

11/9/2018

Exam 3 ~ next Thu!

- Rest of ch 5
- All of ch 6
- Ch. 7, up until WED

- today: all material \leadsto exam 4

MasteringChemistry: this week's homework will be due on WED @ 5pm!

Schrödinger eq (SE)

$$-\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi = E\Psi$$

\hookrightarrow solve for Ψ, E


\nearrow
wavefunction (psi)
orbital


$\Psi^2 \propto \text{prob.}$

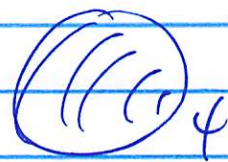
Ψ, E depend on 3 quantum numbers (QN)
+ also a 4th QN (spin) for e^- .

(1) Principal QN, $n=1, 2, 3, \dots$

- det's size + E of ψ

$n=1$ 
 ψ
low E

$n=2$ 
 ψ





$n=3$ 
higher E

$$\text{H-atom: } E_n = -R_H \left(\frac{1}{n^2} \right)$$

(2) Angular momentum QN, $l=0, \dots, n-1$

ex: if $n=3$, $l=0$, or 1 , or 2

- det's shape of ψ

value of l	0	1	2	3
letter designation	s	p	d	f
				

Value of l

Letter Designation

$$l = 0$$

s

$$l = 1$$

p

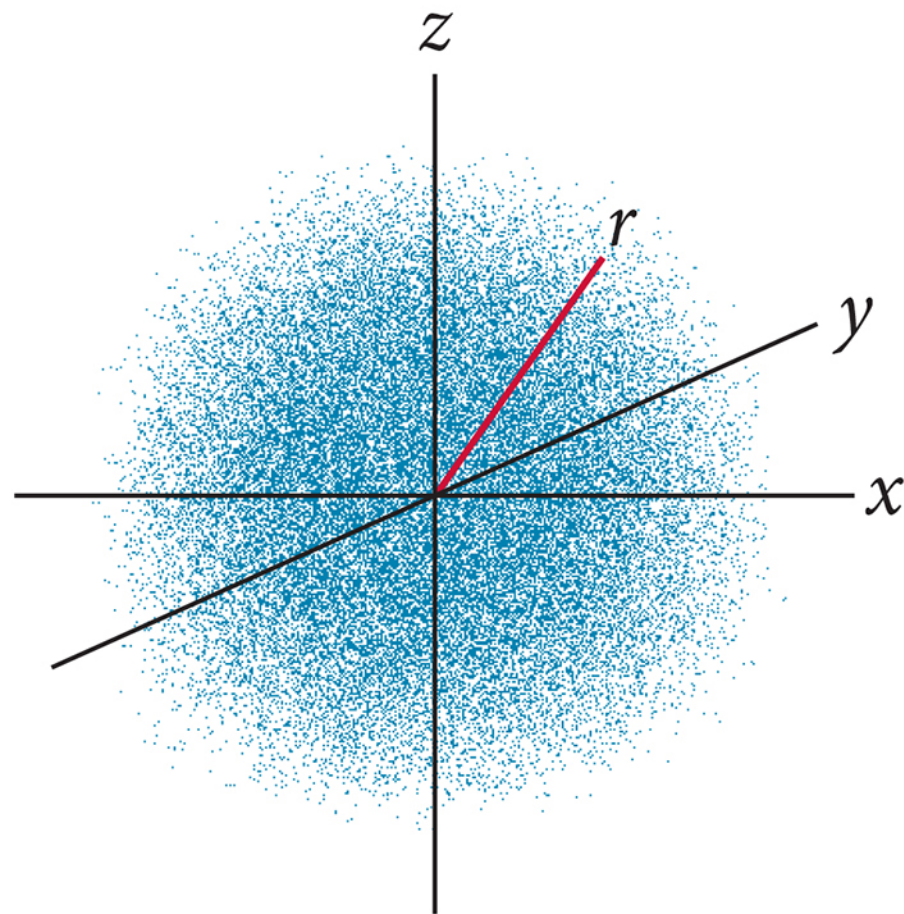
$$l = 2$$

d

$$l = 3$$

f

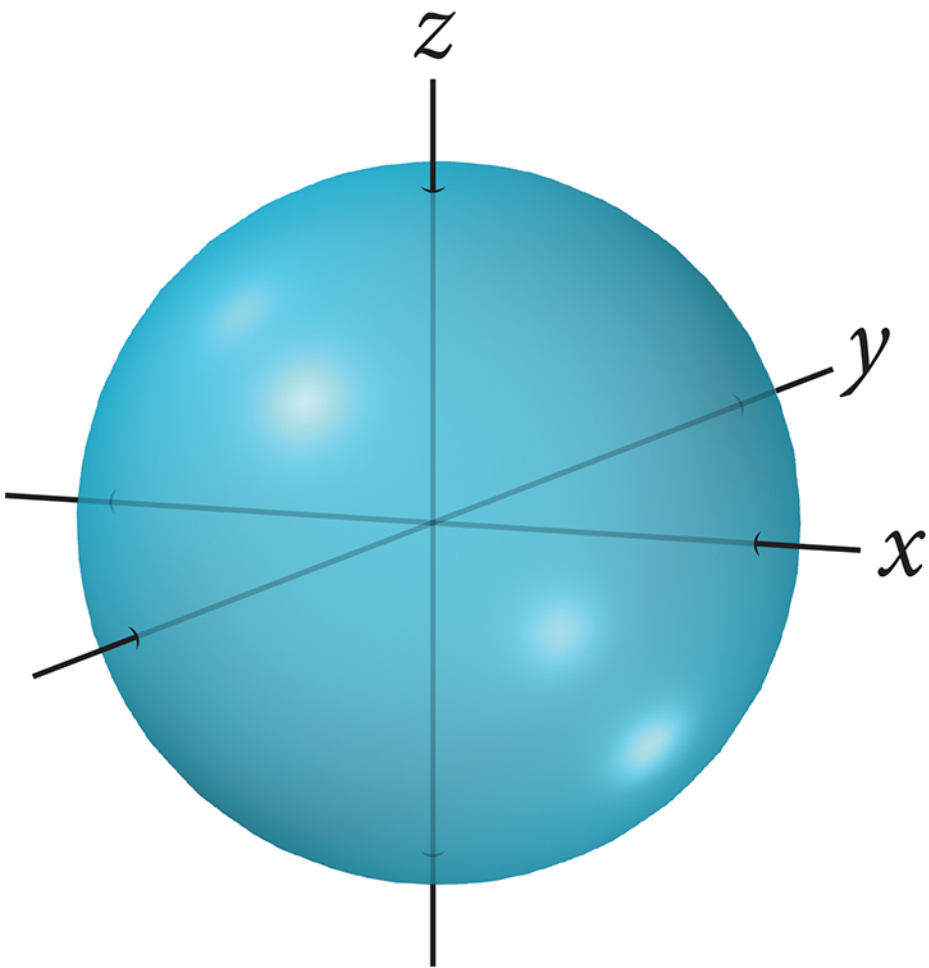
1s orbital



Density of dots
proportional to
probability density (ψ^2).

(a)

1s orbital surface



3) Magnetic QN, $m_l : -l, \dots, 0, \dots, +l$

ex: $l=2$, $m_l = -2, \text{ or } -1, \text{ or } 0, \text{ or } +1, \text{ or } +2$

- def's orientation of ψ

ex: $n=2$, $l=0$, or $+1$

$2s$
(n, l)
 \downarrow
 $m_l = 0$

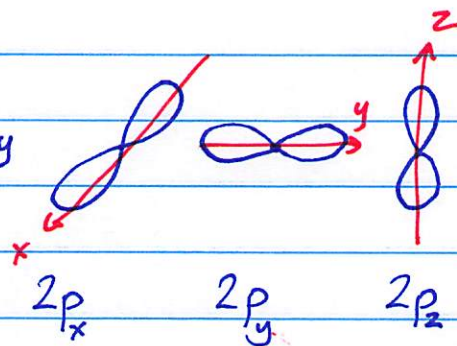
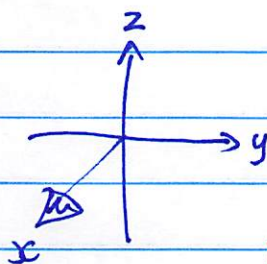
$2p$
(n, l)
 \downarrow
 $m_l = -1, 0, \text{ or } +1$

1-orientation



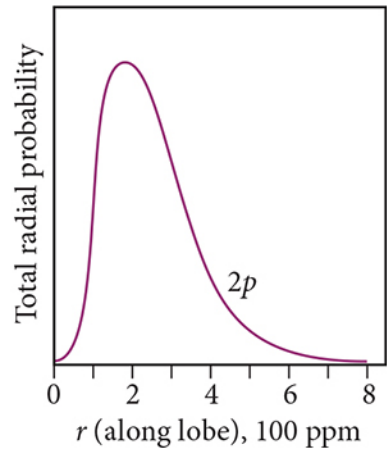
$2s$ -orbital

3 orientations

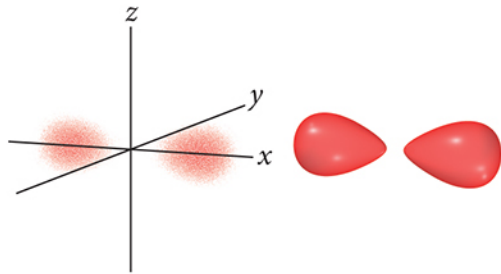


three \times $2p$ orbitals

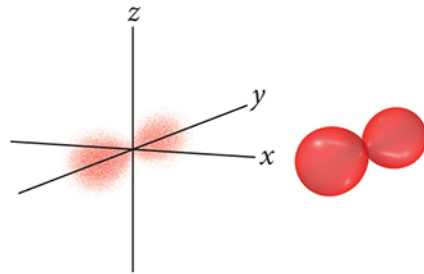
Radial Distribution Function



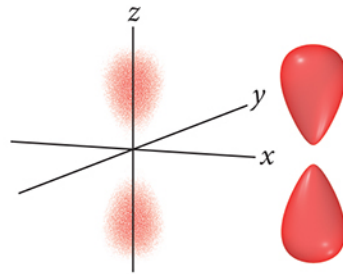
p_x orbital



p_y orbital



p_z orbital



$0, \dots, n-1$

$n=3, l=0, 1, \text{ or } 2$

$M_l=0$

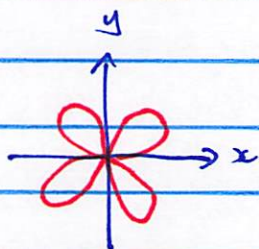
$M_l=-1, 0, +1$

$M_l=-2, -1, 0, +1, \text{ or } +2$

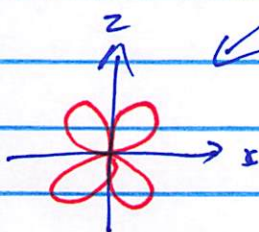
1 x 3s orbital

3 x 3p orbitals

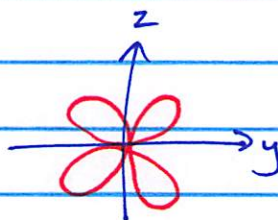
5 x 3d orbitals



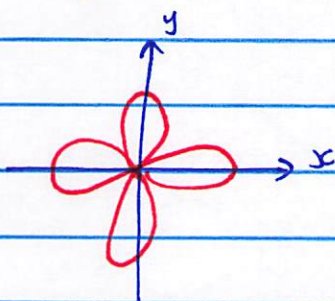
$3d_{xy}$



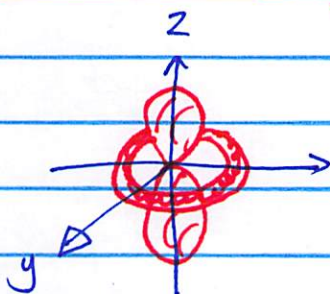
$3d_{xz}$



$3d_{yz}$



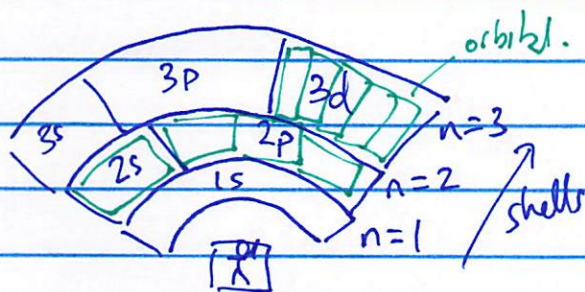
$3d_{x^2-y^2}$



$3d_{z^2}$

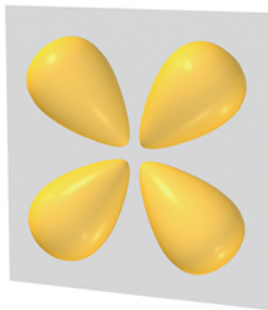
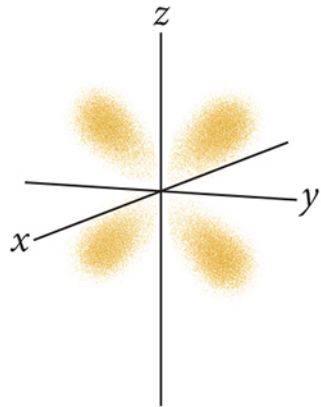
5 orientations

value of n : shell, ex: $n=1$, 1st shell
 value of n, l : sub-shell, ex: $n=3, l=2 = 3d$ subshell
 $n=3, l=1 = 3p$ subshell
 $n=3, l=0 = 3s$ subshell

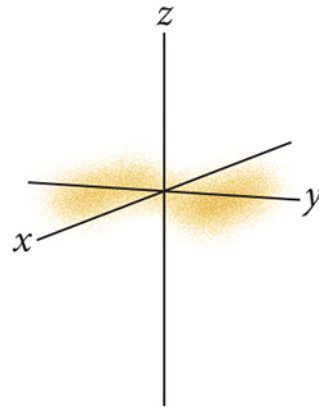


value of n, l, m_l : orbital, ψ

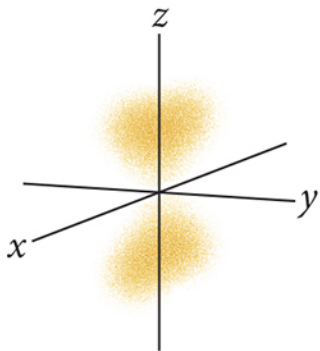
d_{yz} orbital



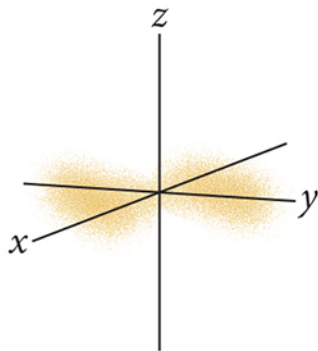
d_{xy} orbital



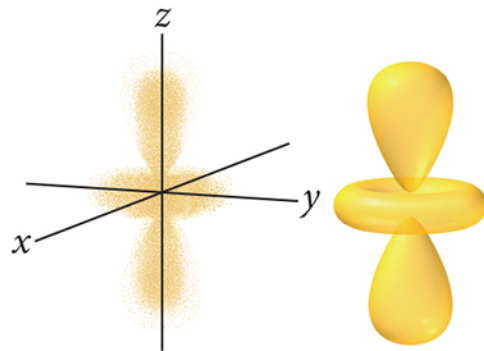
d_{xz} orbital



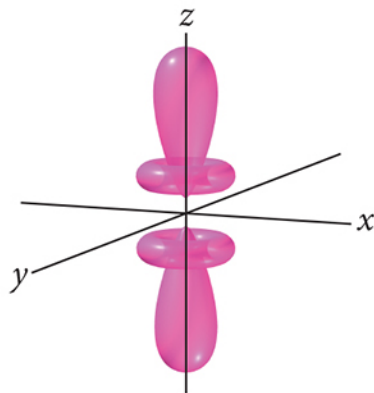
$d_{x^2 - y^2}$ orbital



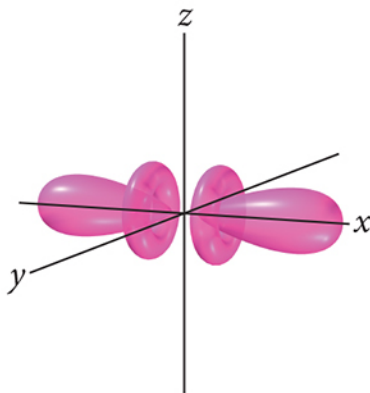
d_{z^2} orbital



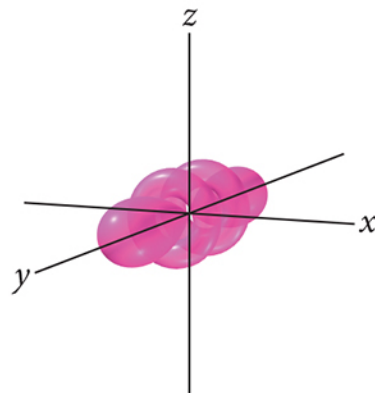
$$f_z^3 - \frac{3}{5}zr^2 \text{ orbital}$$



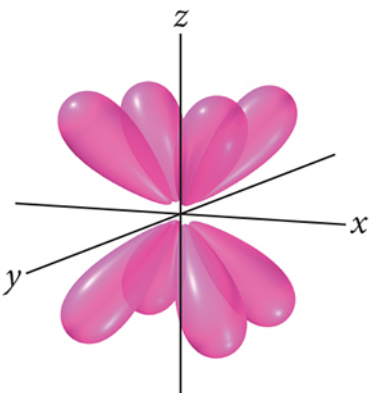
$$f_x^3 - \frac{3}{5}xr^2 \text{ orbital}$$



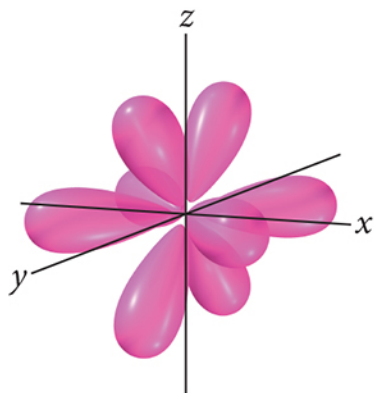
$$f_y^3 - \frac{3}{5}yr^2 \text{ orbital}$$



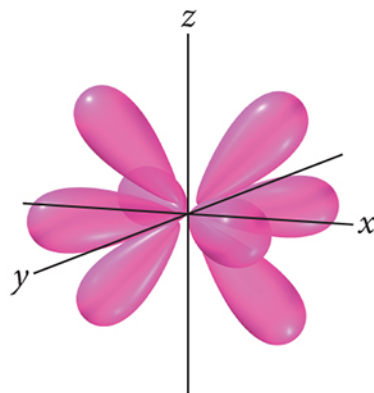
$$f_{xyz} \text{ orbital}$$



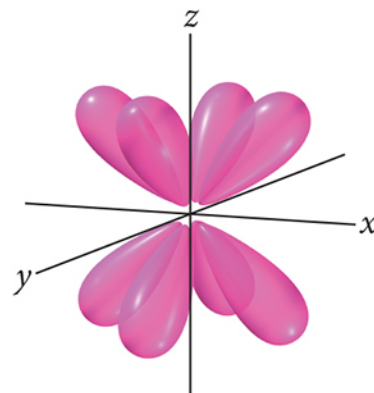
$$f_y(x^2 - z^2) \text{ orbital}$$



$$f_x(z^2 - y^2) \text{ orbital}$$



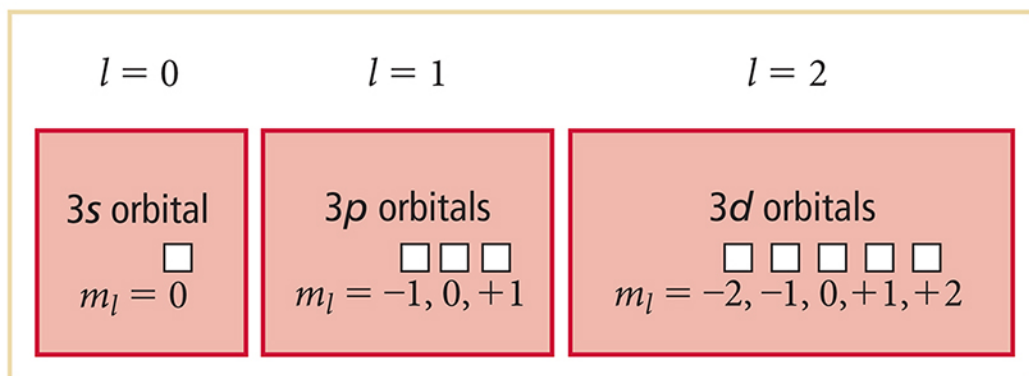
$$f_z(x^2 - y^2) \text{ orbital}$$



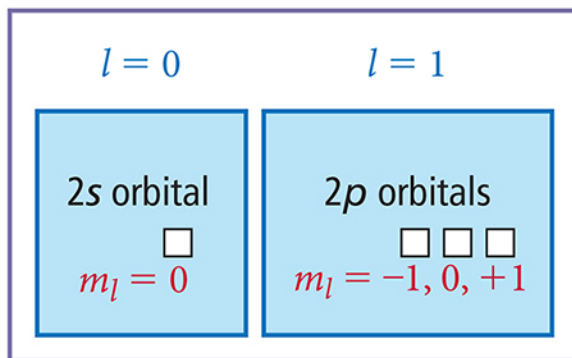
Principal level
(specified by n)

Sublevel
(specified by l)

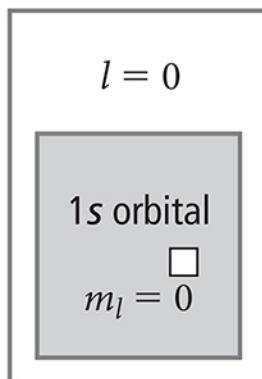
$n = 3$



$n = 2$



$n = 1$



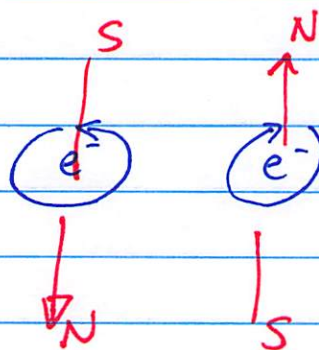
e^- s also have a 4th QN: spin QN

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

"as if e^- is spinning"

- counter-clockwise, $m_s = -\frac{1}{2}$

- clockwise, $m_s = +\frac{1}{2}$



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

"downspin"

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

"upspin"

Hint3: n -subshells per shell

n^2 orbitals per shell

$2l+1$ orbitals per sub-shell.

subshell

$n=1, l=0$ 1s

$n=2, l=0,1$ 2s, 2p

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