The Players

Erwin Schrodinger

Werner Heisenberg

Louis Victor De Broglie

- Neils Bohr

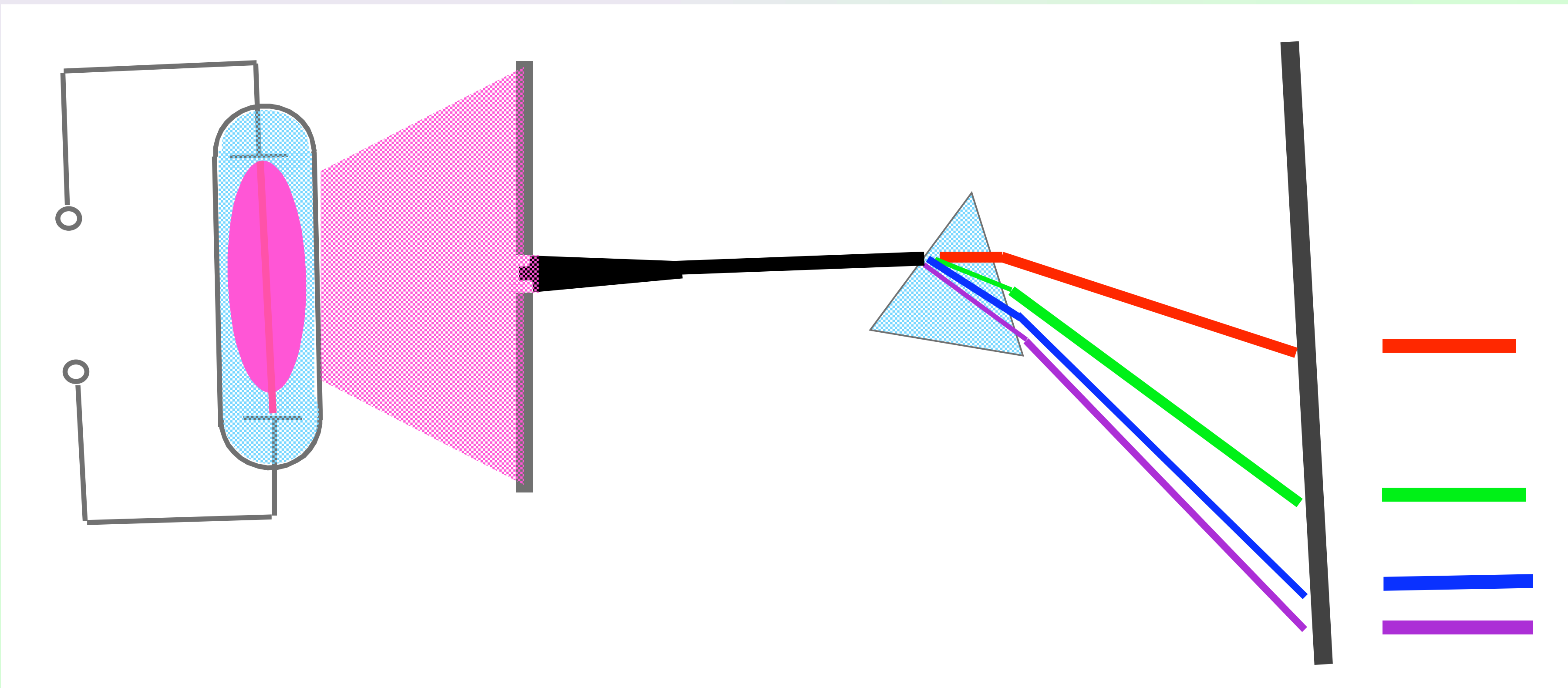
Albert Einstein

Max Planck

James Clerk Maxwell

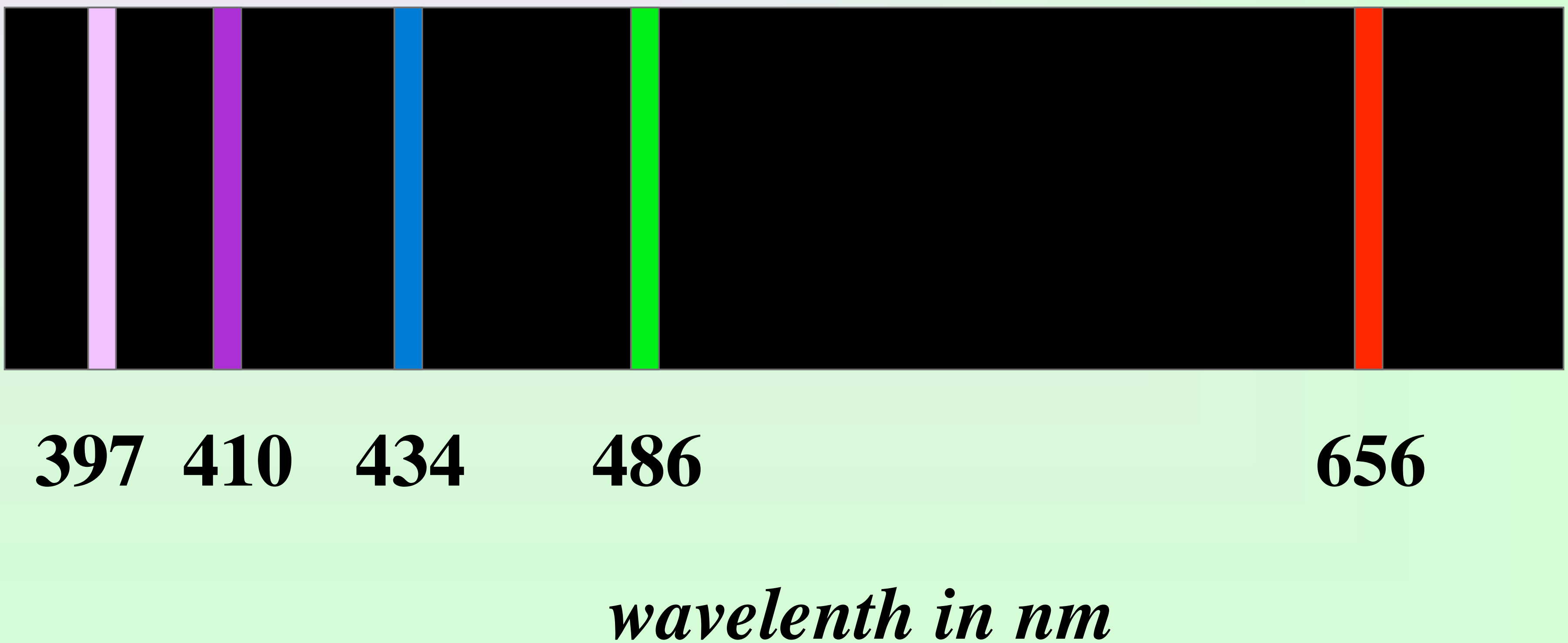
Neils Bohr

Explained the emission spectrum of hydrogen atom on basis of quantization of electron energy.



Emission spectrum

Emitted light is separated into component frequencies when passed through a prism.



Hydrogen, the simplest atom, produces the simplest emission spectrum.

In the late 19th century a mathematical relationship was found between the visible spectral lines of hydrogen

the group of hydrogen lines in the visible range is called the Balmer series

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

Rydberg Constant

$1.0968 \times 10^7 m^{-1}$

Johannes Rydberg

Bohr Solution

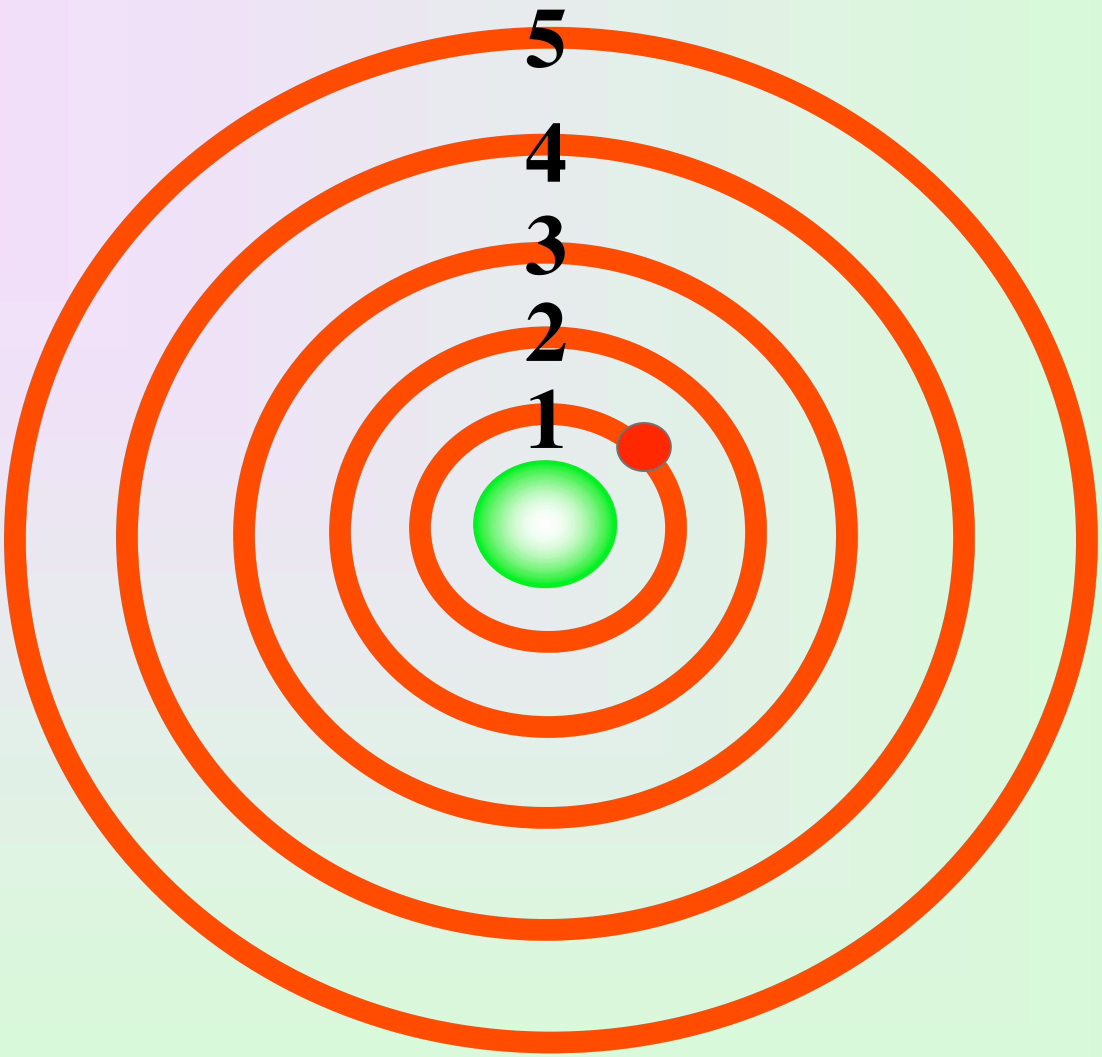
the electron circles nucleus in a circular orbit

imposed quantum condition on electron energy

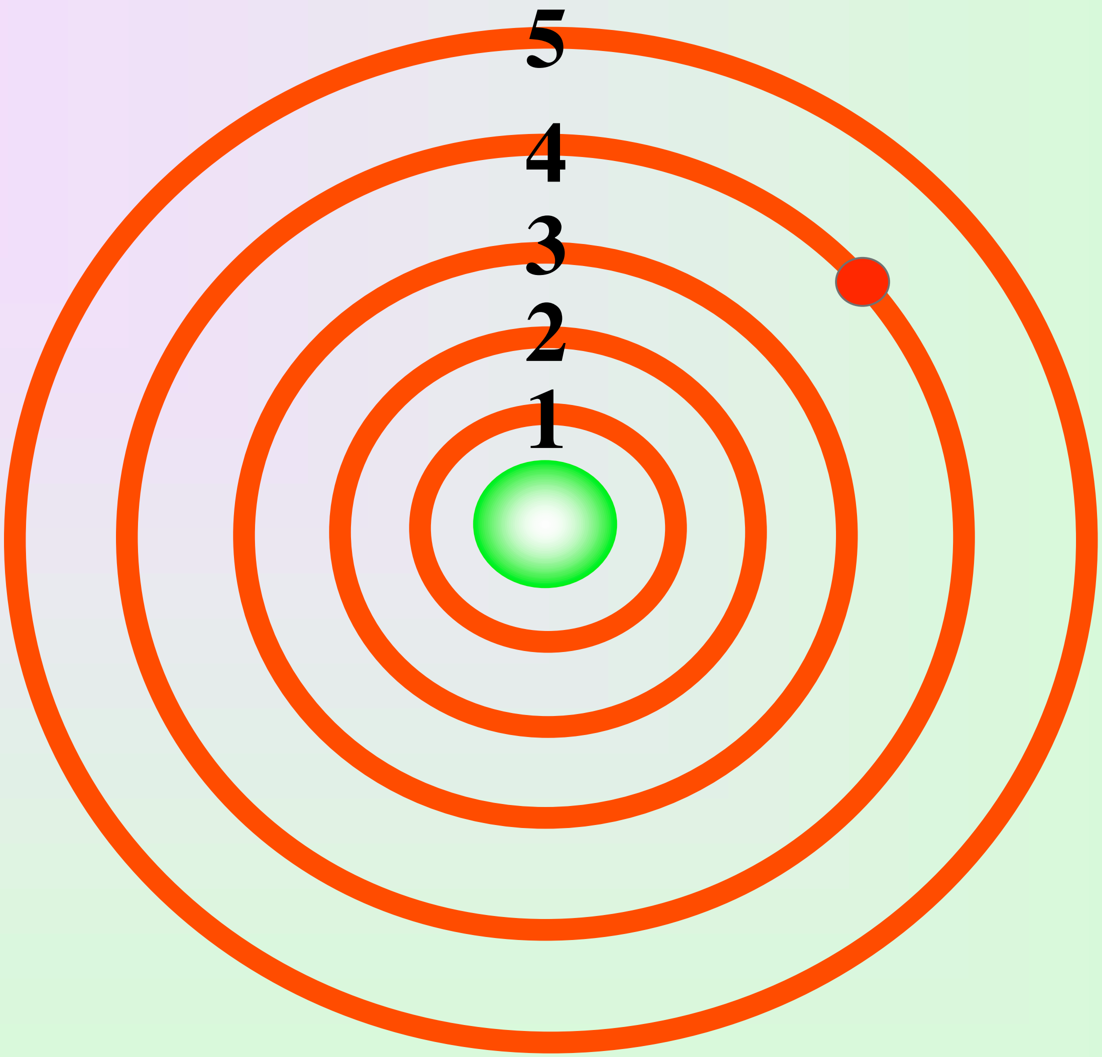
only certain “orbits” allowed

energy emitted is when electron moves from higher energy state (excited state) to lower energy state

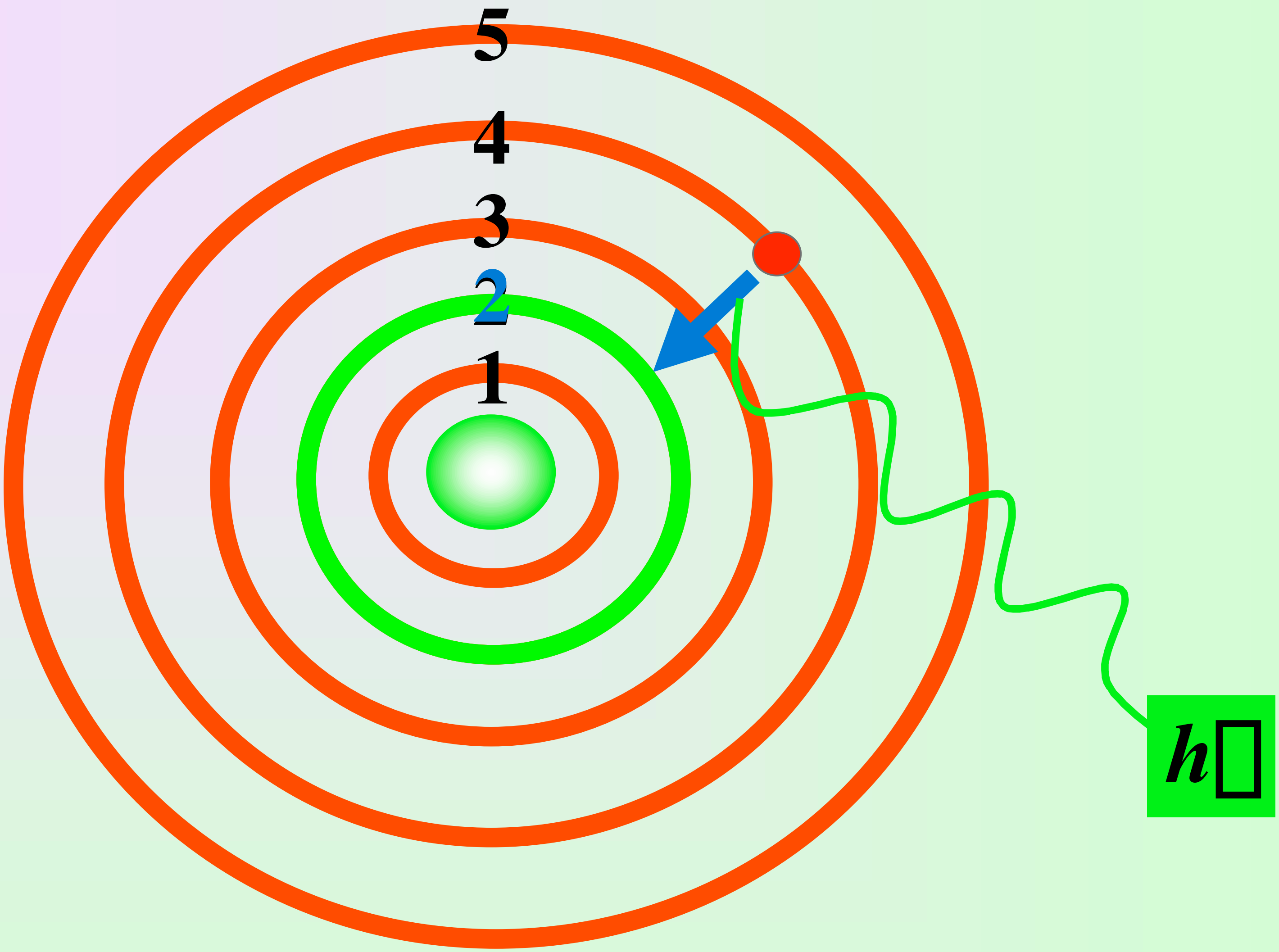
the lowest electron energy state is ground state



Stable state of hydrogen atom ("ground state")



Excited state of hydrogen atom



Which is one of the lines in the Balmer series

$$\frac{1}{\lambda} = R\left(\frac{1}{2^2} - \frac{1}{n^2}\right)$$

Rydberg Constant $1.0968 \times 10^7 m^{-1}$

Rewritten to solve for energy

$$h\nu = \Delta E = -2.178 \times 10^{-18} J \left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Where ΔE is the energy is the released by an excited electron moving to a lower energy level

Example

What is the wavelength of a photon emitted during a transition from the $n_i = 5$ state to the $n_f = 2$ state in the hydrogen atom?

$$\Delta E = -2.178 \times 10^{-18} J \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

Example

What is the wavelength of a photon emitted during a transition from the $n_i = 5$ state to the $n_f = 2$ state in the hydrogen atom?

$$\Delta E = -2.178 \times 10^{-18} \text{J} \left(\frac{1}{2^2} - \frac{1}{5^2} \right)$$

$$\Delta E = h\nu$$

$$\nu = \frac{c}{\lambda}$$

$$\lambda = \frac{hc}{\Delta E} = \frac{(3.00 \times 10^{8} \text{ m/s})(6.63 \times 10^{-34} \text{Js})}{-4.58 \times 10^{-19} \text{J}} = 4.34 \times 10^{-7} \text{m}$$

= 434 nm

A Complex and only Partially Correct Solution

Neils Bohr

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Werner Heisenberg

- **Louis Victor De Broglie**

Neils Bohr

Albert Einstein

Max Planck

James Clerk Maxwell

Wave /Particle Duality

If a light wave has a “particular” nature might not a particle have wave properties.

Albert Einstein - 1905

Theory of special relativity

The laws of science should be the same for all freely moving observers, no matter what their speed (abandoning the idea of absolute time).

- **equivalence of mass and energy (derived from the theory of relativity)**

$$E = m\,c^2$$

energy (E)

mass (m)

speed of light (c): 3.00×10^8 m/s

Louis Victor De Broglie

showed that electrons have wave properties

wave-particle duality

$$E_{\text{(photon)}} = h\nu$$

$$E_{\text{(photon)}} = mc^2$$

$$mc^2 = h\nu$$

$$\nu = c / \lambda$$

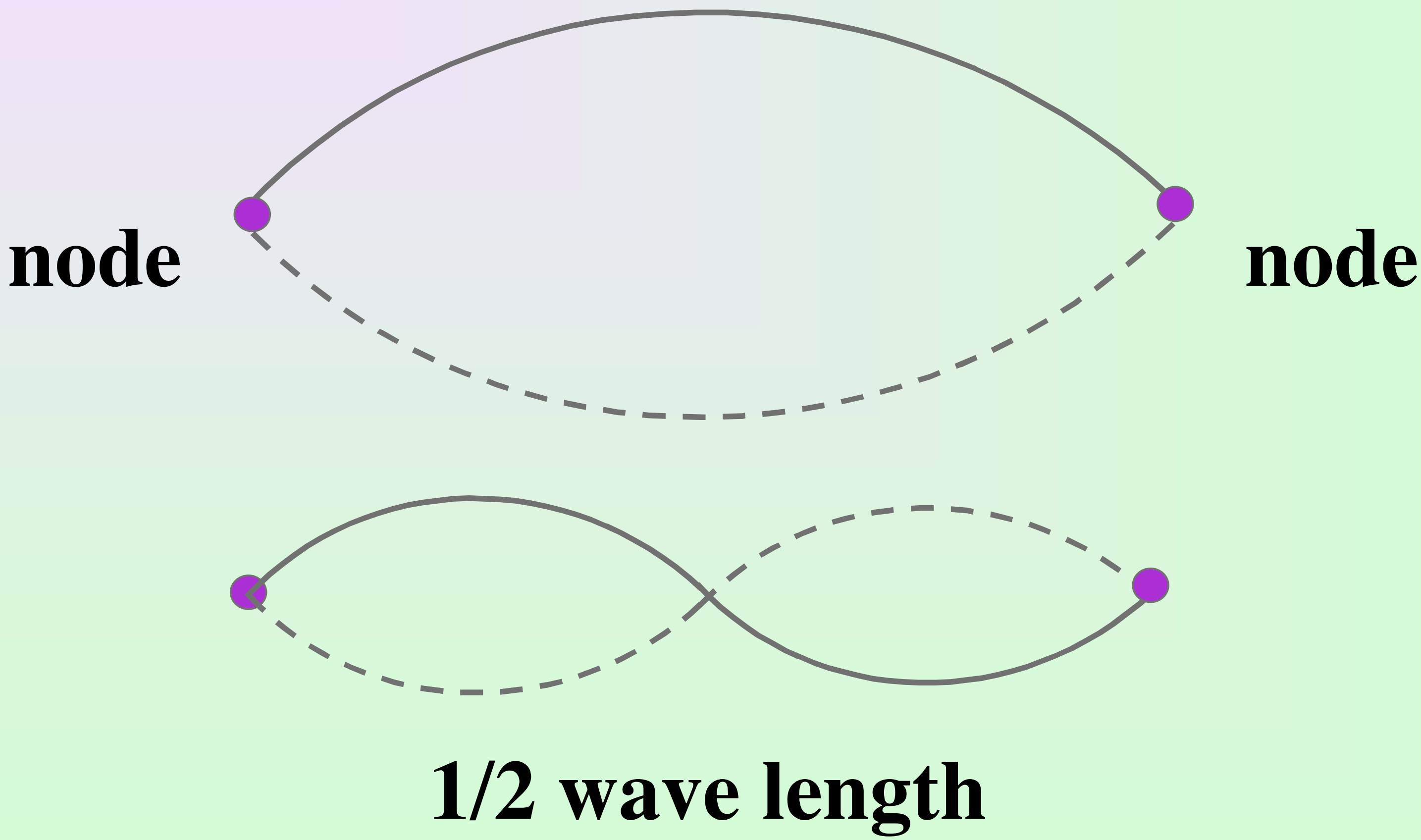
$$mc^2 = h\frac{c}{\lambda}$$

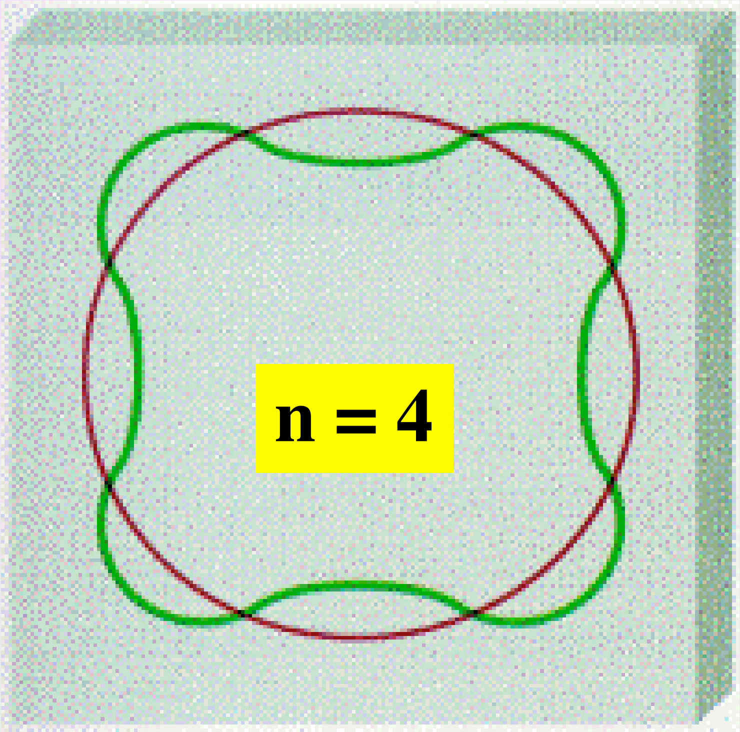
$$\lambda = \frac{h}{mc}$$

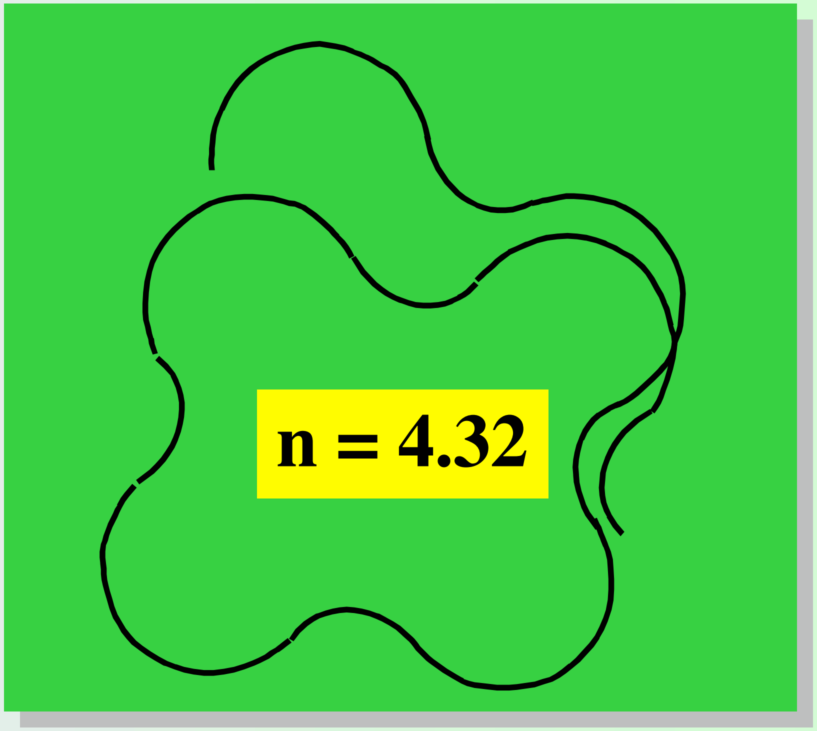
The less massive an object the longer its wavelength

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

Standing Waves







hydrogen electron visualized as a standing wave around the nucleus

the circumference of a particular circular orbit has to correspond to a whole number of wavelengths

Example

compare wavelength for an electron (mass= 9.11 x 10^{-31} kg) ,speed 1.0 x 10^{7} m/s with that of a ball (mass = 0.10 kg) ,speed 35 m/s

$$\lambda = \frac{h}{m\nu}$$

$$\lambda e = \frac{(6.63 \times 10^{-34} kgm^2/s^2)s}{(9.11 \times 10^{-31} kg)\ (1.0 \times 10^{7}\ m/s)} = 7.3 \times 10^{-11} m$$

$$J = kgm^2/s^2$$

$$\lambda ball = \frac{(6.63 \times 10^{-34} kgm^2/s^2)s}{(0.10\ kg)\ (35\ m/s)} = 1.9 \times 10^{-34} m$$

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Werner Heisenberg

Uncertainty principle

position and momentum of a electron cannot
be simultaneously determined

if position is measured accurately, uncertainty
in measuring momentum (speed) is large, vice versa

$$\Delta x \, \Delta P = h/4\pi$$

change in position

change in momentum

The hydrogen atom has a radius on the order of 0. 05 nm. Assuming that we know the position of an electron to an accuracy of 1% of the hydrogen radius, calculate the uncertainty in the velocity of the electron.

□x □P = h/4 π

$$□P = \frac{(6.63 \times 10^{-34} kgm^2 / s)}{4(3.14) \quad (5 \times 10^{-13}\ m)} = 1.05 \times 10^{-22} kg\ m/s$$

$$□P = m□V \qquad □V = \frac{□P}{m} = \frac{1.05 \times 10^{-22} kg\ m/s}{9.11 \times 10^{-31} kg}$$

$$= 5 \times 10^{8}\ m/s$$

Compare this value with the uncertainty in the velocity of a ball of mass 0.2kg and radius 0.05 m whose position is known to an accuracy of 1% of its radius

5×10^{8} m/s

$$\Delta x \, \Delta P = h/4\pi$$

$$\Delta V = \frac{\Delta P}{m} = \frac{h}{(\Delta x)(m)(4\pi)}$$

$$\Delta V = \frac{(6.63 \times 10^{-34} kgm^{2}/s)}{4(3.14)\ (5 \times 10^{-4}\ m)(0.2kg)}$$

$$= 5 \times 10^{-31} \text{ m/s}$$

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wave (quantum) mechanics

<u>Schrodinger Equation</u>

attacks the problem of atomic structure by giving emphasis to the wave properties of the electron

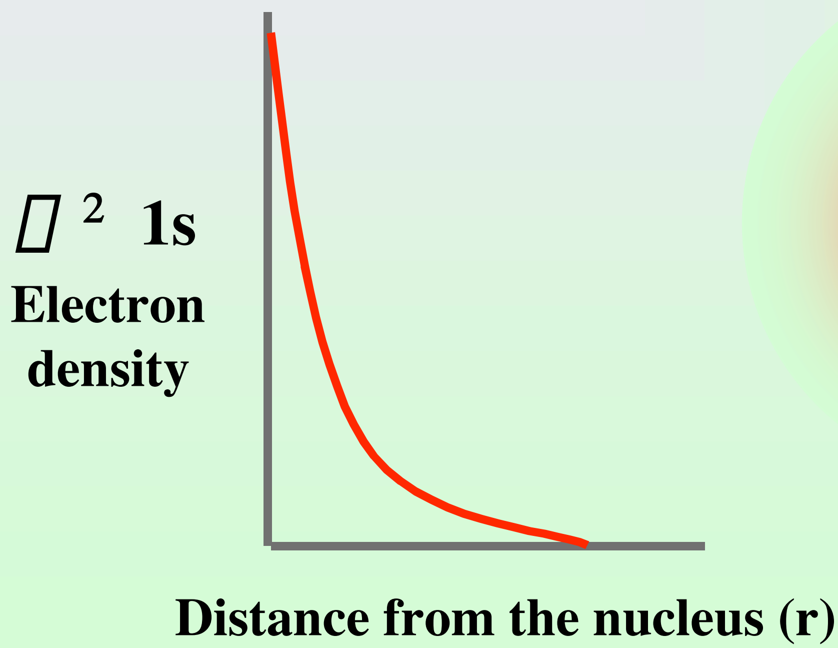
an orbital can be thought of as the wave function of an electron (□) which coordinates the x ,y, and z of an electrons position in a three-dimensional space

Solutions of the Schrodinger Wave Equation for a One-Electron Atom

n	*l*	m_l	orbital	solution
1	0	0	1s	$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$
2	0	0	2s	$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$
2	1	0	$2p_z$	$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$
2	1	± 1	$2p_x$	$\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \cos \phi$
2	1	± 1	$2p_y$	$\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta \sin \phi$

Erwin Schrodinger

the square of the Schrodinger Equation gives us the probability of finding an electron in a certain region of space



Charge-Cloud Model

No orbit path for electrons.

Energy levels or shells are the average points on a probability plot.

Atomic Orbital is the probability distribution of finding an electron with a specific energy level as defined by its quantum numbers.

Neils Bohr

Explained the emission spectrum of hydrogen atom on basis of quantization of electron energy.