

# Orbitals and their Wavefunctions

Shells	Subshells	Orbitals
$M$ $n = 3$	$l = 2$ $d$	$+2 +1 0 -1 -2$ $3d$
	$l = 1$ $p$	$+1 0 -1$ $3p$
	$l = 0$ $s$	$0$ $3s$
$L$ $n = 2$	$l = 1$ $p$	$+1 0 -1$ $2p$
	$l = 0$ $s$	$0$ $2s$
$K$ $n = 1$	$l = 0$ $s$	$0$ $1s$
$n$	$l$	$m_l$

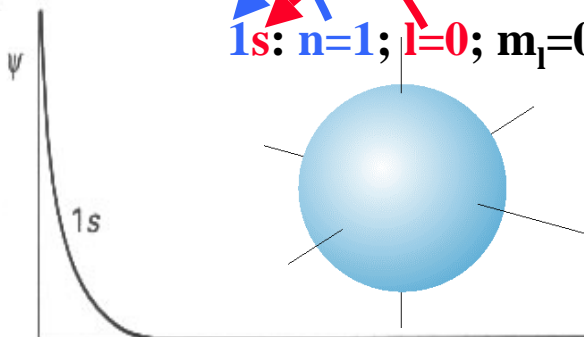
$n^2$  different orbitals

$$\Psi = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}; \quad a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_e e^2}$$

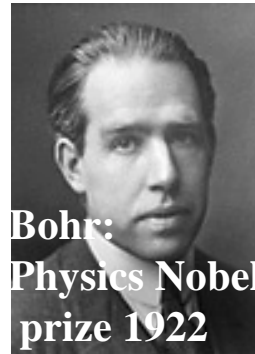
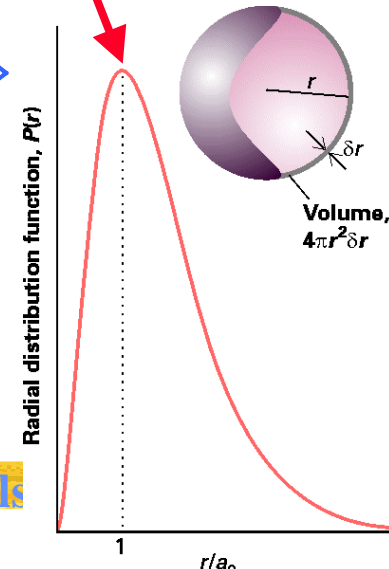
Wave-function

Bohr radius  $a_0 = 52.9\text{pm}$

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



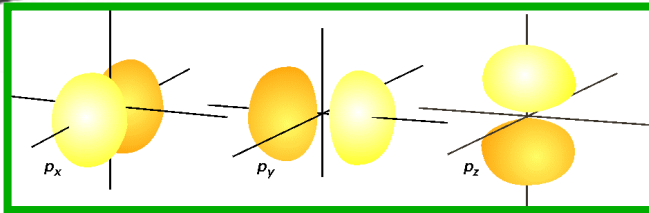
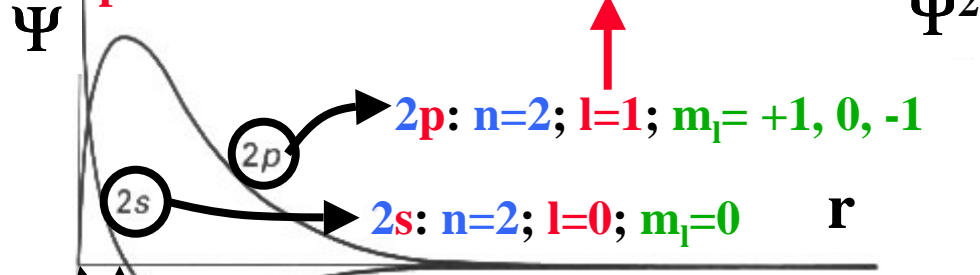
Probability to find electron between two spherical surfaces (area  $4\pi r^2$ ) of thickness  $\delta r$   
 $= 4\pi r^2 \Psi^2 \delta r$



Boundary surface is spherically symmetric

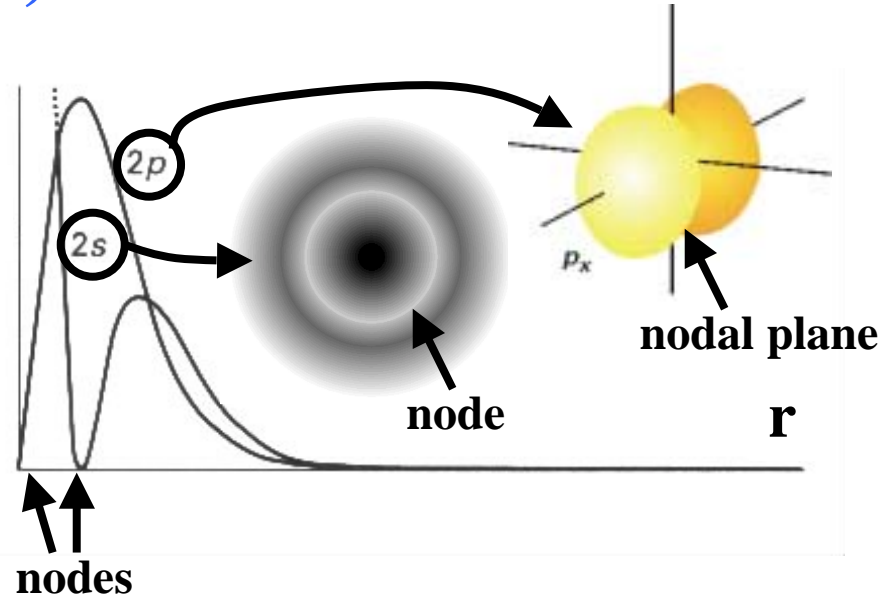
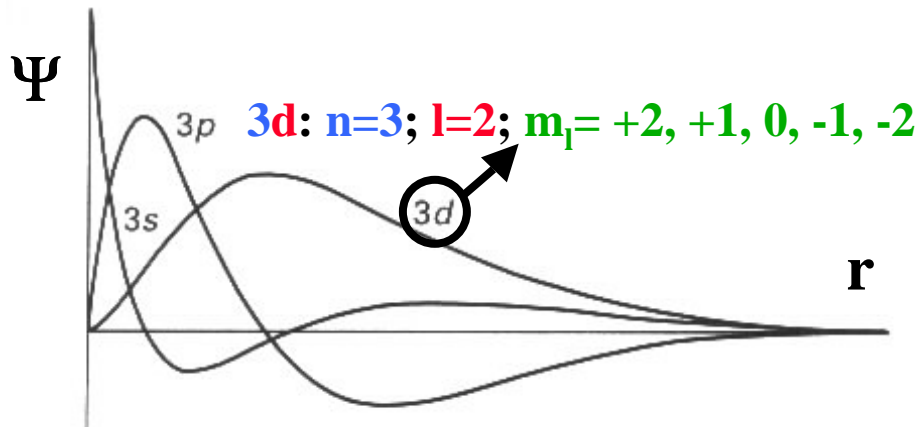
# Wavefunctions: s, p, and d Orbitals

Quantized angular momentum  $= \sqrt{l(l+1)}\hbar$   
 $\Rightarrow$  p electron has node at nucleus

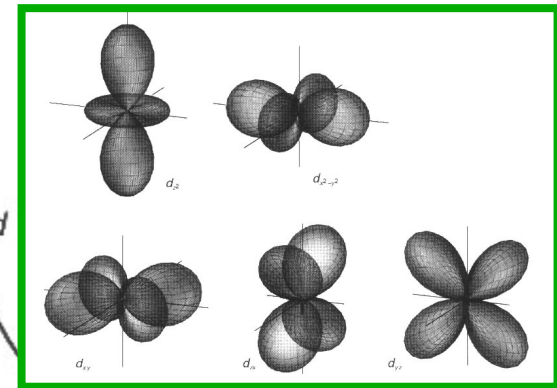


p orbitals:  $m_l = +1, 0, -1$

z component of angular momentum  $= m_l \hbar$



d orbitals:  $m_l = +2, +1, 0, -1, -2$

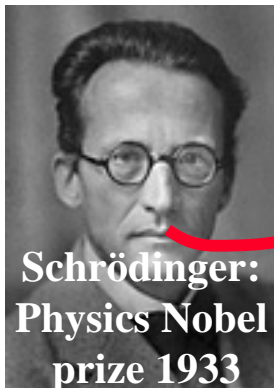


# We Ain't Seen Nothing Yet:

## Many-Electron Atoms

What about atoms  
with 2 electrons  
such as He?

Each electron  
will influence  
all others!



⇒ No analytical, only numerical  
solutions with some “cheating”

⇒ **Orbital approximation:** Each  
electron occupies an **independent**  
orbital, e.g., in He :

$$\Psi = \Psi(1) \times \Psi(2) = \sqrt{\frac{8}{\pi a_0^3}} e^{-2r_1/a_0} \times \sqrt{\frac{8}{\pi a_0^3}} e^{-2r_2/a_0} = \left( \frac{8}{\pi a_0^3} \right) e^{-2(r_1+r_2)/a_0}$$

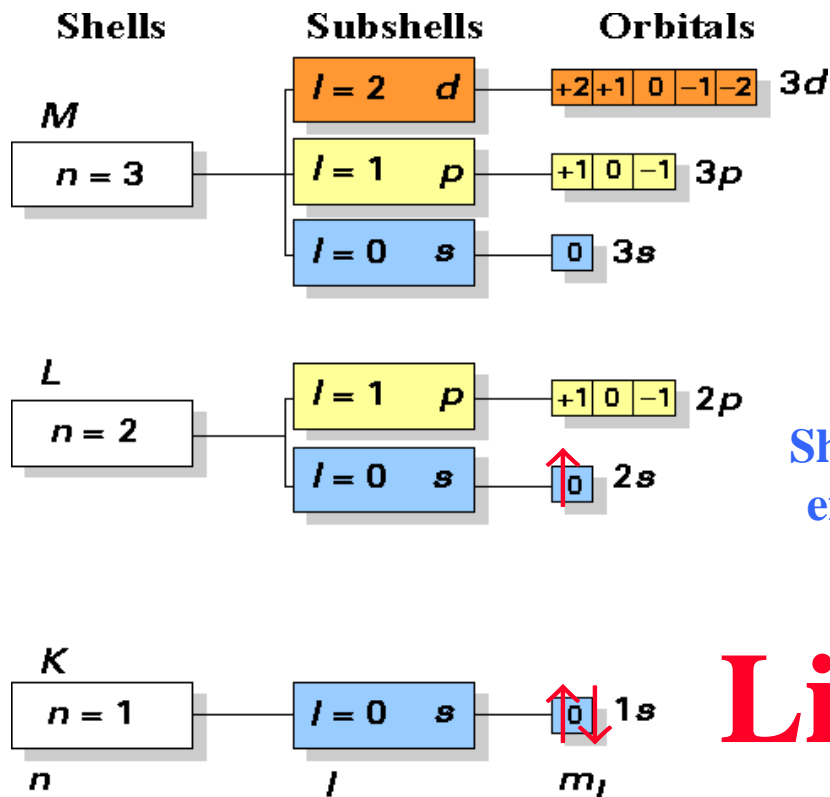
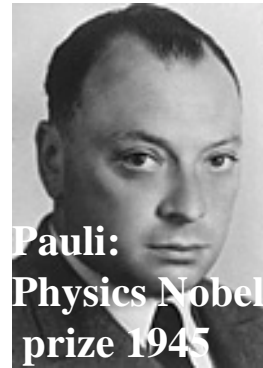
**Overall wavefunction**

**“Configuration”**  
= list of occupied  
orbitals: H =  $1s^1$ ;  
He =  $1s^2$

Li has three electrons with  
configuration  $1s^2 2s^1 = [\text{He}] 2s^1$ ; Why?

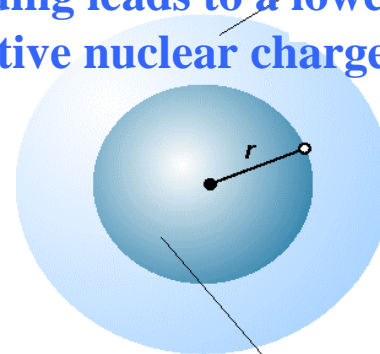
# More and More Electrons

**Pauli Exclusion principle:** No more than 2 electrons may occupy the same orbital; if they do their electrons have to be paired:  $\uparrow\downarrow$ , i.e., one electron is  $m_s = +1/2$ , one  $-1/2$

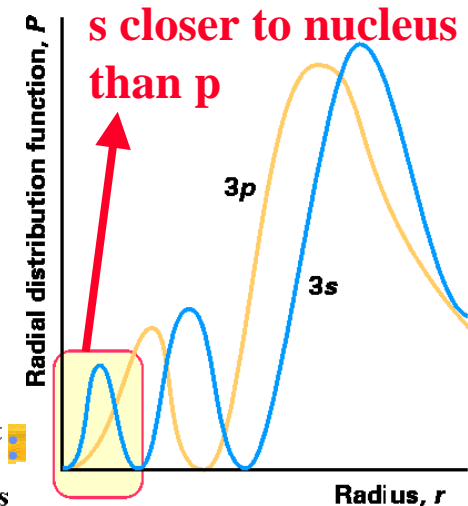


In many-electron atoms orbitals of the same shell are no longer degenerate, i.e., energies:  $s < p < d < f$ , due to their different shielding from the nucleus

Shielding leads to a lower effective nuclear charge



Net effect equivalent to a point negative charge at the nucleus



# Rules for Building up Higher Elements

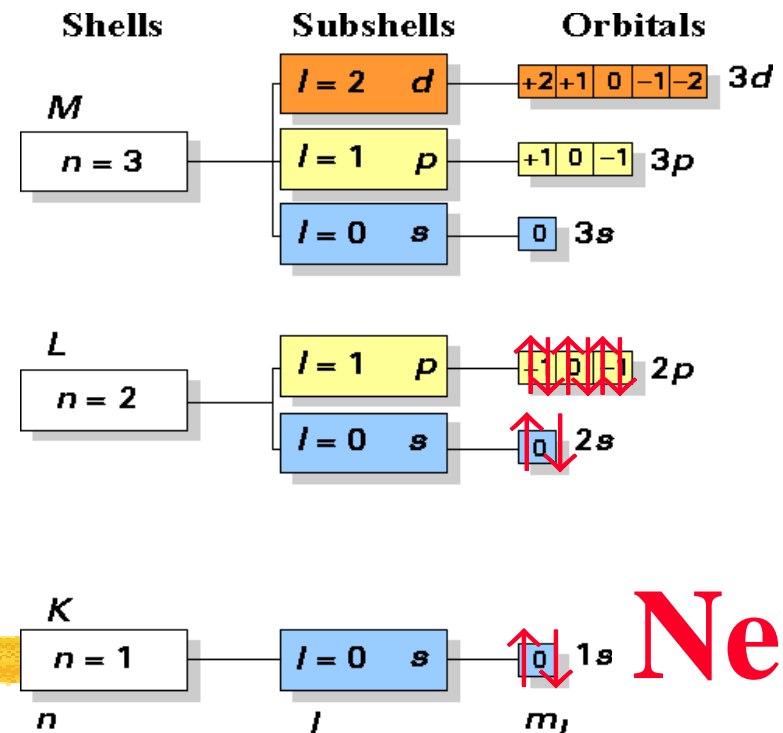
1.) Order of orbital occupation: 1s 2s  
2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 5d 4f 6p...

2.) **Pauli exclusion principle:**  
2 electrons/orbital

3.) Electrons occupy different orbitals of a given subshell before doubly occupying any one of them

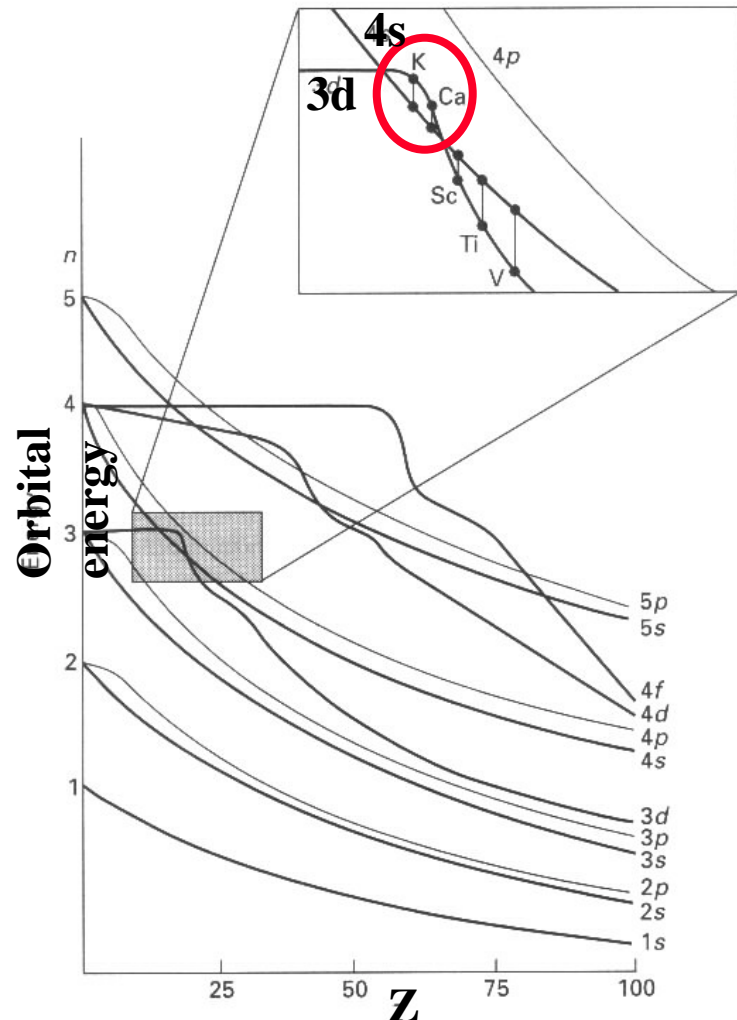
4.) **Hund's rule:**  
In its ground state, an atom adopts a configuration with the greatest number of unpaired electrons

The periodic table shows the order of orbital filling. The s-block includes groups 1 and 2. The p-block includes groups 13-18. The d-block includes transition metals (groups 3-10). The f-block includes lanthanides and actinides. The table is color-coded to show the sequence of filling: 1s (blue), 2s (orange), 2p (yellow), 3s (blue), 3p (yellow), 4s (orange), 3d (blue), 4p (yellow), 5s (orange), 4d (blue), 5p (yellow), 6s (orange), 4f (blue), 5d (blue), 6p (yellow), 7s (orange), 5f (blue), 6d (blue), 7p (yellow).

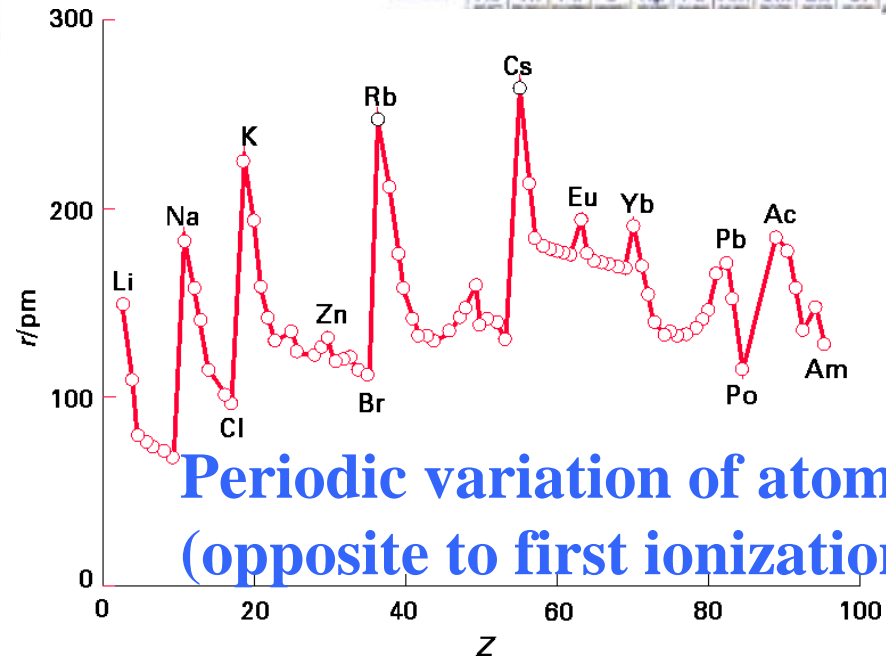


# The Periodic Table of the Elements

Order of orbital occupation: 1s 2s 2p  
3s 3p 4s **3d** 4p 5s 4d 5p 6s 5d 4f 6p...



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36																								
H	He																	Li	Be	B	C	N	O	F	Ne																																		
																		Na	Mg	Al	Si	P	S	Cl	Ar																																		
																		K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr																								
																		Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe																								
																		Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn										
																		Fr	Ra																	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No										



Periodic variation of atomic radius  
(opposite to first ionization energy)

