Quantum Numbers

Quantum Numbers

each orbital is characterized by a unique set of quantum numbers

principal quantum number: $\boldsymbol{n}$

angular momentum quantum number: $\boldsymbol{l}$ **(azimuthal)**

magnetic quantum number: $\boldsymbol{m_l}$

Principal quantum number: *n*

related to size and energy of orbital
shells: integral values: 1, 2, 3, ...

higher *n*

the electron, on average, is farther from nucleus

the electron less strongly bound by nucleus

(higher energy potential)

Angular momentum quantum number: *l*

related to shape of orbital

subshells:

integral values: 0, 1, 2, …, n - 1

l = 0: *s* orbital **l = 2: *d* orbital**

l = 1: *p* orbital **l = 3: *f* orbital**

Relation of n and l

$n = 1$	$l = 0$	1s
$n = 2$	$l = 0, 1$	2s, 2p
$n = 3$	$l = 0, 1, 2$	3s, 3p, 3d
$n = 4$	$l = 0, 1, 2, 3$	4s, 4p, 4d, 4f

Magnetic quantum number: m_l

related to orientation of orbital in space

integral values between l and $-l$

Atomic Orbitals

Relation of l and m_l

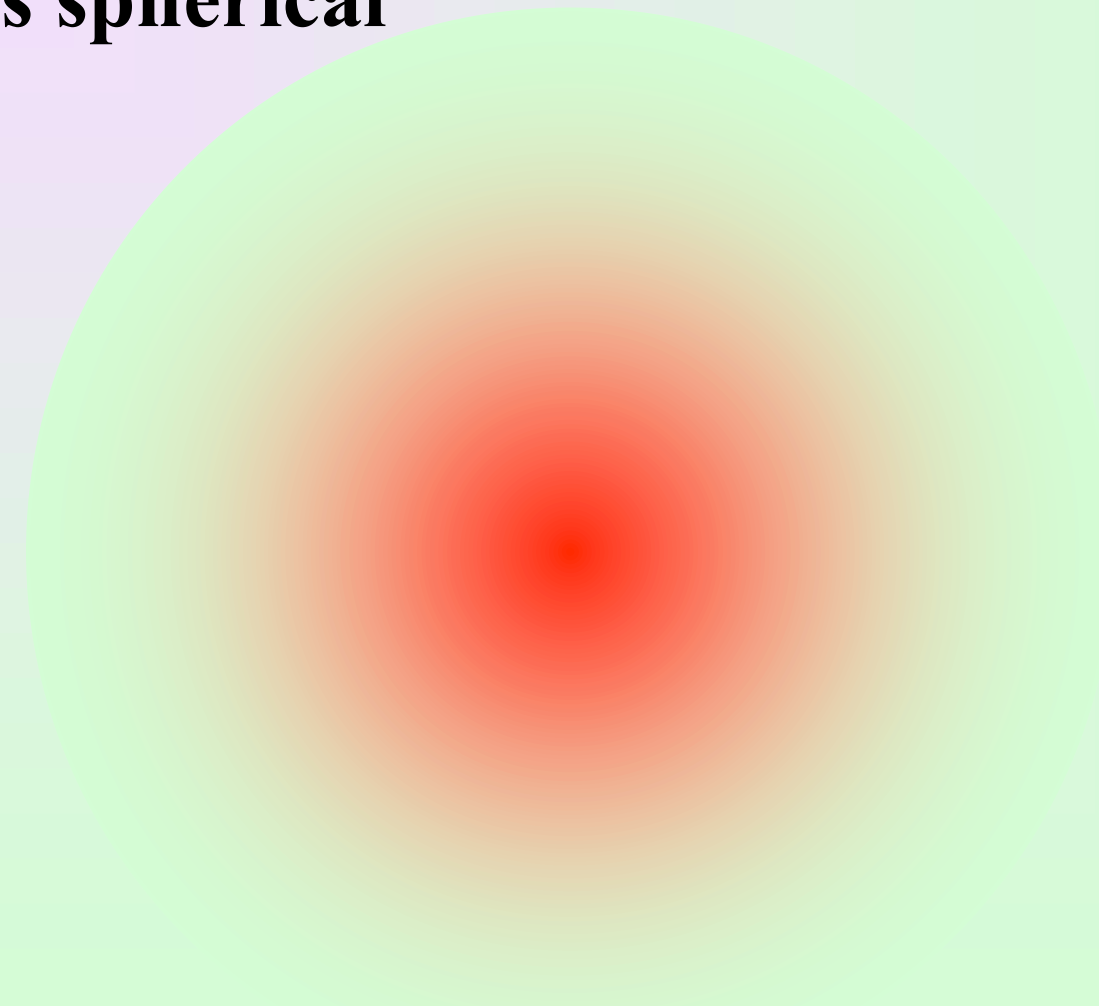
s: $l = 0$ $m_l = 0$

p: $l = 1$ $m_l = -1, 0, 1$

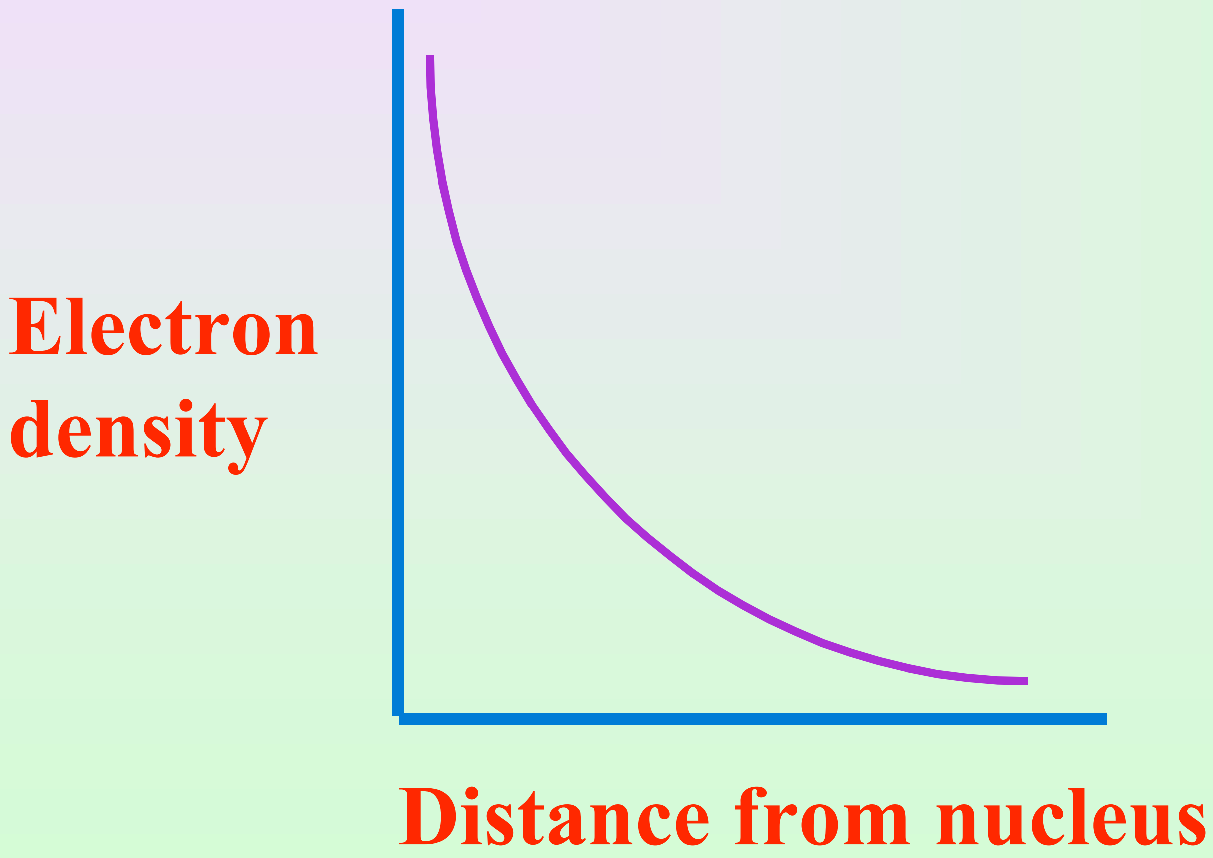
d: $l = 2$ $m_l = -2, -1, 0, 1, 2$

f: $l = 3$ $m_l = -3, -2, -1, 0, 1, 2, 3$

Probability distribution for an electron in a 1*s* orbital is spherical



Probability of finding an electron in a 1*s* orbital at a certain distance on a line originating at the nucleus



Boundary surface encloses 90% of the total electron probability

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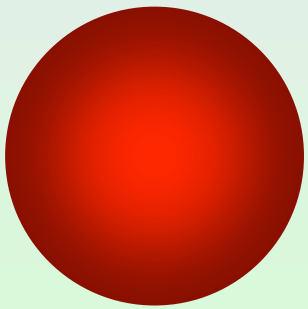
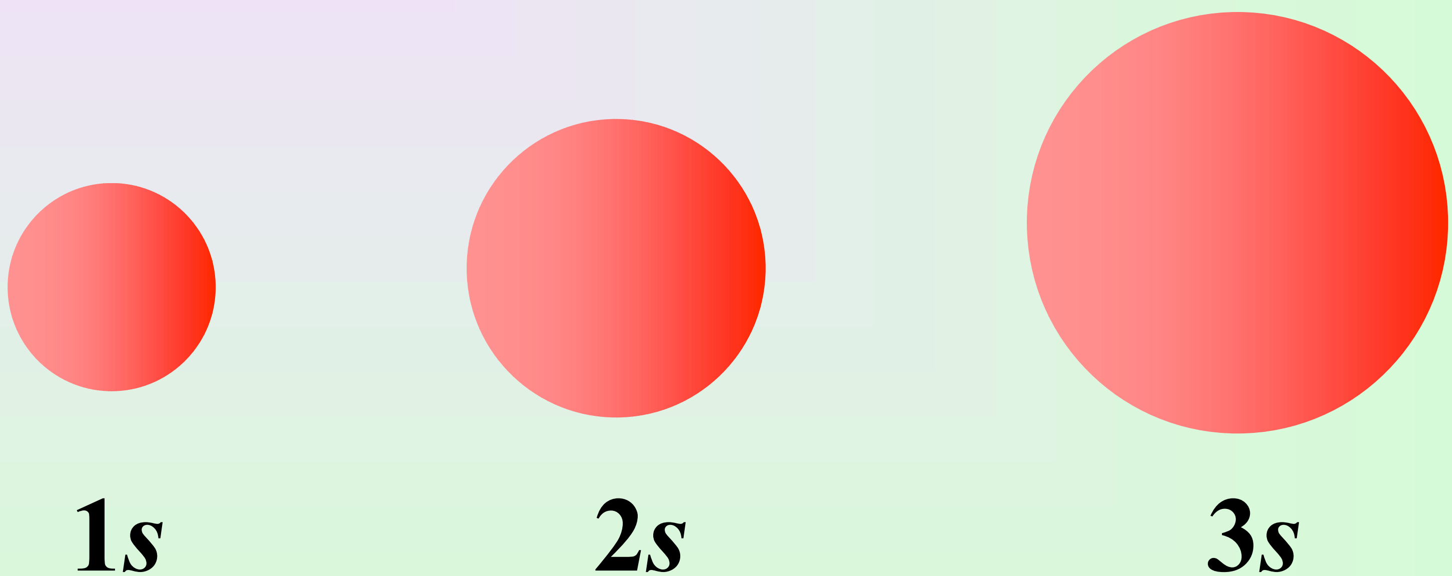
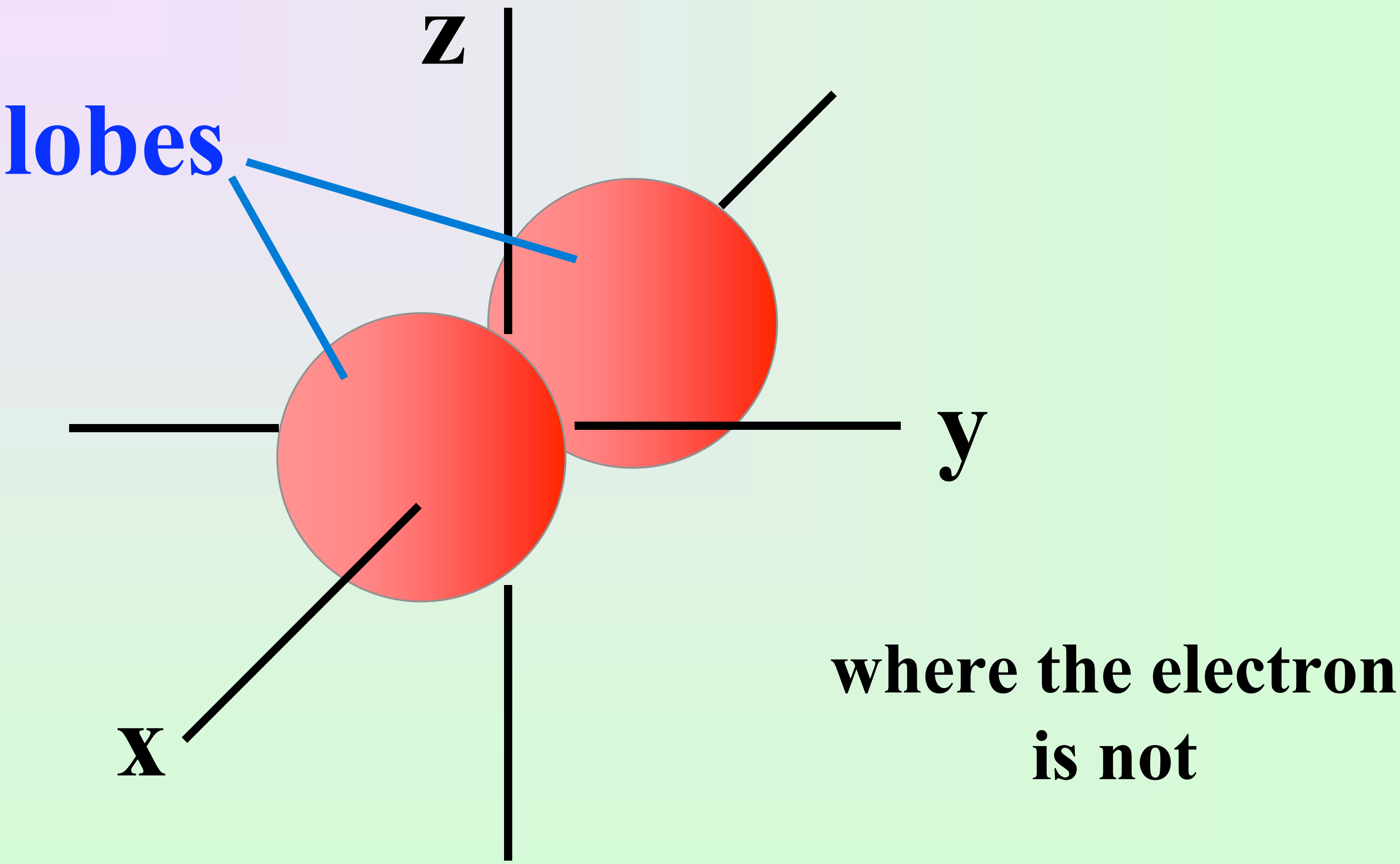
Chemists approximate an orbital by the volume enclosed by the boundary surface



s orbital boundary surfaces

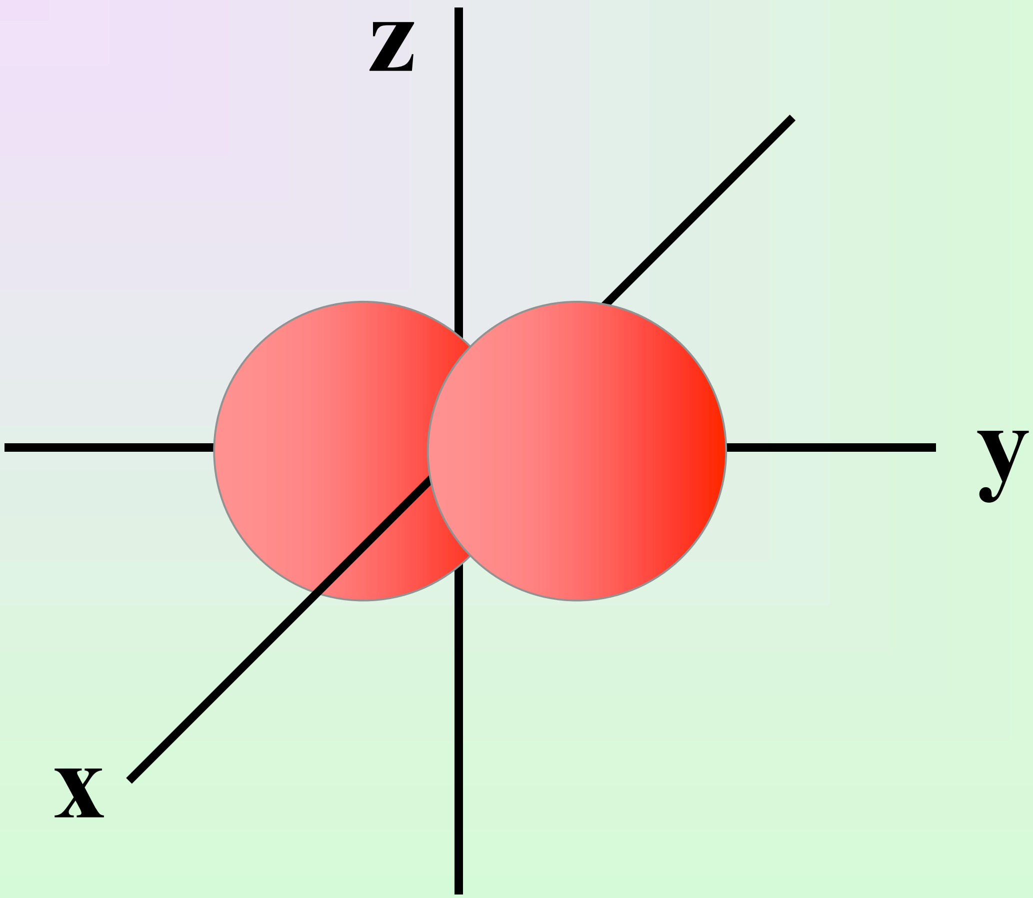


$2p_x$ orbital boundary surface

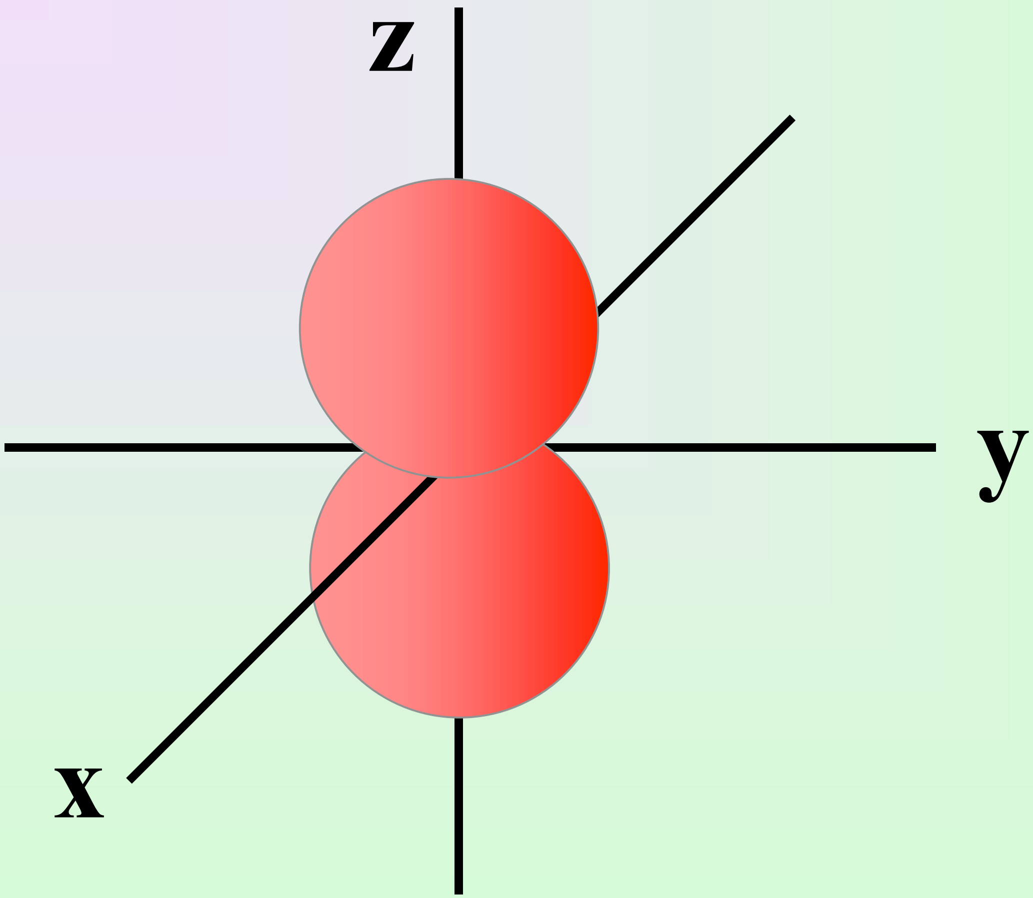


yz plane is a nodal plane

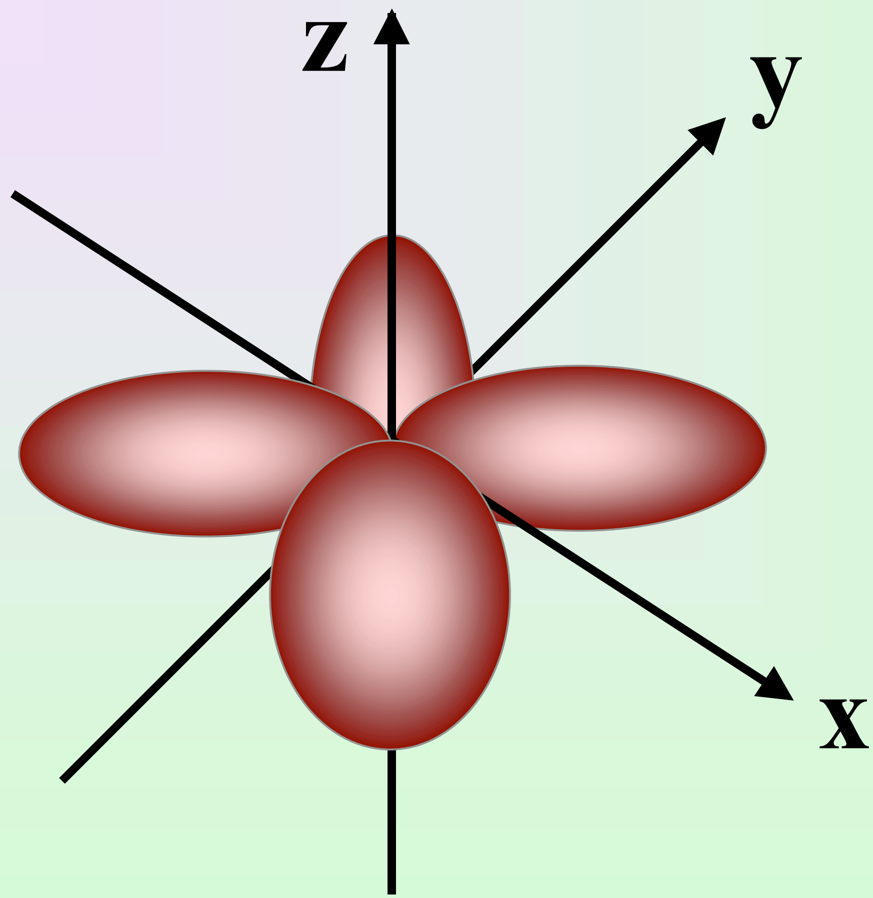
$2p_y$ orbital boundary surface



$2p_z$ orbital boundary surface

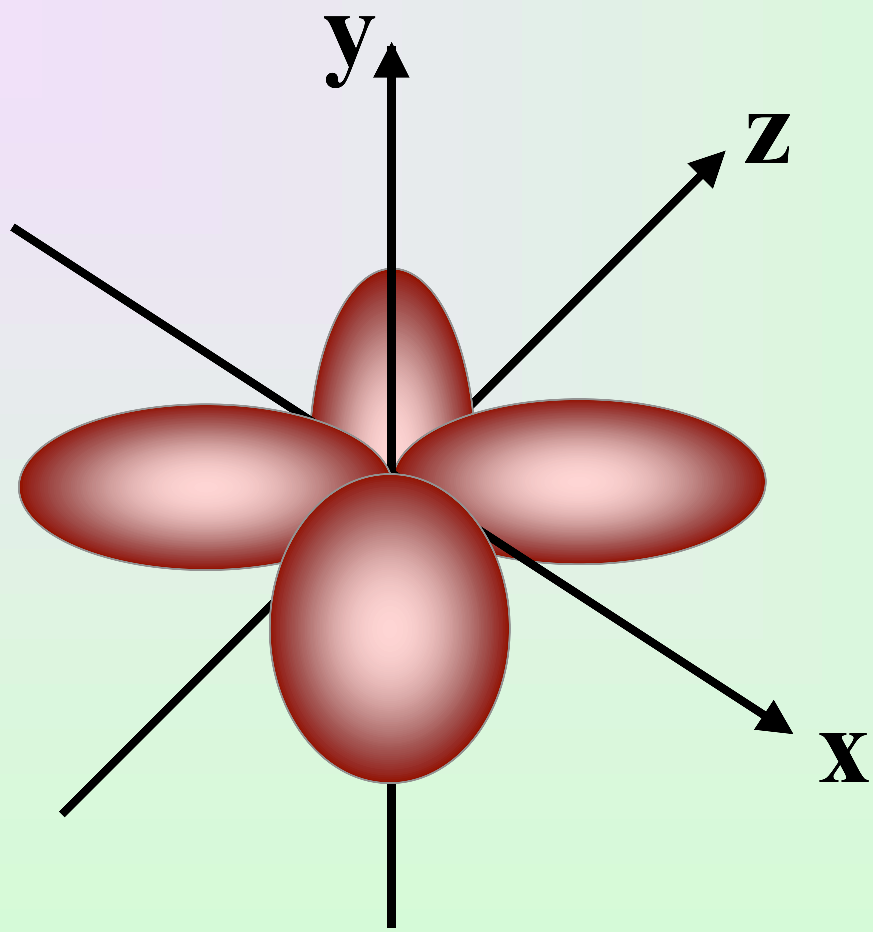


$3d_{xy}$ orbital boundary surface



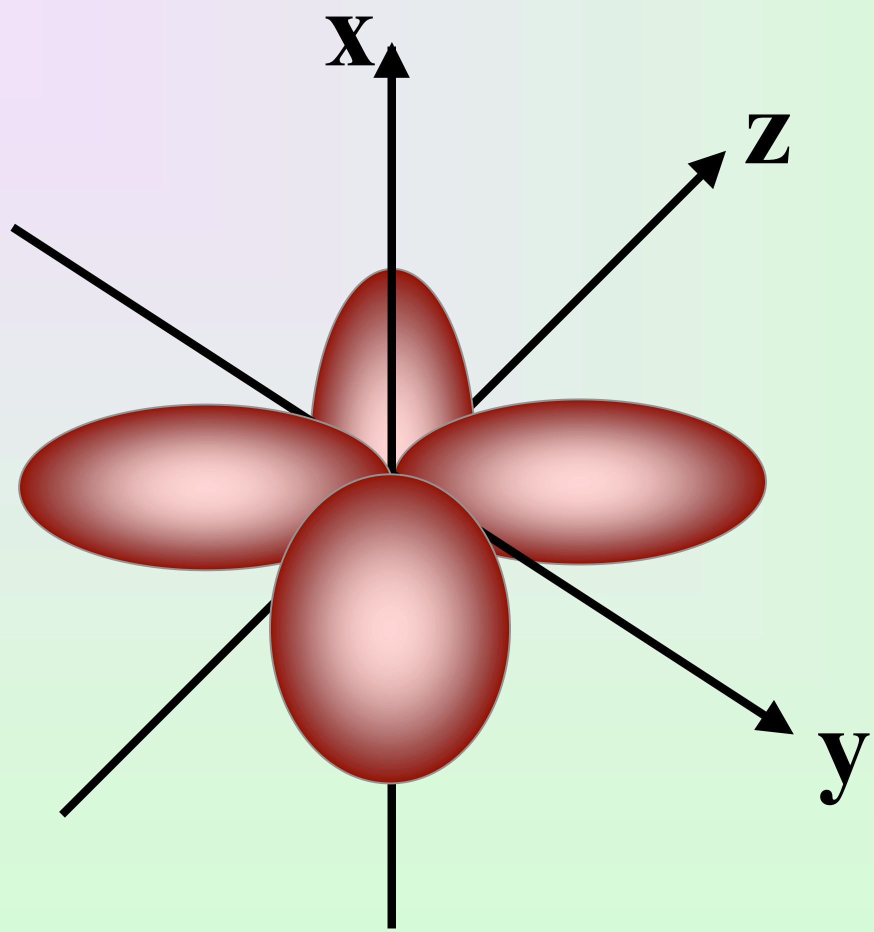
d_{xy}

$3d_{xz}$ orbital boundary surface



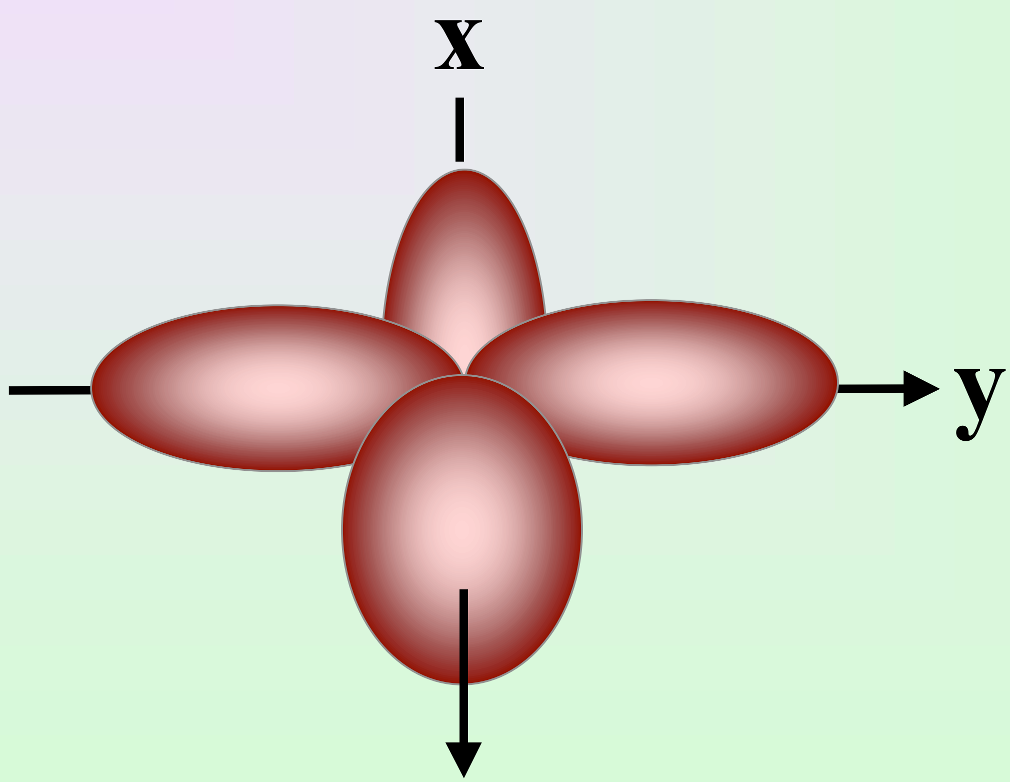
d_{xz}

3d$_{yz}$ orbital boundary surface



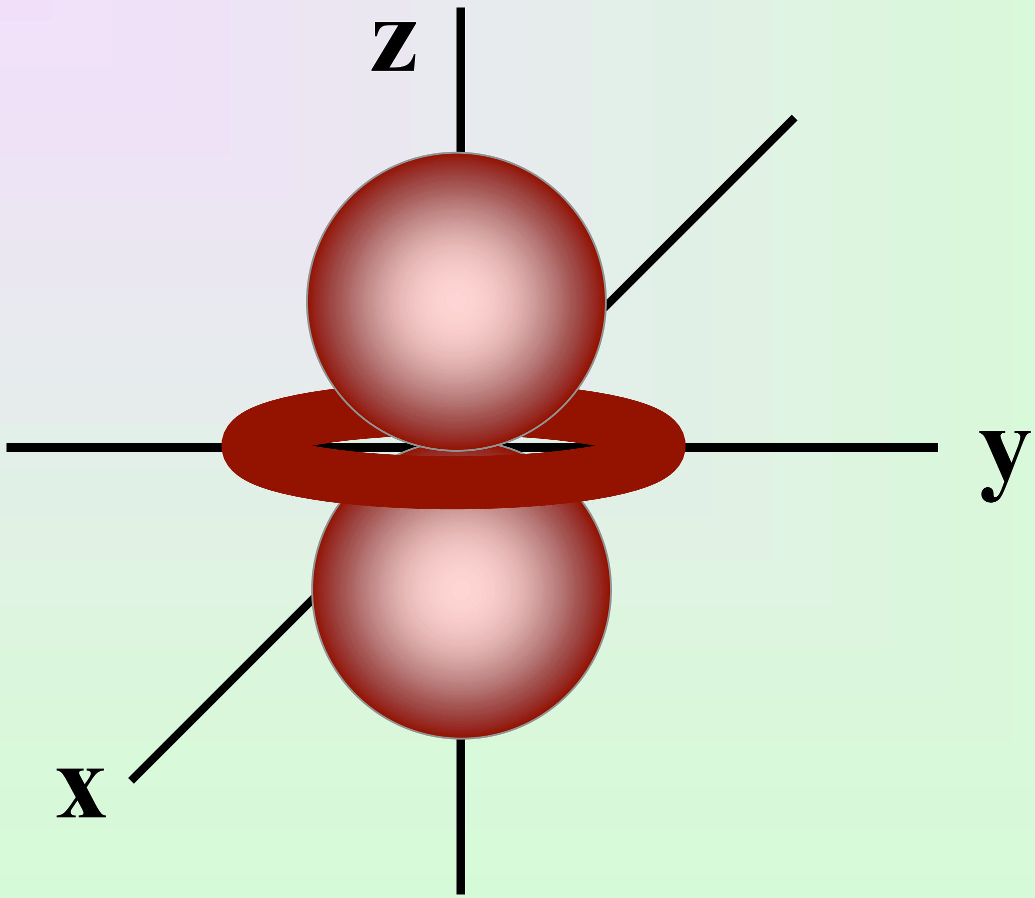
d_{yz}

$3d_{y^2-x^2}$ orbital boundary surface



$d_{y^2-x^2}$

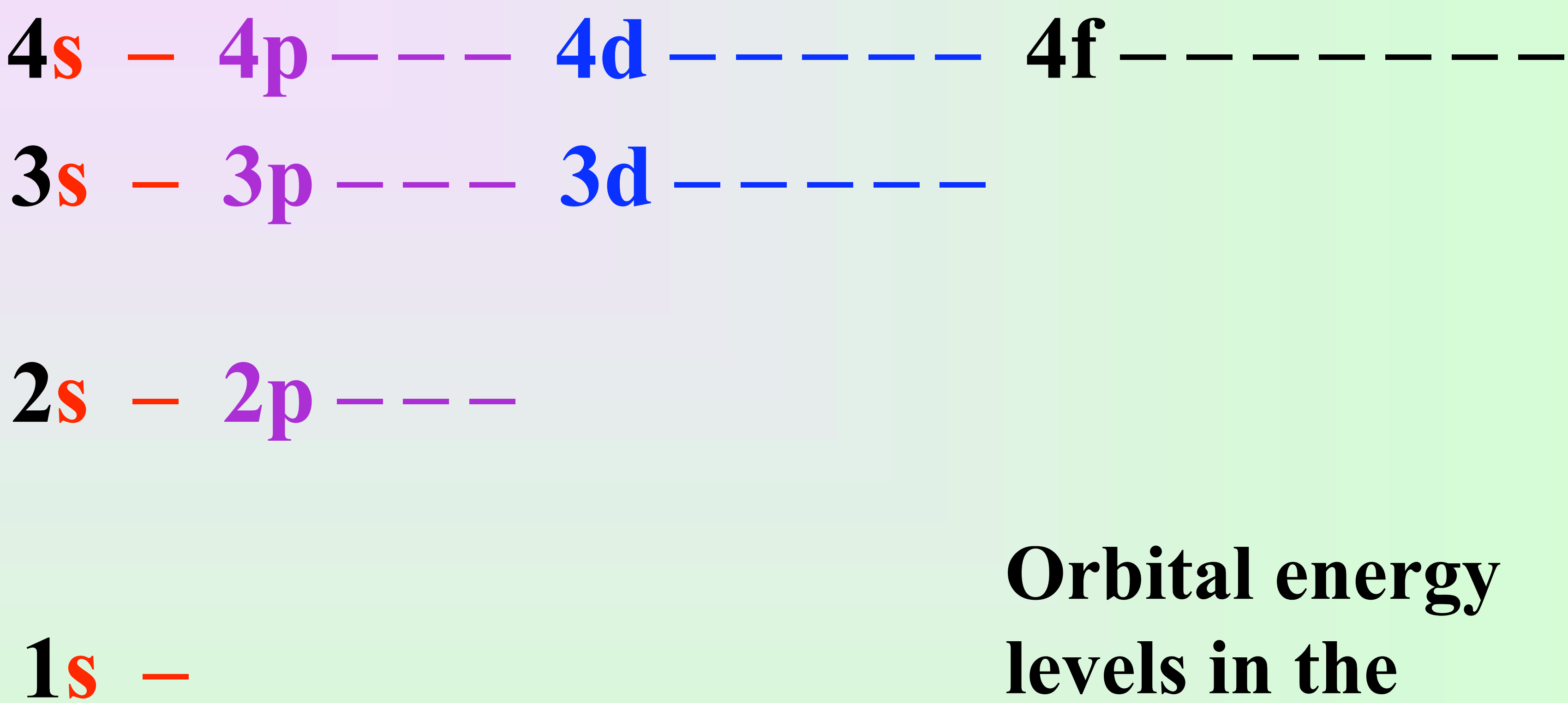
$3d_{z^2}$ orbital boundary surface



energies of hydrogen orbitals

for the hydrogen, all orbitals with the same principal quantum number have the same energy

i.e., they are "degenerate"

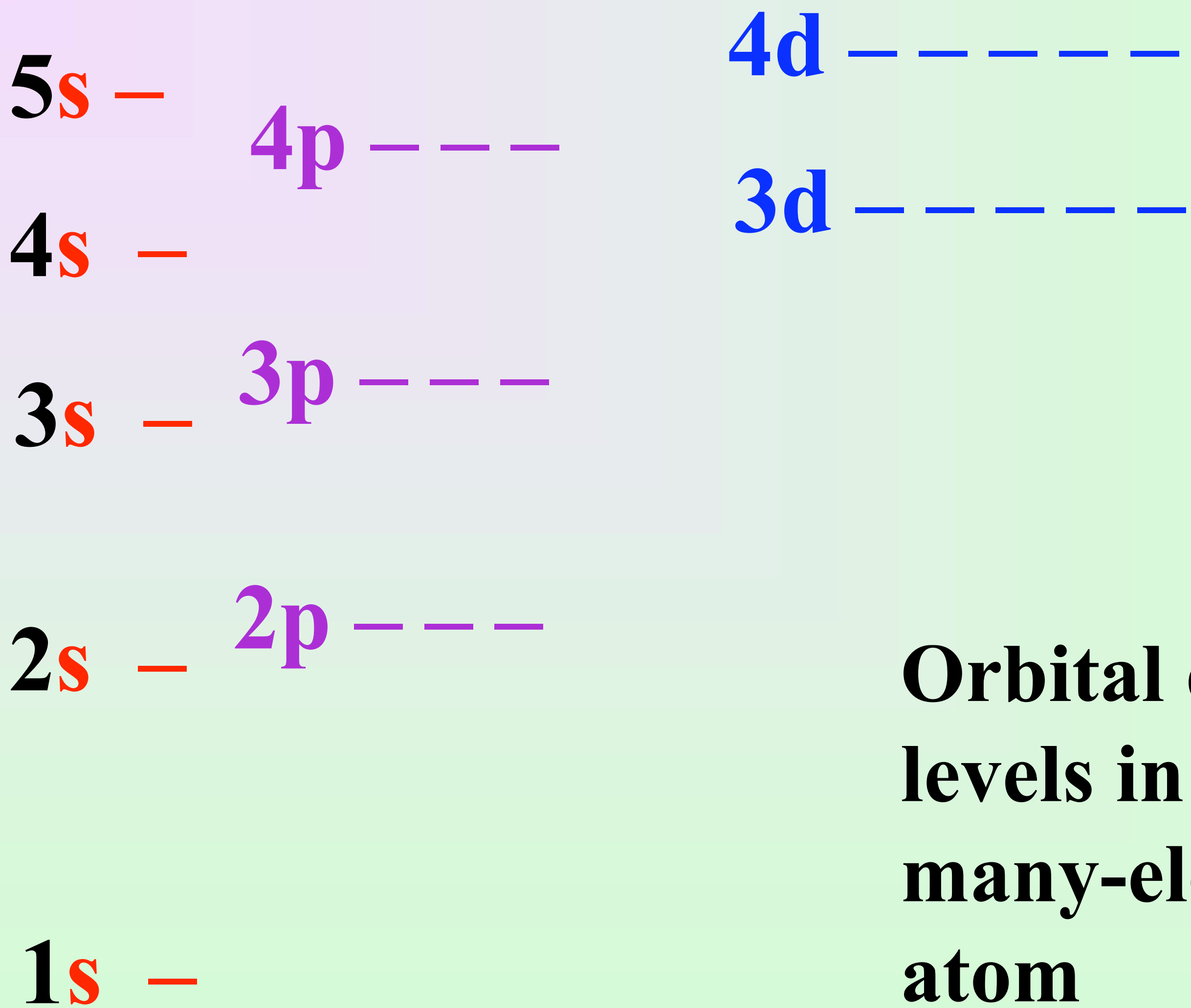


Orbital energy levels in the hydrogen atom

energies of multi-electron orbitals

for a many-electron atom, the energy depends on both the principal quantum number and the angular momentum quantum number

i.e., each subshell represents a different energy in a multi-electron system



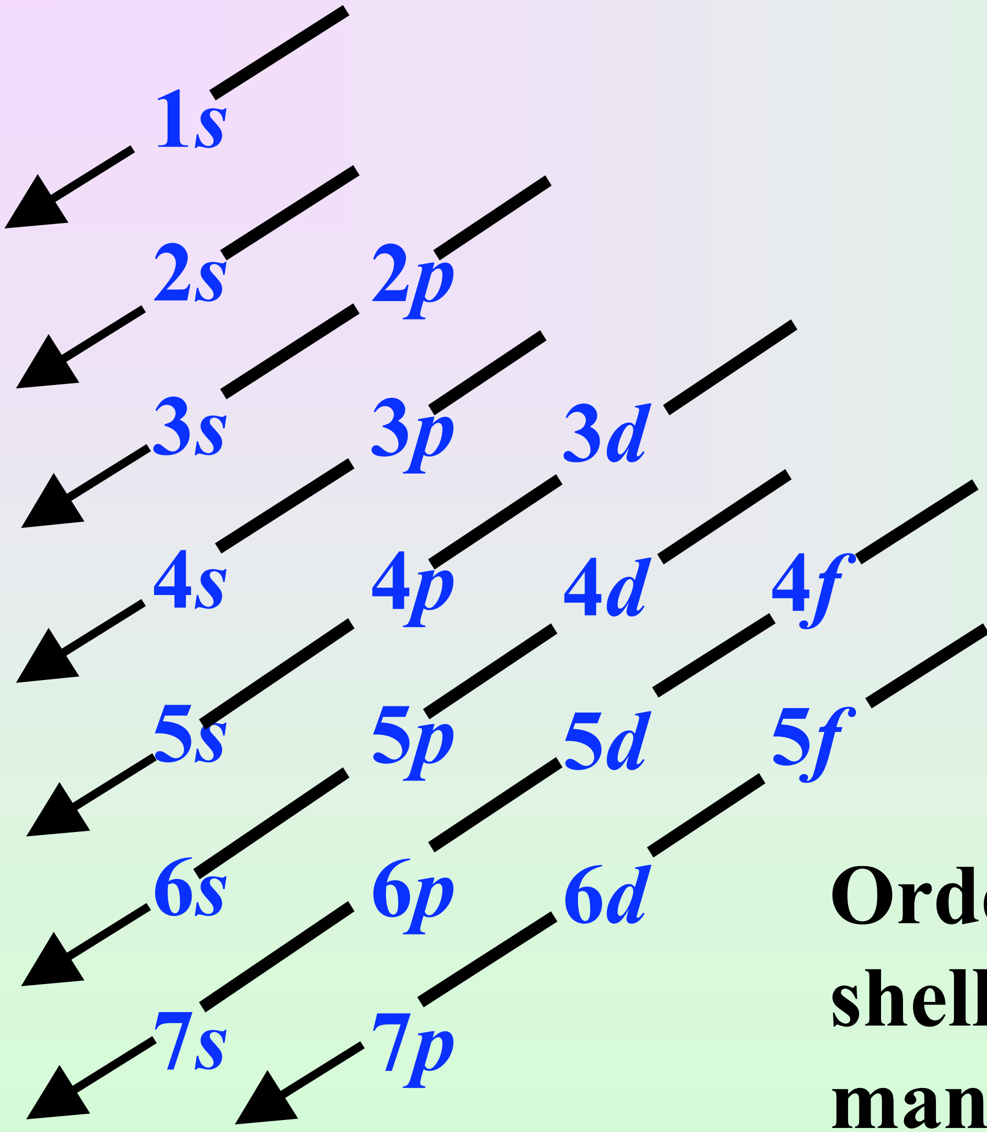
Orbital energy levels in a many-electron atom

Shielding Effect

in a many-electron atom, electrons in the 1*s* orbital shield the electrons located in the 2*s* and 2*p* orbitals from the electrostatic attraction of the protons in the nucleus

2*s* electron density is greater near the nucleus than 2*p* electron density

2*s* orbital is said to be more "penetrating" and is less shielded than the 2*p*



Order in which sub-shells are filled in a many-electron atom