Review

$\sigma \rightarrow r/a_0$

1s $n=1$ $l=0$ $m=0$ ψ_{100} : $e^{-\sigma}=\psi_{1s}$ **F(r) only**

2s $n=2$ $l=0$ $m=0$ ψ_{200} $(2-\sigma)e^{-\sigma/2}=\psi_{2s}$ **F(r) only**

$2p_z$ $l=1$ $m=0$ ψ_{210} $\sigma e^{-\sigma/2}\cos\theta=\psi_{2p_z}$ **F(r,θ)**

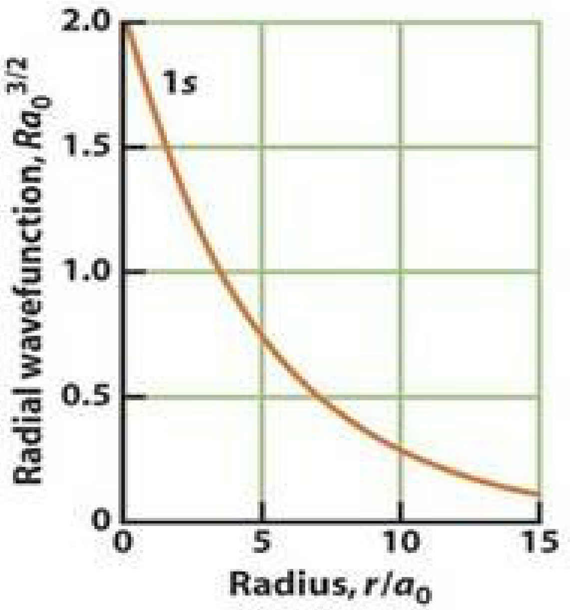
2

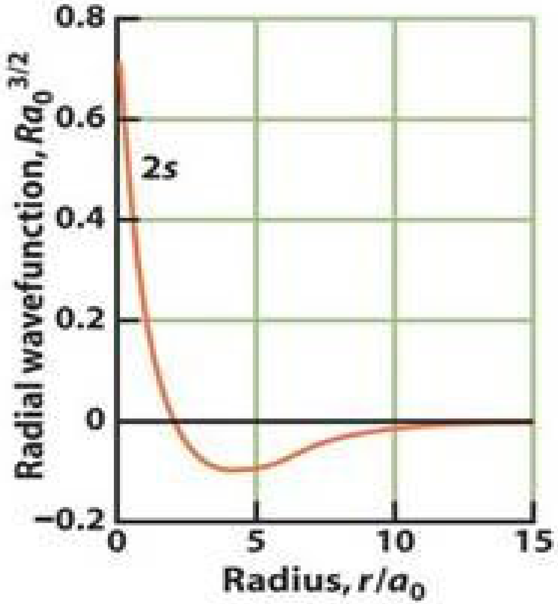
$2p_{x,y}$ $l=1$ $m=\pm1$ $\psi_{21\pm1}$ $\sigma e^{-\sigma/2}\sin\theta\ e^{\pm i\phi}$ **F(r,θ,ϕ)**

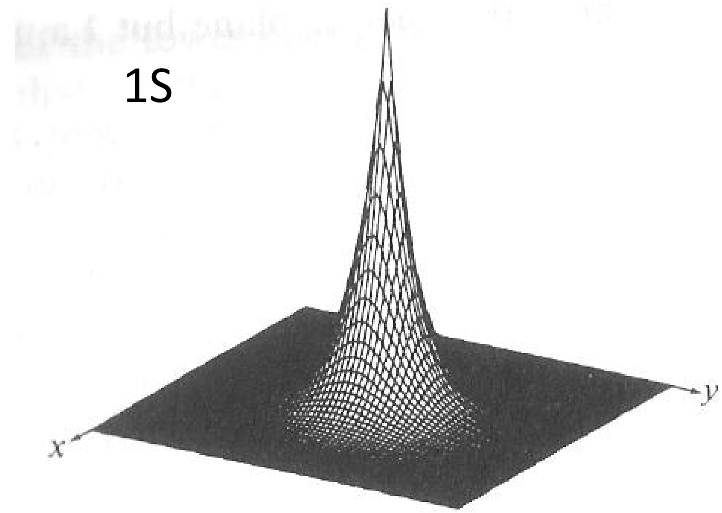
S orbitals are only dependent on “r”- they are radially symmetrical

Review

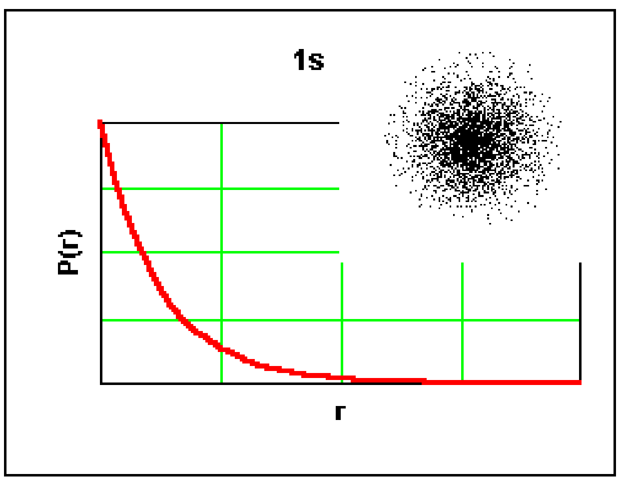
$R_{n,l}$ ⇒ Radial Distribution Function

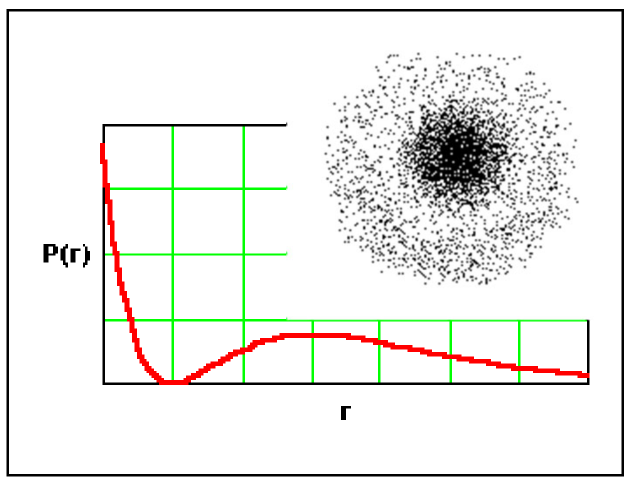


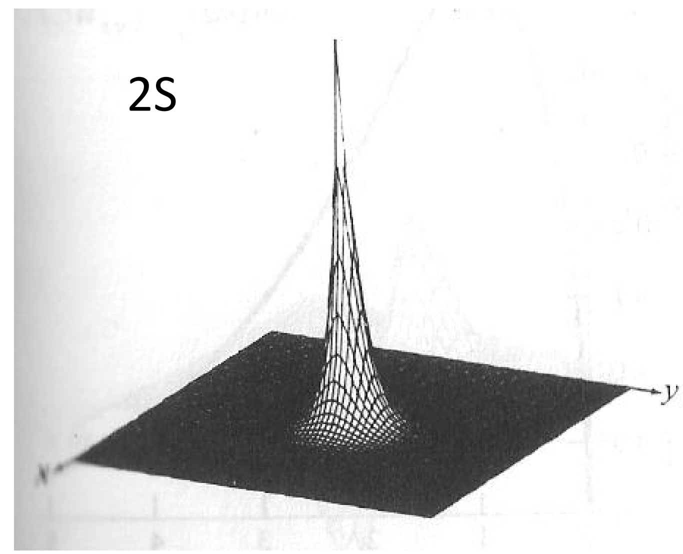




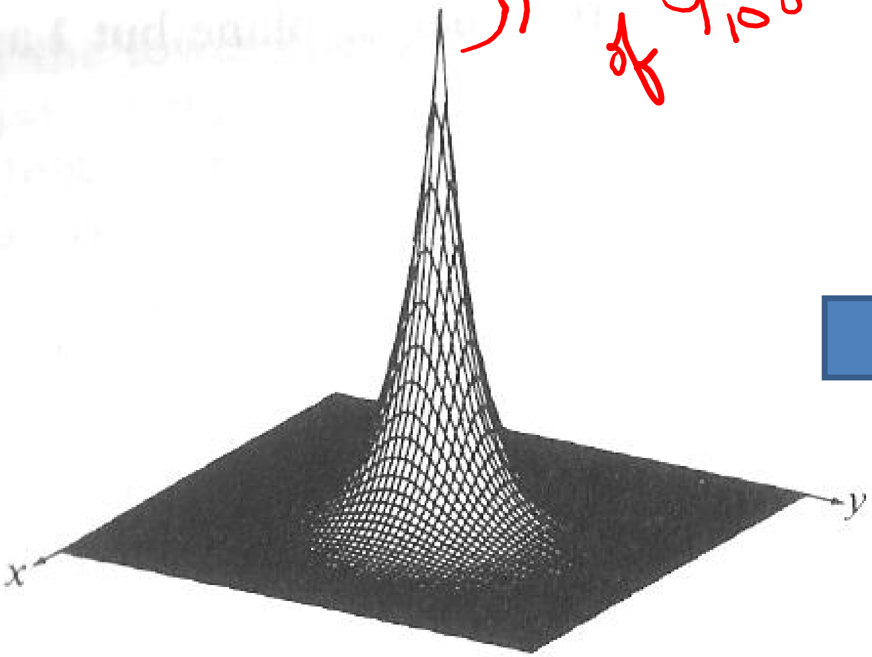
$R^2_{n,l}$

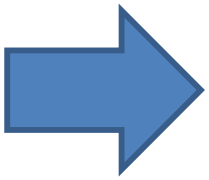


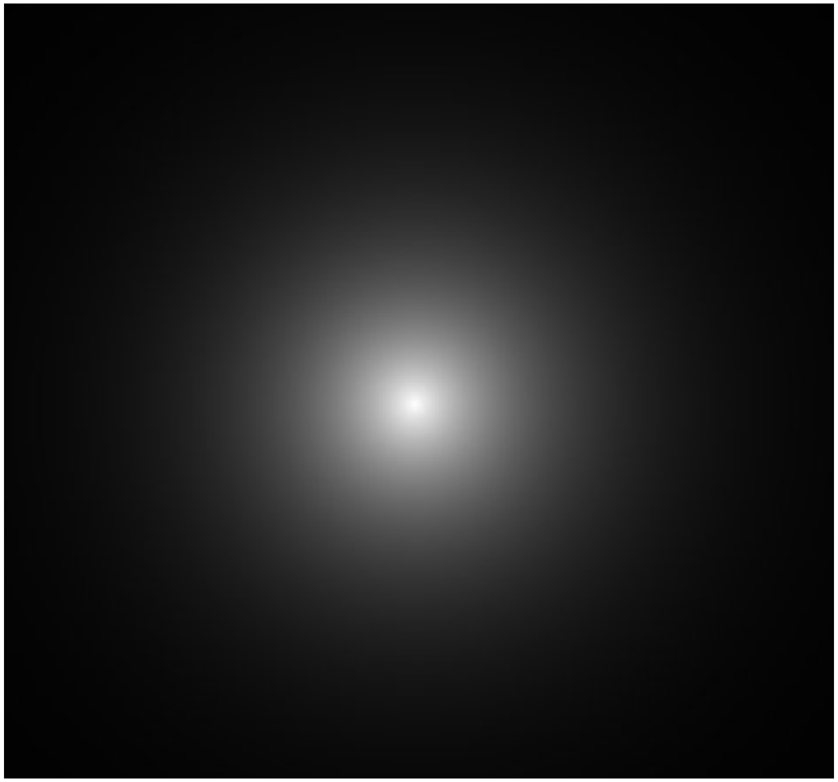




3D visualization of 1s (radial)

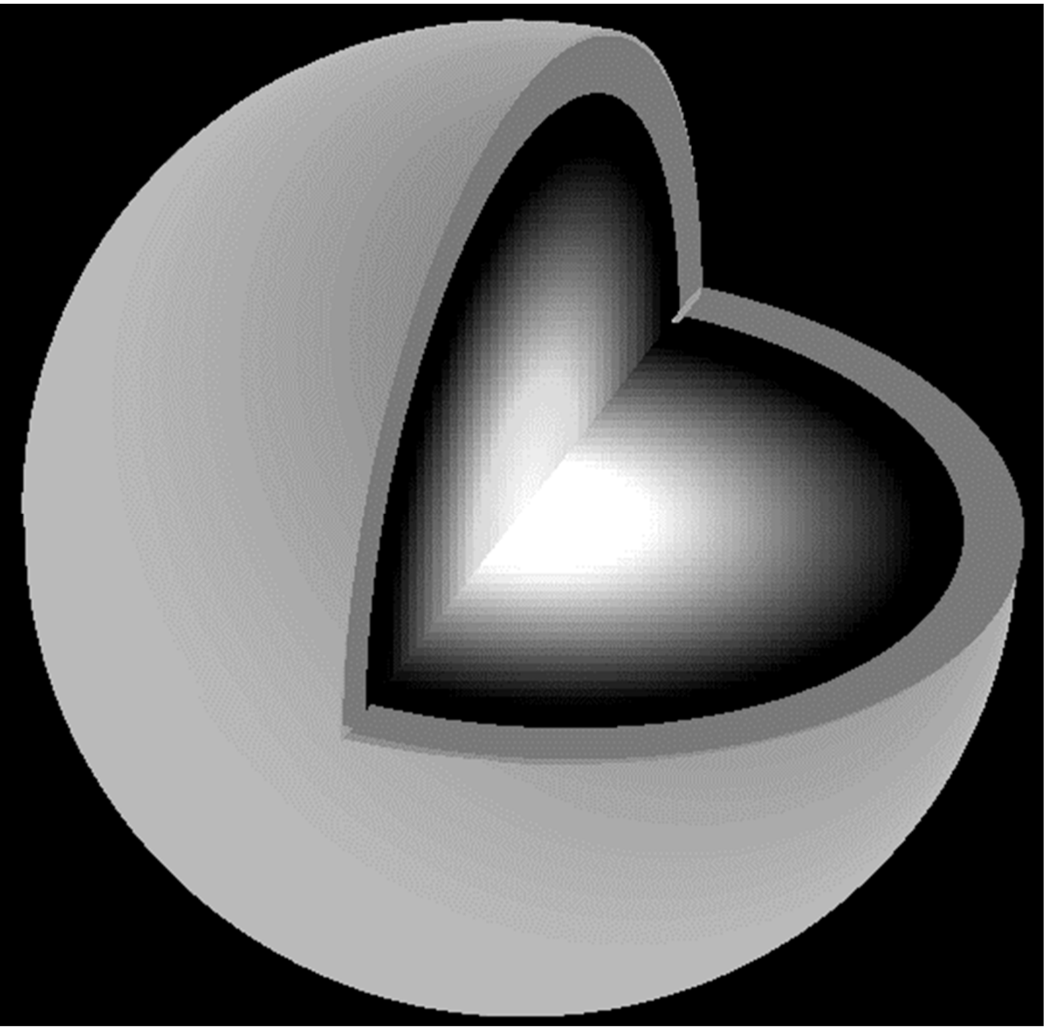




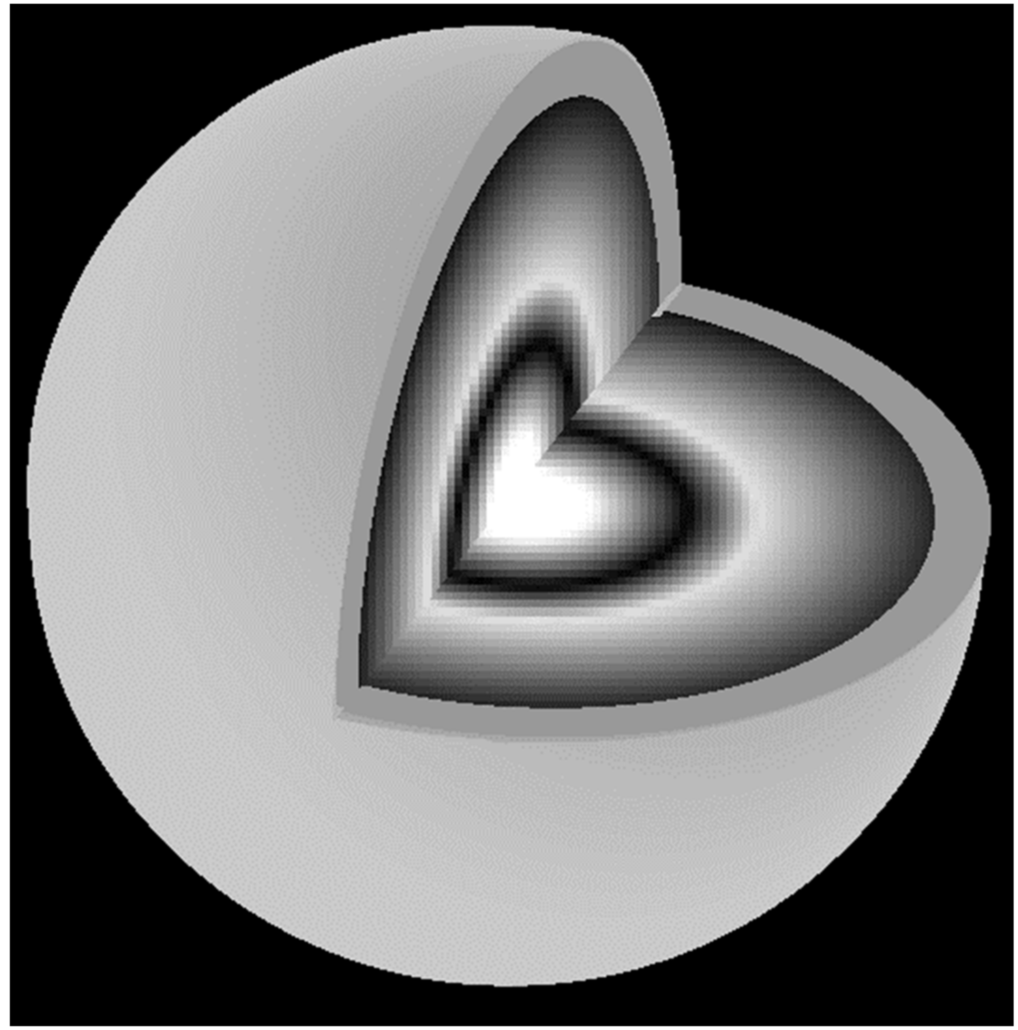


Maximum probability of finding the electron: at nucleus?

3D visualization is non-trivial



$(1s)^2$



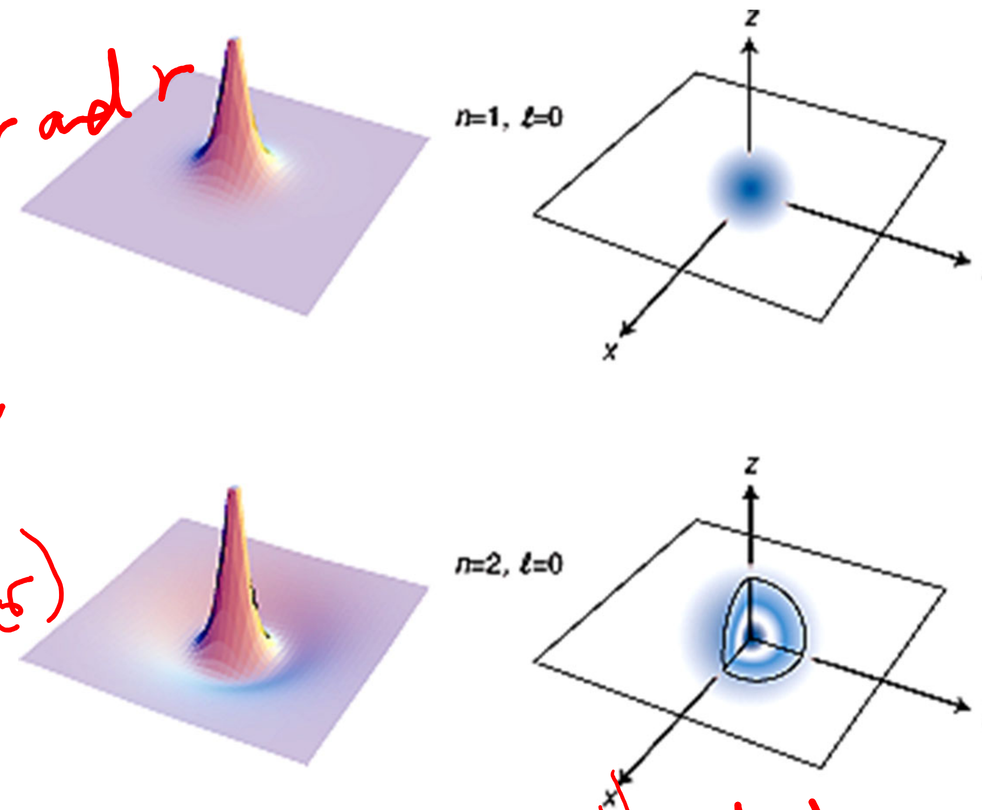
$(2s)^2$

$R^2(r)$ predicts maximum probability at the center of the atom (for s)!!!

Radial Probability Distribution Function

Compute the probability of finding an electron in a thin shell between r+dr and r

dr



P(r)

Probability *of finding the electron anywhere in a shell of thickness dr at radius r is* $4\pi r^2 R_{nl}^2(r)dr$ ($for\ S$)

$r^2 \rightarrow$ increasing *funtion*

$4\pi r^2 R_{nl}^2(r)dr \rightarrow 0\ as\ 4\pi r^2 dr \rightarrow 0$

$4r^2 \delta V$

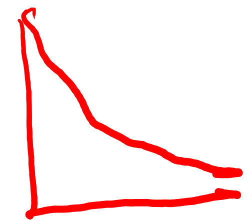
Probability in a small volume δV

$R^2(r)$ predicts maximum probability at the center of the atom (for s)!!!

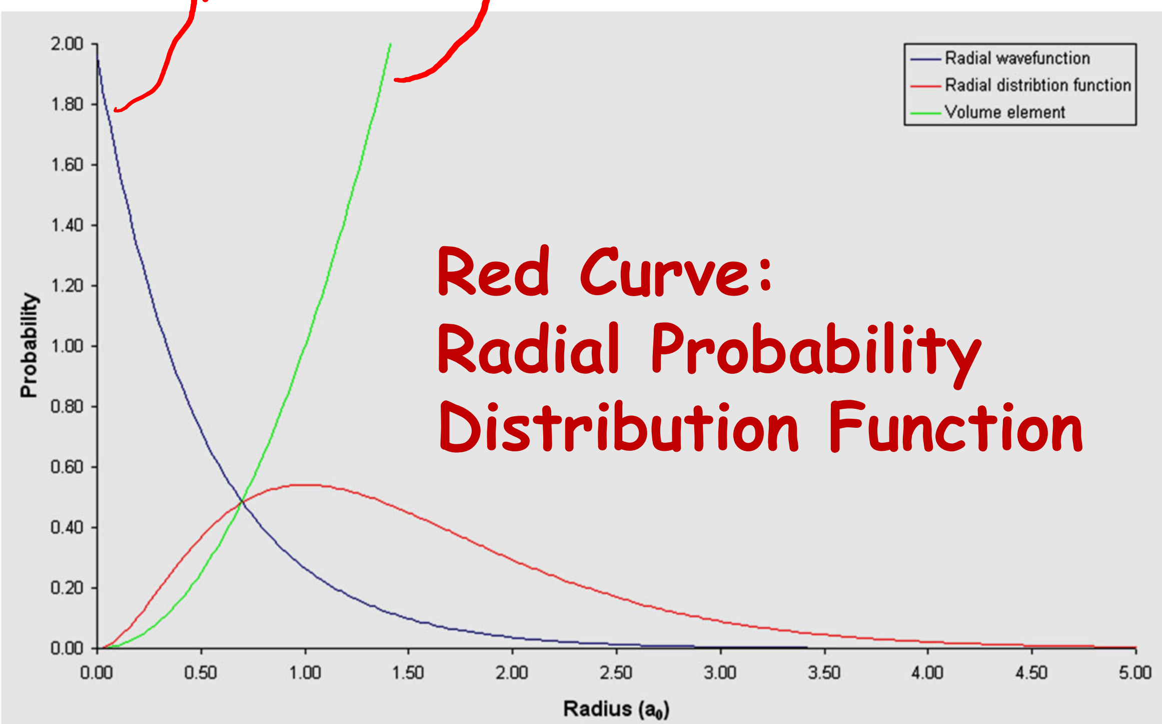
$P(r) \propto r^2 \times R^2_{nl}$

1 2

ψ_{100} or 1s



R^2_{nl} r^2

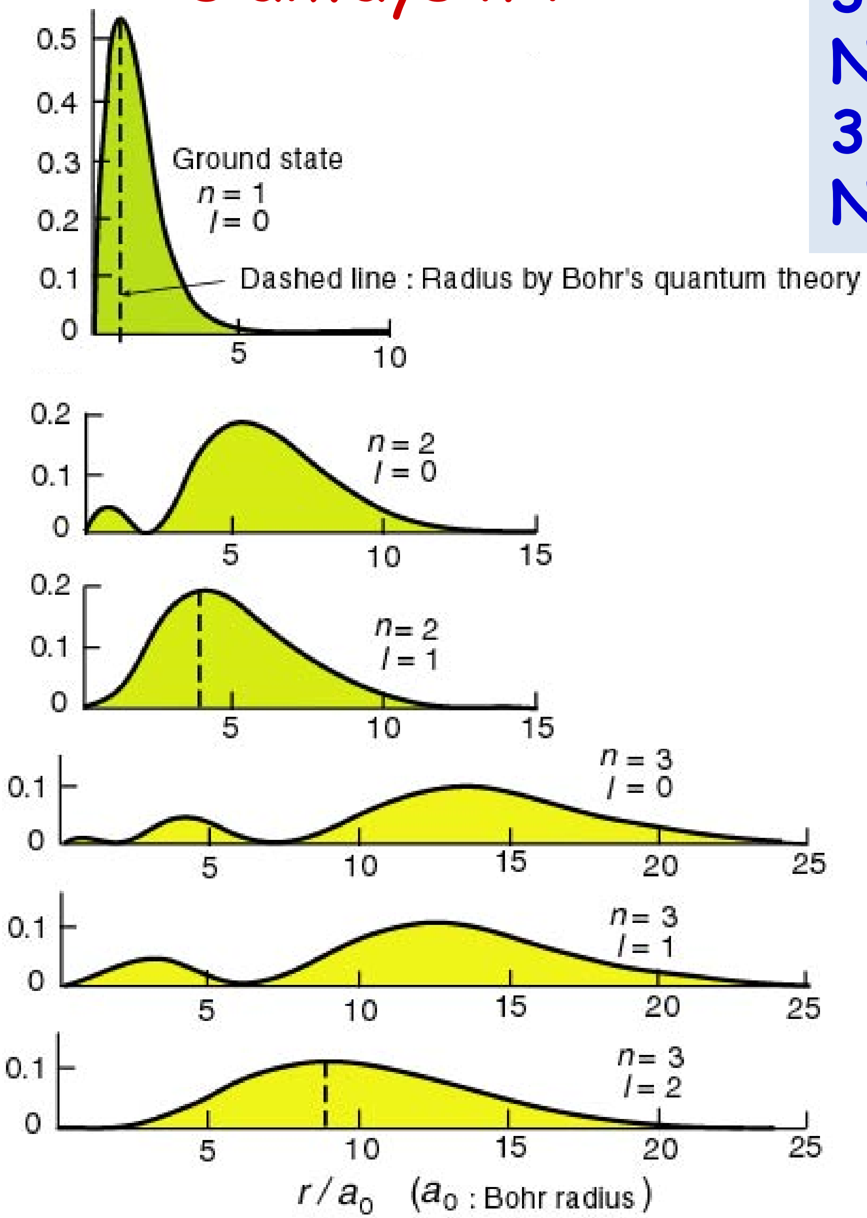


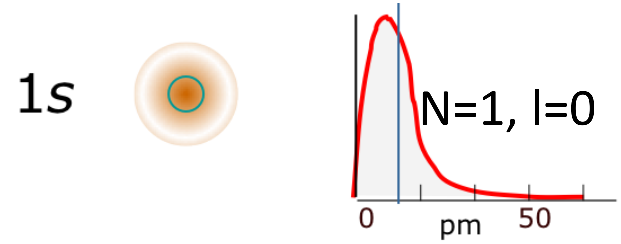
Product of an increasing function and a decreasing function: MAXIMUM

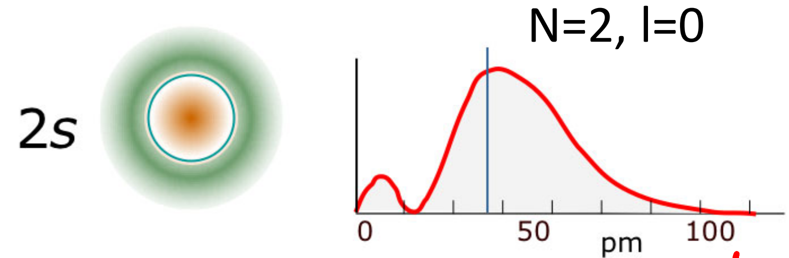
Radial Distribution Functions: $4\pi r^2 R_{nl}^2(r)$

Number of Radial Nodes is always n-l-1

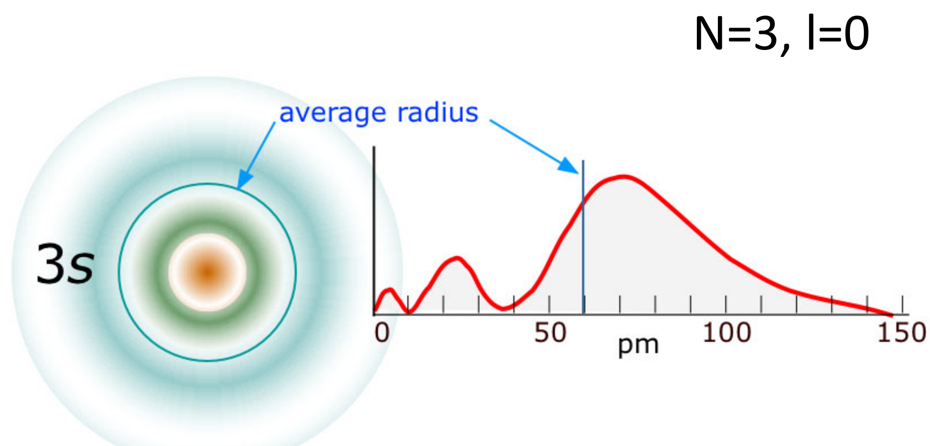
3s: n=3, l=0
Nodes= 2
3p: n=3, l=1,
Nodes= 1
3d: n=3, l=2
Nodes = 0







Max probability of finding the electron closest to nucleus is higher in 1s than in 2s



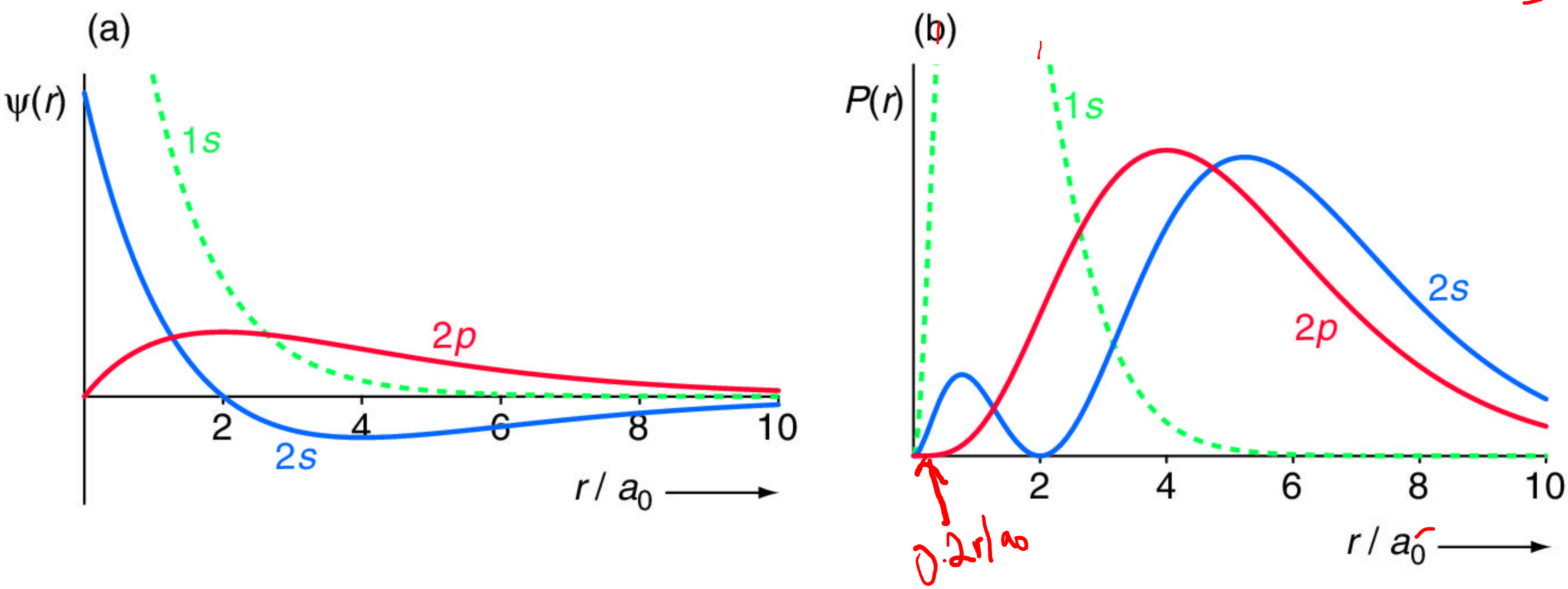
Radial Distribution Function

$\Psi(r)$ vs r

Radial Probability Distribution function

$4\pi r^2\Psi^2(r)$ vs r

$P(r)$



SHAPES AND SYMMETRIES OF THE ORBITALS

S ORBITALS

$$\psi_{1s} = \left(\pi a_0^3\right)^{-1/2} e^{-r/a_0} \qquad \psi_{2s} = \left(32\pi a_0^3\right)\left(2 - r/a_0\right) e^{-r/2a_0}$$

$l = 0$ spherically symmetric

$n - l - 1 = 0$	radial nodes	$n - l - 1 = 1$
$l = 0$	angular nodes	$l = 0$
$n - 1 = 0$	total nodes	$n - 1 = 1$

P ORBITALS: wavefunctions

"Shapes" of orbitals depend on Orbital quantum number l and Magnetic quantum no. m_l

Not spherically symmetric: depend on θ, ϕ

m = 0 case: $\psi_{210} = \psi_{2p_z} = \left(32\pi a_0^3\right)^{-1/2} \left(r/a_0\right) e^{-r/2a_0} \cos\theta$

ψ_{2p_z} independent of ϕ symmetric about z axis

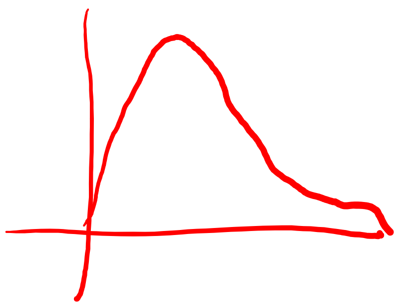
No ϕ dependence: symmetric around z axis

radial nodes	$n - l - 1 = 0$	(note difference from 2s: $R_{nl}(r)$ depends on l as well as n)
angular nodes	$l = 1$	
total nodes	$n - 1 = 1$	

xy nodal plane - zero amplitude at nucleus

Number of Angular Nodes = l

What are we up to?



R_{nl}

$\Downarrow$ → constant r

f(r,θ) at constant r

$$\Psi_{2pz} = (re^{-r})x(Cos\theta)$$

Angular part of Wave Functions

m = 0 case: $\psi_{210} = \psi_{2p_z} = \left(32\pi a_0^3\right)^{-1/2}\left(r/a_0\right)e^{-r/2a_0}\cos\theta$

constant at constant r

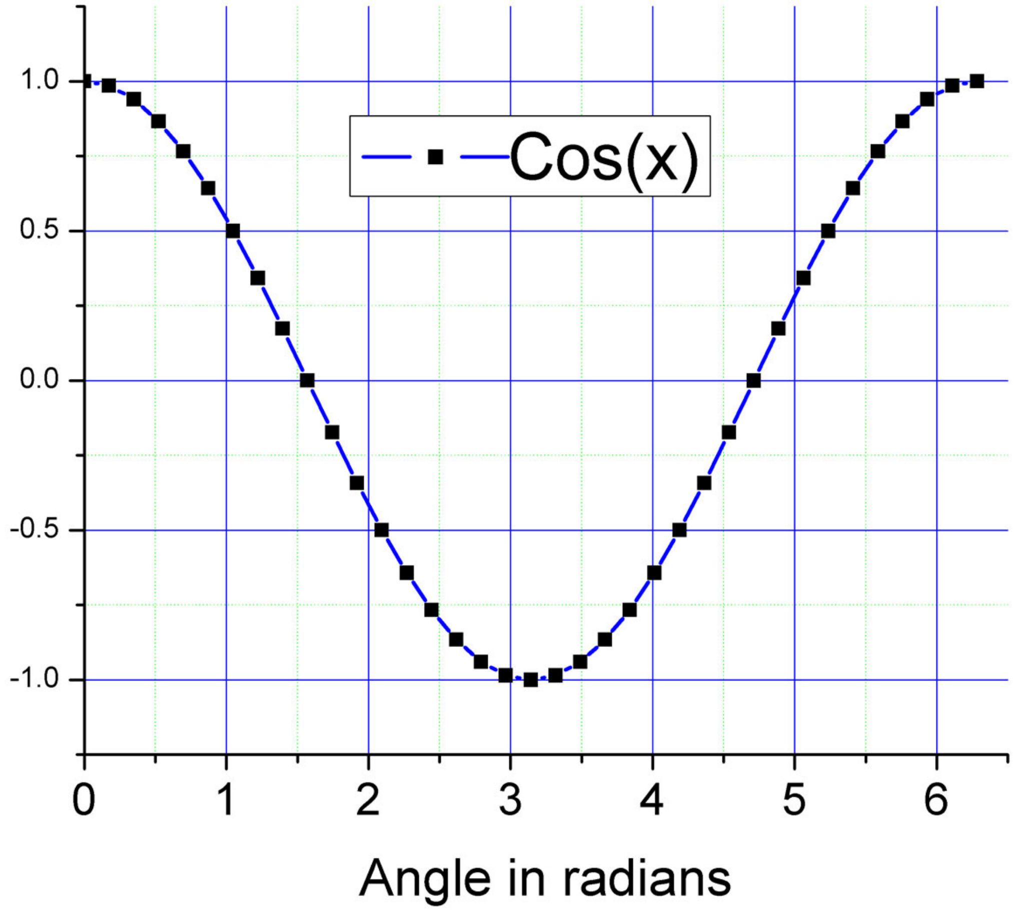
ψ_{2p_z} independent of ϕ symmetric about z axis

$$\Psi_{210}(2p_z) = N\rho e^{-\rho/2}.\cos\theta$$

$$\left|\Psi_{2p_z}(\theta)\right| = Const.\times\left|\cos\theta\right|$$

= -- cos θ

θ	cos θ
10	0.985
20	0.940
30	0.866
40	0.766
50	0.643
60	0.500
70	0.342
80	0.174
120	-0.500
150	-0.866
210	-0.866
240	-0.500



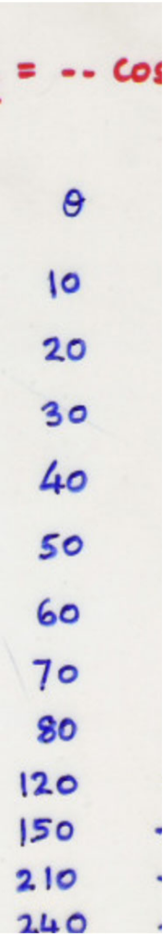
Angular part of Wave Functions

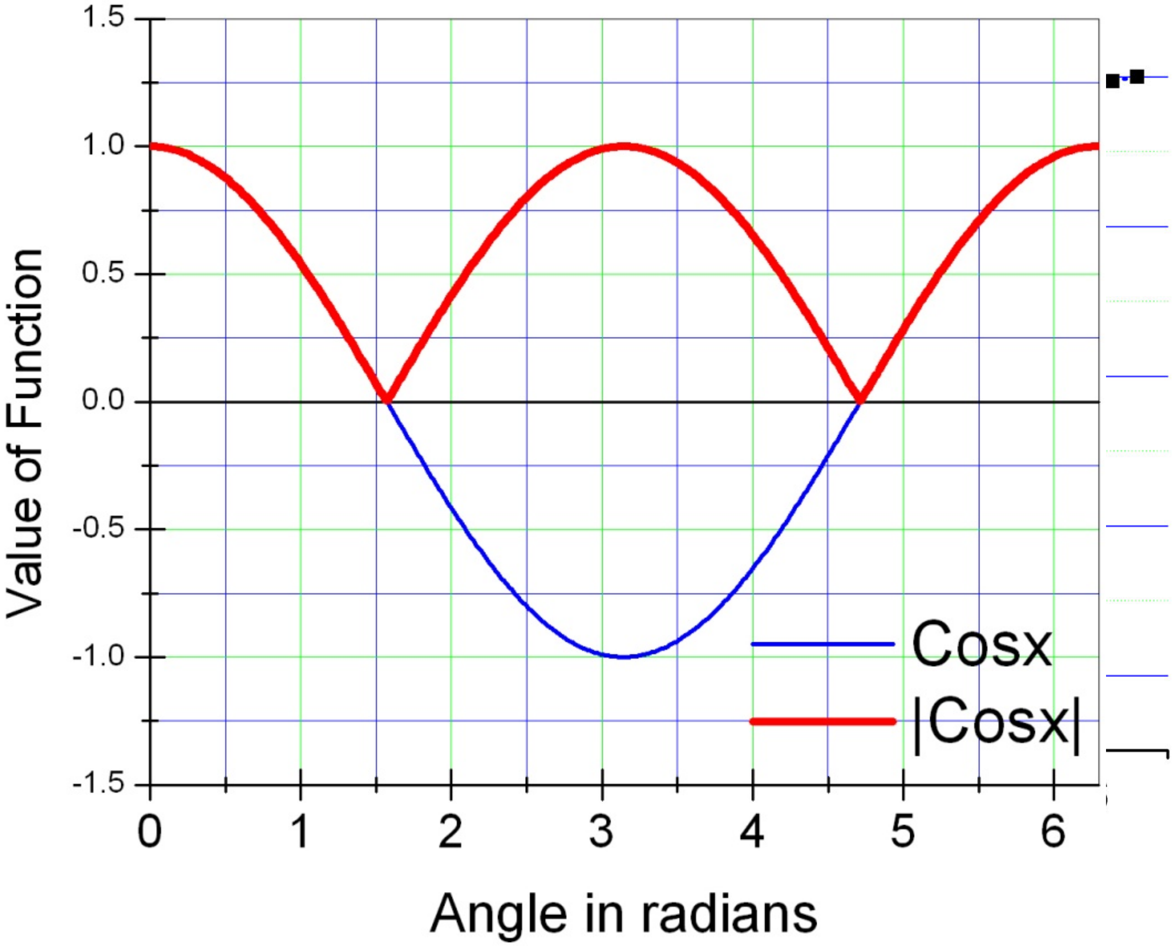
m = 0 case: $\psi_{210} = \psi_{2p_z} = \left(32\pi a_0^3\right)^{-1/2}\left(r/a_0\right)e^{-r/2a_0}\cos\theta$

ψ_{2p_z} independent of ϕ symmetric about z axis

$$\Psi_{210}(2p_z) = N\rho e^{-\rho/2}.\cos\theta$$

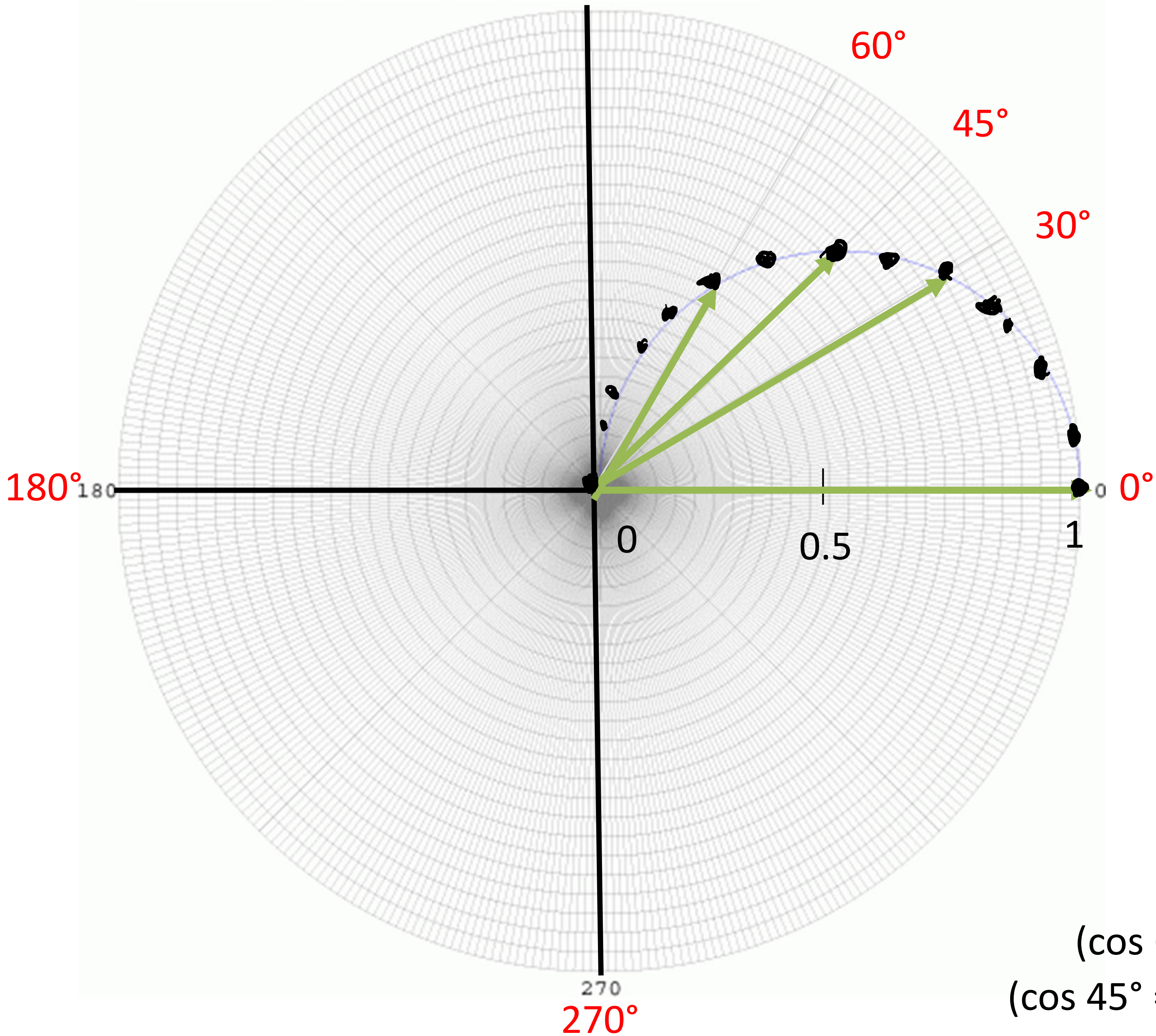
$$\left|\Psi_{2p_z}(\theta)\right| = Const.\times\left|\cos\theta\right|$$





$$\psi_{210} = \psi_{2p_z} = \left(32\pi a_0^3\right)^{-1/2} \left(r/a_0\right) e^{-r/2a_0} \cos\theta$$

$f(x) = \cos\theta$



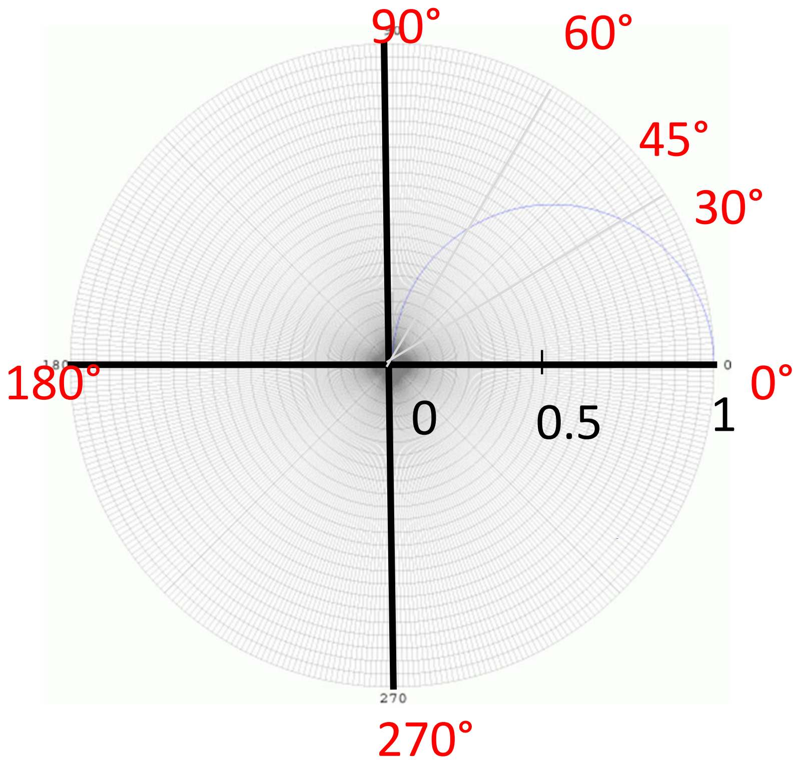
(cos 90° = 0)

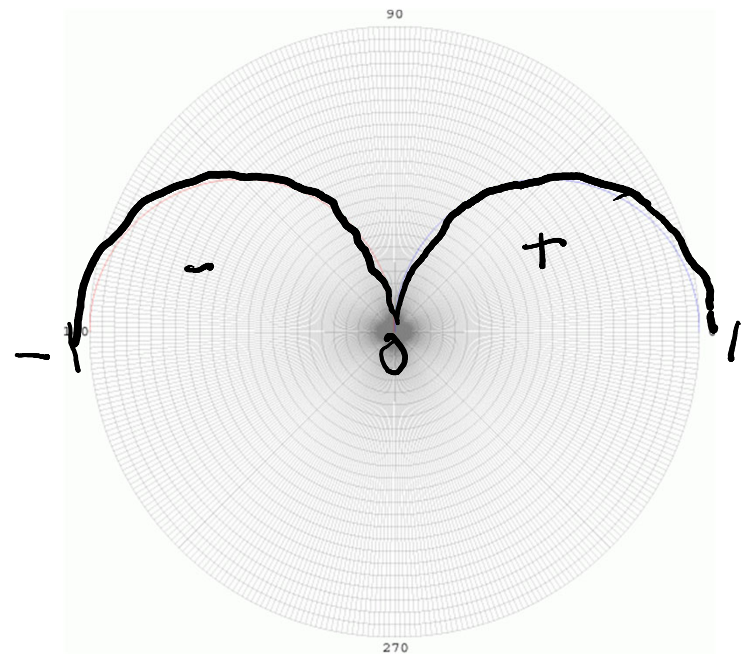
(cos 60° =0.5)

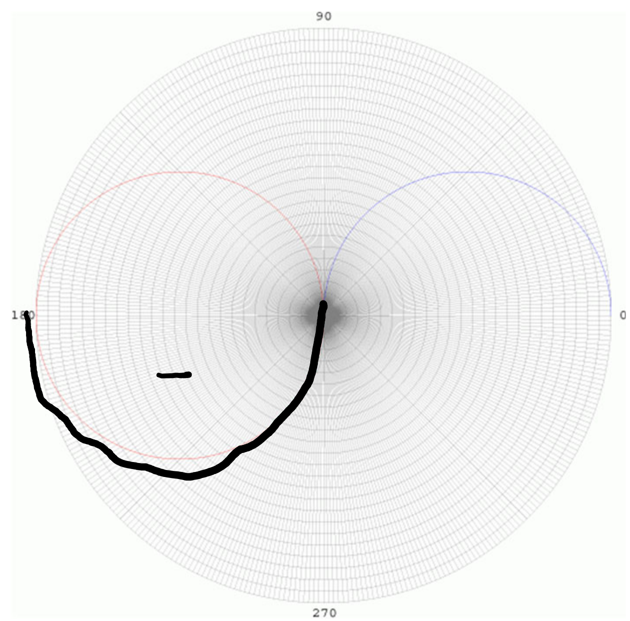
(cos 45° = 0.701)

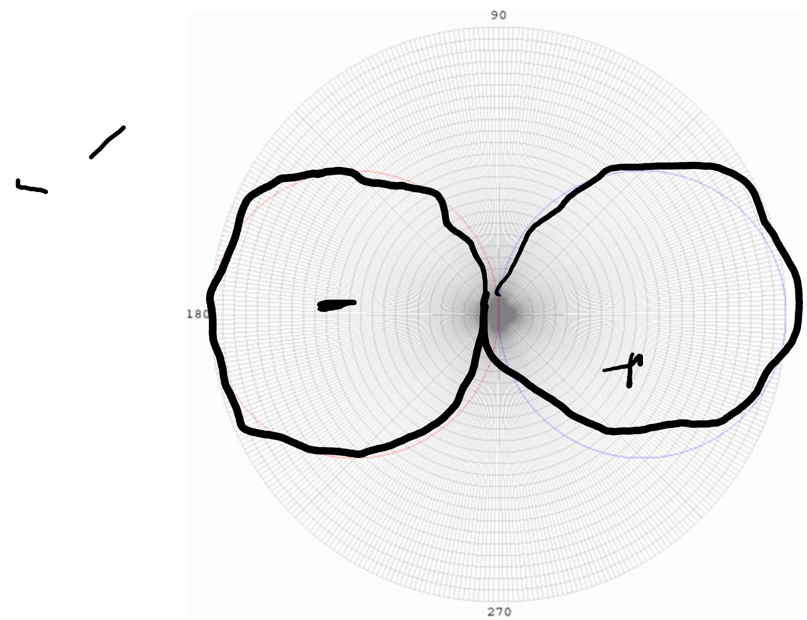
(cos 30° =0.87)

(cos 0° = 1)


90°
60°
45°
30°
180°
0°
0
0.5
1
270°


90
-
+
-1
0
1
270


90
180
0
-
270


90
180
-
+
270

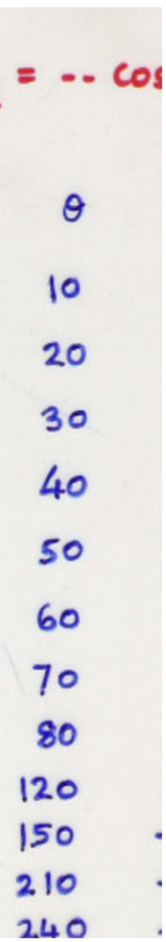
Angular part of Wave Functions

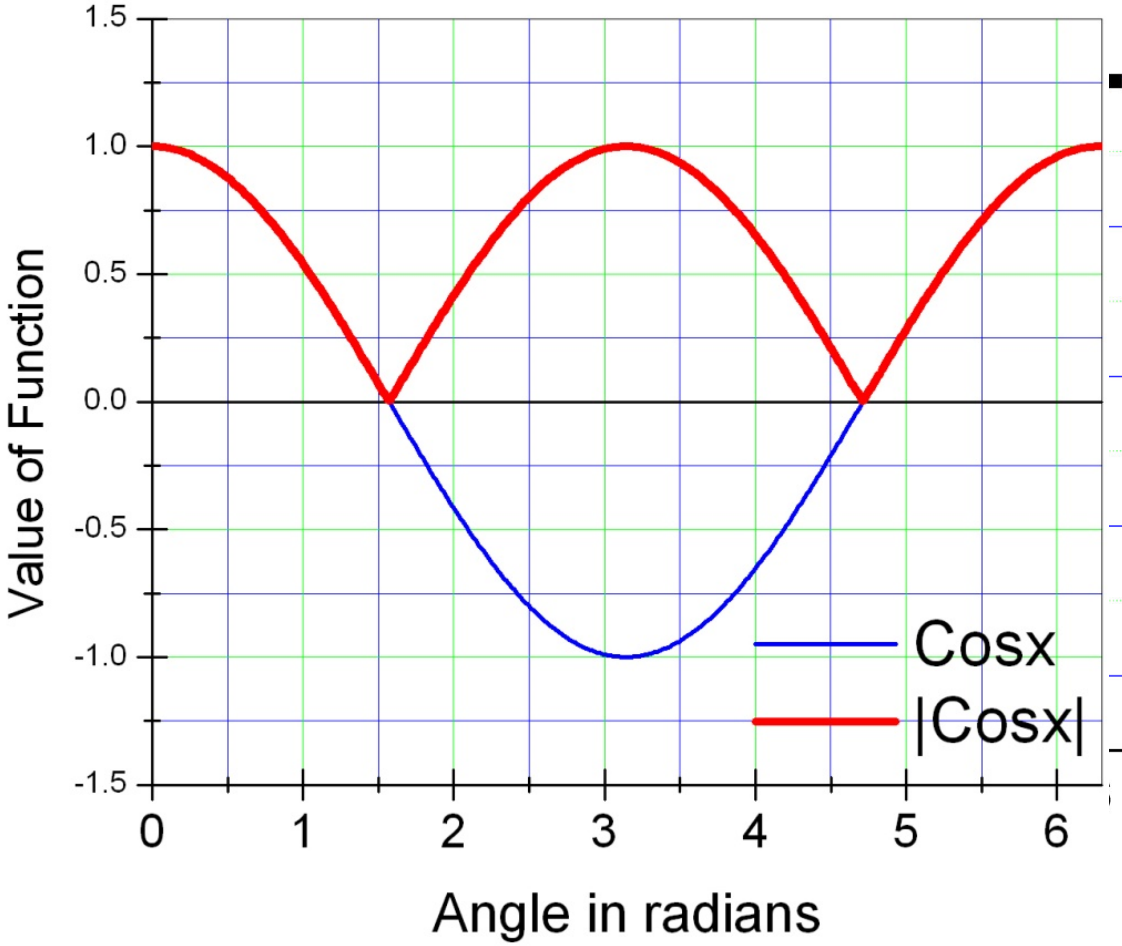
m = 0 case: $\psi_{210} = \psi_{2p_z} = \left(32\pi a_0^3\right)^{-1/2}\left(r/a_0\right)e^{-r/2a_0}\cos\theta$

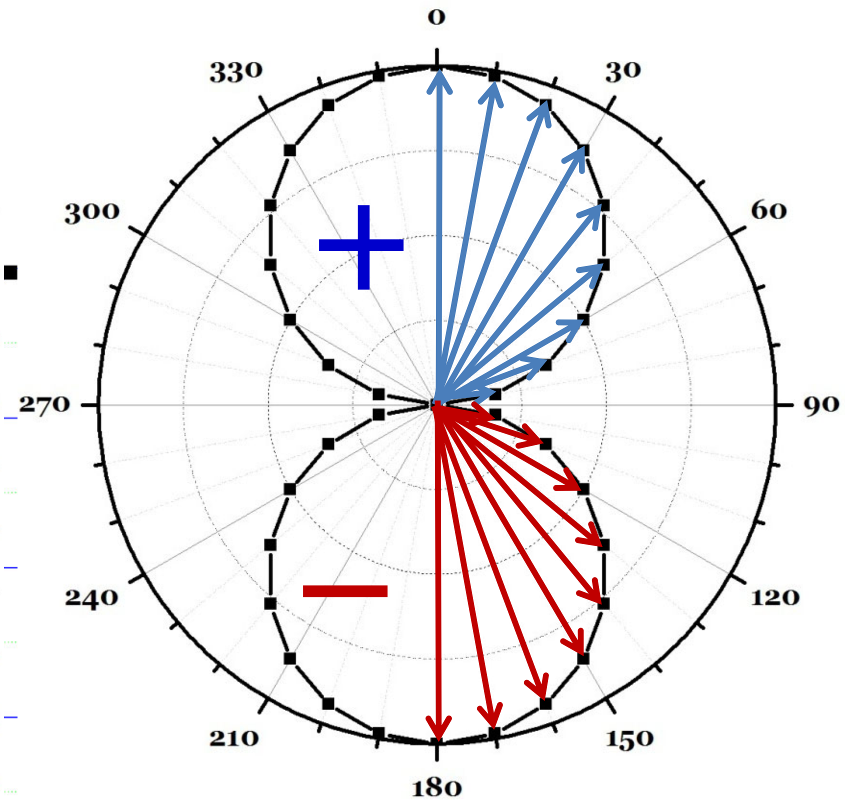
ψ_{2p_z} independent of ϕ symmetric about z axis

$$\Psi_{210}(2p_z) = N\rho e^{-\rho/2}.\cos\theta$$

$$\left|\Psi_{2p_z}(\theta)\right| = Const.\times\left|\cos\theta\right|$$







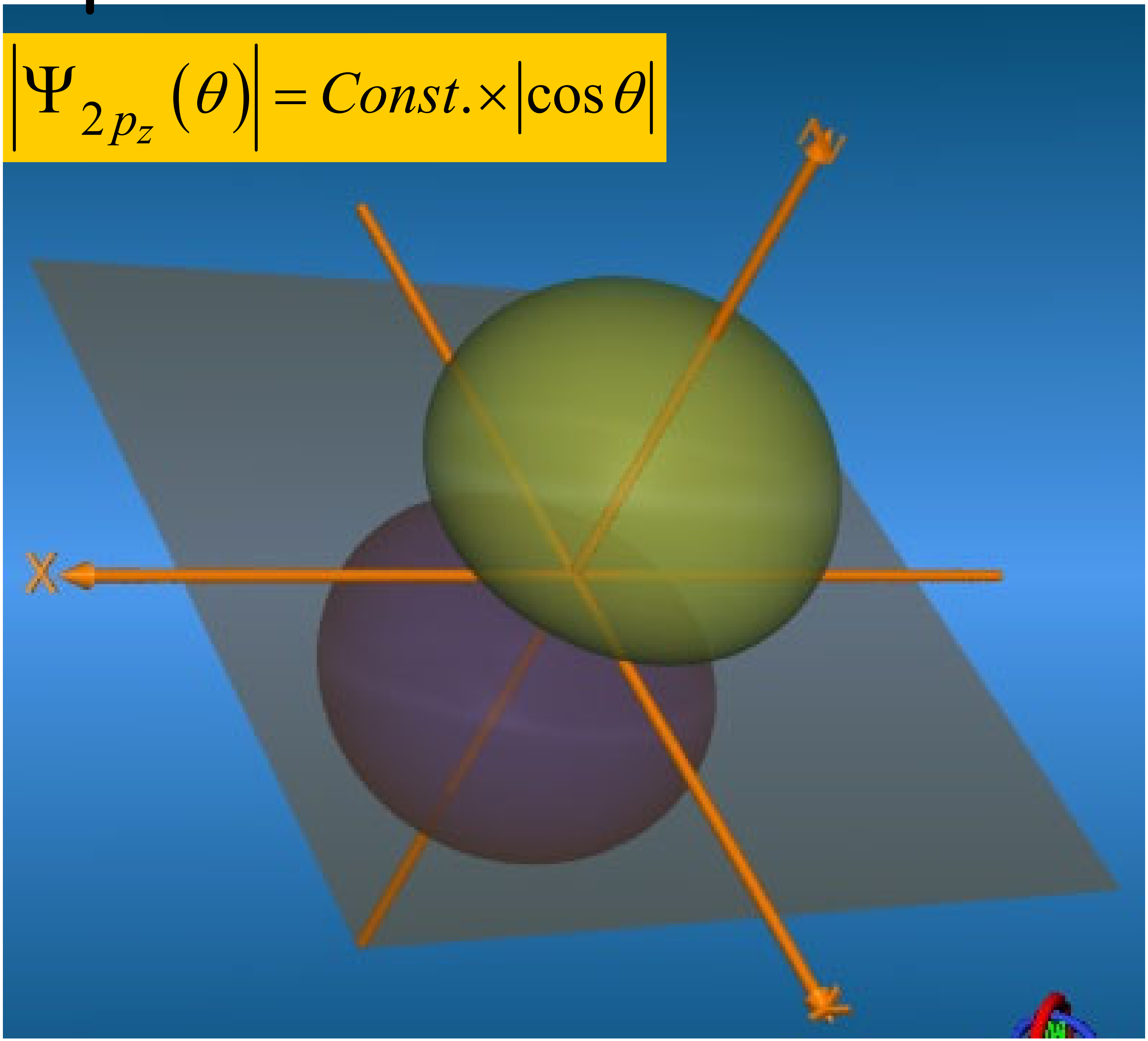
Same logic for p_x and p_y

$$\Psi(2p_x) = N\rho e^{-\rho/2}.\sin\theta.\cos\phi$$

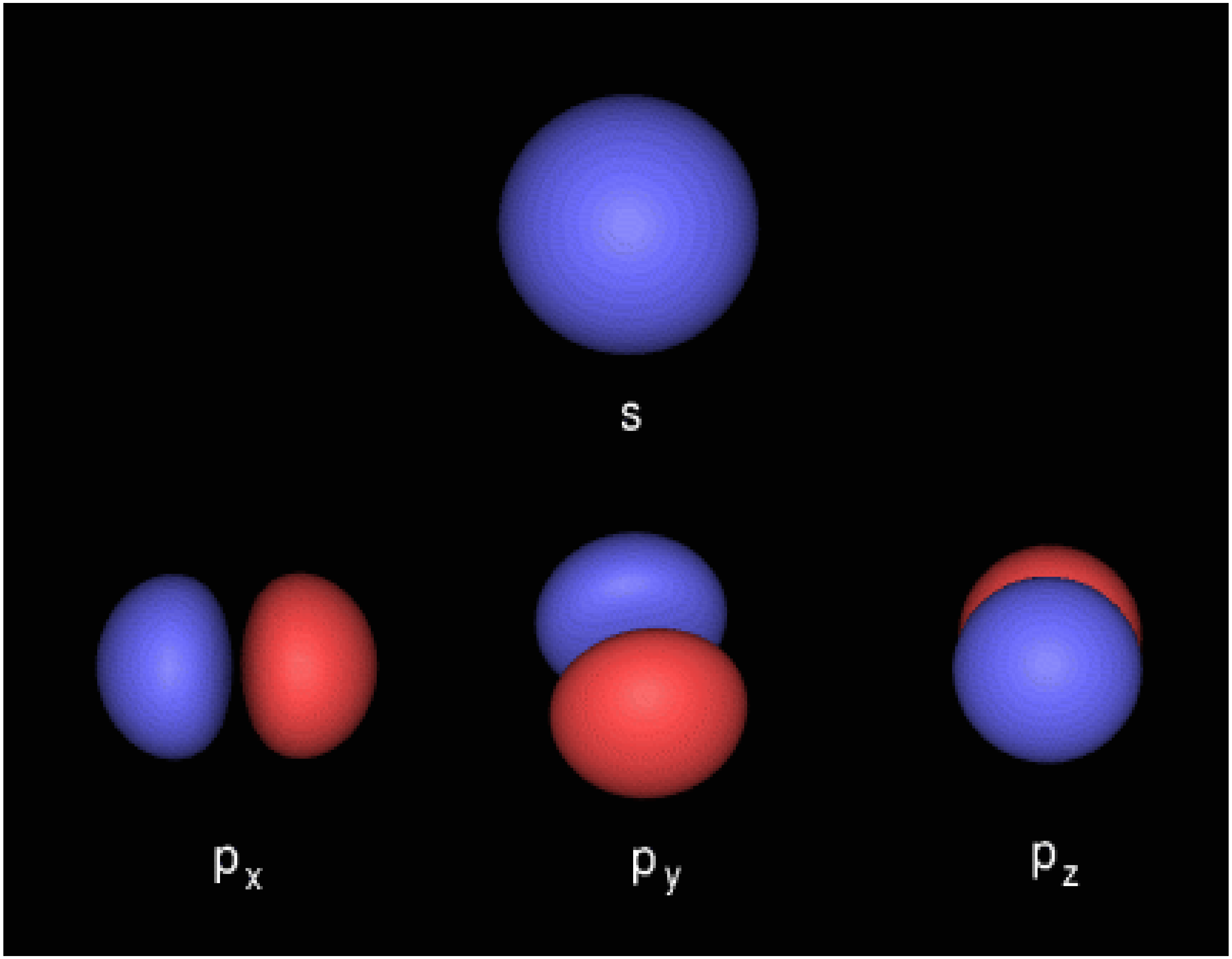
$$\Psi(2p_y) = N\rho e^{-\rho/2}.\sin\theta.\sin\phi$$

Complete Rotation around z-axis

$$\left|\Psi_{2p_z}(\theta)\right| = Const.\times\left|\cos\theta\right|$$



So, what is an orbital?



Are these what chemists refer to as pictures of "Orbitals"?