What did we learn last day?

1. Learnt Electrons are 'Crazy', at times they are waves and when we 'see' those waves they become particles.

2. Learnt Light too is 'Crazy', at times they are waves and when we 'see' those waves they become particles.

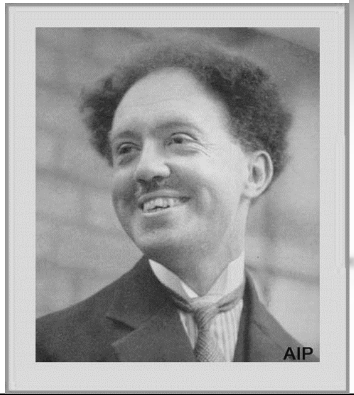
3. Electrons 'make' Atoms and they are 'wavy And particle-like'

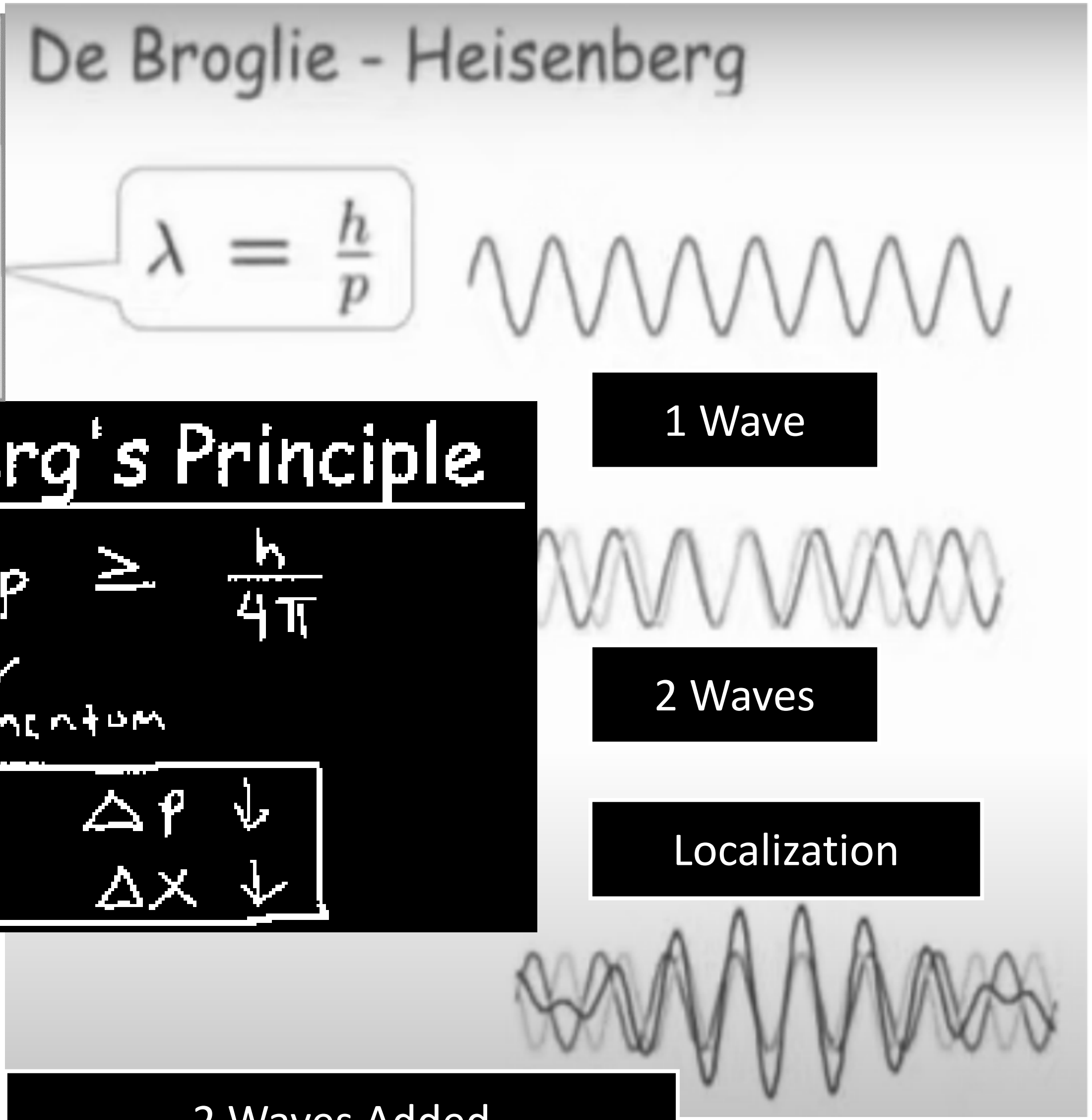
What will we learn today?

Where are the electrons?

What are Atomic Orbitals anyway?

Building on Uncertainty





Heisenberg's Principle

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

Δx ↓ position

Δp ↓ momentum

$$\boxed{\begin{array}{ll} \Delta x \uparrow & \Delta p \downarrow \\ \Delta p \uparrow & \Delta x \downarrow \end{array}}$$

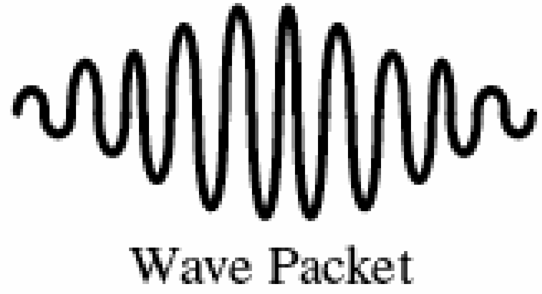
1 Wave

2 Waves

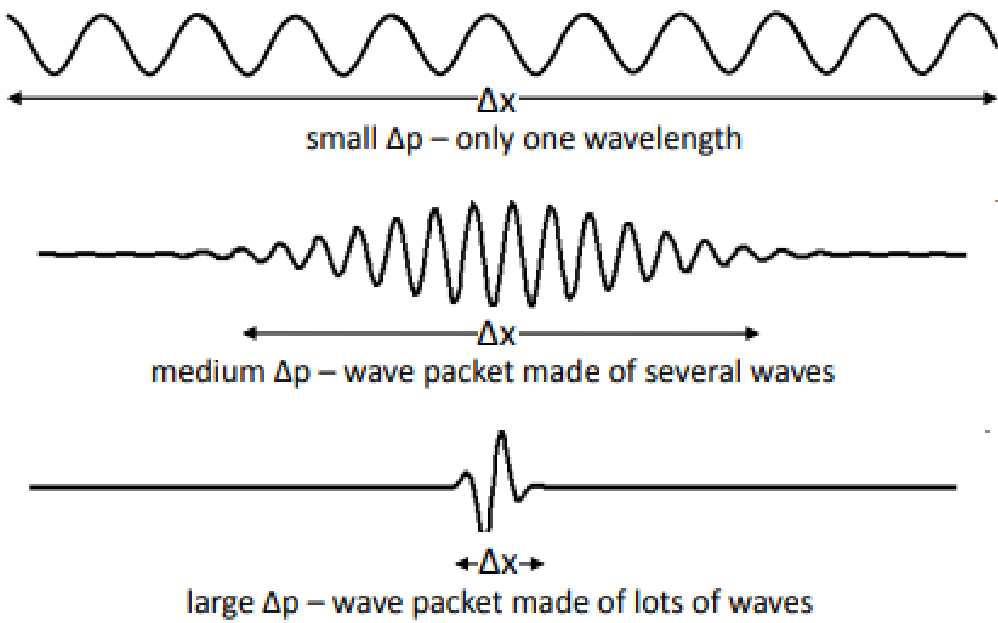
Localization

2 Waves Added

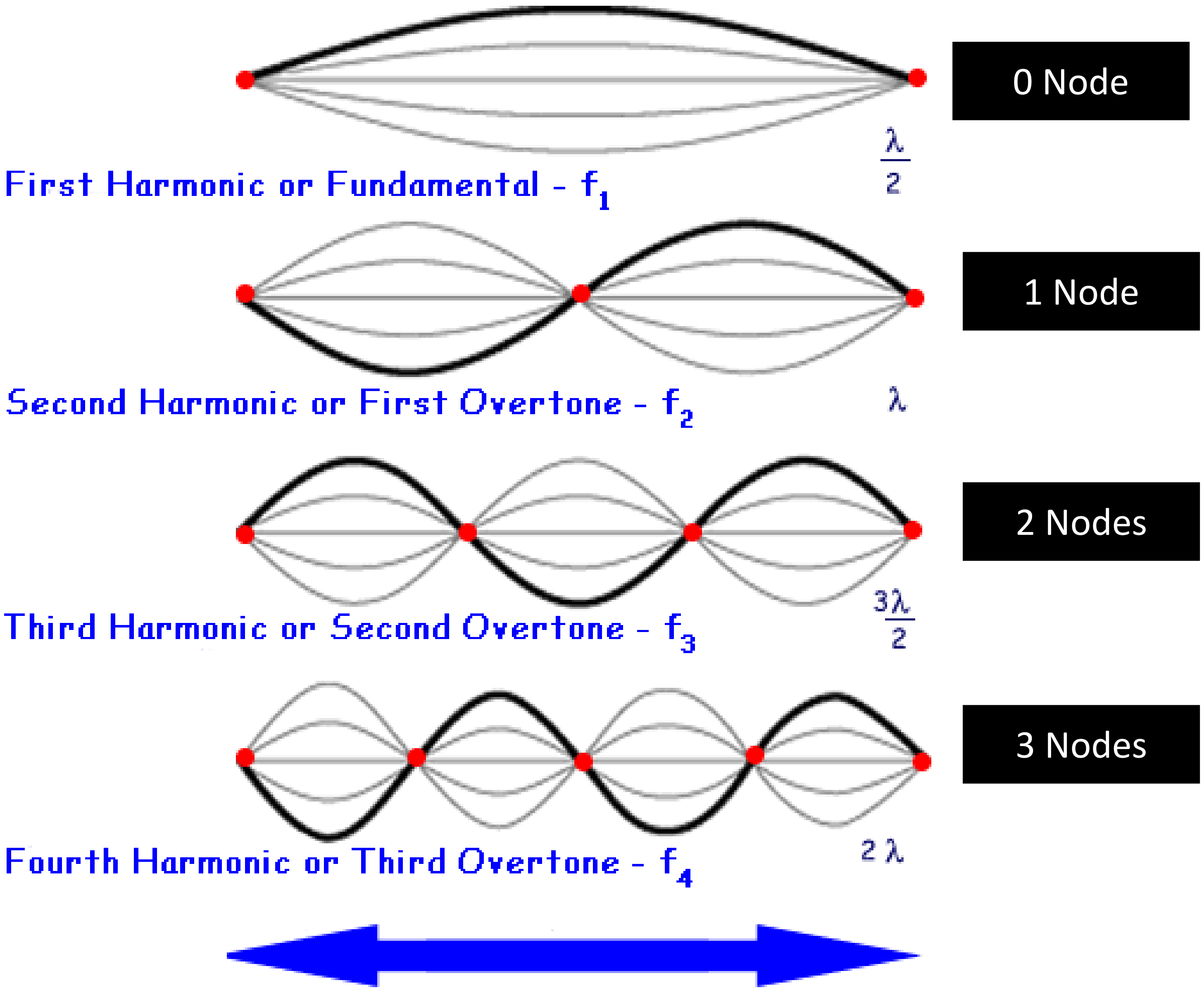
Many Waves Added



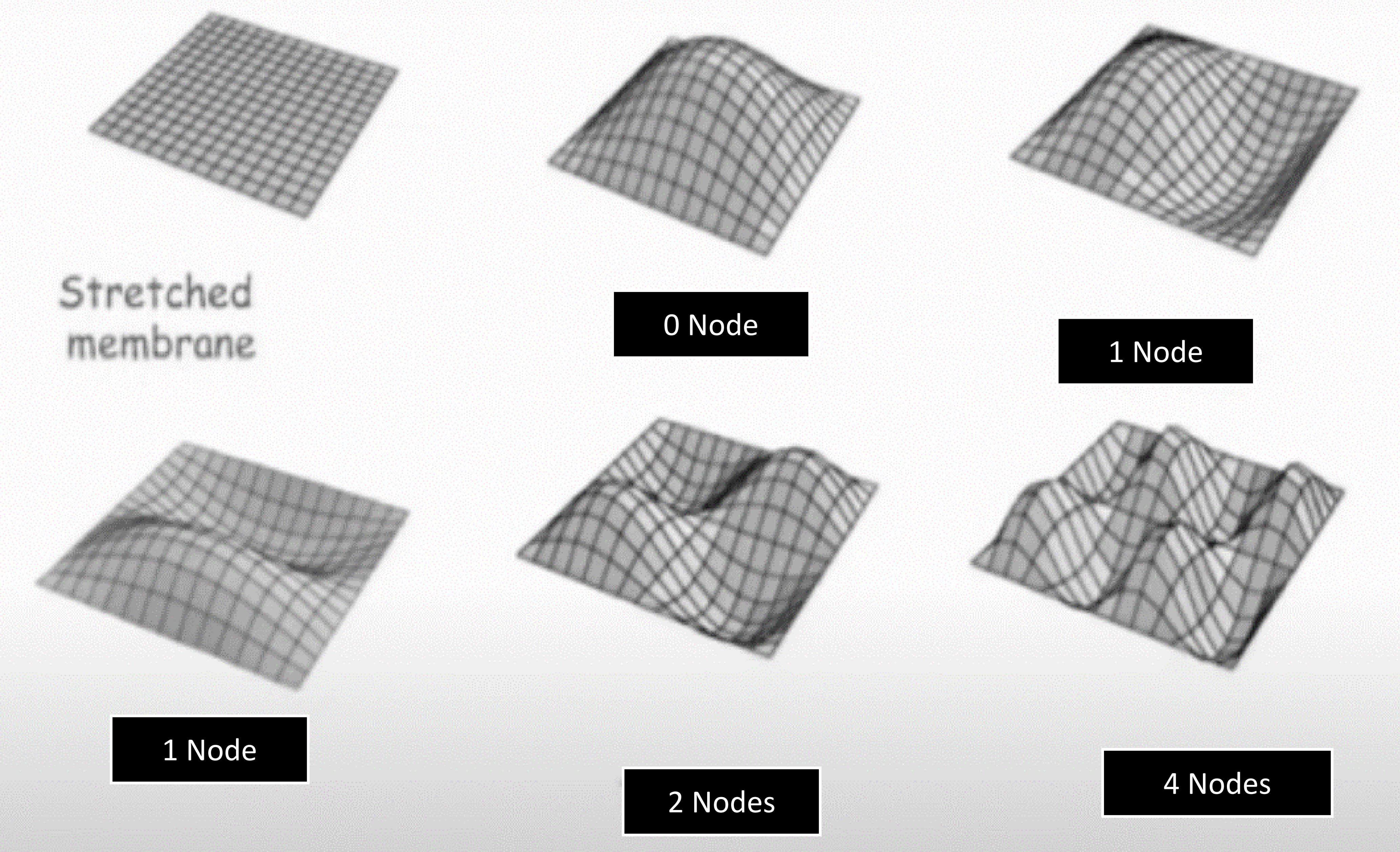
Uncertainty Principle



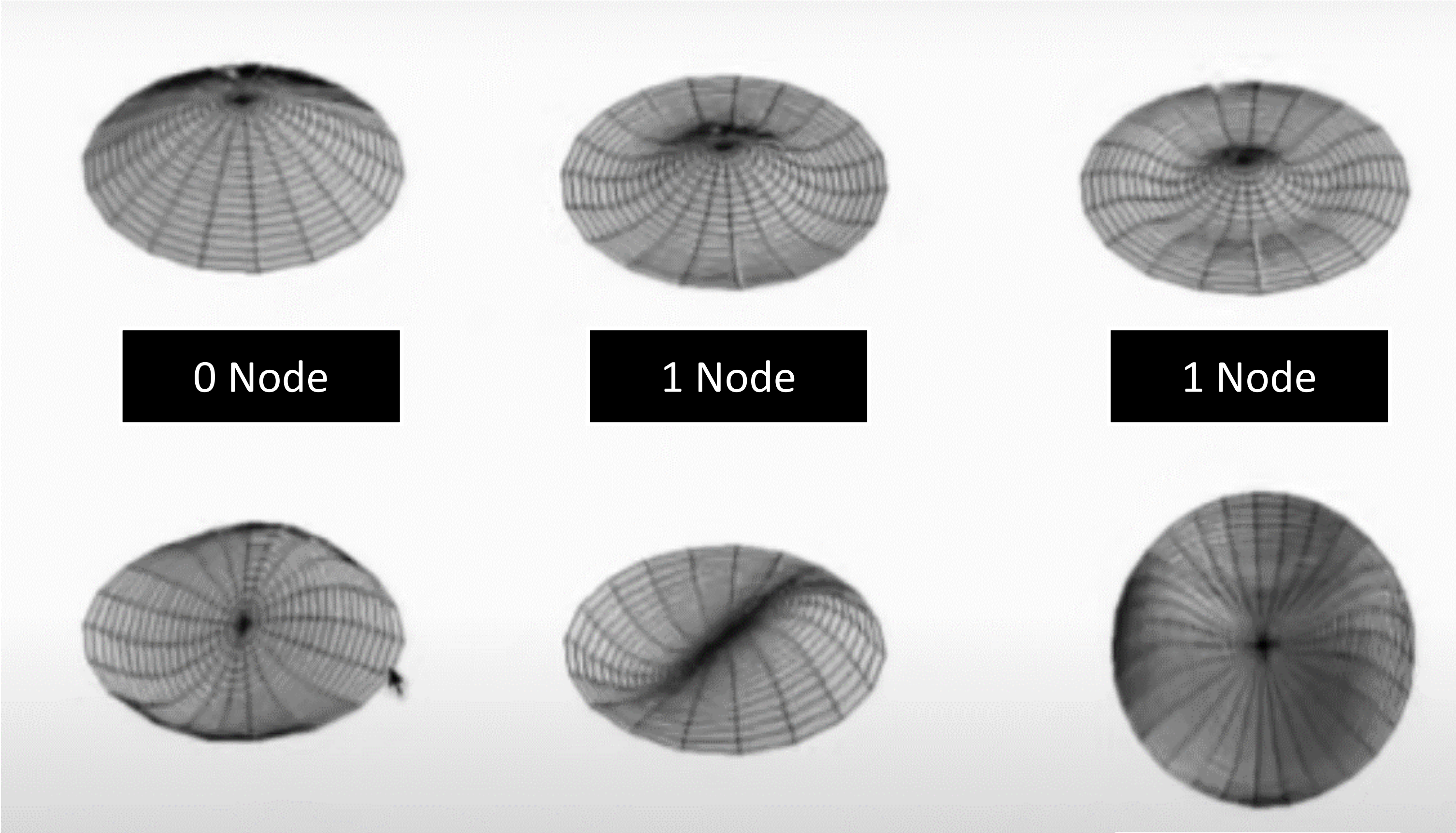
Origin of Nodes (0 D) on a Stretched String (1 D)



Origin of Nodes (1 D) on a Stretched Membrane (2 D)

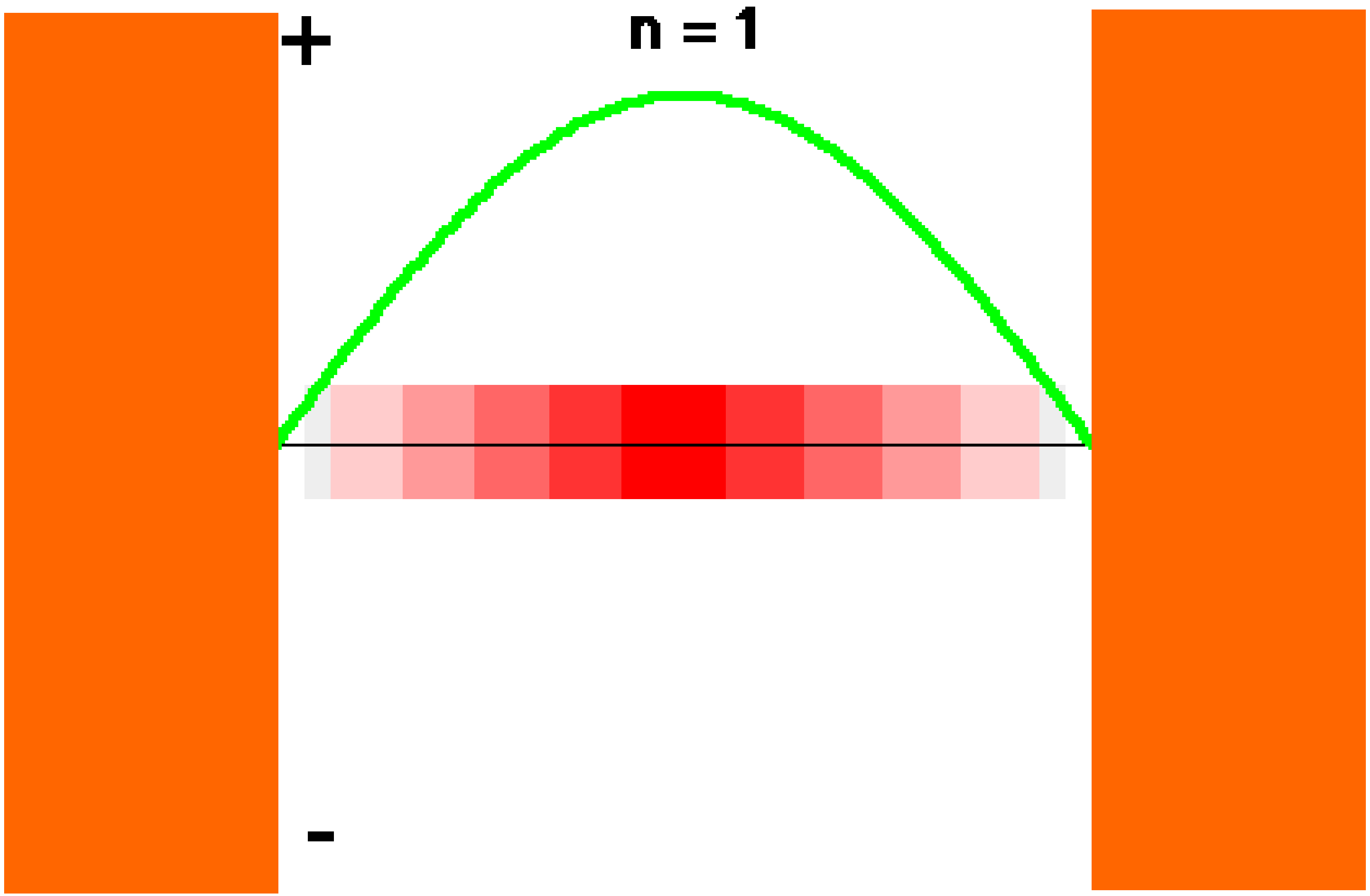


Origin of Nodes (1 D) on a Stretched Membrane (2 D)



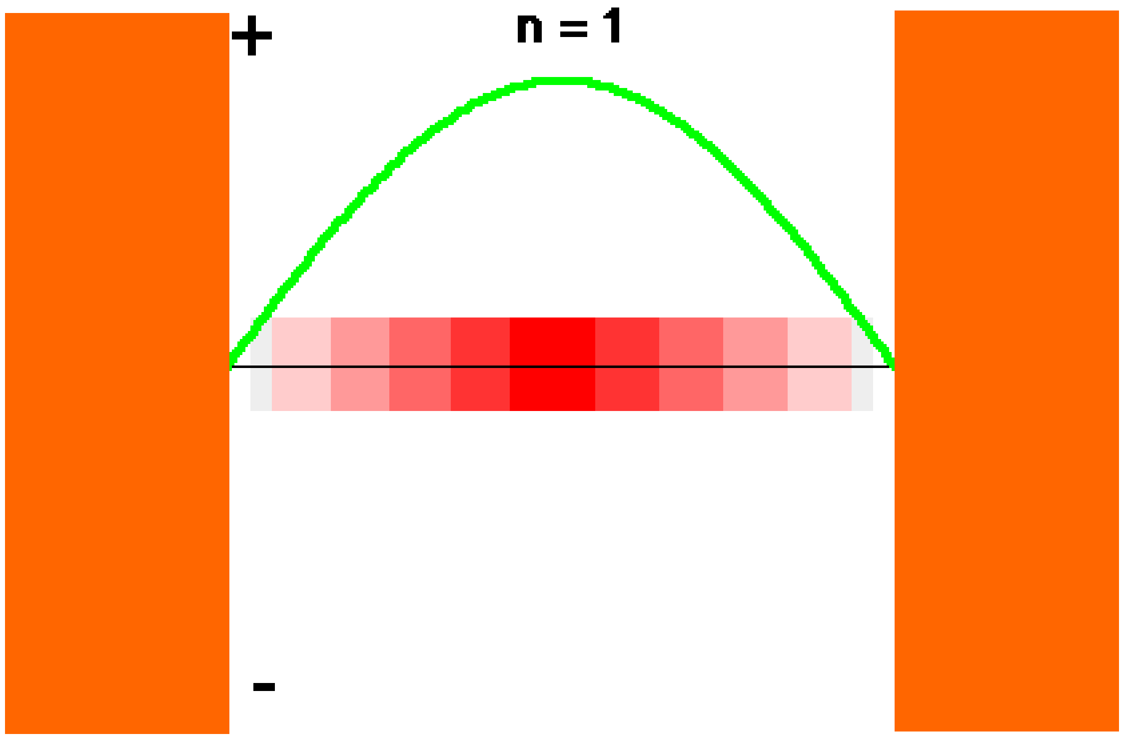
How many nodes possible? INFINITE!

Relevance of Standing Waves in Chemistry: Particle in a box



n = Number of nodes.

Relevance of Standing Waves in Chemistry: Standing Waves are Stationary States: Also known as Atomic Orbitals (AOs)



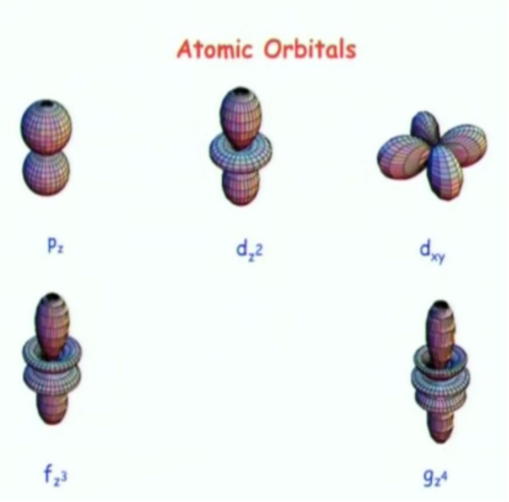
H atom is a proton and an electron

e is confined by the proton: Just like a particle in a box

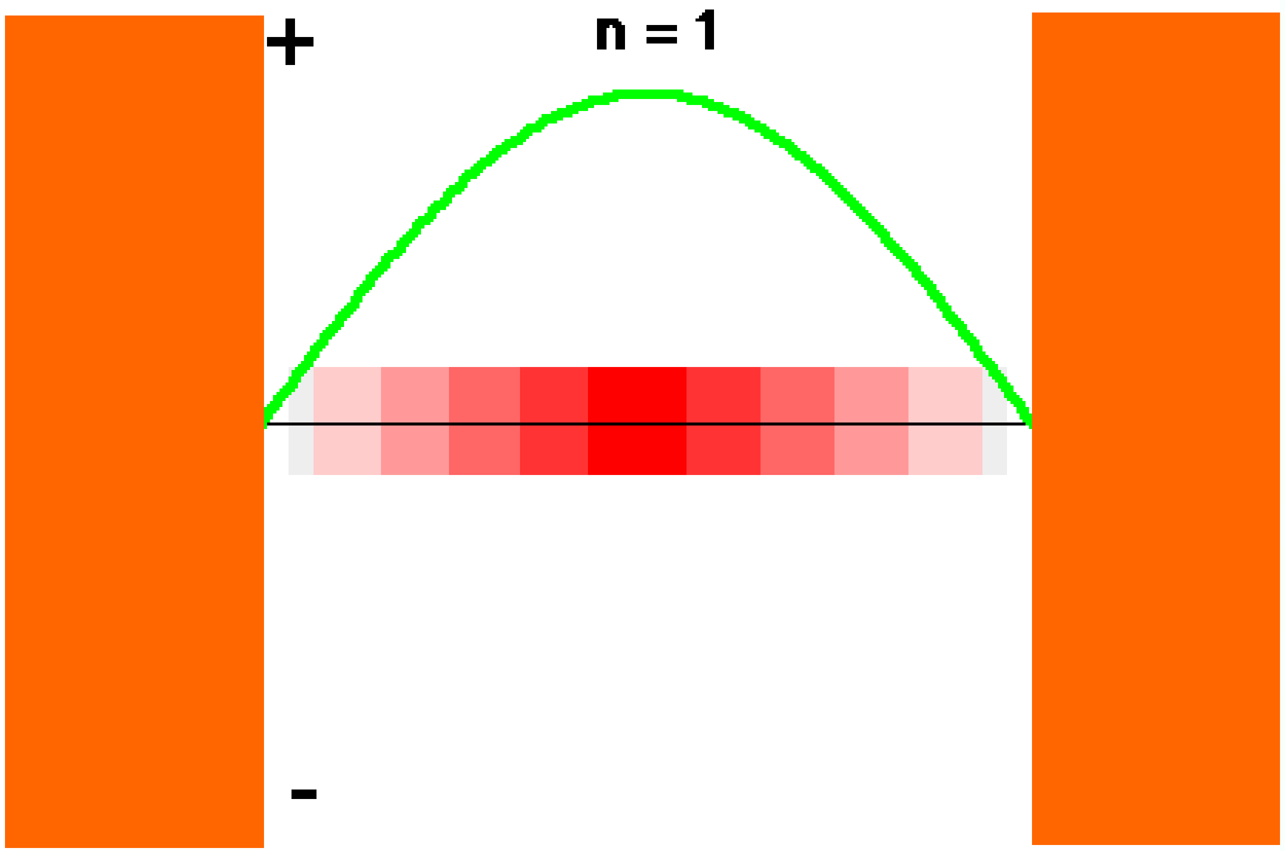
Such e confinement by the proton creates standing wave

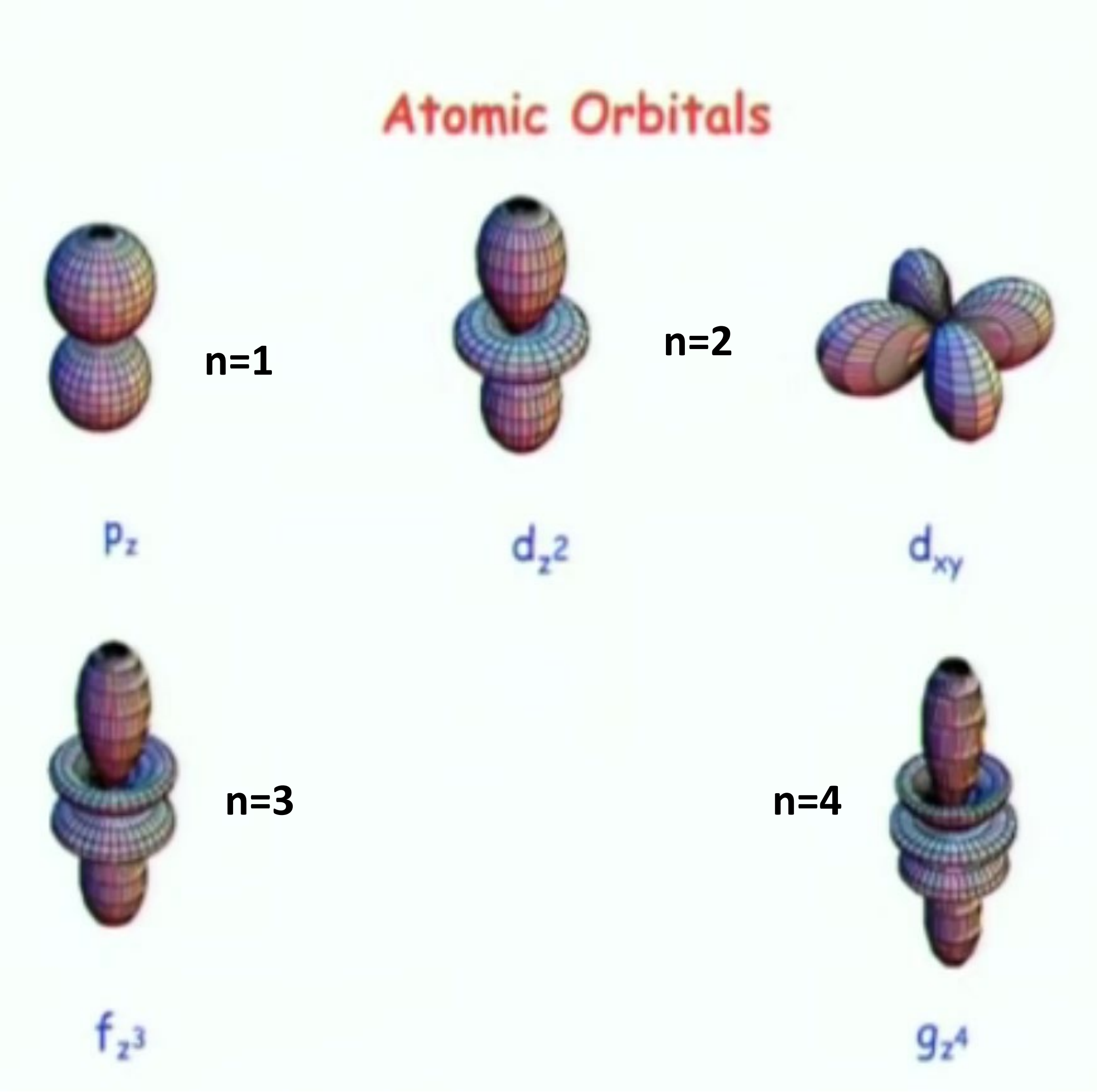
Such standing waves are stationary states

Those stationary states are Atomic Orbitals with varying nodes



Relevance of Standing Waves in Chemistry: Standing Waves are Stationary States: Also known as Atomic Orbitals (AOs)





H atom is a proton and an electron confined

Such e confinement by the proton creates standing wave

Such standing waves are stationary states or Atomic Orbitals with varying nodes (n)

Relevance of Standing Waves in Chemistry: Standing Waves are Stationary States: Also known as Atomic Orbitals (AOs)

Now we apply Schroedinger equation to particle in a box or H atom:

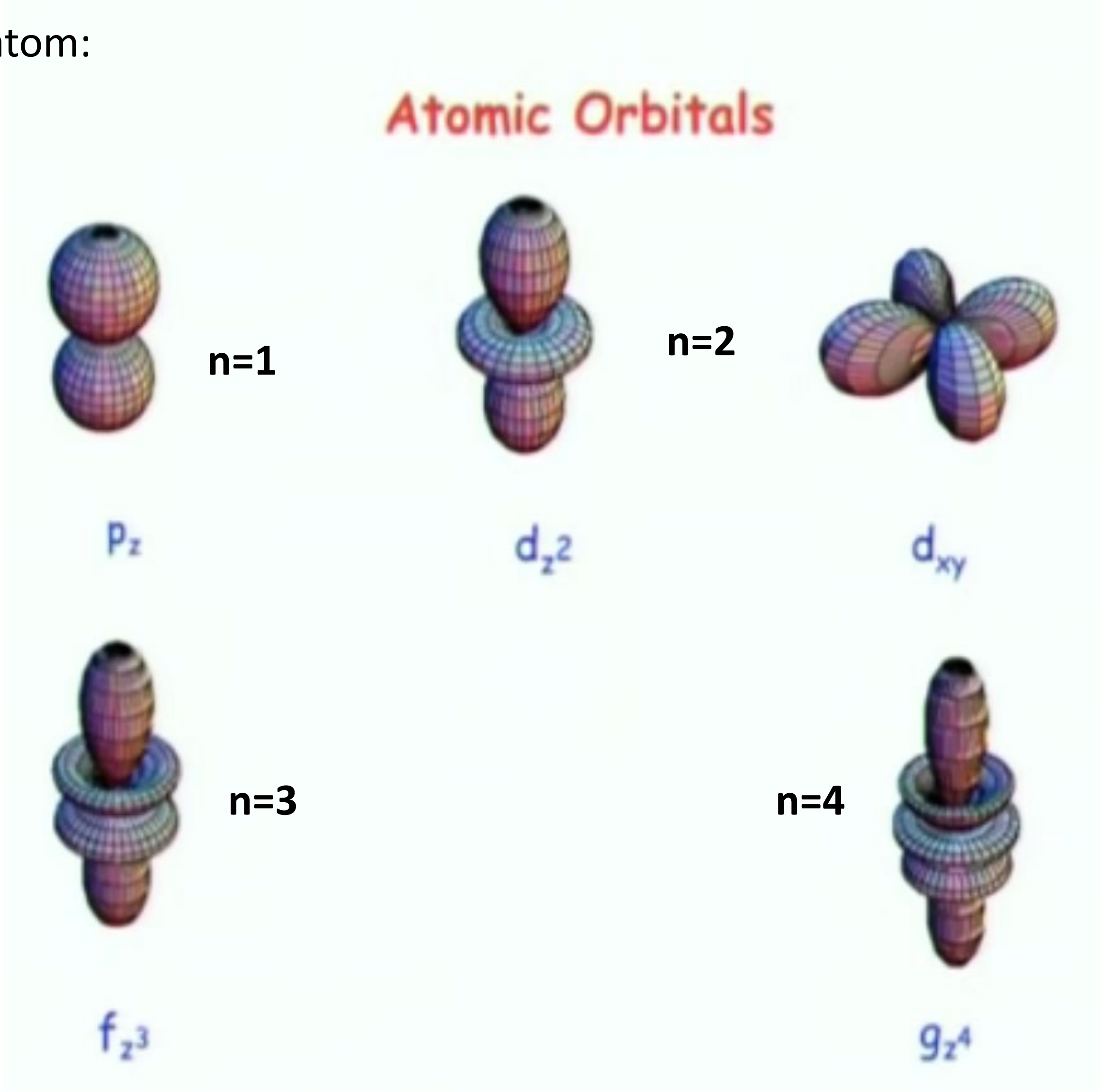
$$\hat{H}\psi = E.\psi$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$

KE we apply Lagranigian (L) to particle in a box or H atom and We apply Action Principle using L and use Path Integral to solve The wave equation for the stationary states (ψ_n) with n nodes as follows:

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \textbf{and} \quad E_n = \frac{n^2h^2}{8mL^2}$$

n are nodes also related to the principal quantum numbers!



H atom is a proton and an electron confined

Such e confinement by the proton creates standing wave

Such standing waves are stationary states or Atomic Orbitals with varying nodes (n)

What did we learn today?

What are Atomic Orbitals?

Relevance of Standing Waves in Chemistry: Standing Waves are Stationary States: Also known as Atomic Orbitals (AOs)

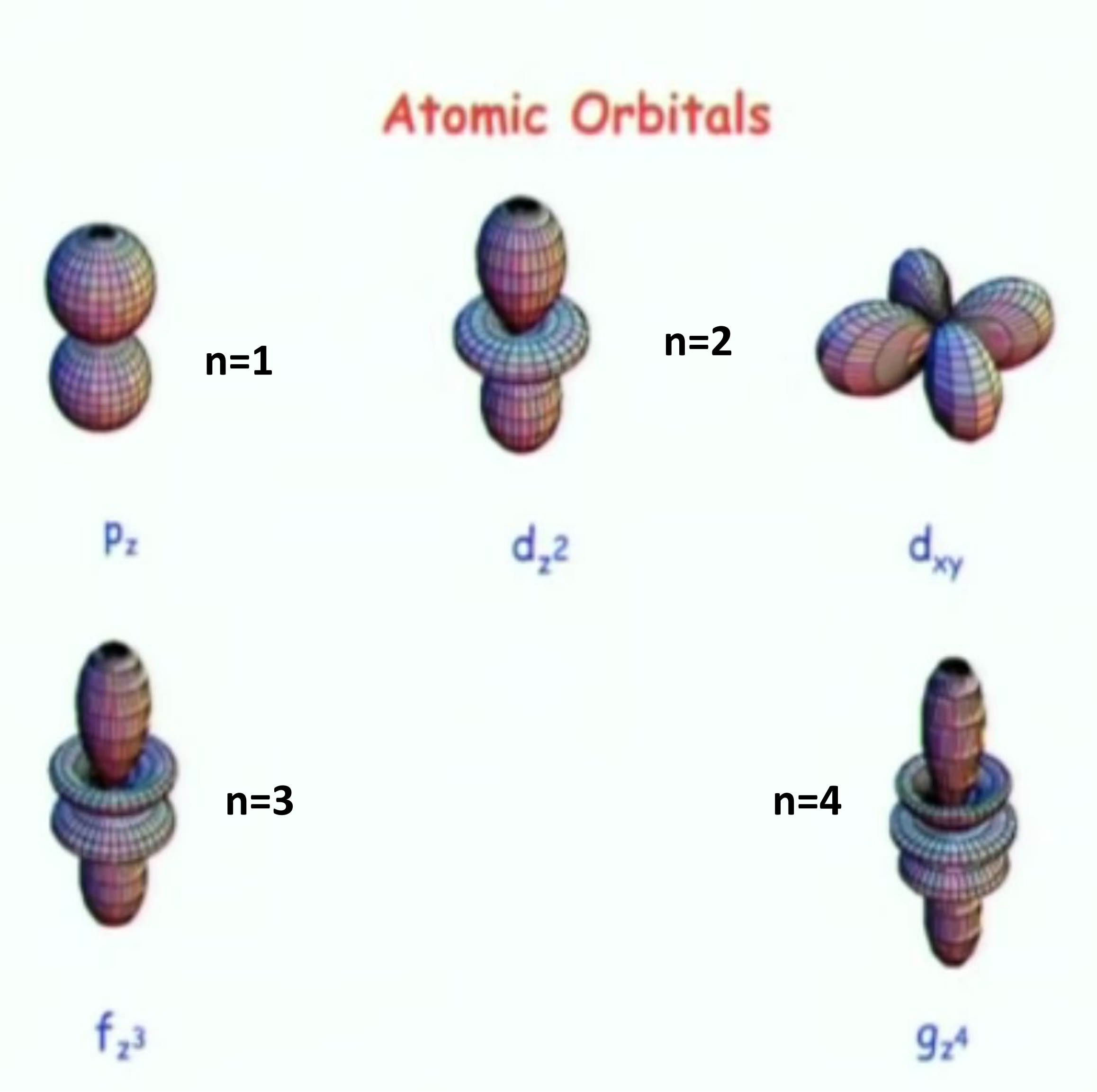
H atom is a proton and an electron confined

Such e confinement by the proton creates standing wave

Such standing waves are stationary states or Atomic Orbitals with varying nodes (n)

Using Schroedinger equation to particle in a box or H atom: $\hat{H}\psi = E.\psi$

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \textbf{and} \quad E_n = \frac{n^2h^2}{8mL^2}$$



n are nodes also related to Angular Quantum Numbers!

What did we learn?

1. Learnt Atomic Orbitals (Aos) are 'Stationary states', corresponding to standing waves created by the confinement of the electron by the proton in H atom model.

2. Learnt what are standing waves and wave packets how they correspond to electrons under confinement using Uncertainty principle and De Broglie relation.

3. Learnt how stationary states correspond to standing waves (AOs) and represent 2D probability surfaces Giving rise to 2D nodes in AOs.

What did we learn?

4. Learnt to use symmetry arguments (Action principle) to arrive at the idea of 'Stationary states', corresponding to standing waves created by the confinement of the electron by the proton in H atom model (approximated by particle in a box).

5. Wrote the Schroedinger equation and came to the idea of principal quantum number (n) from particle in a box.

$$\hat{H}\psi = E.\psi$$

$$\psi_n = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad \textbf{and} \quad E_n = \frac{n^2h^2}{8mL^2}$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) + V(x, y, z)$$