LOCATION OF AN ELECTRON

- Unfortunately, the **Heisenberg uncertainty principle** states that it is impossible to simultaneously measure the momentum and the exact position of an electron.

$$(\Delta x)(\Delta p) \geq h / 4\pi$$

Momentum uncertainty (kg*m/s)

Planck's constant

Position uncertainty (m)

- Instead, we can approximate – we can calculate a probability of finding an electron somewhere

PROBABILITY DENSITY FUNCTIONS

- Since we can't determine precise location of an electron, we have a **wave function Ψ** tells us the **probability** of finding an electron within a volume we specify
- The wave function is a PDF (probability density function). When integrated over a volume V_a, it tells us the probability of finding the electron in that volume.

$$P(e^{-}\ inside\ V_a) = \iiint_{Va} |\psi|^2\, dxdydz$$

- As with any PDF, if we integrate over an infinite space, the probability of finding an electron is 100%

$$\iiint_{\infty} |\psi|^2\, dxdydz = 1$$

WHAT IS A PDF?

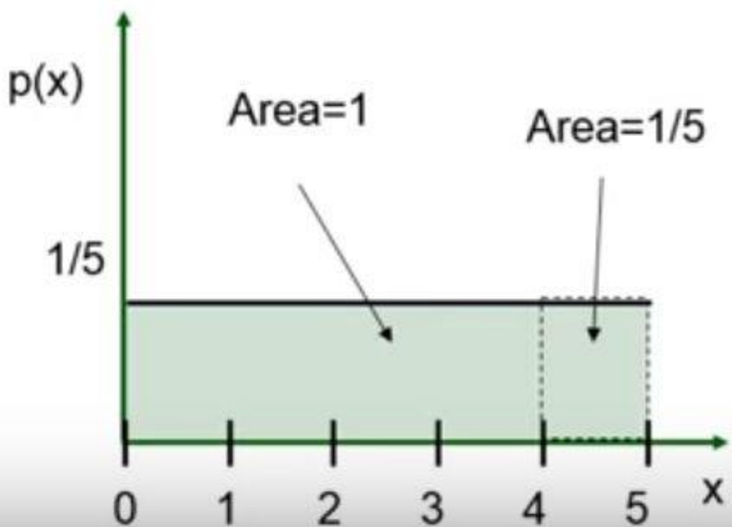
- Let's say we roll a die. What is the probability of rolling a 4?
  - Answer: 1/6 **Discrete System**
- Let's say I can pick any **integer** between 1 and 10. What's the probability of choosing a 6?
  - Answer: 1/10 **Discrete System**
- Now, let's say I pick any **rational number** between 1 and 10. What's the probability of choosing a 6?
  - Answer: Zero! **Continuous System**
- Now, let's say I pick any rational number between 1 and 10. What's the probability of choosing a number *between* 6 and 7?

Real world is analog !

PDF EXAMPLES

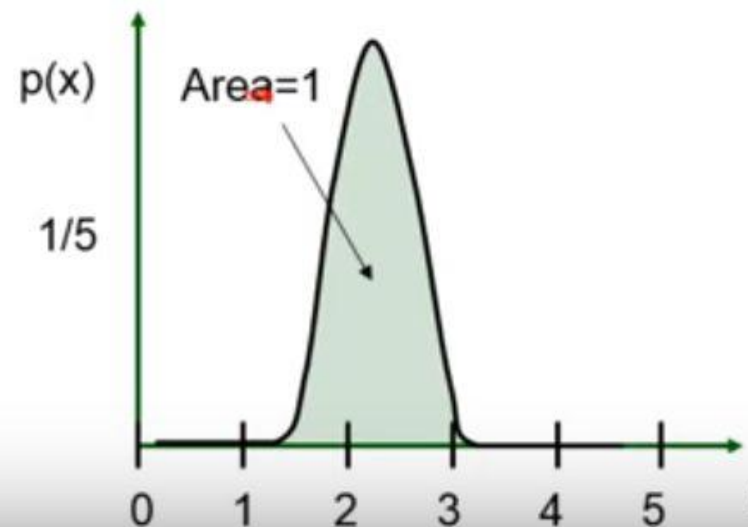
Uniform PDF

- What is the probability that the electron is between x=4 and x=5?
- Answer:



Nonuniform PDF

- What is the probability of that the electron is between x=4 and x=5?
- Answer:



SCHRODINGER EQUATION

- The Schrödinger Equation, which originates from classical mechanics, is a quantum mechanical law describing the energy of an electron. Given a potential field V, it allows us to determine the wave function Ψ.

Energy of an electron (classical mechanics)	Kinetic Energy + Potential Energy = Total Energy $\frac{p^2}{2m} \quad + \quad V \quad = E$

↓ Apply quantum mechanical operators

Quantum Form:	$$\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = -\frac{\hbar}{j}\frac{d\psi}{dt}$$ $$\nabla^2\psi = \frac{d^2\psi}{dx^2} + \frac{d^2\psi}{dy^2} + \frac{d^2\psi}{dz^2}$$ $$(\hbar = h/2\pi)$$

HOW IS THE SCHRODINGER EQUATION USED?

- *Given some potential field, the solution of the Schrödinger equation is a wave function Ψ which describes the location of an electron*

Boundary conditions
V(x,y,z)

V is the electrostatic potential field

→ Schrödinger Equation →

Wave Function
Ψ(x,y,z)

Describes the location of an electron

The atomic structure of the material determines the potential field ↑

↓ The electron configuration determines the electronic properties of a material

EXAMPLE SCHRODINGER EQUATION 1D POTENTIAL WELL

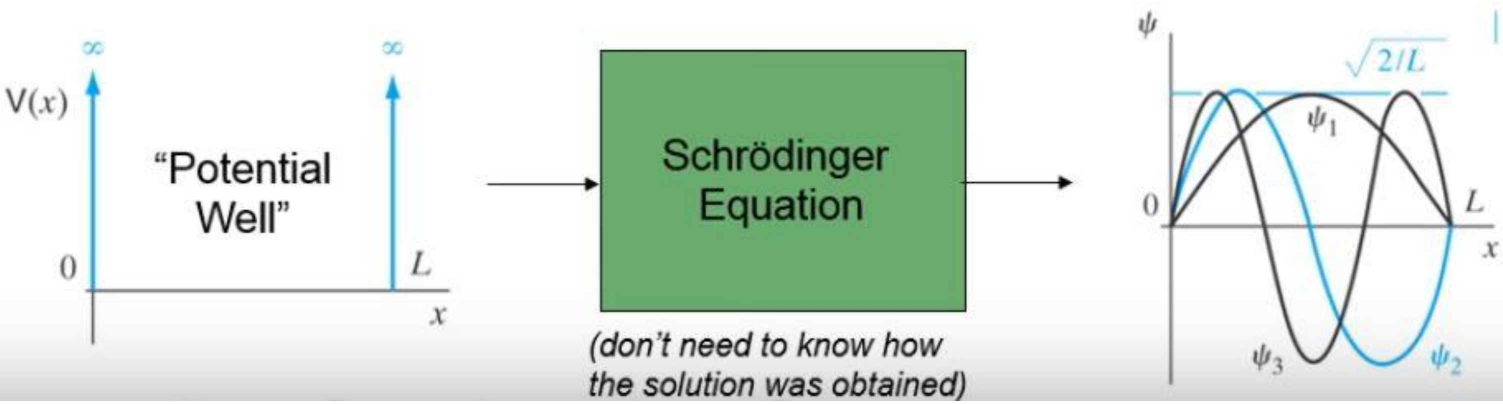
- This is a one dimensional example
- Note that there are multiple solutions!
- Each solution has a corresponding quantum number *n*

Boundary condition

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & x = 0, L \end{cases}$$

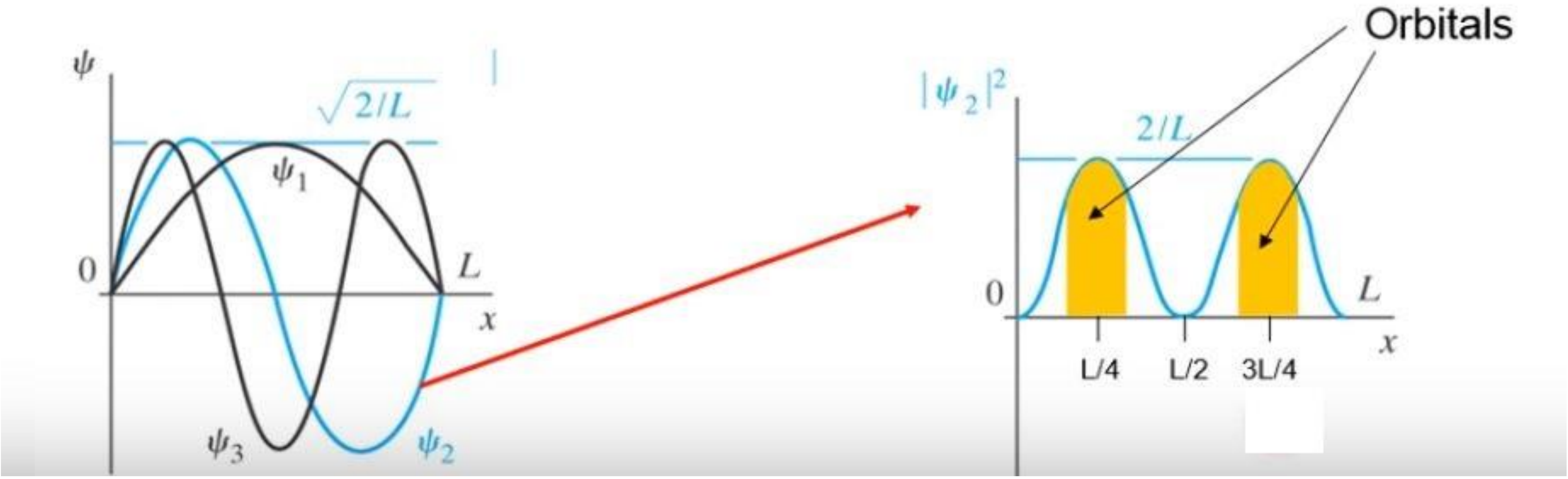
Wave Function

$$\psi = \frac{2}{L} \sin \frac{n\pi}{L} x, \quad n = 1,2,3,\ldots$$



WHAT DOES THE SOLUTION MEAN?

- **Physical meaning**: Each solution corresponds to an energy state which can be occupied by an electron. The higher frequency solutions correspond to a higher energy state.
- ***Multiple solutions means that there are multiple ways an electron can orbit the nucleus.*** Each energy state corresponds to a specific **orbital,** a region where the electron is likely to be found.
- For example, If we choose an energy state n=2 (Ψ_2) we can plot the PDF $|\Psi_2|^2$ which describes the likelihood of finding an electron at some point x. The plot on the right shows that the electron is most likely to be found near L/4 and 3L/4.



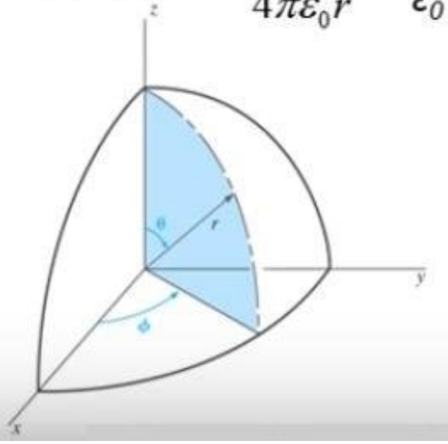
SOLUTION FOR SE FOR SINGLE ATOM

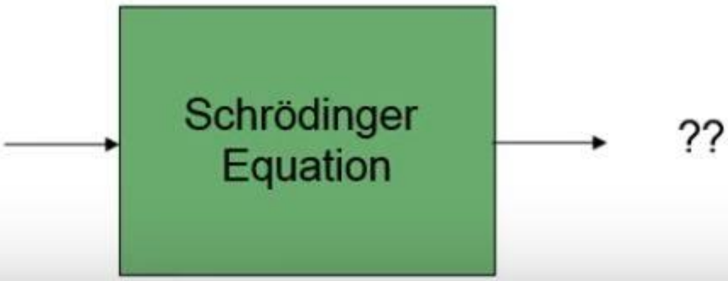
- To solve the SE for an atom, we need a potential field. In an atom, the potential field is created by the protons in the nucleus
- Like before, it is possible to find the corresponding electron wave functions by solving the SE.
- Note this is a 3 dimensional problem in spherical coordinates

Boundary condition (Coulomb's Law)

$$V(r,\theta,\phi) = -\frac{q^2}{4\pi\varepsilon_0 r}$$

q = Nucleus charge
ε_0 = permittivity of free space





SOLUTION TO SE FOR SINGLE ATOM CONT.,

- The solution is a set of *3 dimensional* wave functions describing the location of the electron
- As before, there are multiple solutions, each corresponding to an energy state an electron can occupy (see orbital configuration in the following slides)
- **Pauli Exclusion Principle**: Each electron can occupy only a single energy state. Electrons fill up the lowest energy states first.
- An energy state is defined by 4 quantum numbers
  - **n** = 1,2,3,… [Energy level]
  - **l** = 0,1,2,… (n-1)
  - **m** = -l,…,-2,-1,0,+1,+2,…,+l
  - **s** = +/- 1/2 [Electron spin].