Quantum Numbers

Quantum Numbers

principal quantum number: n

angular momentum quantum number: l
(azimuthal)

magnetic quantum number: m_l

Principal quantum number: *n*

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

higher *n*

the electron 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

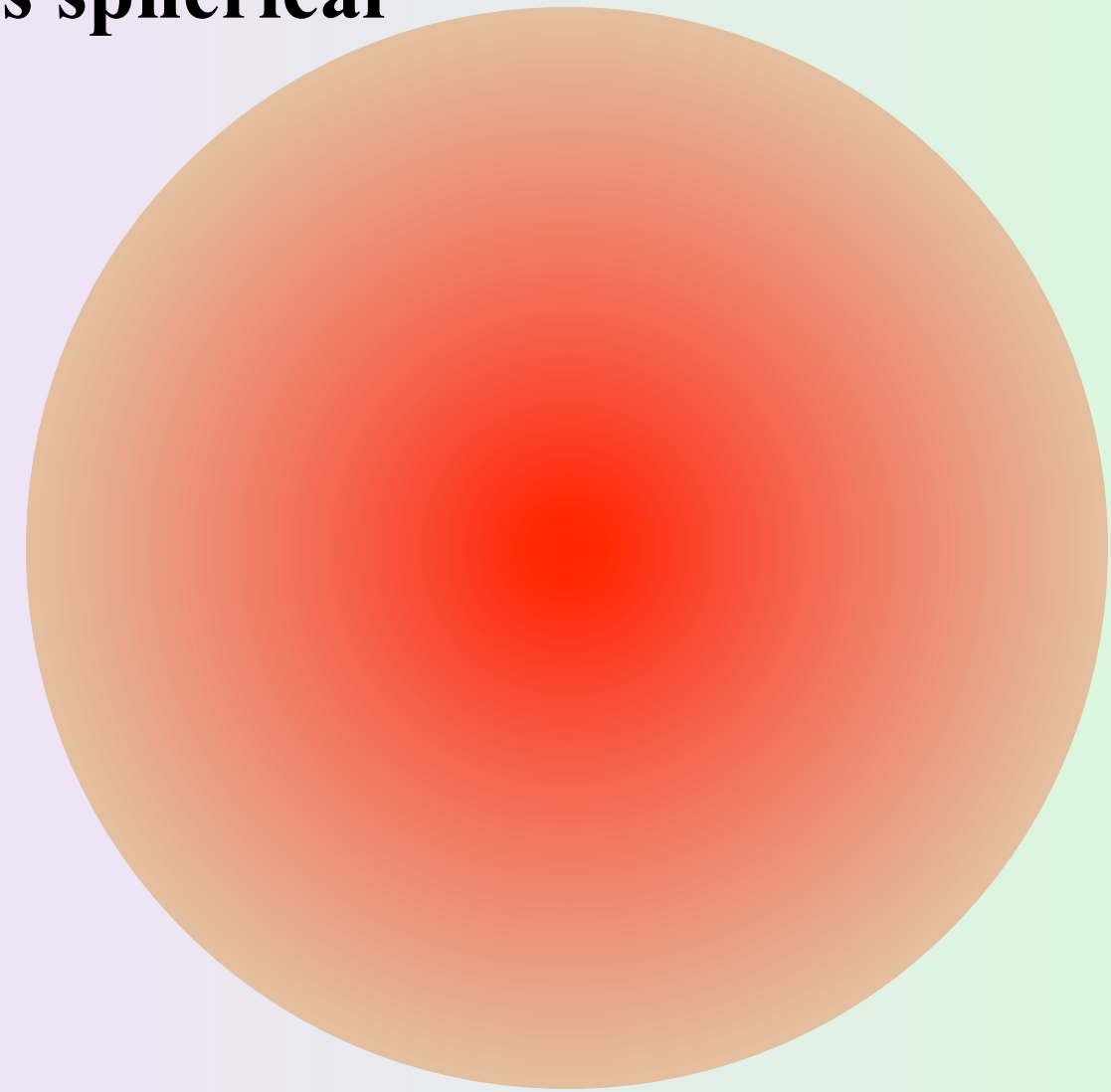
related to the three-dimensional orientation of orbital in space

integral values between *l* and -*l*

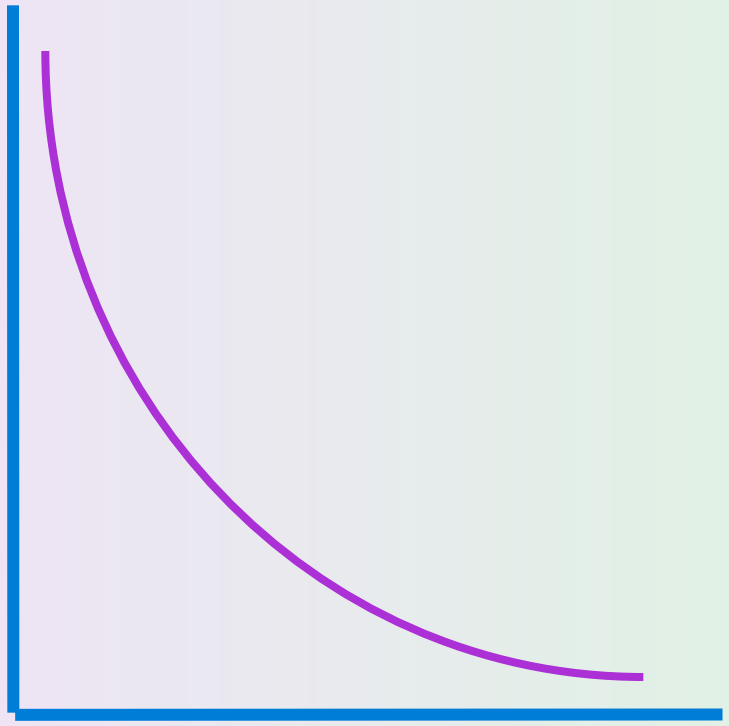
Relation of l and m_l

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

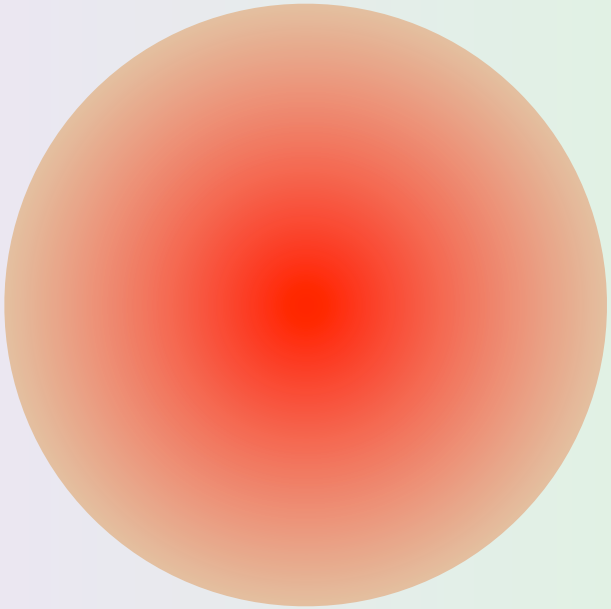
Probability distribution for an electron in a 1*s* orbital is spherical



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

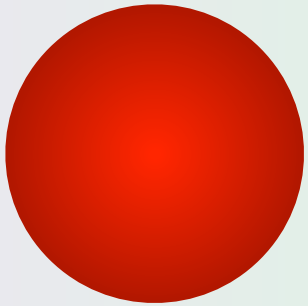


Boundary surface encloses 90% of the total electron probability

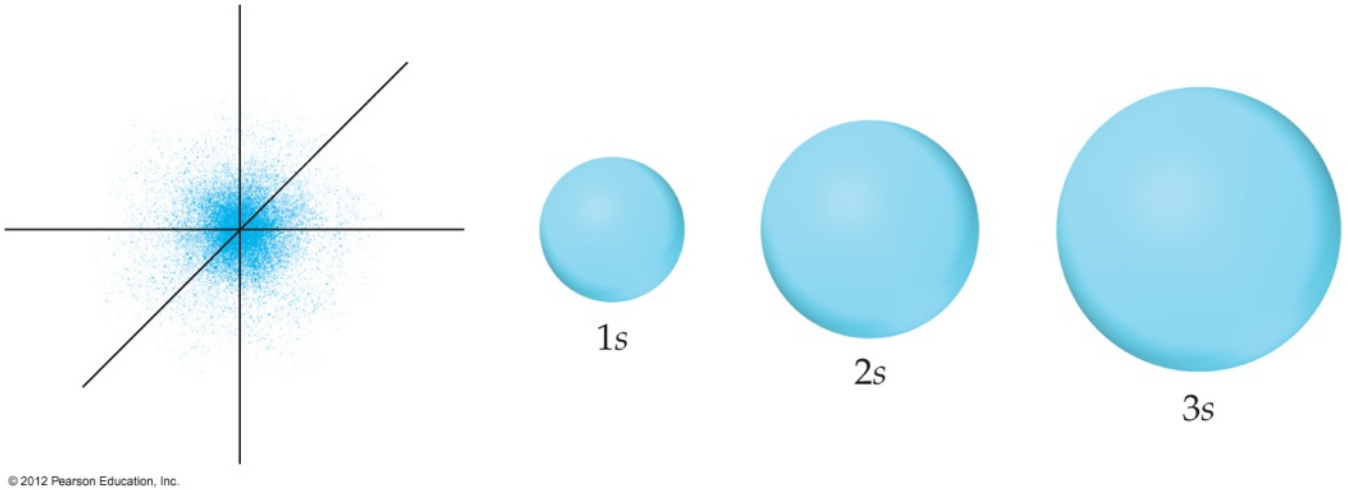


Boundary surface encloses 90% of the total electron probability

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



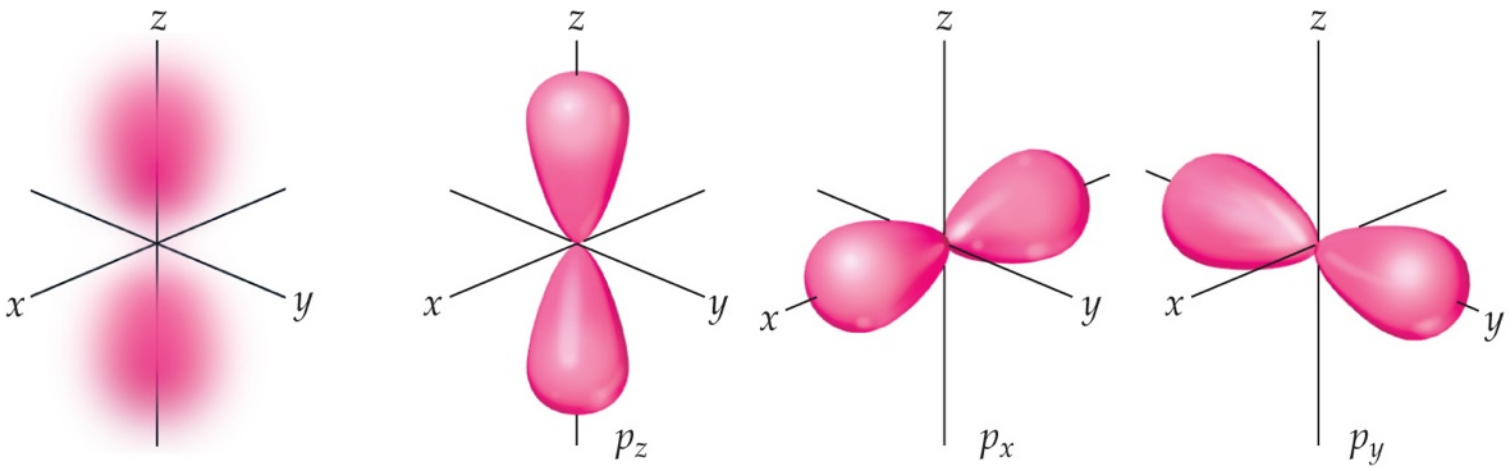
s Orbitals



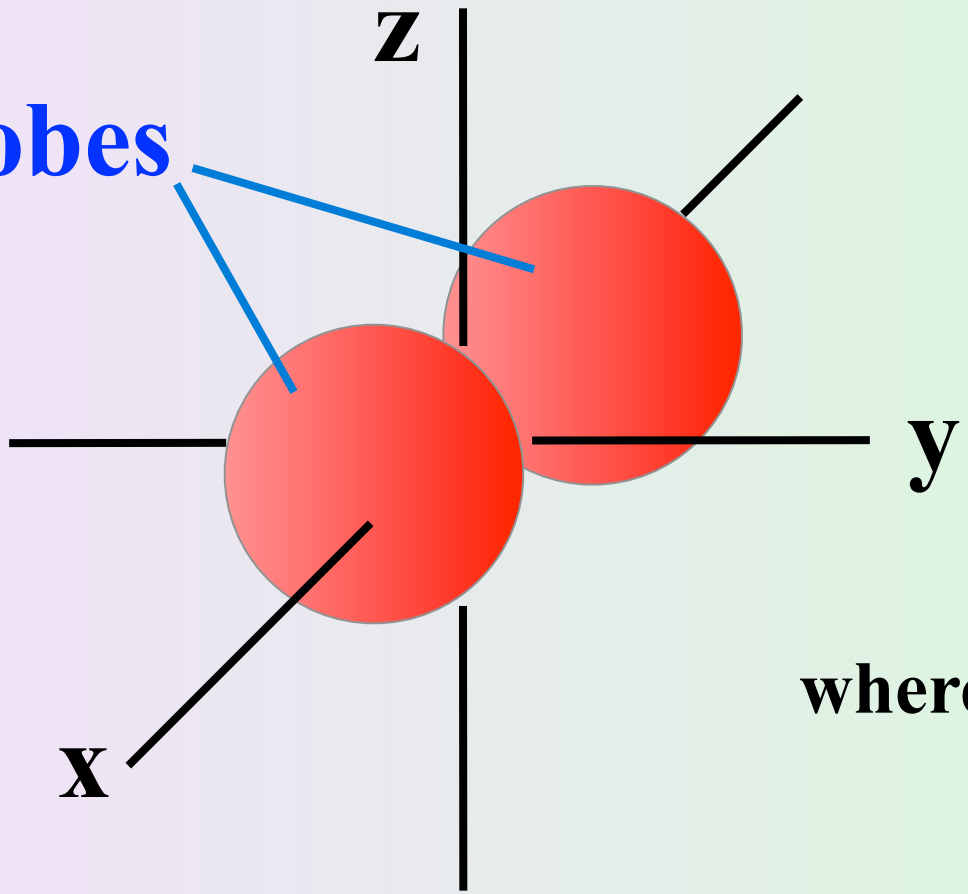
- The value of *l* for *s* orbitals is 0.
- They are spherical in shape.
- The radius of the sphere increases with the value of *n.*

p Orbitals

- The value of *l* for *p* orbitals is 1.
- They have two lobes with a node between them.



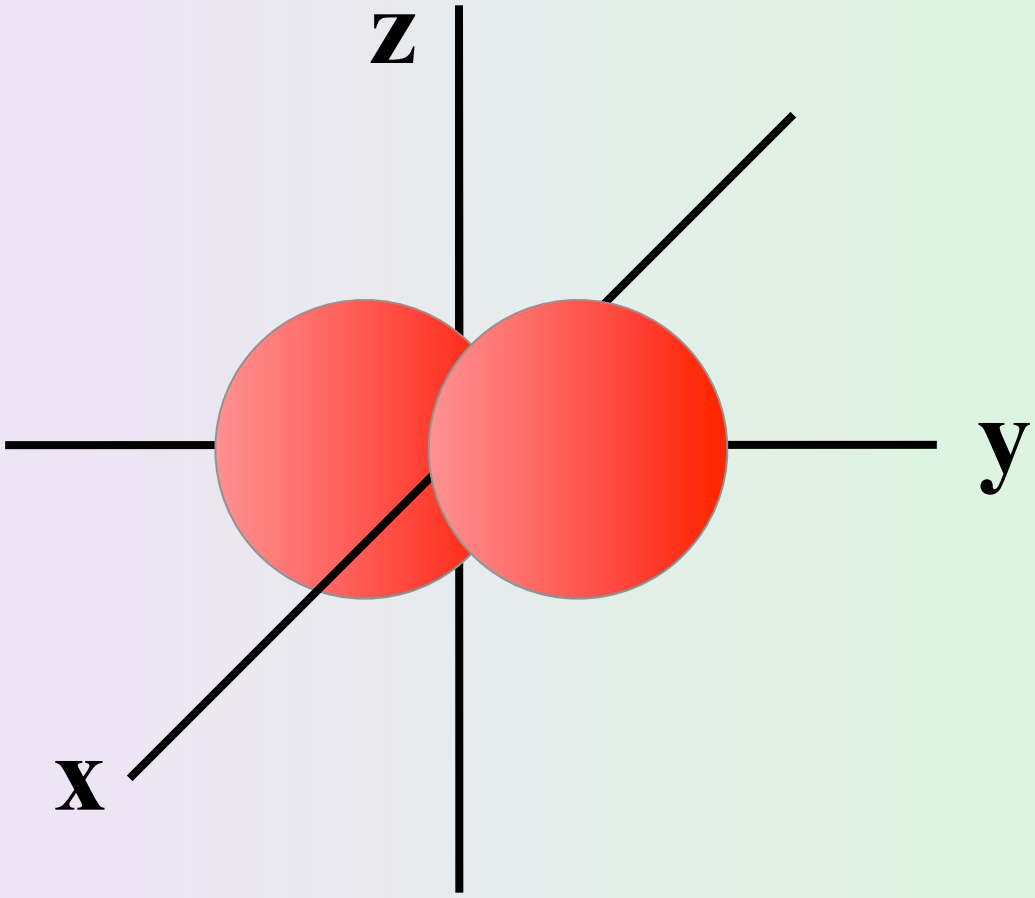
$2p_x$ orbital boundary surface



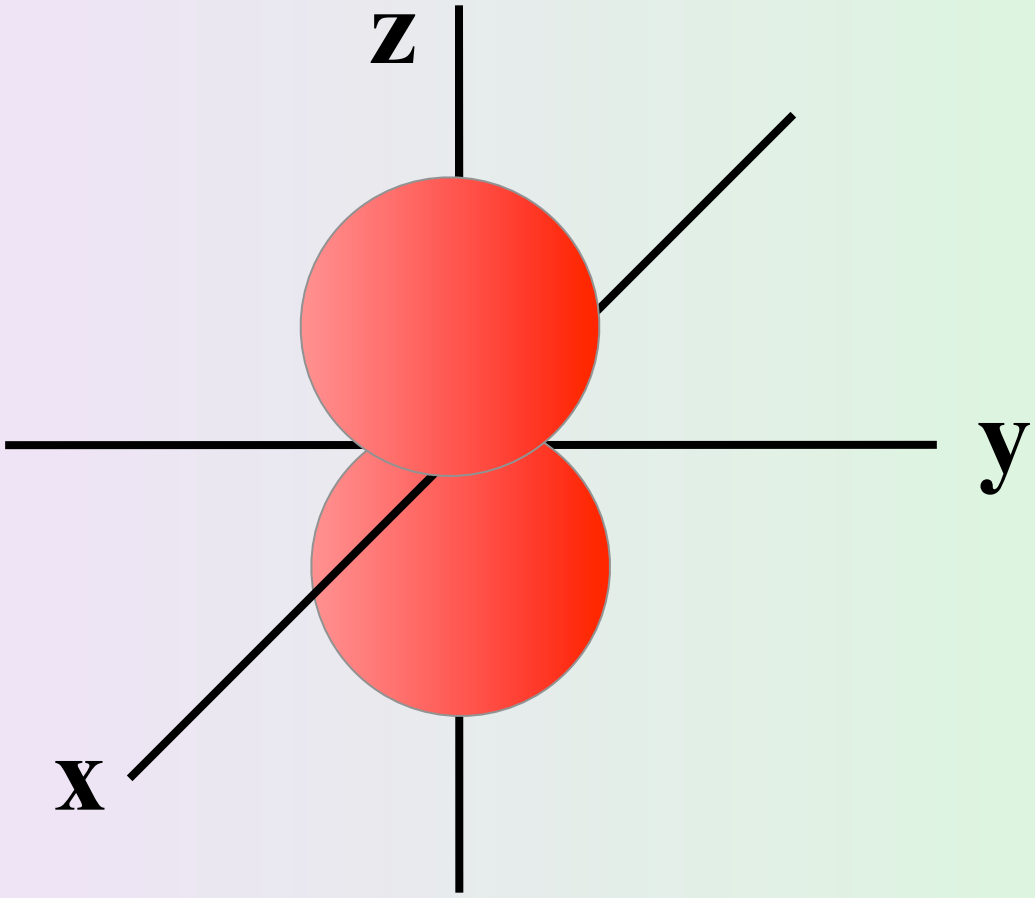
where the electron is not

yz plane is a nodal plane

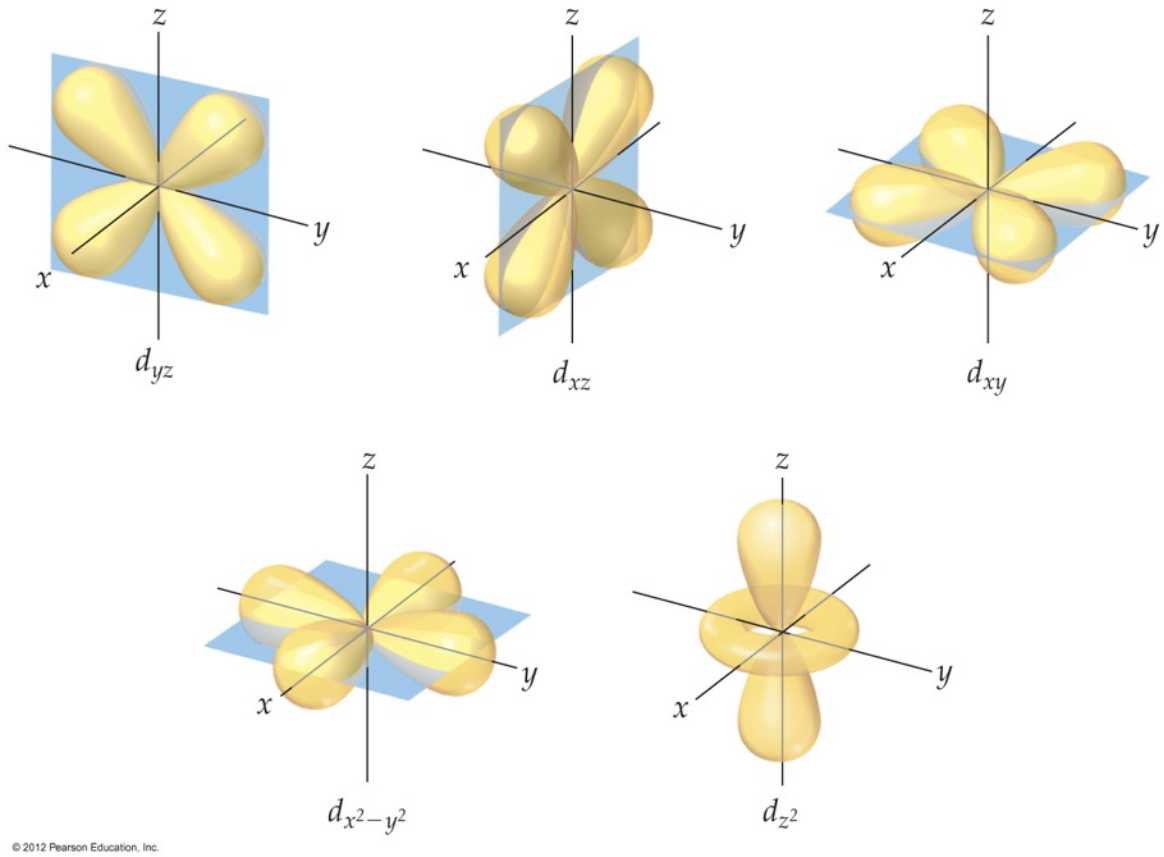
$2p_y$ orbital boundary surface



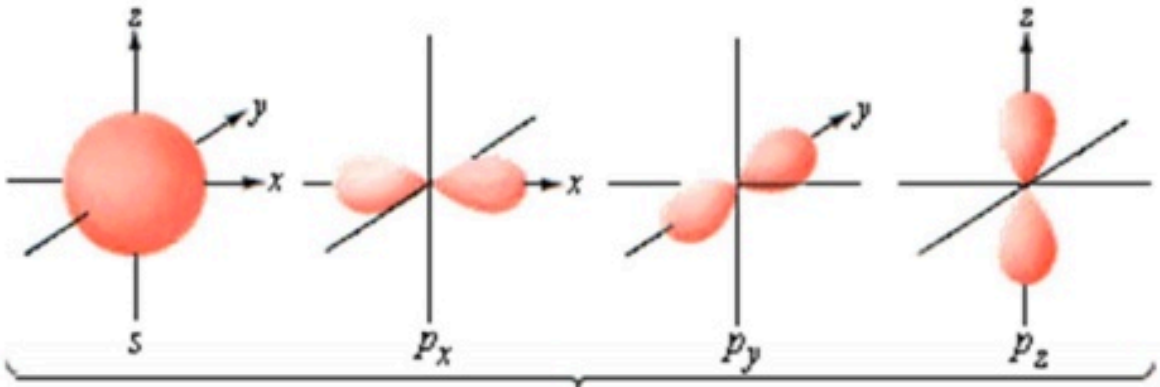
$2p_z$ orbital boundary surface



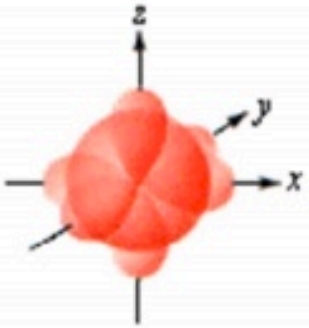
d Orbitals

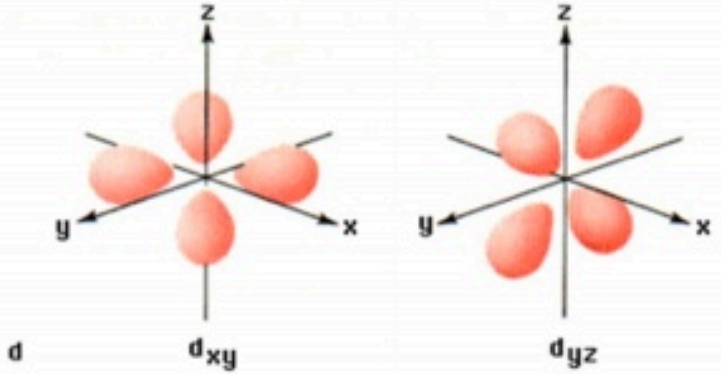


- The value of *l* for a *d* orbital is 2.
- Four of the five *d* orbitals have 4 lobes; the other resembles a *p* orbital with a doughnut around the center.

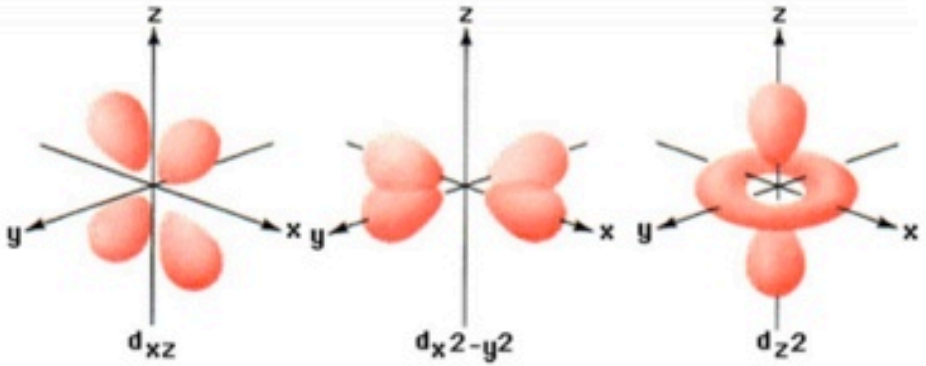


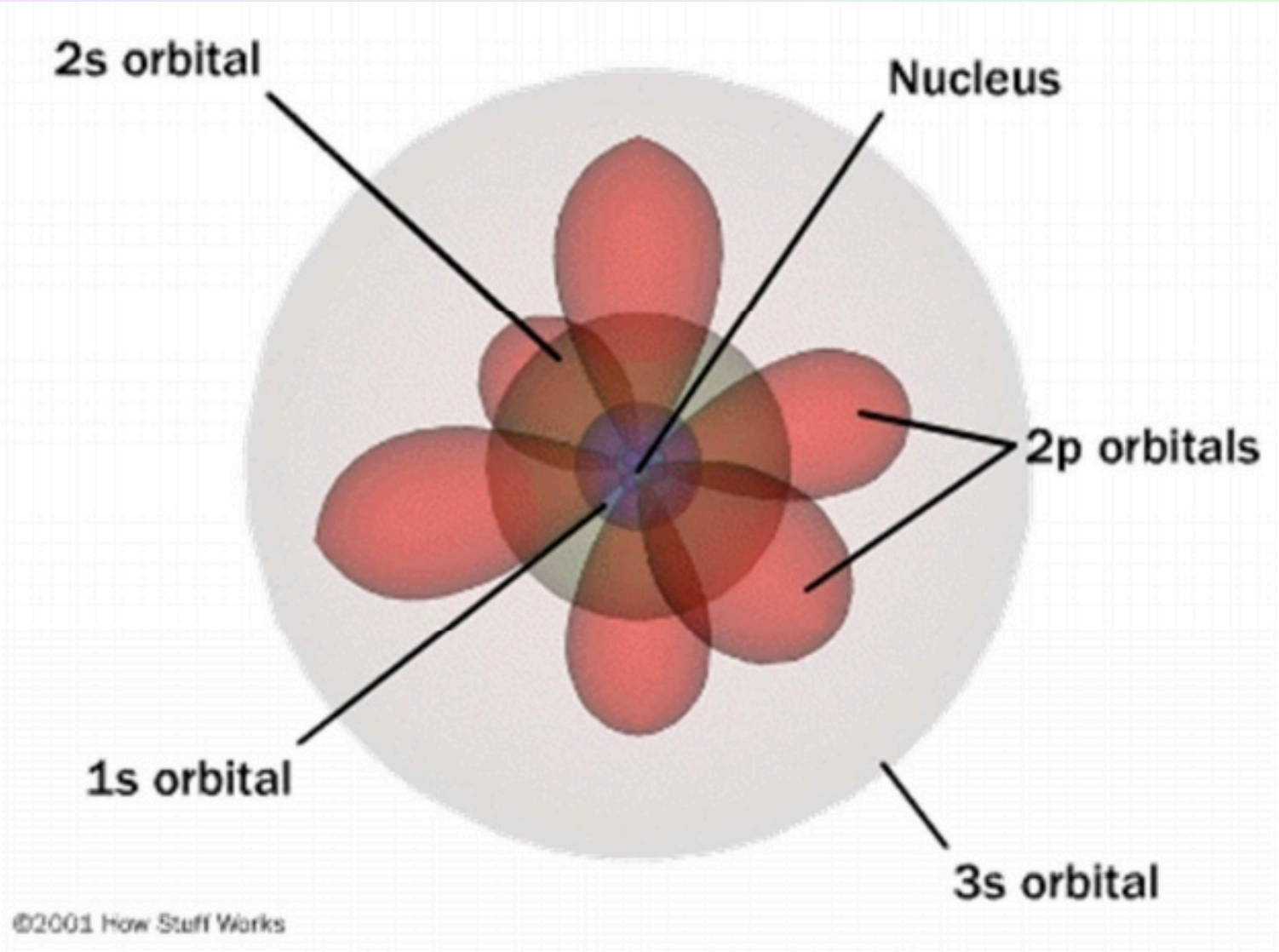
s and p sublevels





d sublevels




2s orbital
Nucleus
2p orbitals
1s orbital
3s orbital
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Atomic Orbitals

each orbital is characterized by a unique set of quantum numbers

principal quantum number:

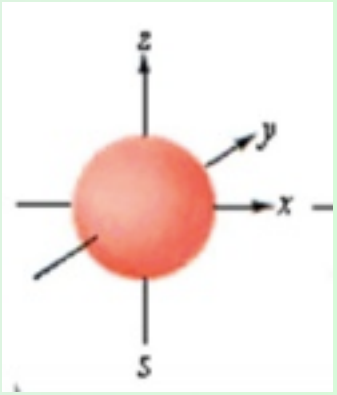
angular momentum quantum number:

magnetic quantum number:

n l m_l

(1, 0, 0)

1s



each orbital is characterized by a unique set of quantum numbers

principal quantum number:

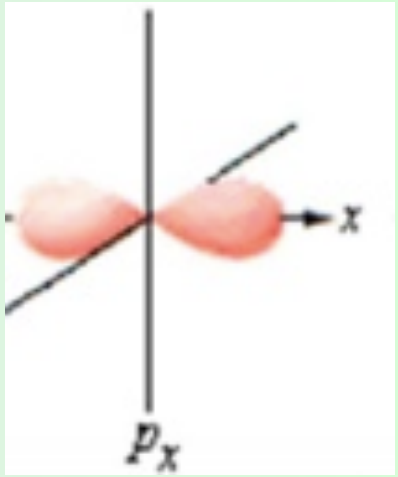
angular momentum quantum number:

magnetic quantum number:

n l m_l

(2, 1, 1)

$2p_x$



each orbital is characterized by a unique set of quantum numbers

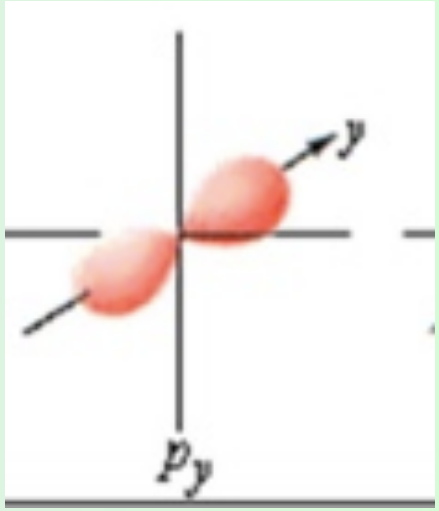
principal quantum number:

angular momentum quantum number:

magnetic quantum number:

n	l	m_l
(2,	1,	0)

$2p_y$



each orbital is characterized by a unique set of quantum numbers

principal quantum number:

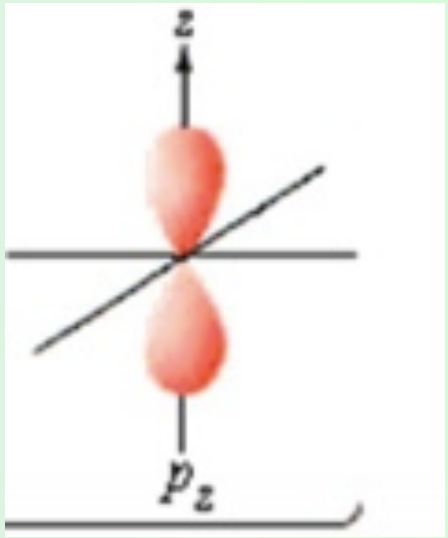
angular momentum quantum number:

magnetic quantum number:

n l m_l

(2, 1, -1)

$2p_z$



each orbital is characterized by a unique set of quantum numbers

principal quantum number:

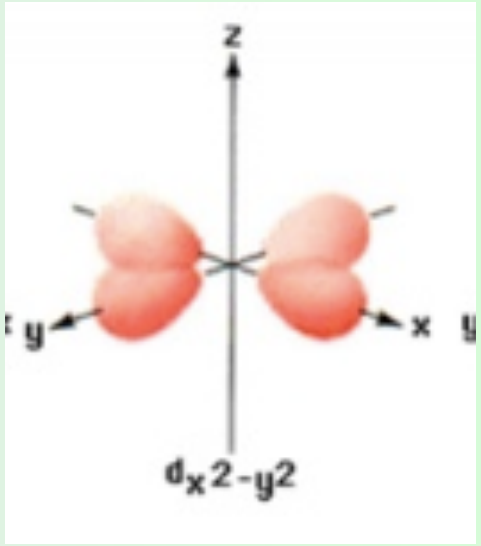
angular momentum quantum number:

magnetic quantum number:

n l m_l

(3, 2, 1)

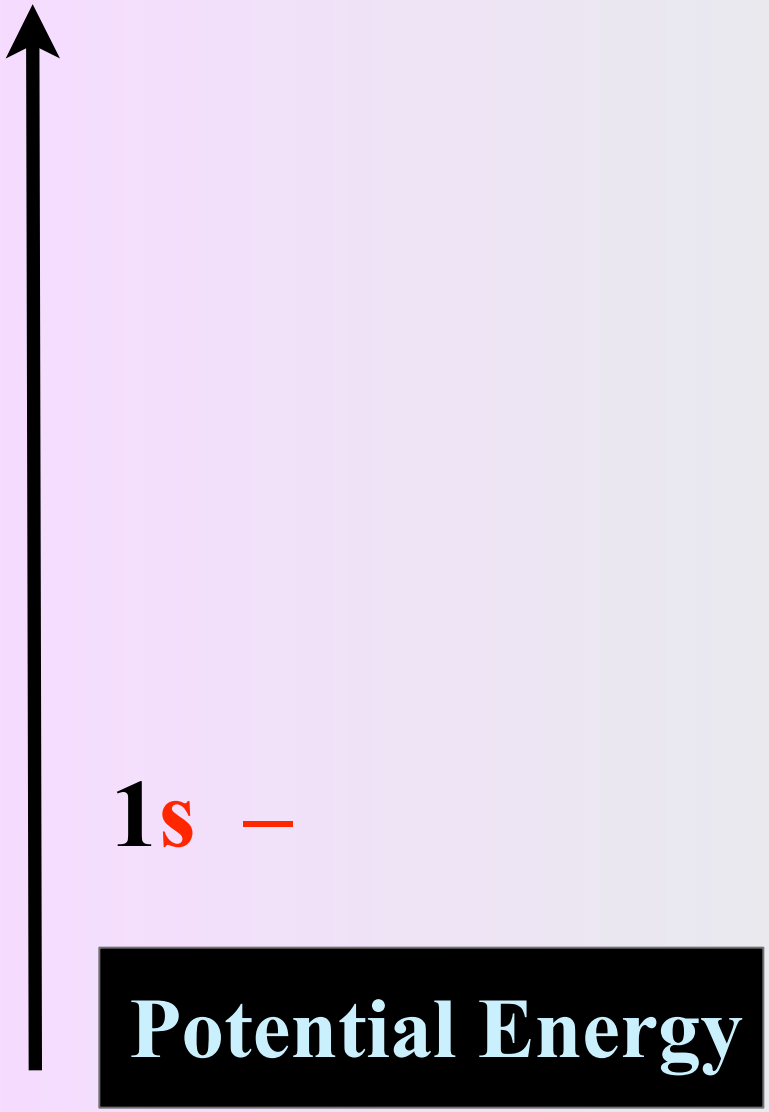
$3d_{x^2-y^2}$



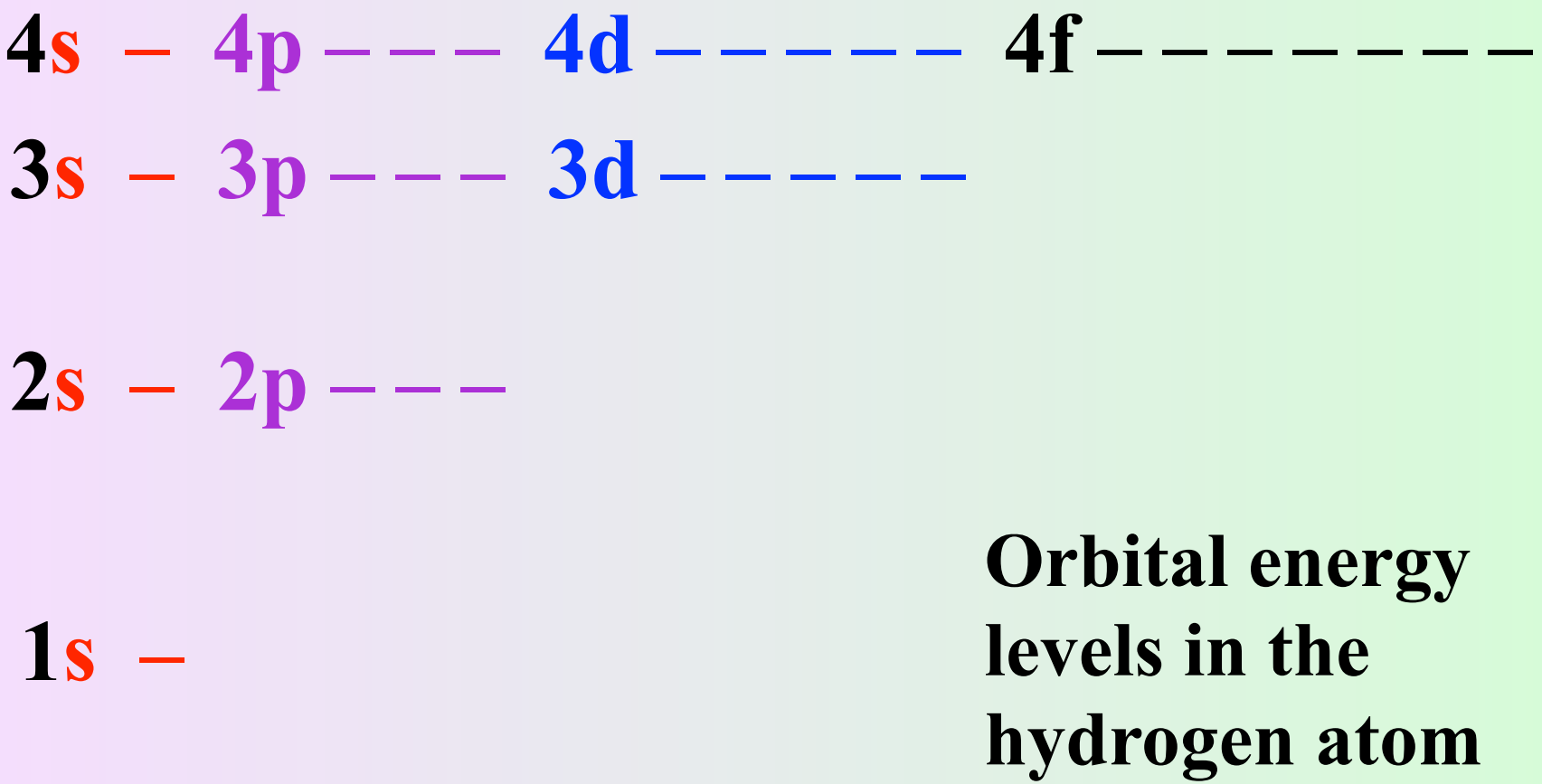
energies of hydrogen orbitals

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

i.e., they are "degenerate"



Orbital energy levels in the hydrogen atom

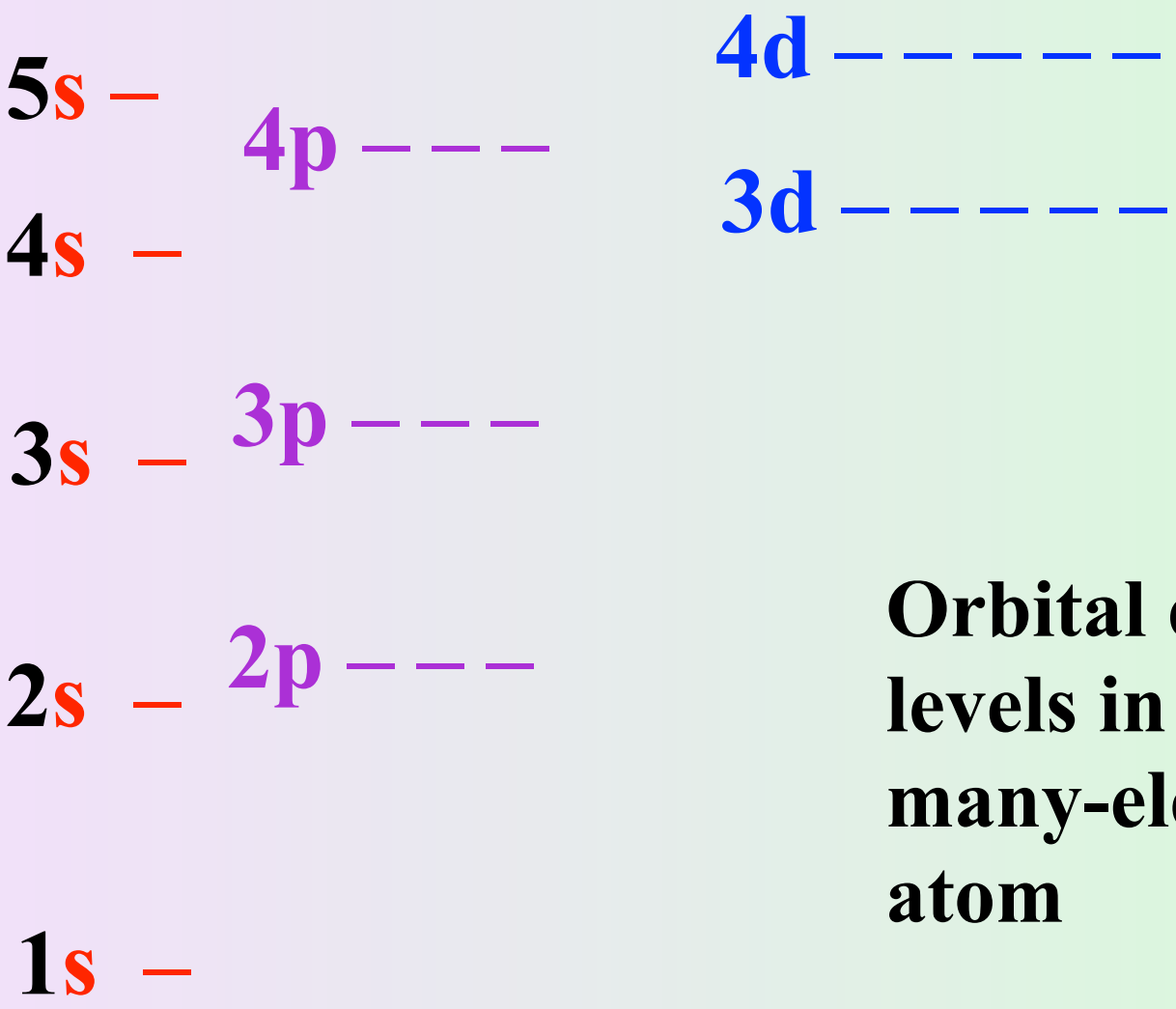


Orbital energy levels in the hydrogen atom

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

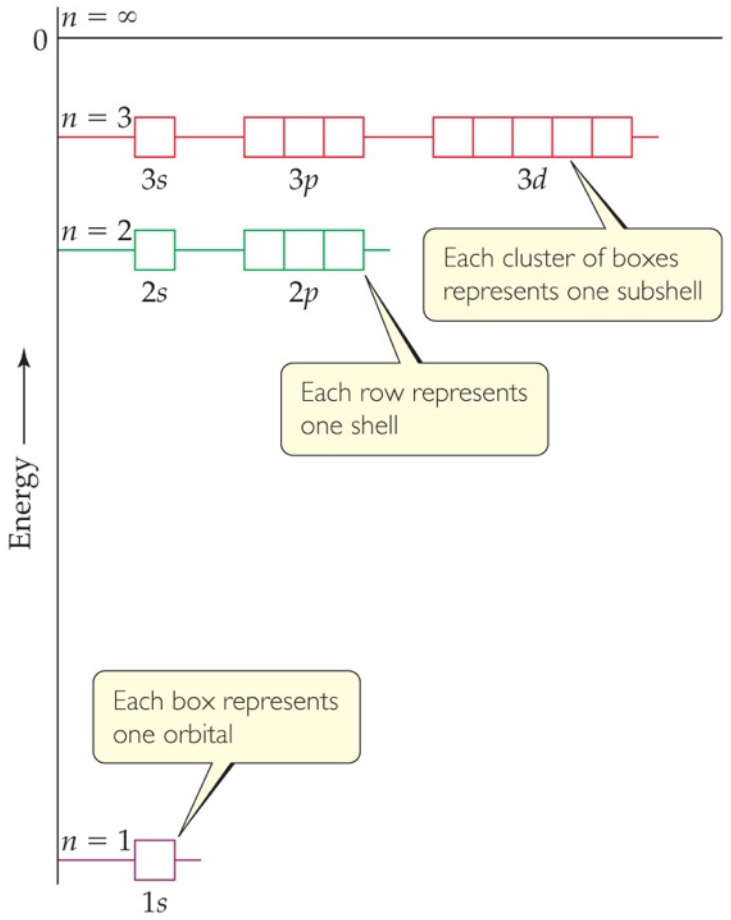
in a many-electron atom, electrons in the 1*s* orbital shield the electrons located in the 2*s* and 2*p* orbitals from the electrostatic attraction of the protons in the nucleus

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

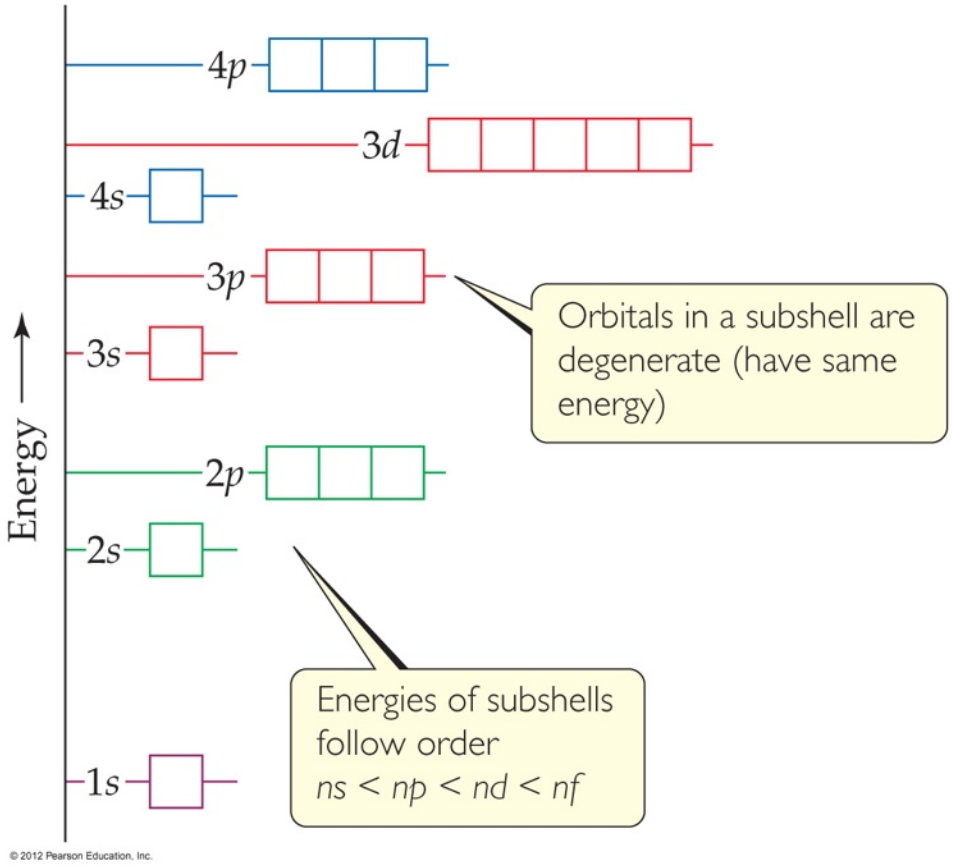
2*s* orbital is said to be more "penetrating" and is less shielded than the 2*p*

Energies of Orbitals

- For a one-electron hydrogen atom, orbitals on the same energy level have the same energy.
- That is, they are **degenerate**.



Energies of Orbitals



- As the number of electrons increases, though, so does the repulsion between them.
- Therefore, in many-electron atoms, orbitals on the same energy level are no longer degenerate.

Electronic Structure of Atoms