

11/6/2019

## Heisenberg Uncertainty Principle

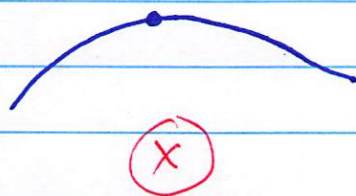
$$\underbrace{\Delta x}_{\text{uncertainty in position}} \times m \cdot \underbrace{\Delta v}_{\text{uncertainty in speed}} \geq \frac{h}{4\pi}$$

$6.626 \times 10^{-34} \text{ J}\cdot\text{s}$

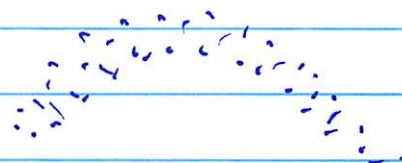
- can't know exactly where something is!

" ————— " how fast something is going!

classical  
trajectory



QM



prob. wave (✓)

de Broglie:  $\lambda = h/m \cdot v$

matter:

## Schrödinger Equation

$$\text{H-atom. } e^- \quad -\frac{\hbar^2}{2me} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi - \frac{e^2}{4\pi\epsilon_0 r} \psi = E \psi$$

psi

$\psi$

: wave function

ORBITAL (chemistry)

wave function

Energy

Max Born:  $\psi^2 \propto \text{prob. of finding } e^-$

Math:

- 4 Quantum Numbers (QN)  
associated w/  $\psi$ .


- determine  $E$ , shape, size, orientation of  $\psi$

① Principal QN :  $n$  : 1, 2, 3, 4, ...

determines  $E$ , size of  $\psi$

$$\hookrightarrow E_n = -\frac{R_H}{n^2} \quad (\text{H-atom})$$

ex:  $n=1$   low  $E$

$n=2$  

$n=3$  

↑  
higher  $E$



② Angular momentum QN :  $l$


$l: 0, 1, \dots, n-1$

ex:  $n=5, \quad \left. \begin{array}{c} l=0 \\ 1 \\ 2 \\ 3 \\ 4 \end{array} \right\} \text{any one!}$

\* slightly diff  $E$  for atoms w/ 2 or more  $e^-$   
 $1e^- \sim$  no effect on  $E$ . (H)

diff the shape of  $\psi$

ex:  $l=0$             letter  
s

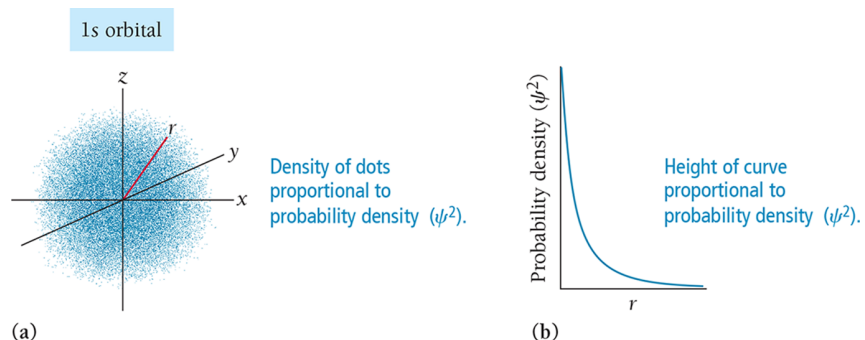
$l=1$             p

$l=2$             d

$l=3$             f

## Probability Density for s Orbitals ( $l = 0$ )

The probability density function represents the total probability of finding an electron at a particular point in space.



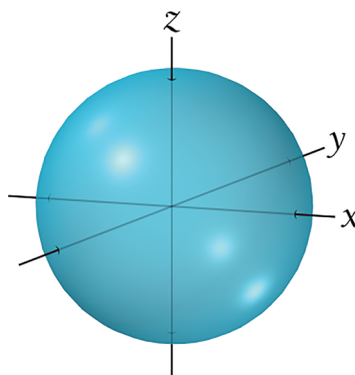
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## $l = 0$ , the s Orbital

- Each principal energy level has one **s** orbital.
- Lowest energy orbital in a principal energy state
- Spherical
- Number of nodes =  $(n - 1)$

1s orbital surface



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③ Magnetic QN:  $m_l$

$$m_l: -l, \dots, 0, \dots, +l$$

$$\text{ex: } l=2, \quad m_l = \left. \begin{array}{c} -2 \\ -1 \\ 0 \\ +1 \\ +2 \end{array} \right\}$$

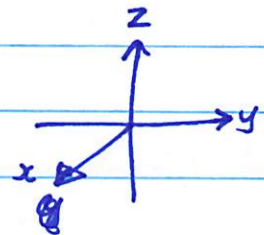
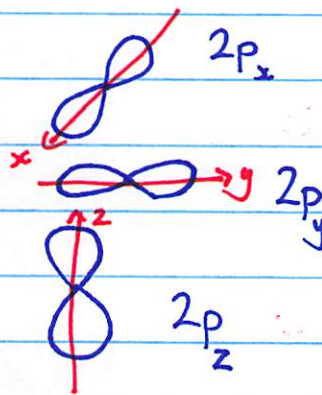
- doesn't affect E (unless there's a magnetic field)  
dets orientation of  $\psi$

$$\underbrace{n=1, l=0, m_l=0}_{1s}$$

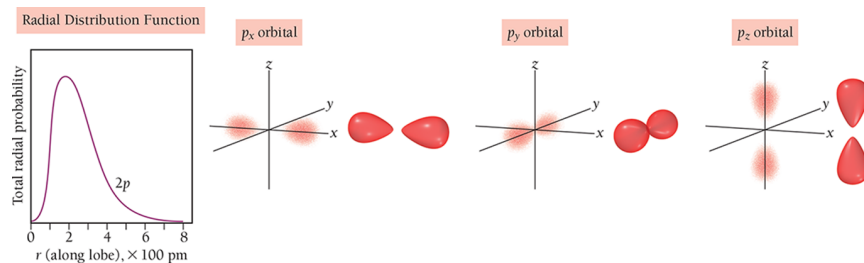


1s

$$\underbrace{n=2, l=1, m_l = \begin{cases} -1 \\ 0 \\ +1 \end{cases}}_{2p}$$

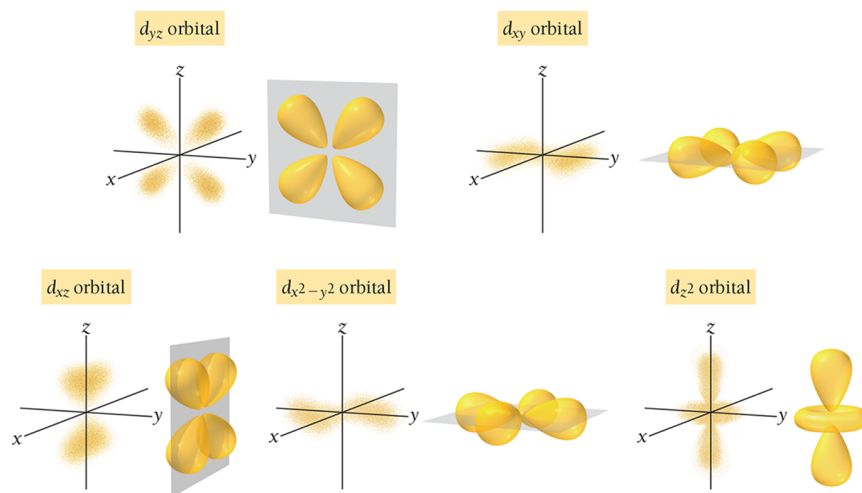


## $p$ Orbitals ( $l = 1$ )



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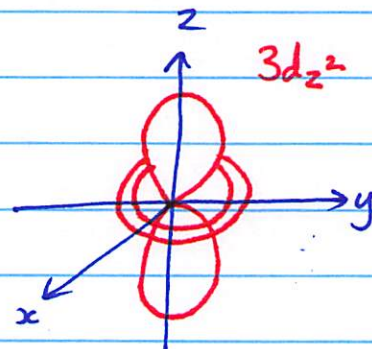
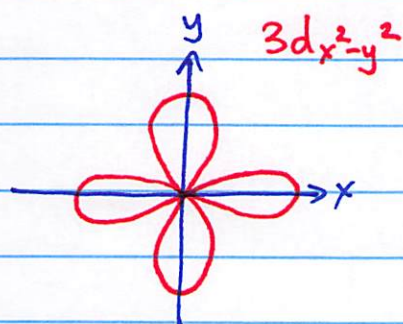
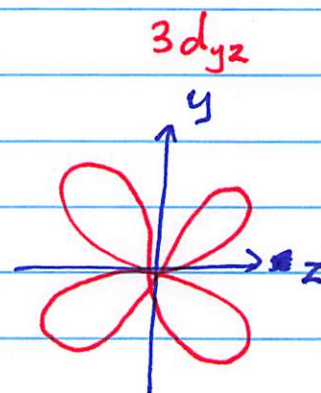
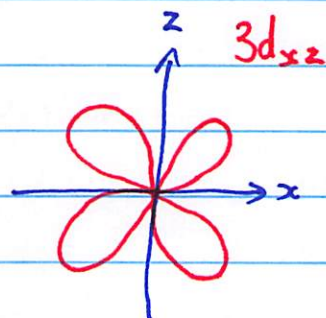
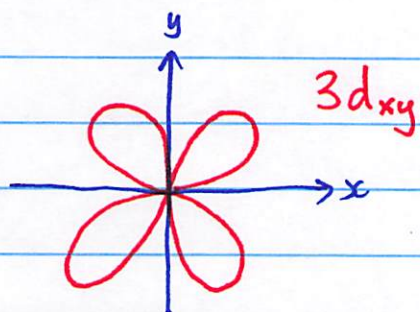
## $d$ Orbitals ( $l = 2$ )



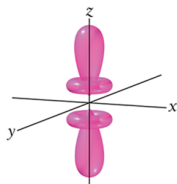
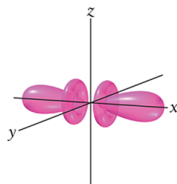
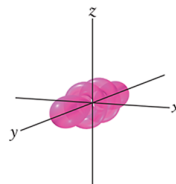
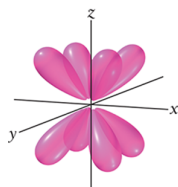
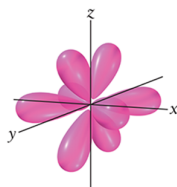
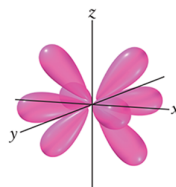
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$$\begin{array}{l}
 n=3, l=2, m_l = -2 \\
 \underbrace{\hspace{1.5cm}} \\
 3d
 \end{array}
 \begin{array}{l}
 -1 \\
 0 \\
 +1 \\
 +2
 \end{array}$$



## $f$ Orbitals ( $l = 3$ )

 $f_{z^3 - \frac{3}{2}zr^2}$  orbital

 $f_{x^3 - \frac{3}{2}xr^2}$  orbital

 $f_{y^3 - \frac{3}{2}yr^2}$  orbital

 $f_{xyz}$  orbital

 $f_{y(x^2 - z^2)}$  orbital

 $f_{x(z^2 - y^2)}$  orbital

 $f_{z(x^2 - y^2)}$  orbital
