CH 431 8/30/2016 Lecture 02

ψ psi → wave function → atomic orbitals

1s
↑
n=1 (principal quantum number

larger n = larger energy

l (angular momentum quantum #)
0 ... n-1

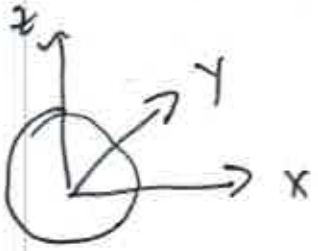
m_l 0 ... $\pm l$

$l=1$ $m_l = -1, 0, +1$

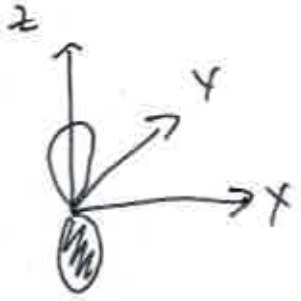
m_s $\pm \frac{1}{2}$

→ every electron has a unique set of quantum numbers

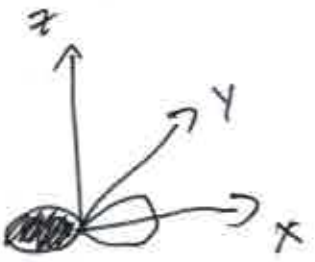
s orbital $\ell = 0$ $m_\ell = 0$



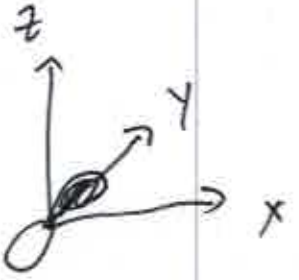
p orbitals $\ell = 1$ $m_\ell = -1, 0, +1$



P_z

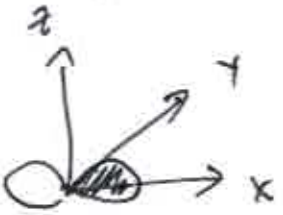


P_x



P_y

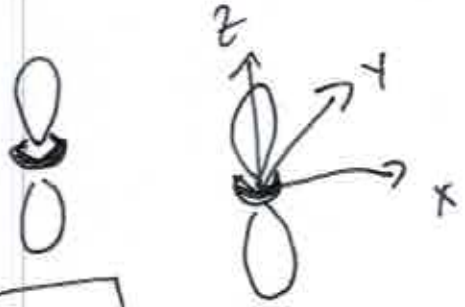
111



d orbitals $\ell = 2$ $m_\ell = -2, -1, 0, 1, 2$

5 d orbitals

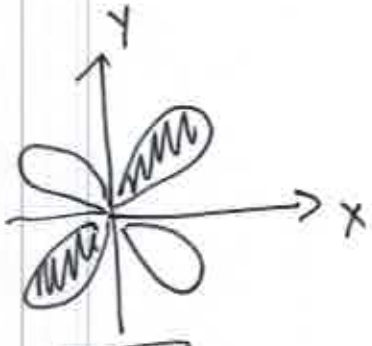
Two basic shapes



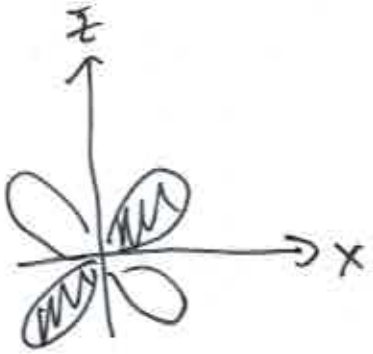
d_{xy}, d_{xz}, d_{yz}

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

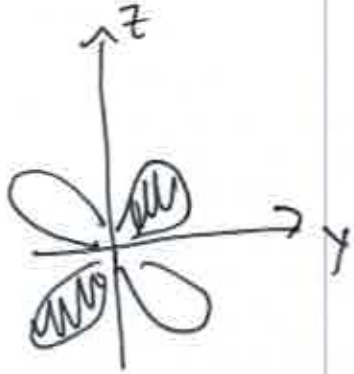
d_{z^2}



d_{xy}

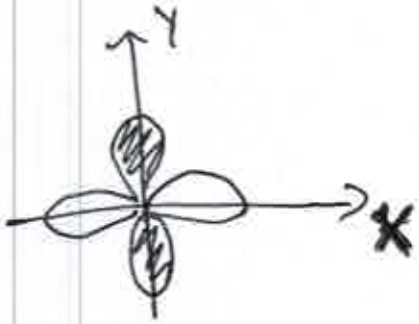


d_{xz}



d_{yz}

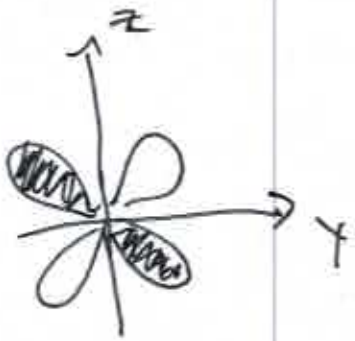
in xy plane, lobes pointed in between axes



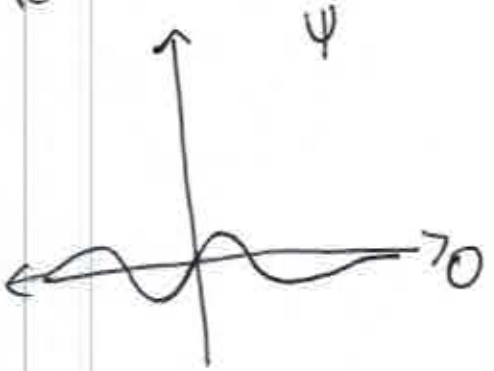
$d_{x^2-y^2}$

in xy plane, lobes are pointed along the axes

III

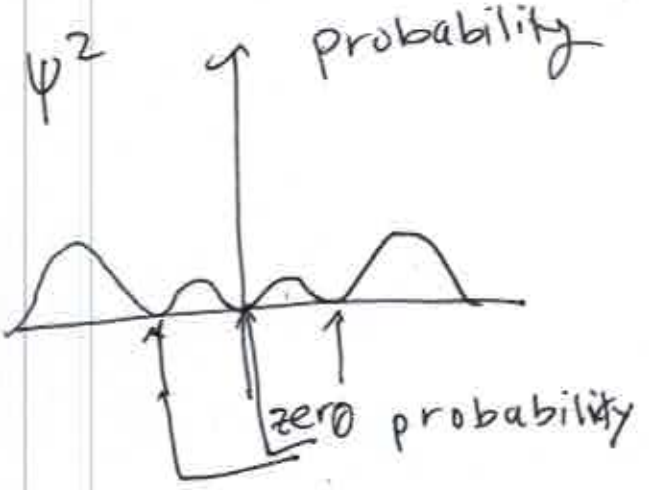


Radial wavefunction



can be ⊕ or ⊖

→ origin of orbital shading



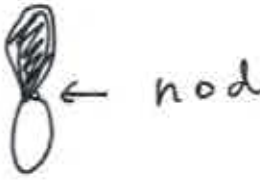
orbitron website

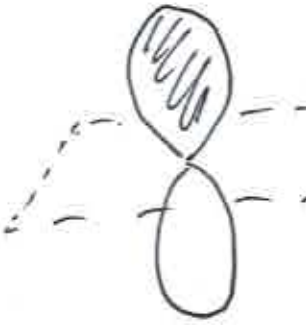
Electron density, tab = probability

Angular Nodes

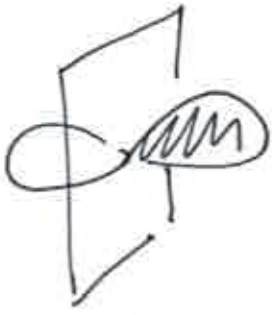
s orbital $\ell = 0$ no angular nodes

p orbital $\ell = 1$ 1 angular node

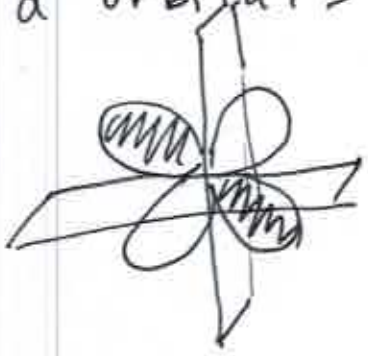




node → plane that goes ~~through center~~ in between two lobes



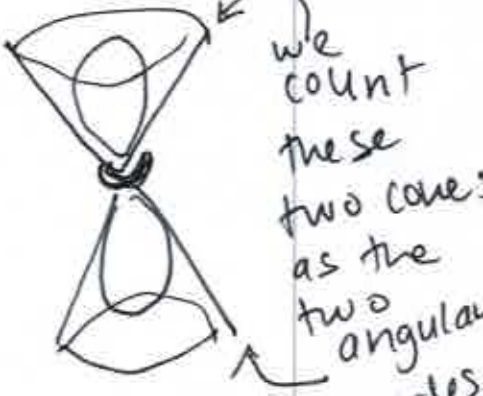
d orbitals $\ell = 2$ 2 angular nodes



d_{xy}, d_{xz}, d_{yz}

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

↑ nodal plane (angular node)



d_{z^2}

Radial node

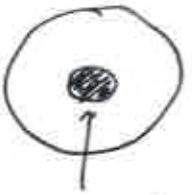
→ think of this as a sphere-~~spal~~ shaped node

1s vs 2s vs 3s

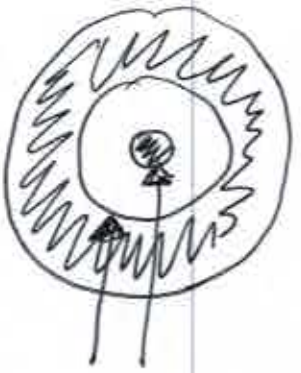
Probability functions ψ^2

- 2s : 1 node (zero probability)
- 3s : 2 nodes

1s 

2s 

1 radial node in between two shaded regions

3s 

2 radial nodes

2p vs 3p

convert 2p to 3p orbital

1) make orbital bigger

2) add in a radial node

radial node

3p orbital

radial node

angular node

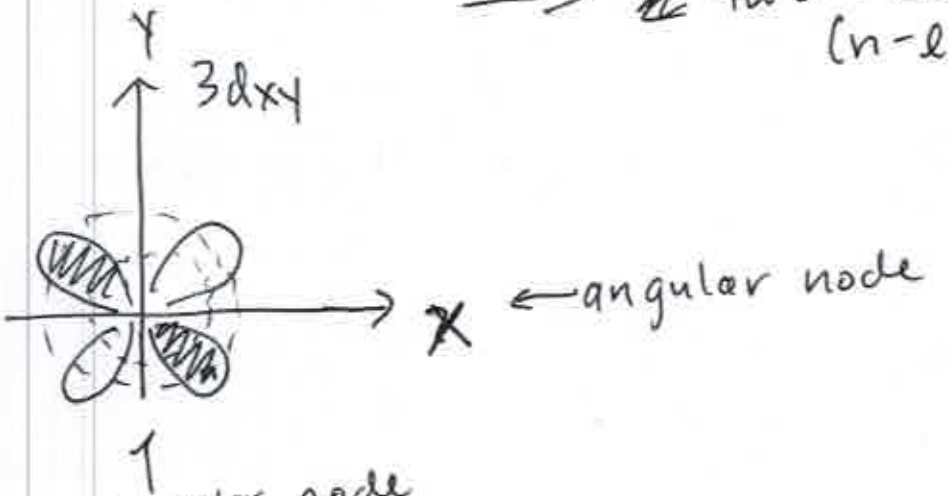
3dxy has 2 total nodes, both are angular because $\ell = 2$

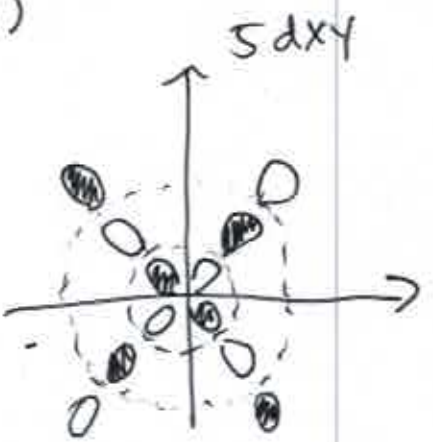
Example $5d_{xy}$ orbital

$n = 5$ → there should be 4 total nodes $(n-1)$

$\ell = 2$ → two of the nodes are angular

⟹ two radial nodes $(n-\ell-1)$





- shading will always change ~~in the~~ as you cross a node (applies to both angular and radial nodes)

Aufbau

P electron configuration

$1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^3$

$[Ne]\ 3s^2\ 3p^3$

Cr

$[Ar]\ 4s^2\ 3d^4$ ✗ NO

$[Ar]\ 4s^1\ 3d^5$ YES

Cu

$[Ar]\ 4s^1\ 3d^{10}$ not $4s^2\ 3d^9$ ✗

Cu^+ $4s^0$

$[Ar]\ 3d^{10}$

Cu^{2+}

$[Ar]\ 4s^0\ 3d^9$

N

↑↓	↑ ↑ ↑	YES ←
2s	2p	
↑↓	↑↓ ↑ —	NO
2s	2p	
↑↓	↑ ↑ ↑	NO
2s	2p	

5s $\ell = 0$

4 nodes

↑

radial