Today (3)

2.2 The Schrödinger Equation

2.2.1: The Particle in a Box

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

Next Class (4)

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

2.3 Periodic Properties

Second Class from Today (5)

2.2.2 Quantum Numbers and Atomic Wave Functions

2.2.3 The Aufbau Principle and Shielding

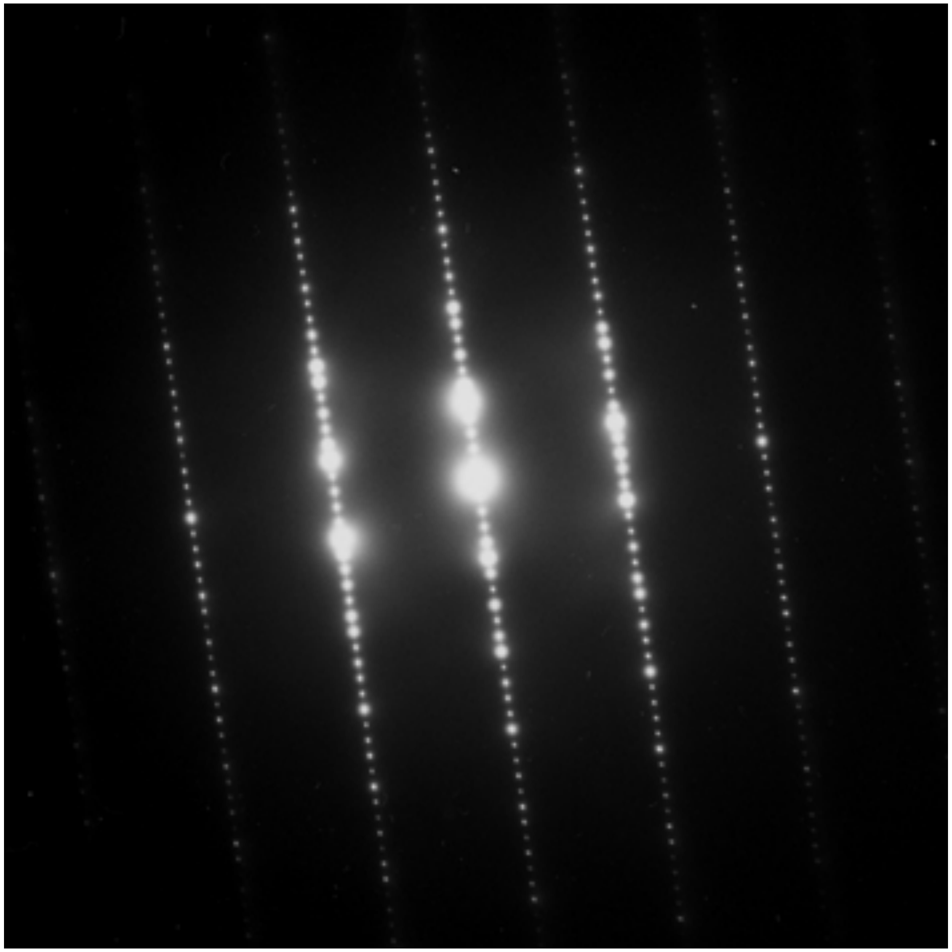
2.3 Periodic Properties

Third Class from Today (6)

3.1 Lewis Structures

3.2 VSEPR

Wave-Particle Duality



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

the wavelength of a particle

de Broglie $\lambda = h/mv$

with mass m + velocity v

Heisenberg $\Delta x \, \Delta p_x \geq h/4\pi$

$h \sim 6 \times 10^{-34}$ for large objects like people

λ is very small

small energetic objects have a larger wavelength wave function

$$H\Psi = E\Psi$$

when the Hamiltonian operator operates on a wave function

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

the wave function comes back out & it is multiplied by the energy of the system

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	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)

as distance approaches infinity $\Psi^*\Psi$ approaches 0

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

Since,

KE

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

PE between 2 charged particles

e = charge of e^-

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

Z = atomic # charge of nucleus

E = KE + PE

$= \frac{1}{2}mv^2 + \frac{q_1 q_2}{r} k$

$\frac{m^2}{s^2}$

$\frac{(\text{charge } e^-)\cdot(\text{nuclear charge})}{r}$

constants

distance

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

$\overset{x}{\cos}, \overset{y}{\sin}$ — $(\cos, \sin)$

model any wave

$$\Psi = A \sin rx + B \cos sx$$

simplify

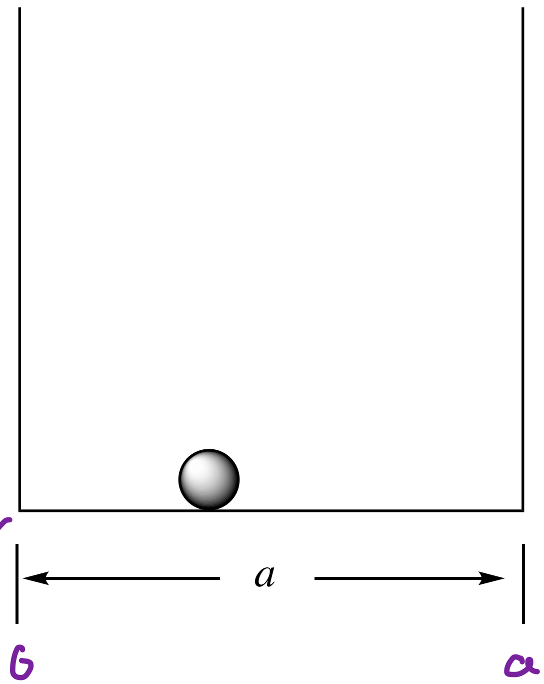
$\cos(0) = 1$

$\sin(0) = 0$

set $B = 0$

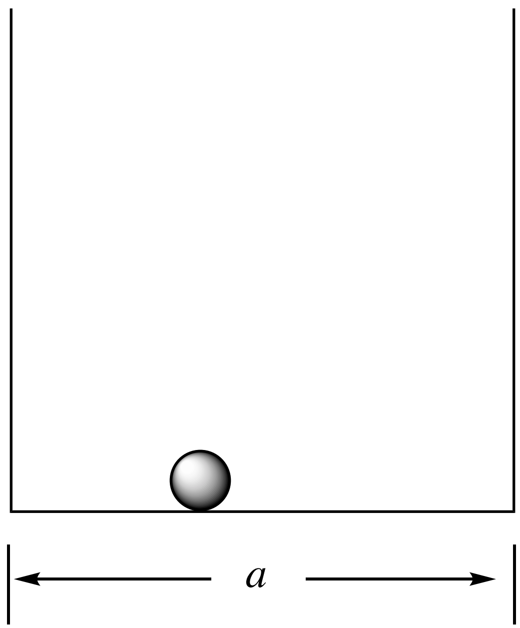
model my wave

$$\Psi = A \sin rx$$



probability of finding my particle in the wall? 0 so wave function at $x=0$ must be 0

So the electron is a particle/wave trapped in an atom… Section 2.2.1



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

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

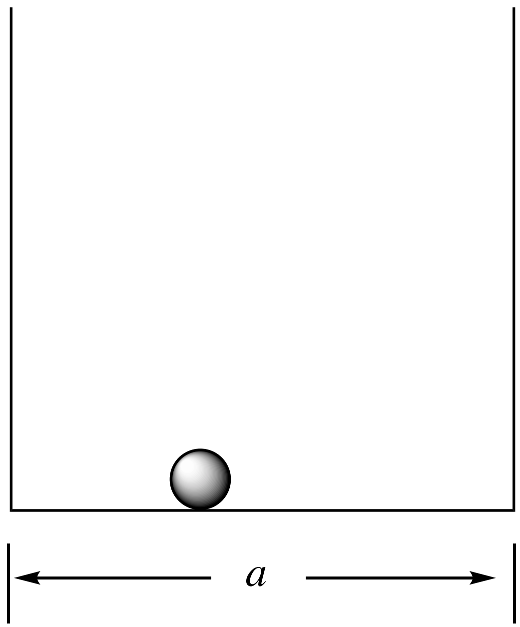
?

$$H\Psi = E\Psi$$

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

simplified because our particle is not charged, so no contribution to E from Coulombs law.

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

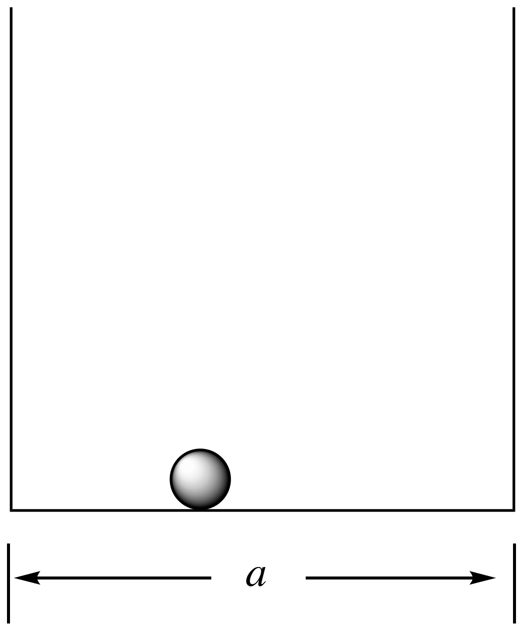


$$\frac{-h^2}{8\pi^2 m}\left(\frac{\delta^2}{\delta x^2}\left(A \sin rx\right)\right) = E\left(A \sin rx\right)$$

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

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

So the electron is a particle/wave trapped in an atom… Section 2.2.1

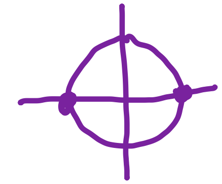


$$\frac{-h^2}{8\pi^2 m}\,(-Ar^2)\,(\sin rx) = E\ \ A \sin rx$$

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

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

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



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

cos, sin
x y

at π radians
sin(π) = 0

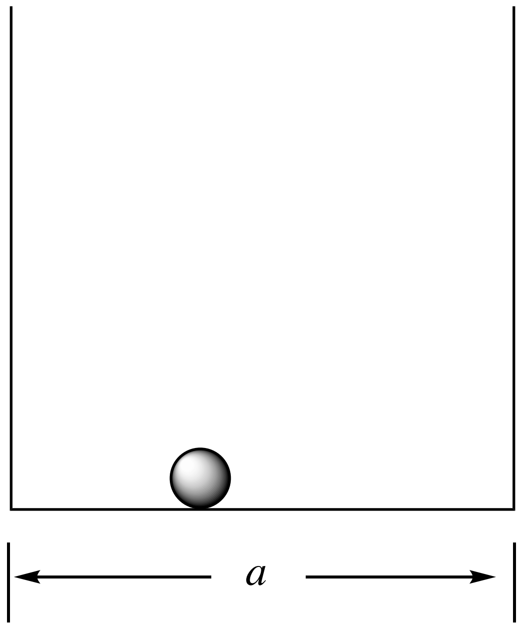
But remember $\Psi = A \sin rx$

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

x = a rx = π

So,

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

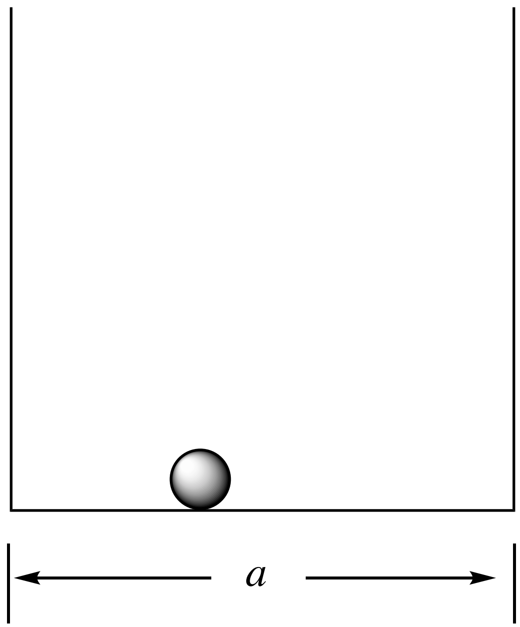


when is sin(x) = 0

whole #

value of ψ when x = a must be 0.
The particle can't exist in the wall.

the energy is quantized because the wave function has many n's where the function goes to 0.

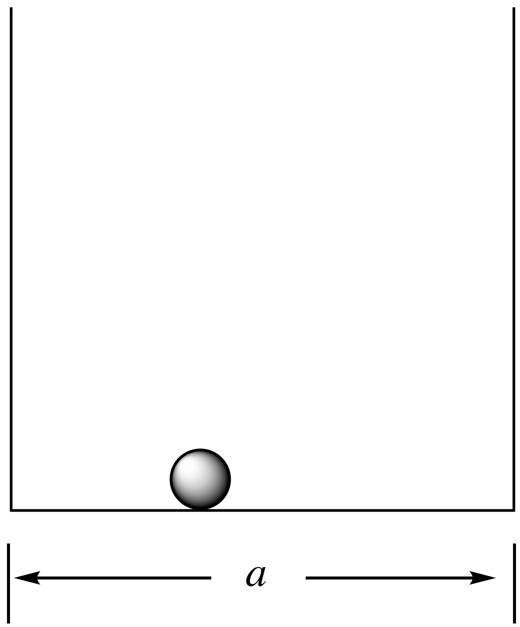


$$\Psi = \mathbf{A\ sin\ rx}$$

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

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

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



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

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

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

Equations

https://www.westfield.ma.edu/cmasi/advinorg/angular_distribution_functions/text_and_graphics_containe.htm

Pictures

https://www.westfield.ma.edu/cmasi/advinorg/quant_orbital_surfaces/orbital_surfaces.htm

Models

s and p
https://www.westfield.ma.edu/cmasi/organic/mo-plain/aos.html

d orbitals
https://www.westfield.ma.edu/cmasi/advinorg/dorbs/dorbsp.html

One quantum number wasn't enough to model the electrons in an atom

n is the principal quantum number

$n = 1, 2, 3, 4, 5$

quantum mechanics n is kindof like Bohr's shells

l shells are sub shells inside an n shell

l is the Angular momentum quantum number

describes the shape of the orbitals in the l sub shells

m_l is the magnetic quantum number

· experimental observation

m_s is the spin quantum number e^-'s can align with or against a magnetic field

e^-'s have 2 spin states | spin up or spin down | $m_s = \frac{1}{2}$ or $-\frac{1}{2}$

For a given n allowed values for l are n−1 down to 0

$n=1 \quad l=0 \qquad n=2 \quad l=1,0$

For a given l allowed values for m_l are $+l$ to $-l$ in whole # steps

$n=1 \quad l=0 \quad m_l=0 \qquad n=2 \quad l=1 \quad m_l=1,0,-1 \qquad l=0, \; m_l=0$

1 s

p type orbital three 2p orbitals one 2s

Periodic Table of the Elements

	1	2															3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H**																															2 **He**
2	3 **Li**	4 **Be**																									5 **B**	6 **C**	7 **N**	8 **O**	9 **F**	10 **Ne**
3	11 **Na**	12 **Mg**																									13 **Al**	14 **Si**	15 **P**	16 **S**	17 **Cl**	18 **Ar**
4	19 **K**	20 **Ca**															21 **Sc**	22 **Ti**	23 **V**	24 **Cr**	25 **Mn**	26 **Fe**	27 **Co**	28 **Ni**	29 **Cu**	30 **Zn**	31 **Ga**	32 **Ge**	33 **As**	34 **Se**	35 **Br**	36 **Kr**
5	37 **Rb**	38 **Sr**															39 **Y**	40 **Zr**	41 **Nb**	42 **Mo**	43 **Tc**	44 **Ru**	45 **Rh**	46 **Pd**	47 **Ag**	48 **Cd**	49 **In**	50 **Sn**	51 **Sb**	52 **Te**	53 **I**	54 **Xe**
6	55 **Cs**	56 **Ba**	57 **La**	58 **Ce**	59 **Pr**	60 **Nd**	61 **Pm**	62 **Sm**	63 **Eu**	64 **Gd**	65 **Tb**	66 **Dy**	67 **Ho**	68 **Er**	69 **Tm**	70 **Yb**	71 **Lu**	72 **Hf**	73 **Ta**	74 **W**	75 **Re**	76 **Os**	77 **Ir**	78 **Pt**	79 **Au**	80 **Hg**	81 **Tl**	82 **Pb**	83 **Bi**	84 **Po**	85 **At**	86 **Rn**
7	87 **Fr**	88 **Ra**	89 **Ac**	90 **Th**	91 **Pa**	92 **U**	93 **Np**	94 **Pu**	95 **Am**	96 **Cm**	97 **Bk**	98 **Cf**	99 **Es**	100 **Fm**	101 **Md**	102 **No**	103 **Lr**	104 **Rf**	105 **Db**	106 **Sg**	107 **Bh**	108 **Hs**	109 **Mt**	110 **Ds**	111 **Rg**	112 **Cn**	113 **Nh**	114 **Fl**	115 **Mc**	116 **Lv**	117 **Ts**	118 **Og**

https://en.wikipedia.org/wiki/Periodic_table

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

Factors determining the energy of the electron

Penetration and effective nuclear charge

Π_c = coulomb repulsion
- -bad
- -number of paired electrons

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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,