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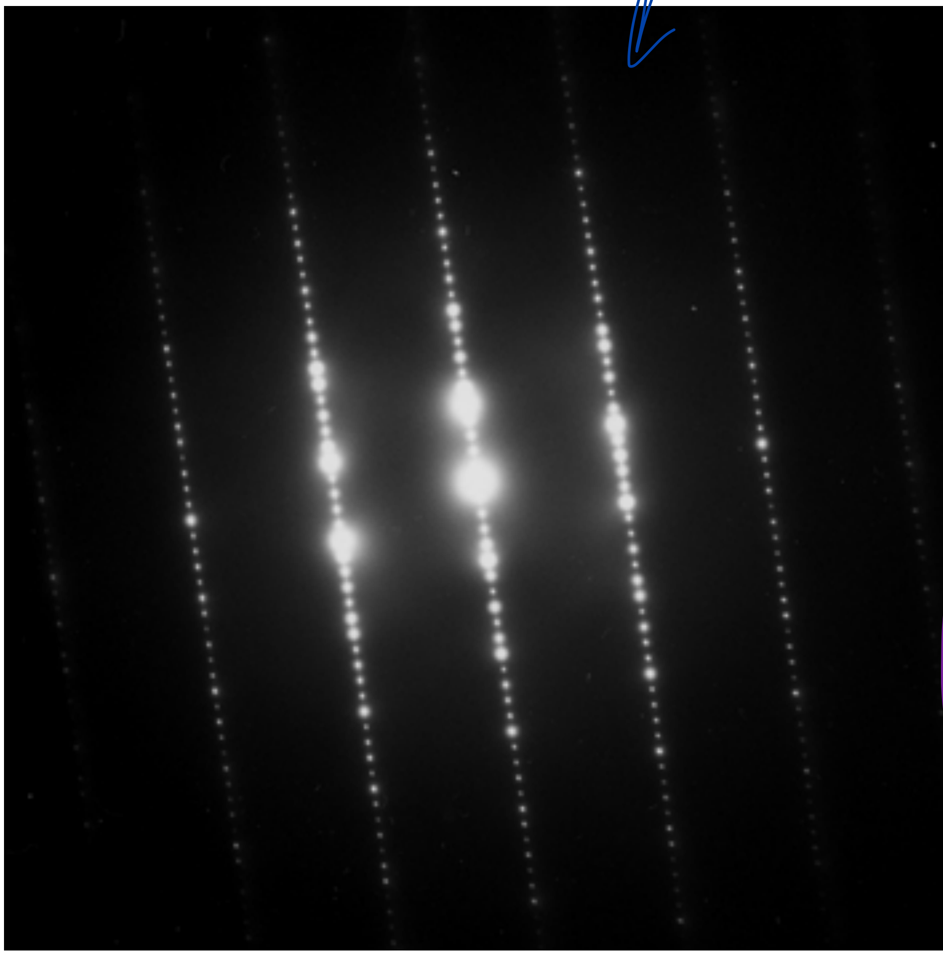
2.2 The Scrödinger Equation	~~2.1.2 The Bohr Atom~~
The Particle in a Box, Quantum Numbers, The Aufbau Principle and Shielding	~~2.2 The Scrödinger Equation~~
	~~2.1.1 The Periodic Table~~
2.3 Periodic Properties	2.3 Periodic Trends

Wave-Particle Duality



https://en.wikipedia.org/wiki/Electron_diffraction#/media/File:DifraccionElectronesMET.jpg

de Broglie $\lambda = h/mv$ (wavelength) matter has wave like properties

Heisenberg $\Delta x \, \Delta p_x \geq h/4\pi$ (Δx: 2 ft; m) $\Delta p_x \geq \frac{h}{2 \cdot 4\pi}$

Bohr model treated the e^- as a particle.

we can't tell where the e^- is. uncertainty in position

diffraction pattern produced by a beam of e^-'s ..... waves make diffraction patterns ⇒ treat the e^- as a wave

Hamiltonian Operator

the wave function

$$H\Psi = E\Psi$$

Energy

Squaring the wave function gives use the probability of finding a the electron at a given location in space

The wave function must be an eigenfunction

Math-speak	English
1. The wave function must be single valued.	Cannot have two probabilities for finding the electron at a given point
2. The wave function and its first derivatives must be continuous.	The probability must be defined at all points in space and cannot change abruptly
3. The wave function must approach 0 as r approaches infinity	The probability must get smaller at large distances of the atom. The atom must be finite.
4. Integrating $\Psi_A\Psi_A^*$ over all space must equal 1	The electron must be somewhere in space. Process is called normalizing the wave function
5. Integrating $\Psi_A\Psi_B^*$ over all space must equal 0	The orbitals must be orthogonal (mutually exclusive)

Hamiltonian is a mathmatical function we use to find the energy of the e.

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}}$$

Since,

$$r = \sqrt{x^2+y^2+z^2}$$

planks

$$H = \left[\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right)\right] - \left[\frac{Ze^2}{4\pi\varepsilon_0 r}\right]$$

PE

Bohr

$KE = \frac{1}{2}mv^2$

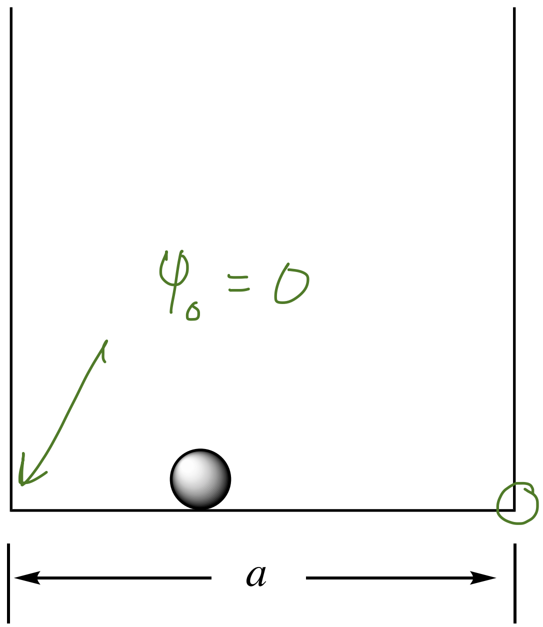
$PE = \frac{Ze^2}{r}$

$v \cdot v$

Like this marble is trapped in a box

$A \sin(r\,0)$ $B\cos(s\,0) = 1$

$$\Psi = A \sin rx + \sout{B \cos sx}$$



$\psi = 0 + B$ an $\psi_0 = 0$

so

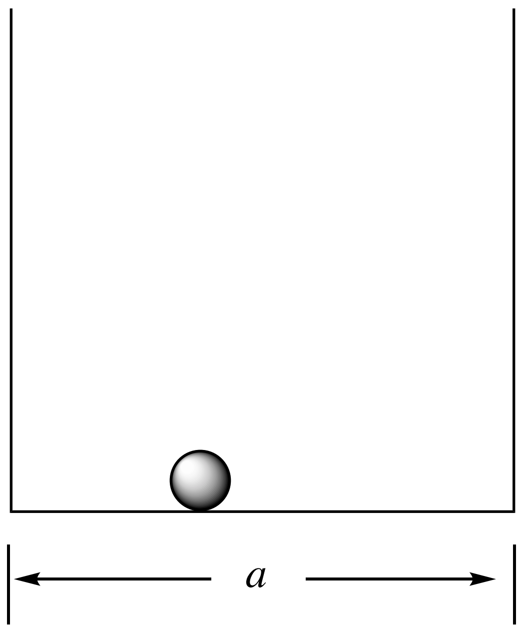
$0 = 0 + B$ or $B = 0$

$$\Psi = A \sin rx$$

at $x = 0$
my wavefunction
must go to 0

Wave functions come from mathematical experience

So the electron is a particle/wave trapped in an atom…



$$\Psi = \mathbf{A\ sin\ rx}$$

particle not moving in y or z so we don't need this part

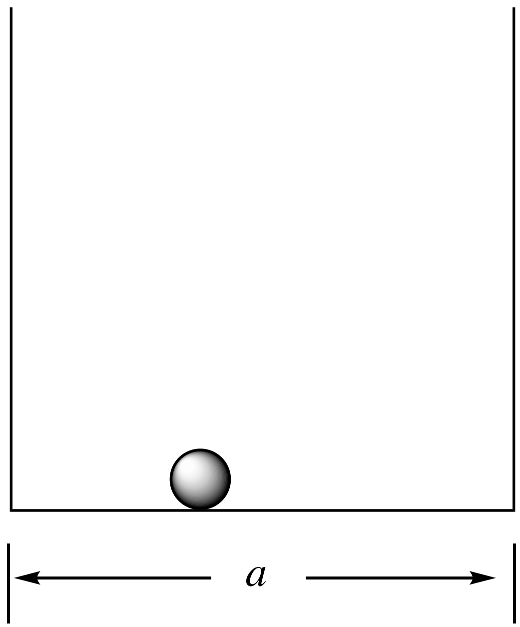
our particle is not charged

$$H = \frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2} + \frac{\delta^2}{\delta y^2} + \frac{\delta^2}{\delta z^2}\right) - \frac{Ze^2}{4\pi\varepsilon_0 r}$$

$$H\Psi = E\Psi$$

$$\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2}\left(A \sin rx\right)\right) = E\left(A \sin rx\right)$$

ψ? ψ?

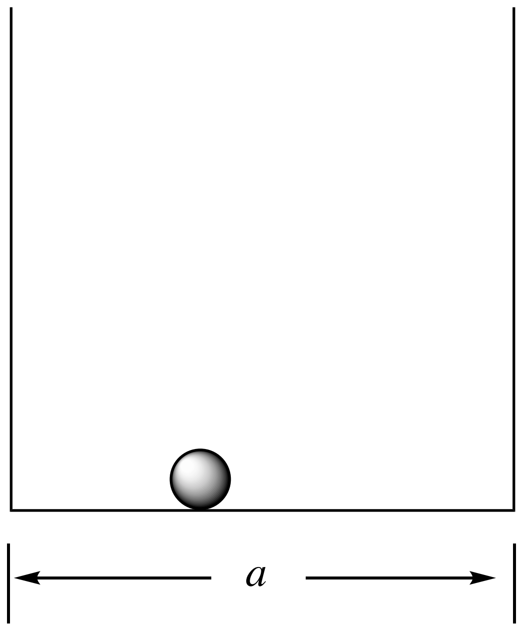


$$\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2}\left(A \sin rx\right)\right) = E\left(A \sin rx\right)$$

$$\frac{-h^2}{8\pi^2 m}\left(\ Ar\right)\left(\frac{\delta}{\delta x}\left(\cos rx\right)\right) = E\left(A \sin rx\right)$$

$$\frac{-h^2}{8\pi^2 m}\left(-Ar^2\right)\left(\sin rx\right) = E\ A \sin rx$$

So the electron is a particle/wave trapped in an atom…



$$\frac{-h^2}{8\pi^2 m}(\cancel{-}Ar^2)\,\cancel{(\sin rx)} = E\ \cancel{A \sin rx}$$

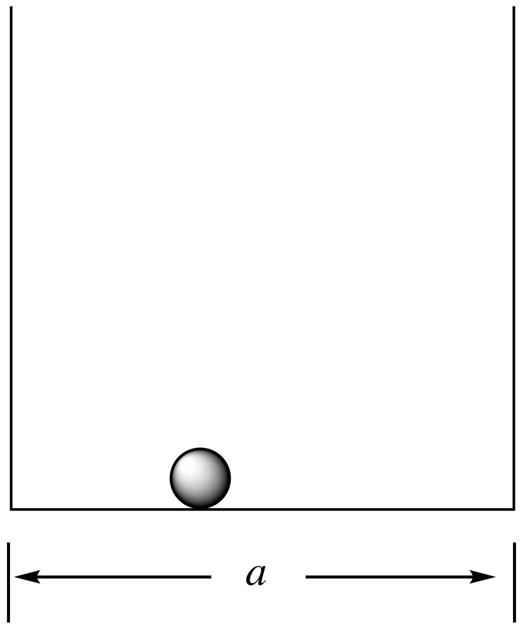
$$\frac{-h^2}{8\pi^2 m}(-r^2) = E$$

$$r^2 = E\,\frac{8\pi^2 m}{h^2}$$

$$r = \frac{2\pi}{h}\sqrt{2mE}$$

this is the r in

A sin(rx)



$\psi_0 = 0$ $\psi_a = 0$

$$r = \frac{2\pi}{h}\sqrt{2mE}$$

But remember $\Psi = A \sin rx$

has to make sin go to 0, so r must get r · x to values of $\pi, 2\pi, 3\pi, 4\pi, 5\pi \ldots$

r must also equal $n\dfrac{\pi}{a}$

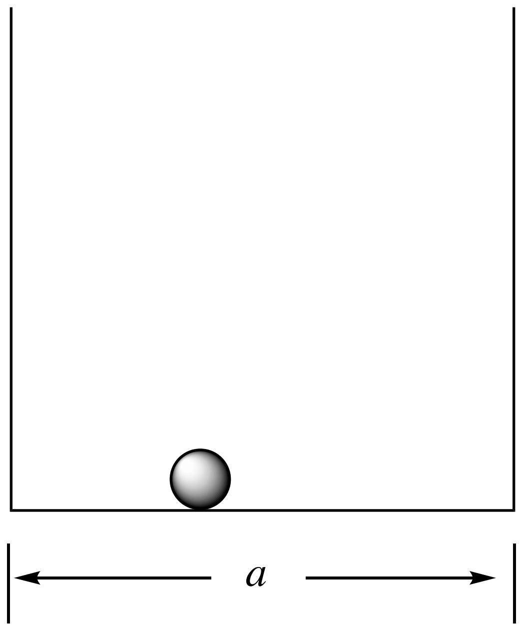
So,

$$E = \frac{n^2h^2}{(8a^2m)}$$

$A \sin(r a) = 0$

$A \sin\left(n\frac{\pi}{a} \cdot a\right) = 0$

r

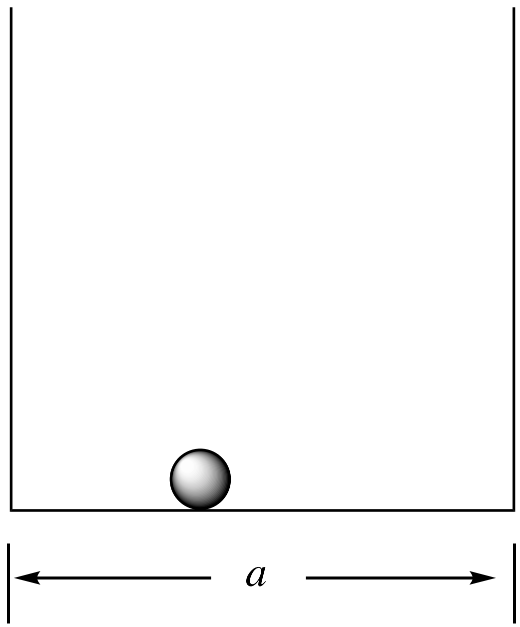


$$\Psi = \mathbf{A\ sin\ rx}$$

$$r = n\frac{\pi}{a}$$

$$\Psi = \mathbf{A\ sin}(n\frac{\pi}{a}\ \mathbf{x})$$

So the electron is a particle/wave trapped in an atom…



$$\Psi = \mathbf{A}\ \mathbf{sin}(\ n \frac{\pi}{a}\ \mathbf{x})$$

$$(\Psi\Psi^*) = 1$$

$$\Psi = (2/a)1/2\ \mathbf{sin}\ (n\pi/a)\mathbf{x}$$

The Aufbau Principle

1. start in lowest quantum levels
2. Pauli exclusion principle---comes from experiment, not the Schrödinger Equation
3. Hund's Rule of Multiplicity--Multiplicity is the number of unpaired e^{-}'s + 1

Penetration/effective nuclear charge

Π_c = coulomb repulsion
- bad
- number of paired electrons

Π_e = exchange energy
- good in the case of parallel electrons in an atom
- number of exchanges that can be made and produce identical electron configurations

Exchange energy is **NOT** the exchanges between all possible arrangements (states). Rather, it is the number of possible exhanges of electrons in a single state; thus,