This Class

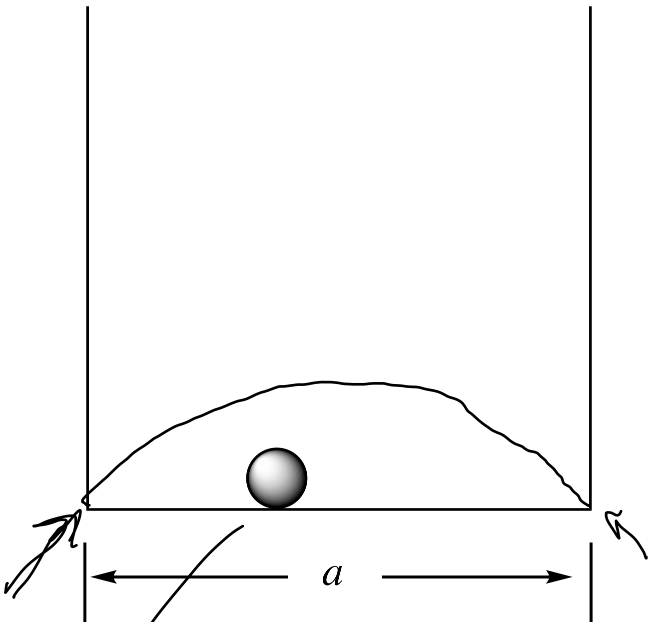
Finish The Particle in a Box, Quantum Numbers, The Aufbau Principle and Shielding

Next Class

Shielding and

2.3 Periodic Trends

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



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

when $x = a$

$\sin(ra) = 0$

But remember $\Psi = A \sin rx$

~~cos~~

$\sin \pi = 0$

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

$\sin 2\pi = 0$

$\sin 3\pi = 0$

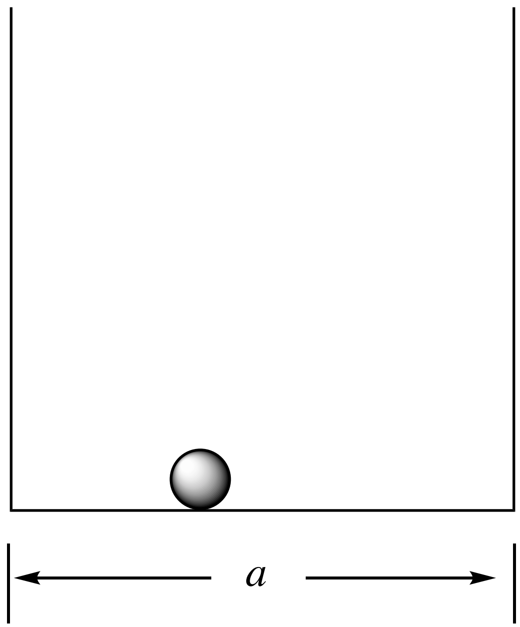
what is A?

this makes it so when $x = a$, $\sin(n) = 0$

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

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

Instead of assuming we can put any amount of energy into this particle in a box we decided to treat it like a standing wave and that causes the energy of the particle to be quantized*.



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

$$\int_0^a (\Psi\Psi^*) = 1$$

This is called normalizing the wavefunction... The probability of finding the particle is 1 somewhere between 0 and 1

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

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 tells us about the # of orbitals available in a shell n can be 1, 2, 3, 4, 5 ... higher # means more orbitals

l is the Angular momentum quantum number

l can be $n-1$ down to 0. The l # is the orbital type

m_l is the magnetic quantum number

m_l # of orbitals of a given type

$m_l = +l \ldots -l$

m_s is the spin quantum number

$m_s = +\frac{1}{2}$

$m_s = -\frac{1}{2}$

$l = 2$ $m_l = ?$

d: 2, 1, 0, −1, −2

in n=1

$n=1$ $l=0$ $m_l=0$ 1s

in n=2

$n=2$ $l=0$ $m_l=0$ 2s

$n=2$ $l=1$ $m_l=1$ $2p_x$

$m_l=0$ $2p_y$

$m_l=-1$ $2p_z$

in $n=4$ l can be 3, 2, 1, 0

f, d, p, s

Orbitals (n, l, and m_l)

$n=1 \quad l=0 \quad m_l=0 \quad m_s=+\frac{1}{2}$

$n=1 \quad l=0 \quad m_l=0 \quad m_s=+\frac{1}{2}$

$n=1 \quad l=0 \quad m_l=0 \quad m_s=-\frac{1}{2}$

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

$n=1$

$n=2$

f $l=3$

d $l=2$

1 2 3 4 5 6

p

$l=0$

Be

$n=1$	$l=0$	$m_l=0$	$m_s=+\frac{1}{2}$	e_1
$n=1$	$l=0$	$m_l=0$	$m_s=-\frac{1}{2}$	e_2
$n=2$	$l=0$	$m_l=0$	$m_s=\frac{1}{2}$	e_3
$n=2$	$l=0$	$m_l=0$	$m_s=-\frac{1}{2}$	e_4

$1s^2 \; 2s^2$

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/effective nuclear charge

Π_c = coulomb repulsion

-bad

-number of paired electrons

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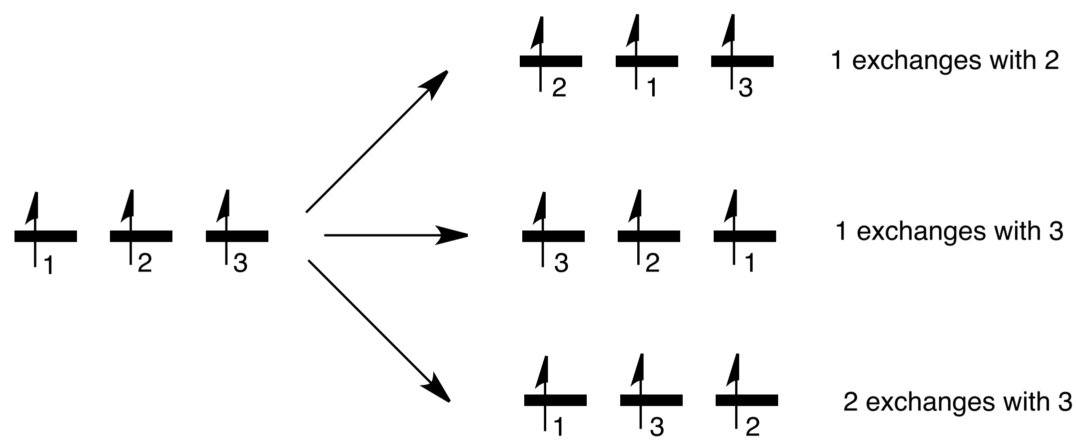
Π_e = exchange energy
-good in the case of parallel electrons in an atom
-number of exchanges that can be made and produce identical electron configurations

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,



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Wave Functions

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