0$

$$\hat{T} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

$$-\frac{\hbar^2}{2m} \frac{d^2\Psi}{dx^2} = E\Psi$$

Rearranging,

$$\frac{d^2\Psi}{dx^2} = \frac{-2mE}{\hbar^2} \Psi$$

Note that $m, E,$ and \hbar are all constants.

This is called a second order ordinary differential equation. We guess the solution,

$$\Psi(x) = A \sin(kx)$$

$$\frac{d}{dx} A \sin(kx) = Ak \cos(kx)$$

$$\frac{d^2\Psi}{dx^2} = \frac{d}{dx} \left(\frac{d}{dx} A \sin(kx) \right)$$

$$\frac{d^2\Psi}{dx^2} = \frac{d}{dx} (Ak \cos(kx)) = -Ak^2 \sin(kx) = -k^2 (A \sin(kx)) = -k^2\Psi$$

Notice that what we wanted was:

$$\frac{d^2\Psi}{dx^2} = \frac{-2mE}{\hbar^2} \Psi$$

By inspection, our trial solution works so $\Psi(x) = A \sin(kx)$ and

$$-k^2 = \frac{-2mE}{\hbar^2}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

But what are the constants A and k ?

The role of boundary conditions

At the walls of the box, the wavefunction must be zero. Why?

So,

$$\Psi(x = 0) = A \sin(0) = 0$$

$$\Psi(x = L) = A \sin(kL) = 0$$

$$\sin(kL) = 0$$

$$k = \frac{n\pi}{L} \quad \text{where} \quad n = 1, 2, 3, \dots$$

$$\Psi(x) = A \sin\left(\frac{n\pi}{L} x\right)$$

What is the value of A?

Consider the fact that the particle **MUST** be in the box. That is to say, the probability of finding the particle in the box is 100%.

Total probability of finding the Particle in the box

$$= \int_0^L \Psi^2(x) dx = 1$$

$$\Psi(x) = A \sin\left(\frac{n\pi}{L} x\right)$$

$$\int_0^L A^2 \sin^2\left(\frac{n\pi}{L} x\right) dx = 1$$

$$A^2 \int_0^L \sin^2\left(\frac{n\pi}{L} x\right) dx = 1$$

$$\int_0^L \sin^2\left(\frac{n\pi}{L} x\right) dx = \frac{1}{A^2}$$

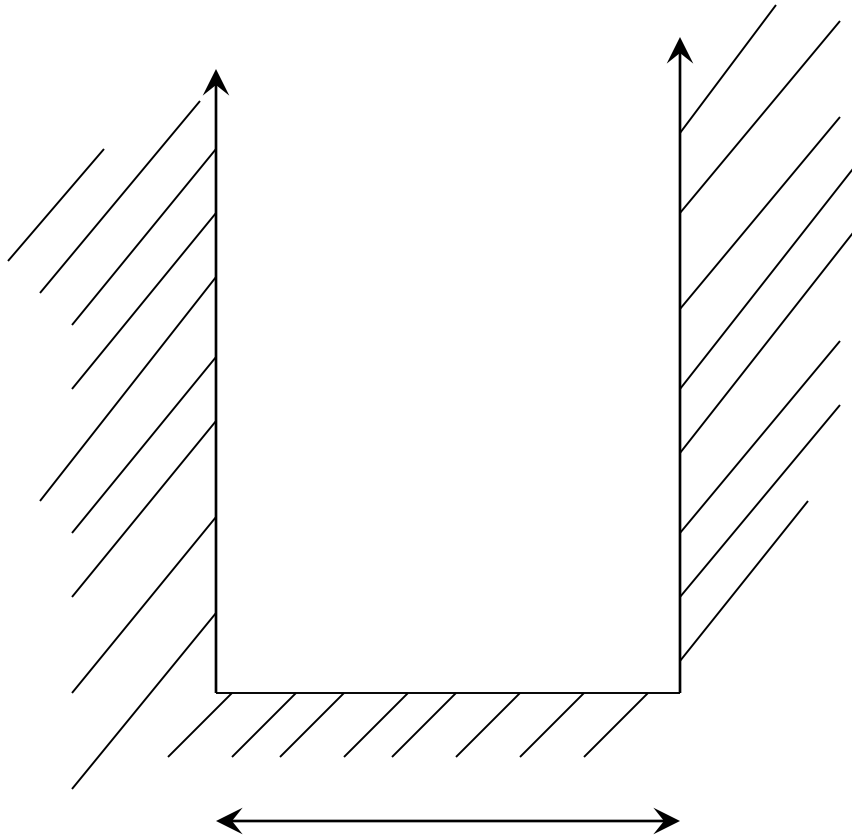
Value of integral = L/2

$$\frac{L}{2} = \frac{1}{A^2} \quad \text{So,} \quad A = \sqrt{\frac{2}{L}}$$

$$\left\{ \begin{array}{l} \Psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right) \\ E = \frac{n^2 h^2}{8mL^2} \quad n=1,2,3,\dots \end{array} \right.$$

Schrodinger solution for Particle in a 1D box

What wave can exist inside the box?

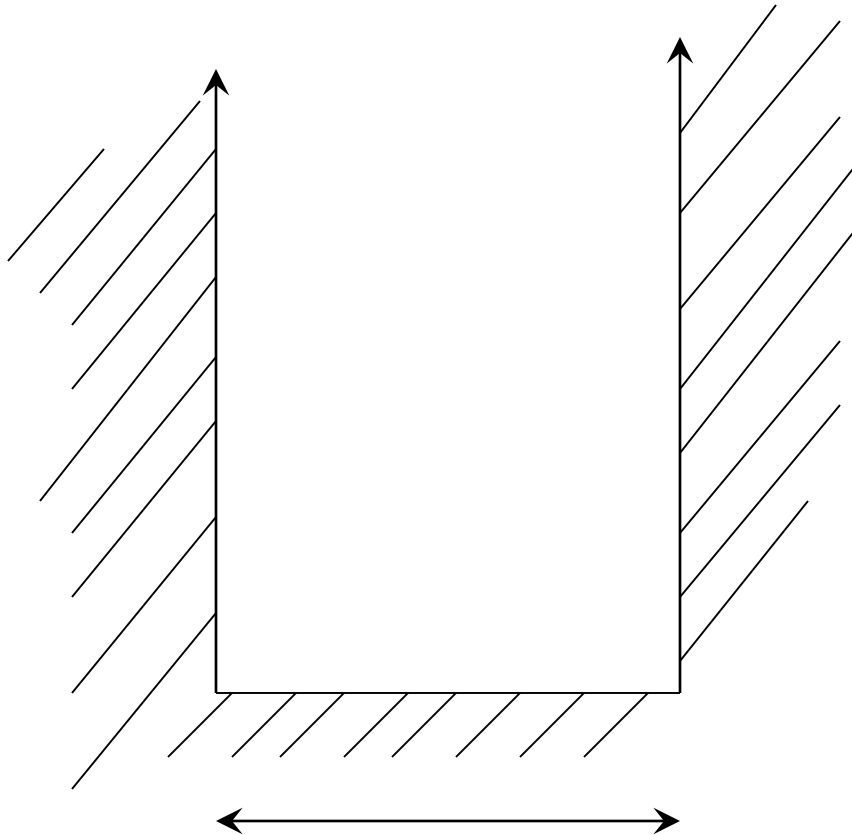


- a) What is the shape (functional form) of $\Psi(x)$?
- b) What is the value of Ψ at the walls?
- c) What is the value of Ψ at the middle of the box.

Is this the only possible solution ?

Schrodinger solution for Particle in a 1D box

Other solutions for the particle in the box



How does the energy of the second solution compare with the energy of the first solution?

The lowest energy state is called the *ground state*

The first state higher in energy than the ground state is called the *first excited state*.

IDEA: The general solution is an integer number of half sine waves.

Schrodinger solution for Particle in a 1D box

Probability for finding the electron at a given location is $|\Psi(x)|^2$

$\Psi(x)$ is the amplitude of the wavefunction at position x . The larger Ψ is the larger the probability of finding the particle at that location.

A node is a position (aside from the walls) where the wavefunction is equal to zero.

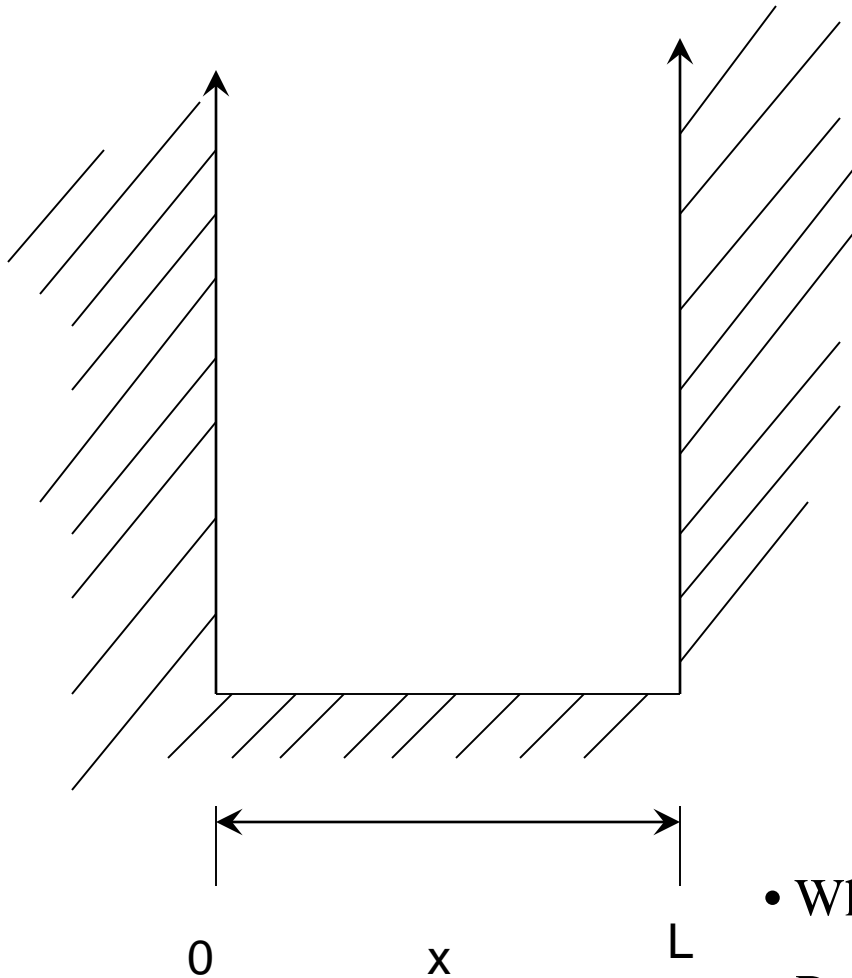
The larger the number of nodes, the higher the energy.

Questions to consider

Where is it most likely to find the electron when the electron is in the lowest energy state ?

What is the probability for finding the electron in the middle of the box when the electron is in the first excited state?

Particle in a box



This is the lowest energy state
(ground state)

$$\psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = \frac{n^2 h^2}{8mL^2}$$

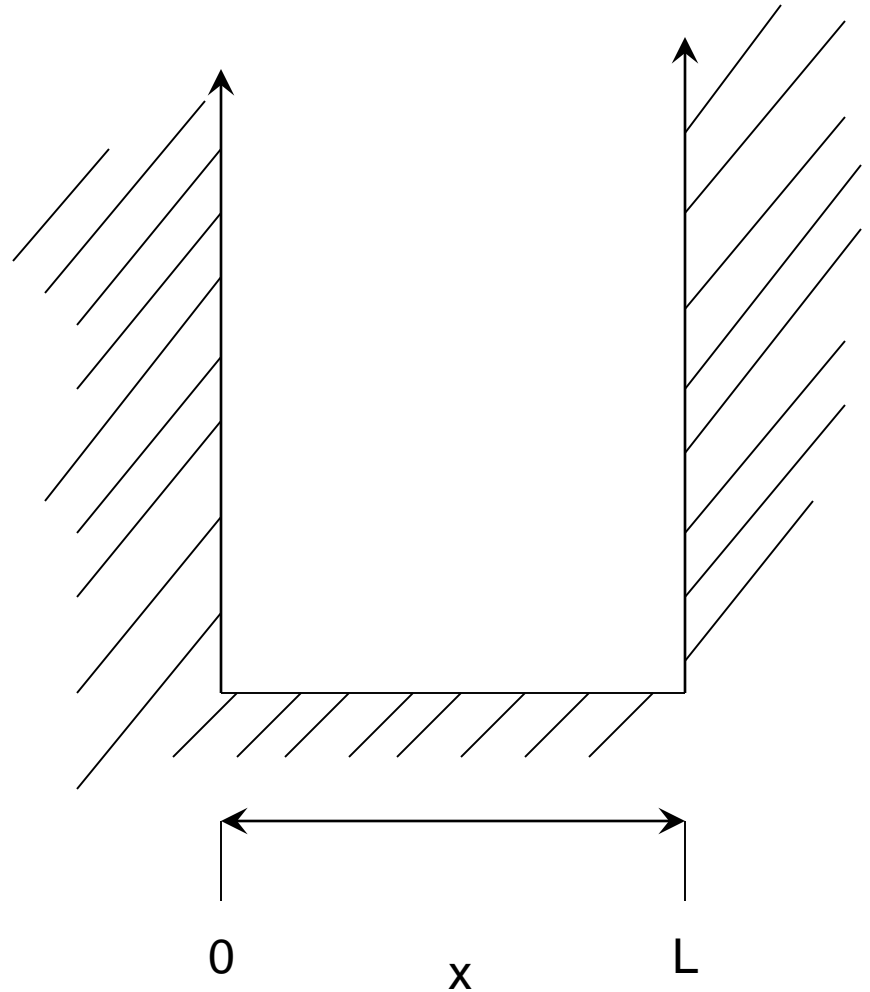
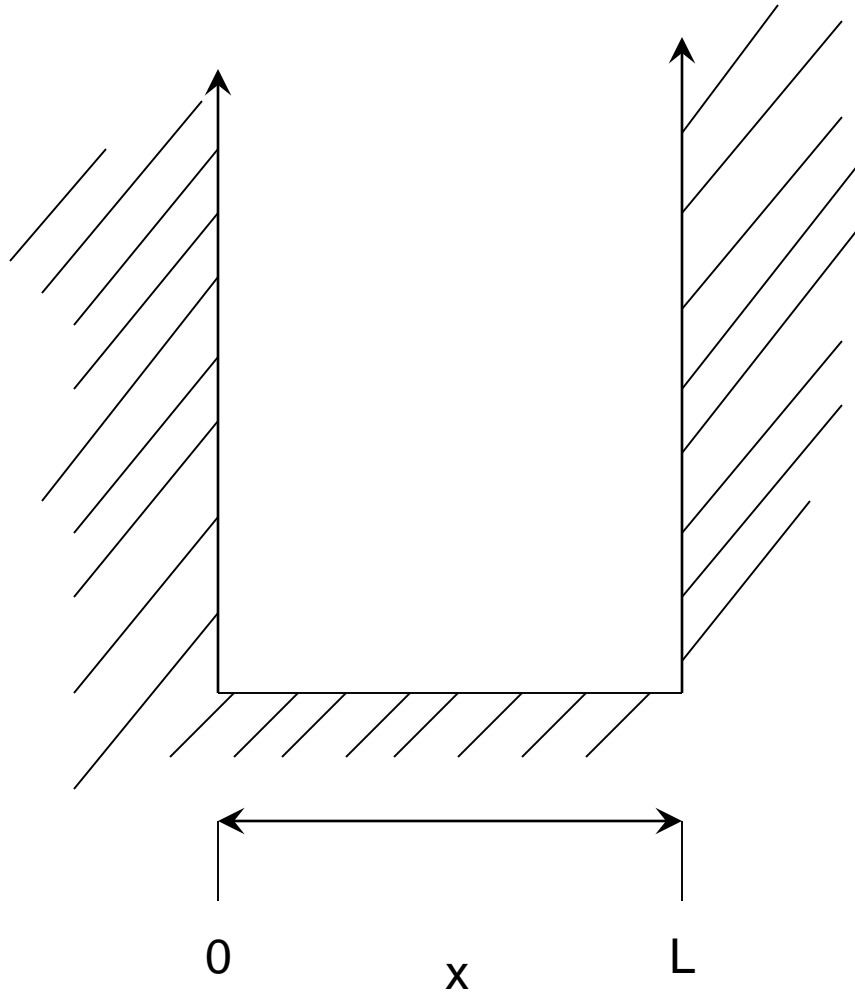
- Where is $\psi(x)$ maximum?
- Probability of finding the electron $\propto |\psi(x)|^2$

Is the electron at the middle of the box?

One quantum number, n , is necessary to specify the state of the electron

Particle in the first excited state

- What is the probability of finding the electron at $x=L/2$ (middle of the box)?
- Probability of finding the electron $\propto |\psi(x)|^2$



Where is $\psi(x)$ maximum?

Things to remember...

In solving Schrodinger's equation $H\psi=E\psi$ you get two pieces of information:

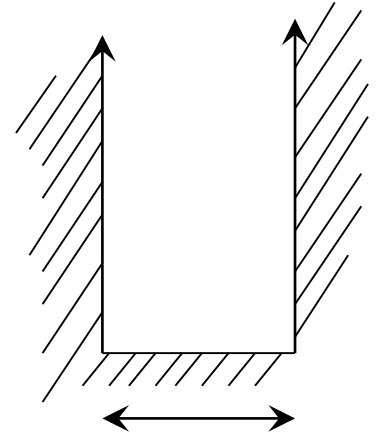
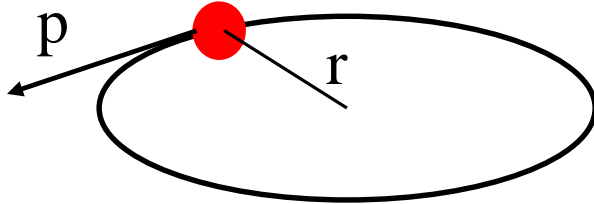
- ψ the wavefunction – this is KEY as from it you can calculate not only the probability but any other observable quantity (e.g. dipole moment, etc.)
- E_n -- the energy states (also called *eigenvalues*)

- levels get further & further apart as we go up in n .
- particle **must** have the minimum energy E_1 (called the zero point energy) otherwise $n = 0 \rightarrow$ particle is not in the box. All solutions to a Schrödinger eqn. where the wave funct. is "bounded" has:

- ◆ quantized energy levels
- ◆ a zero point energy

- number of nodes increases with n .
- note that the WF is continuous and differentiable
derivative of the WF is continuous and differentiable
everywhere within the box.

Particle on a ring



Particle on ring is simply the particle in a box wrapped on itself.

The hydrogen atom and Schrodinger's equation

$$\hat{H}\Psi = E\Psi$$

In the hydrogen atom the electron is attracted by the nucleus. The potential depends on the distance between the electron and the nucleus.

$$V(r) = \frac{(-Ze)(e)}{r}$$

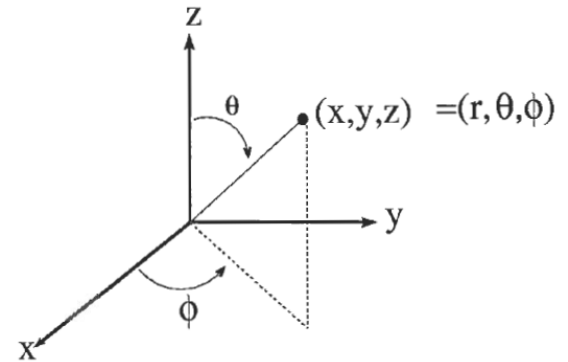
Where (Ze) is the charge of the nucleus and (e) is the charge on the electron. The distance between the nucleus and the electron is r .

You can see that this potential depends on only the distance between the nucleus and the electron and not the coordinates (x,y,z) . Such a "central potential" suggests we work with the SPHERICAL POLAR coordinate system (r,θ,ϕ) rather than the Cartesian (x,y,z) .

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$\theta = \cos^{-1}(z/r)$$

$$\phi = \tan^{-1}(y/x)$$



Moreover the solution to the Schrodinger equation is SEPARABLE that is:

$$\Psi(r, \theta, \phi) = R(r)\Theta(\theta)\Phi(\phi)$$

When we solve Schrodinger's equation we get :

- a) Eigenenergies
- b) Wavefunctions

Eigenenergies

$$E_n = -\frac{Z^2}{n^2} \left(\frac{me^4}{8\epsilon_0^2 h^2} \right) = -2.178 \times 10^{-18} \text{ J} \left(\frac{Z^2}{n^2} \right)$$

$n=1,2,3,4,\dots$ and
is called the
**PRINCIPAL
QUANTUM
NUMBER**

- Notice that for hydrogen ($Z=1$) or a hydrogen-like atom (only one electron) the eigenenergies depend only on the principal quantum number n .
- Since n is integer, the energy levels are quantized.
- This is the same equation as determined by Balmer et al and later Niels Bohr.

The hydrogen atom

The hydrogen atom and Schrodinger's equation

Four quantum numbers are needed to describe the state of the electron

1. n : principal quantum number ; $n = 1, 2, 3, 4, \dots$
2. l : azimuthal quantum number ; $l = 0, 1, 2, \dots, (n-1)$
3. m_l : magnetic quantum number ; $m_l = -l, (-l+1), (-l+2) \dots 0, 1, 2, \dots, l$

Orbital : The region in an atom within which an electron can be found

Orbital : a valid set of the quantum numbers (n, l, m_l)

Shell : A group of orbitals with the same principal quantum #, n

Total number of orbitals in a shell : n^2

Notice that m_l has $(2l + 1)$ possible values

Nodes and energy in the hydrogen atom

Hydrogen wavefunctions in more detail

$$\sigma = \frac{Zr}{a_0} \quad \text{Scaled distance } r$$

$$a_0 = \frac{\epsilon_0 h^2}{\pi m e^2} = 5.29 \times 10^{-11} \text{ m} \quad \text{Bohr orbit}$$

Lowest energy level:

$n=1, l=0$ (s), $m_l=0$; 1 s orbital

$$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$$

Now look at the 2s wavefunction

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$$

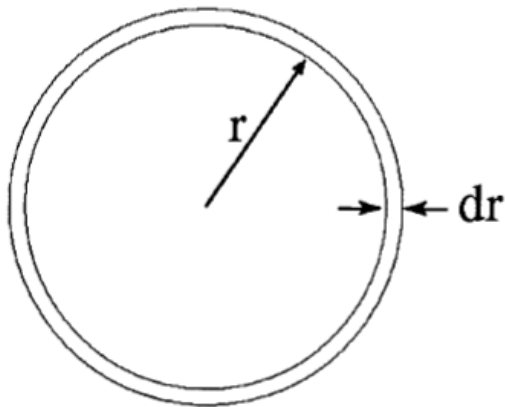
- When is the wavefunction (and therefore the probability) zero?
- How does the wavefunction fall off as compared to the 1s wavefunction?

The Physical Meaning of a wave function

From the uncertainty principle we know there is no way to describe the detailed “motion” of the electron in the atom. (In fact, is it even correct to think of the motion of an electron in the atom as this implies trajectories ?)

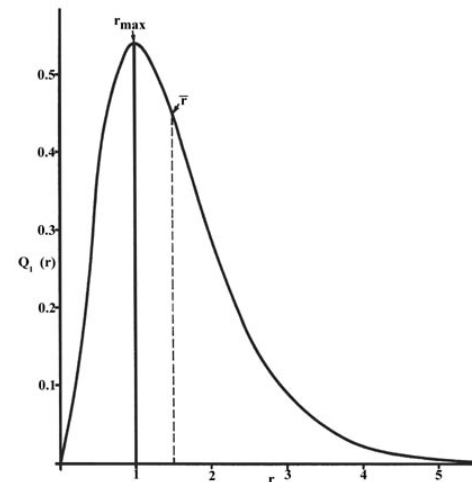
The square of the function evaluated at a particular point in space indicates the probability of finding the electron at that point.

What is the probability of finding the electron at some distance from the nucleus?



Surface of inner sphere = $4\pi r^2$
Thickness of shell = dr
Volume of shell = $4\pi r^2 dr$

Radial Probability distribution



Pauli exclusion principle

Statement #1 : No more than two electrons can be assigned to any orbital, and they must have opposite spins.

Statement #2 : No two electrons in the same atom can have the same set of four quantum numbers $n, l, m_l,$ and m_s .

Hund's Rule (the bus rule)

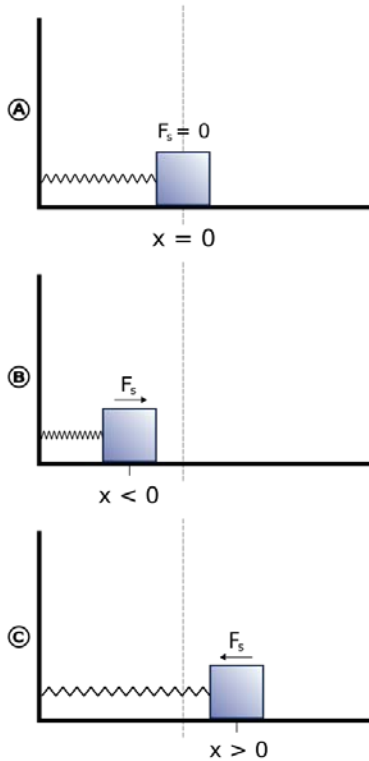
Electrons pair only after each orbital in a sub-shell is occupied by a single electron.

Why ?

Nobel gas notation: Write the electron configuration using the preceding noble gas to represent filled subshells.

Example: Mg : $1s^2 2s^2 2p^6 3s^2$ → [Ne] $3s^2$

The harmonic oscillator



The classical harmonic oscillator:

$$V(x) = \frac{1}{2}kx^2$$

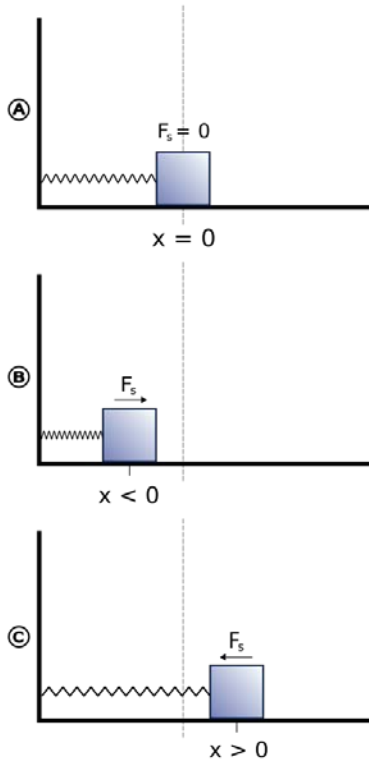
$$F = -\frac{dV}{dx} = -kx$$

What is form of the potential?

- k is the spring constant
- k is the curvature of the potential

- The mass can have zero kinetic energy (be at rest at the equilibrium position)
- The mass can have any energy (classical)

The harmonic oscillator



The **quantum** harmonic oscillator:

$$V(x) = \frac{1}{2}kx^2$$

$$F = -\frac{dV}{dx} = -kx$$

Solving Schrodinger's equation with this potential yields (as always) ψ and eigenenergies.

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, 2, 3, \dots \quad \omega = \sqrt{\frac{k}{m}}$$

- The potential is a parabola
- The mass cannot have zero kinetic energy – it must have at least the zero point energy
- The mass cannot have any energy – the energy levels are quantized

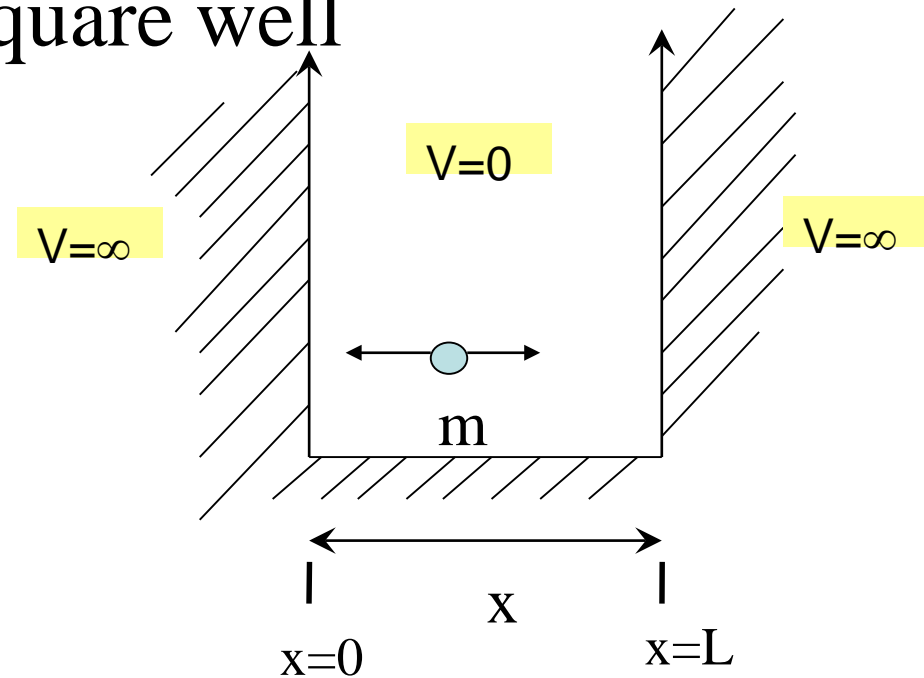
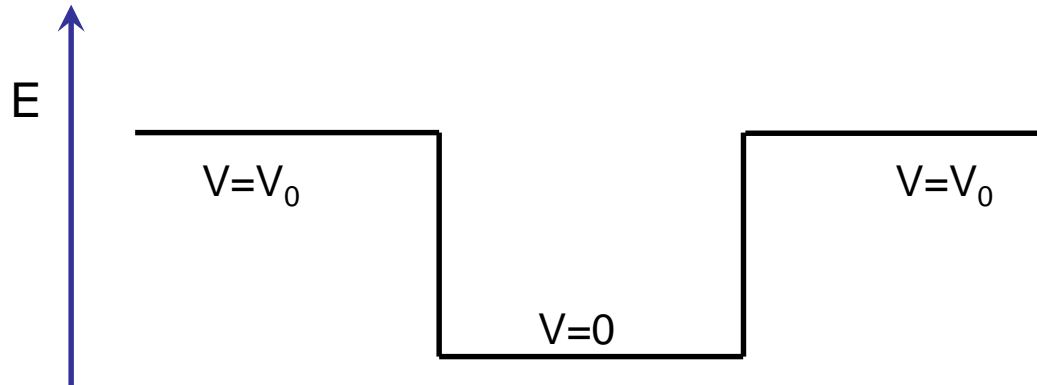
The finite square well

What is the consequence of a square well not being infinite?

Recall,

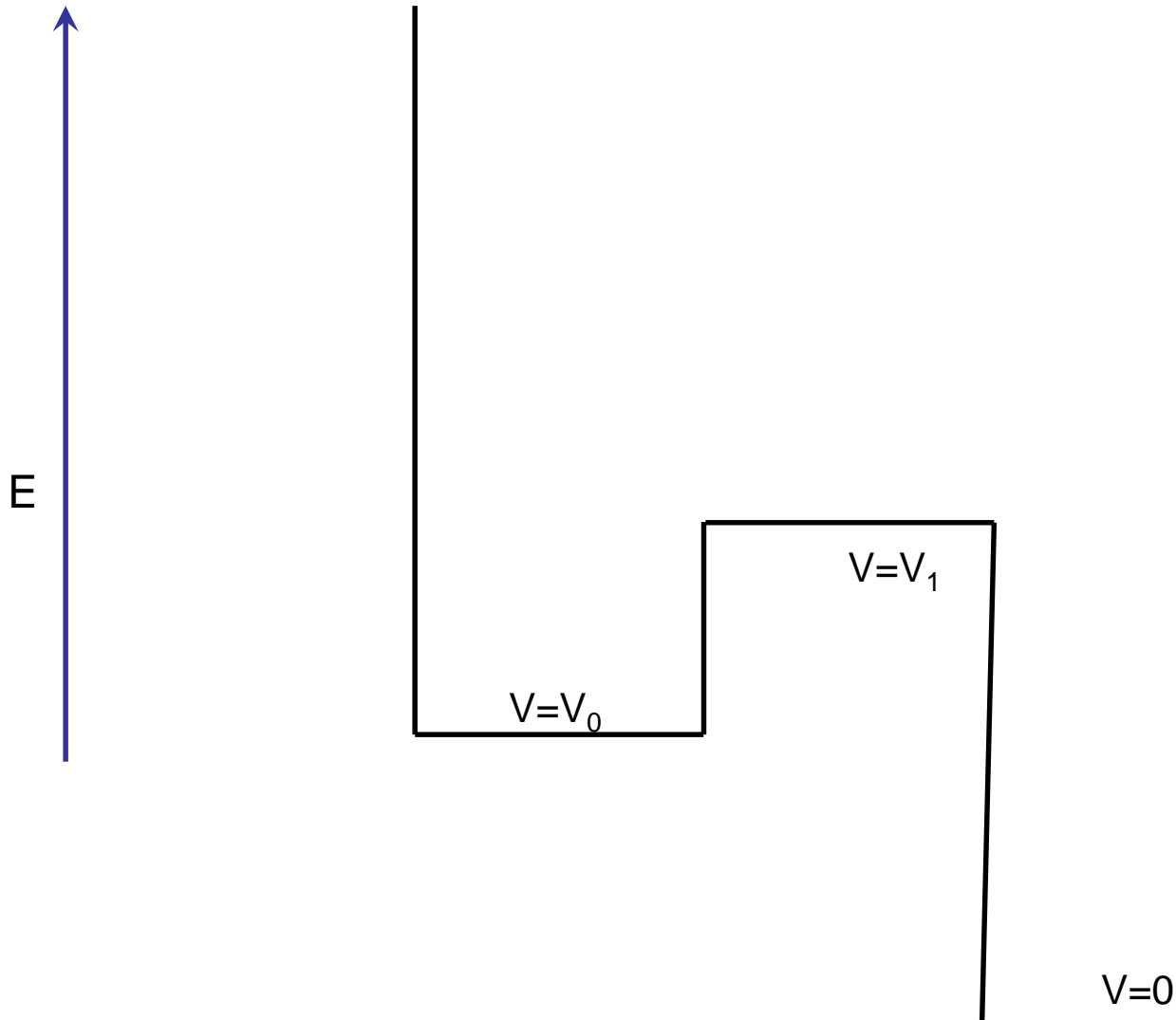
$$\lambda = \frac{h}{p}$$

$$E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$



- Consider a particle with energy, $E > V_0$ approaching from the left. What is its KE?
- What happens to the particle when it is over the finite well?
- Imagine a particle of zero kinetic energy incident from the left. What can we say?
- Imagine a particle with an energy $E < V_0$ that is in the well. What can we say?

Quantum tunneling and alpha decay



Bottom line

- A potential is a “box”
- Boxes hold things, in this case particles
- When microscopic particles are bounded they behave as waves
- The boundaries (“walls”) of the box define the discrete energy levels (“quantization”)
- Solution of Schrodinger’s equation gives not only the energy states (“eigenenergies”) but the wavefunction
- The wavefunction is useful not only for calculating the probability of where the particle exists but ANY observable quantity.

With this background in mind, let’s turn to the nuclear case.