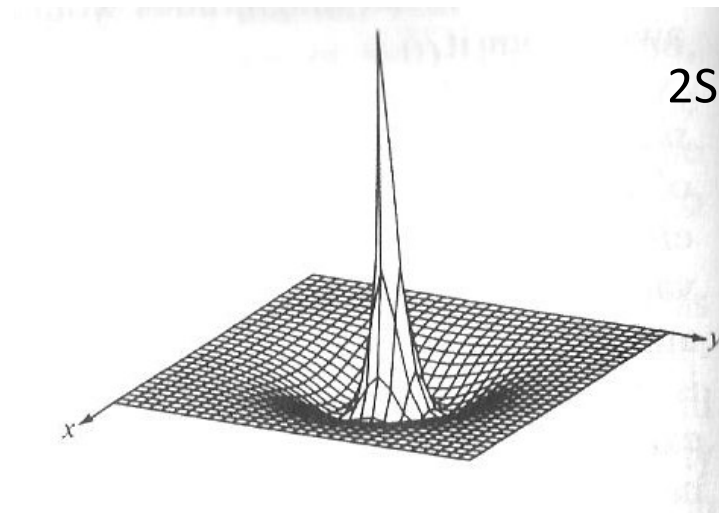
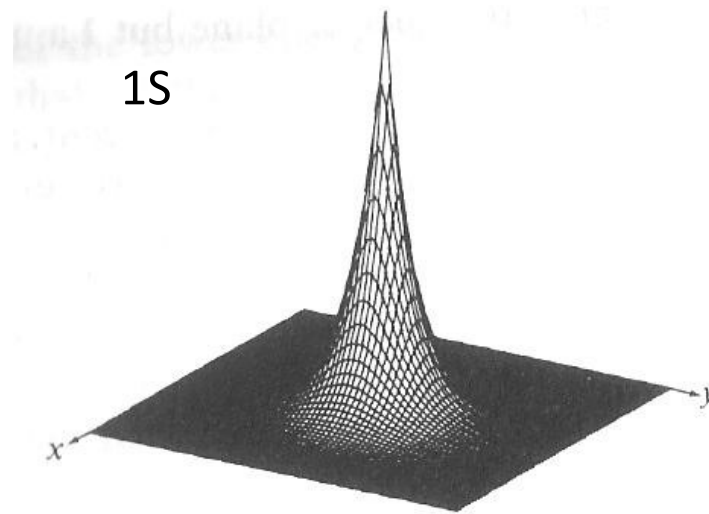
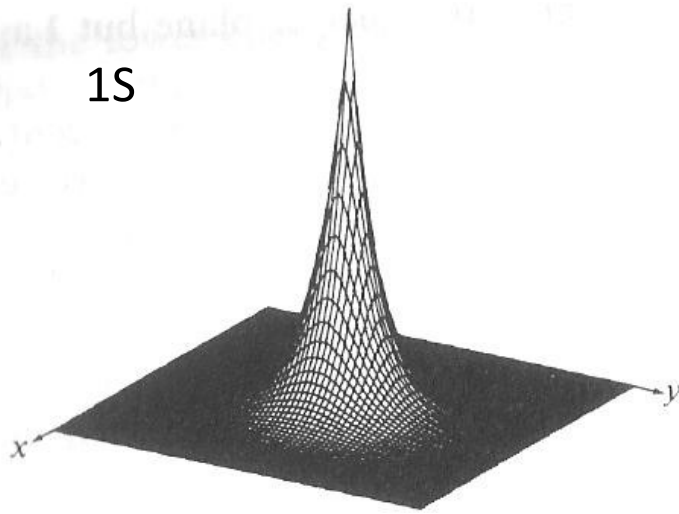


# Surface plot of $\Psi$ for $S$

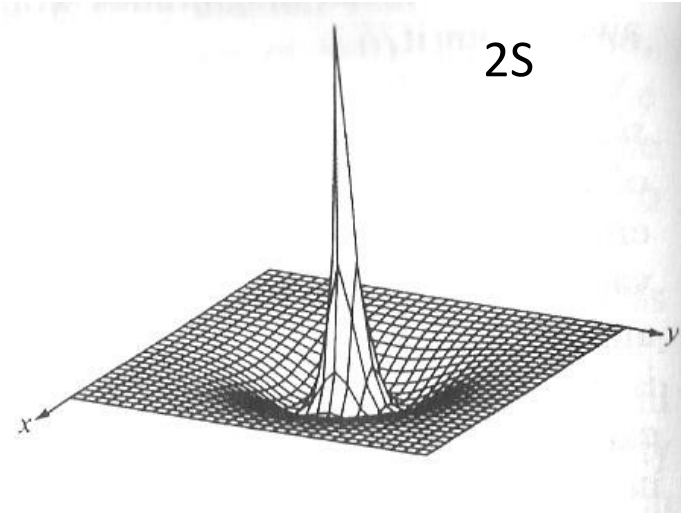


# Surface plot of $\Psi^2$ for S

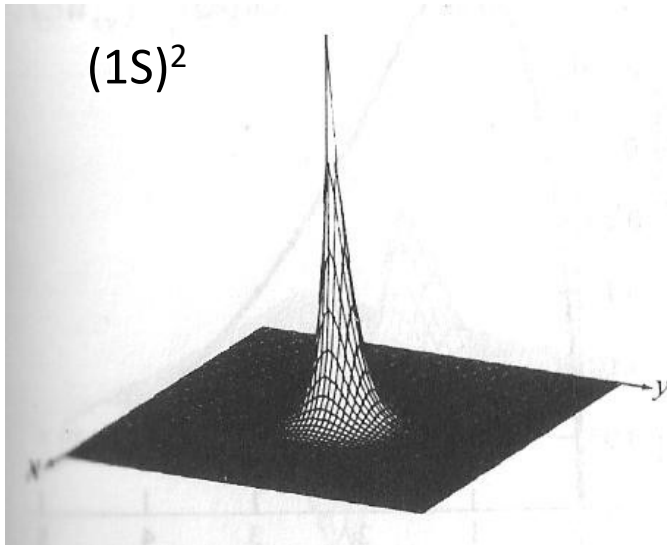
1S



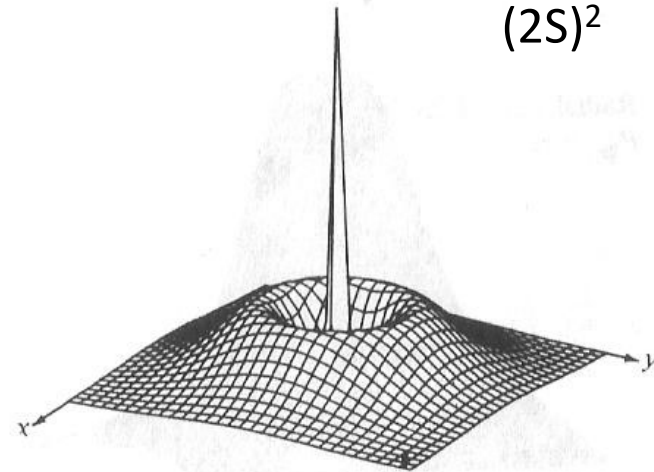
2S



$(1S)^2$

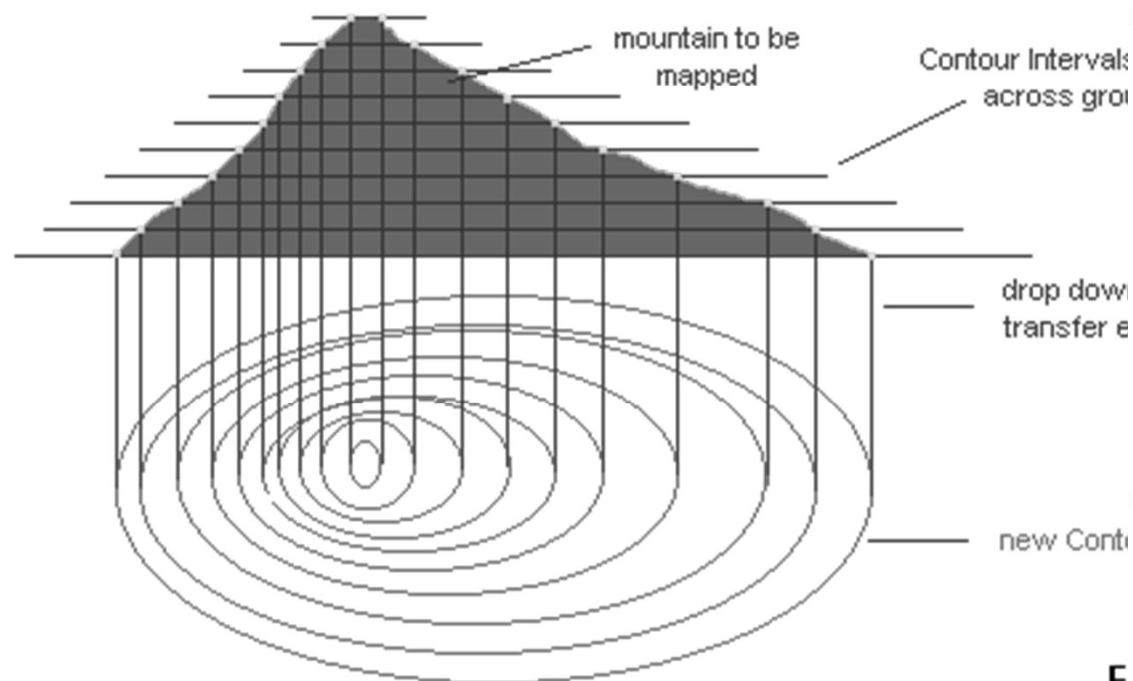
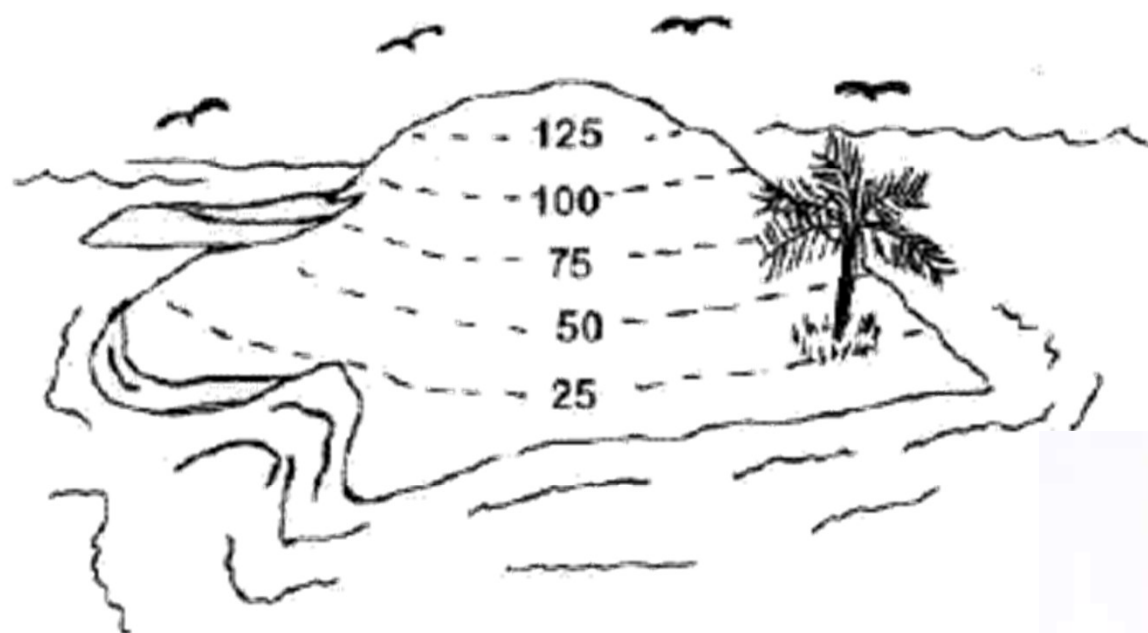


$(2S)^2$

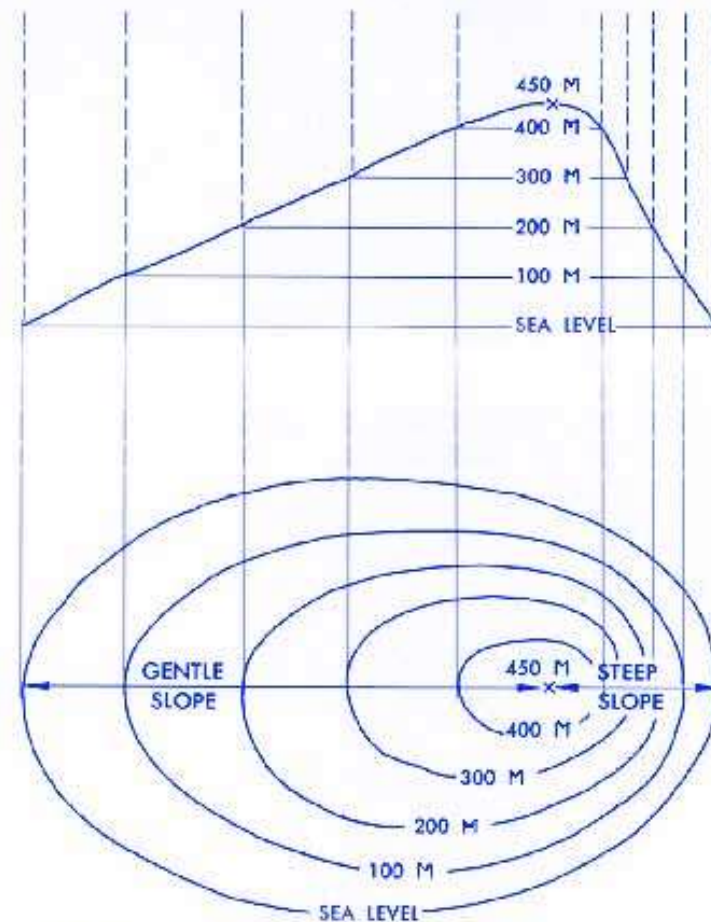


**Maximum probability density of finding the electron?**



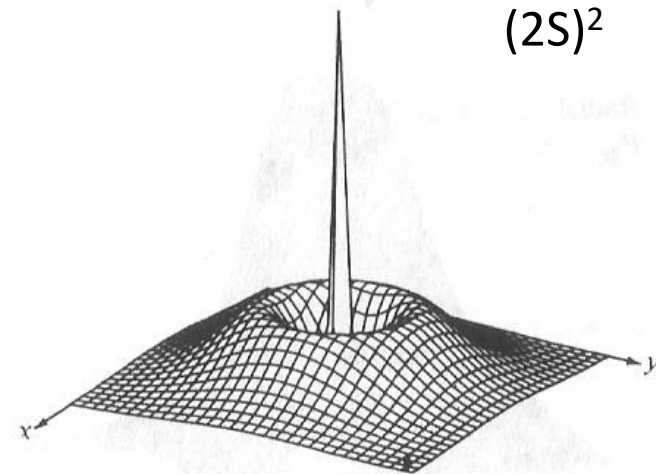
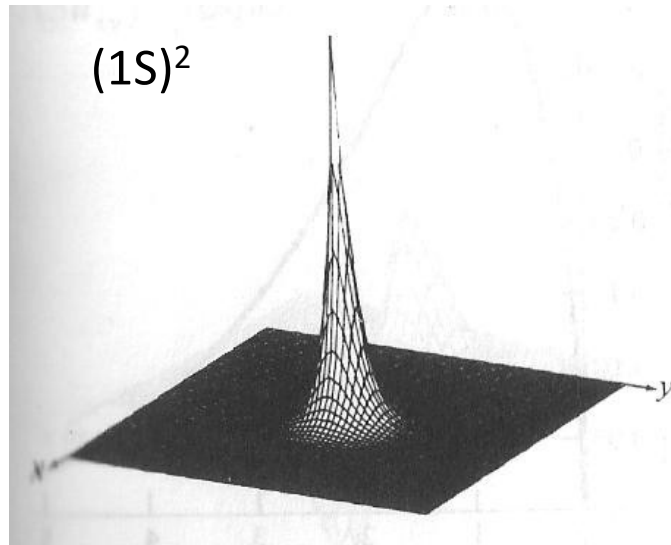
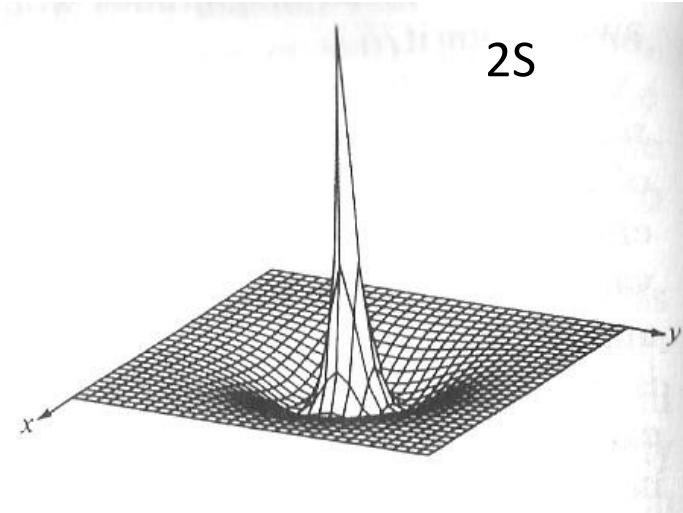
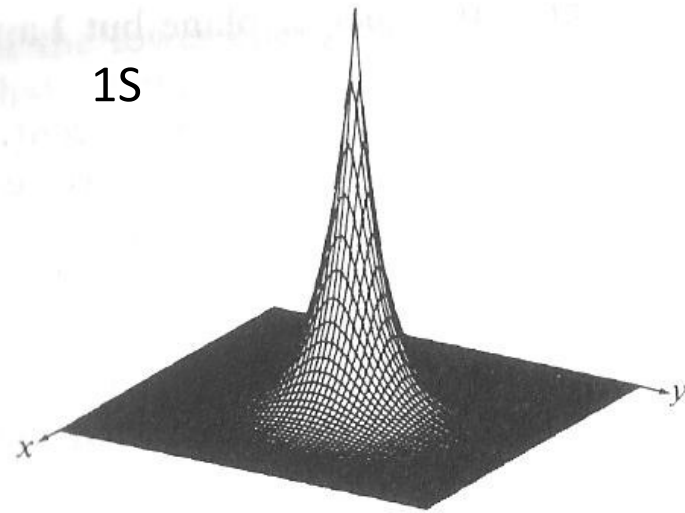


F



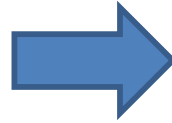
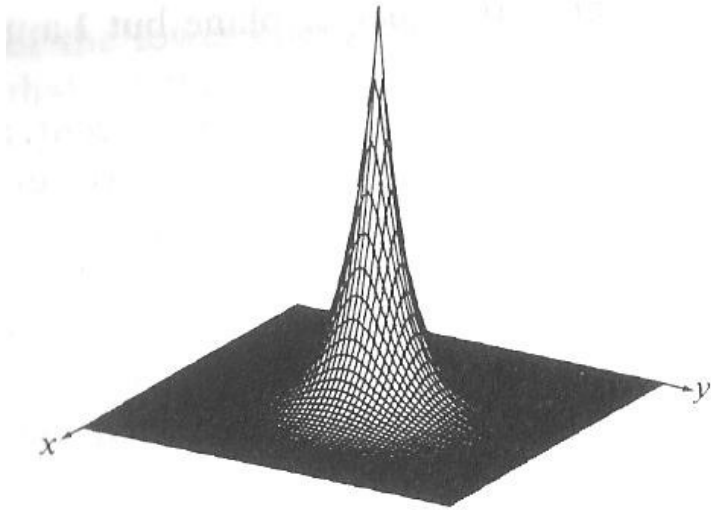
CONTOUR INTERVAL, 100 M

# Surface plot of $\Psi$ and $\Psi^2$ for S

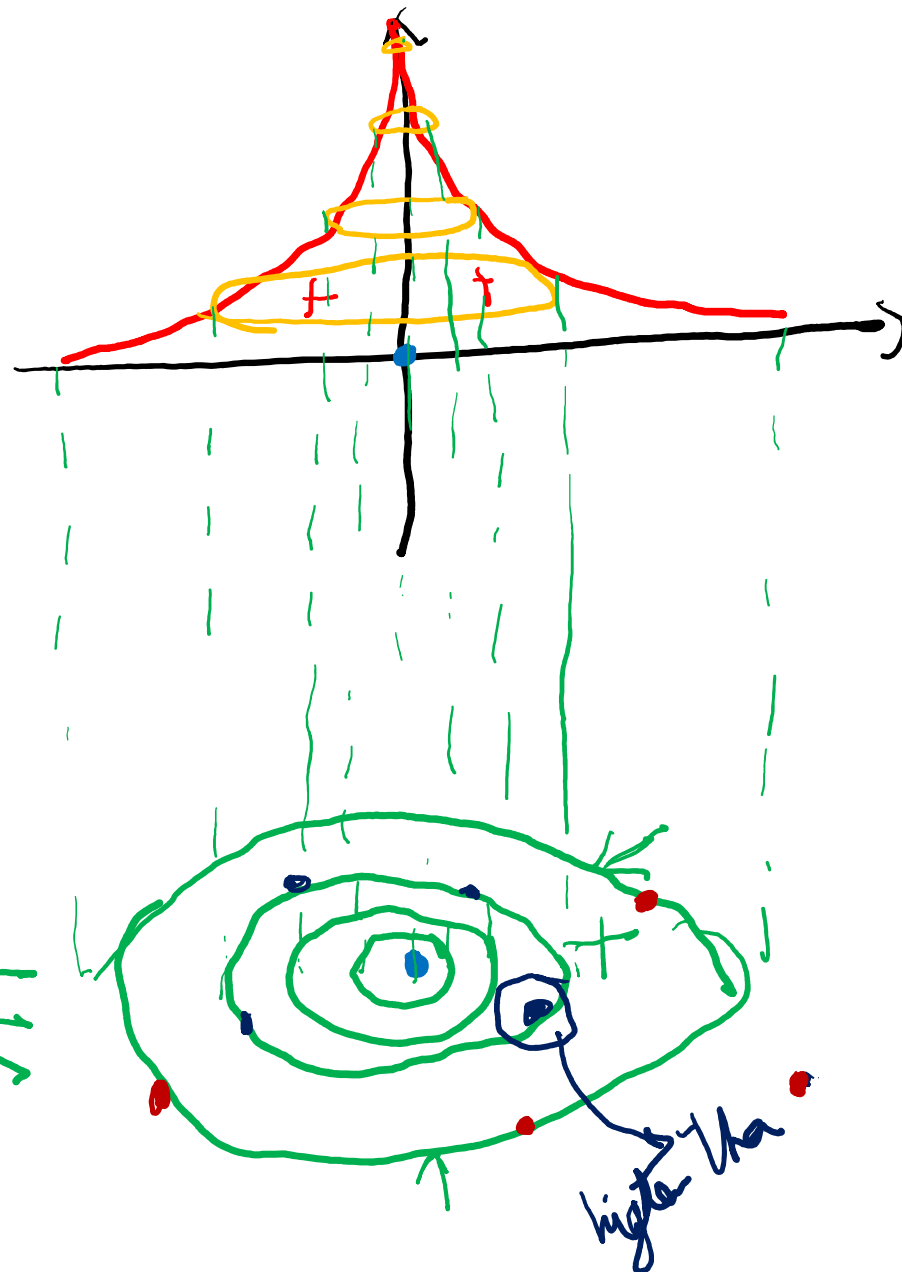
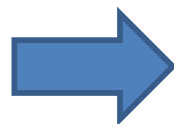
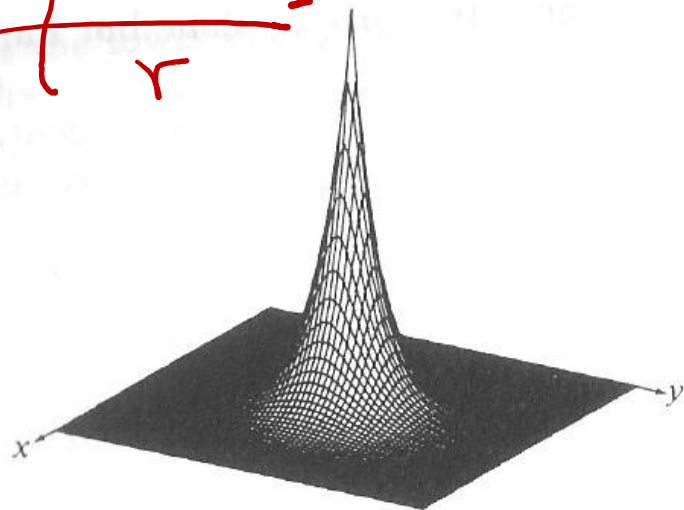


**Maximum probability of finding the electron?**

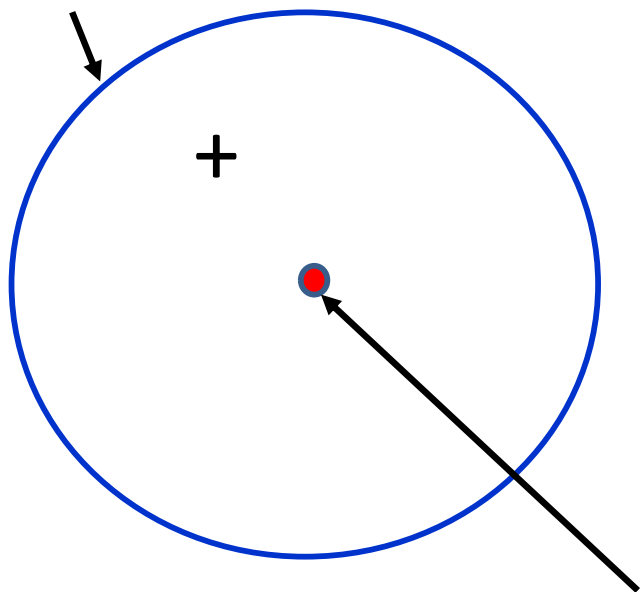
# Surface plot of 1s



# Surface plot of 1s



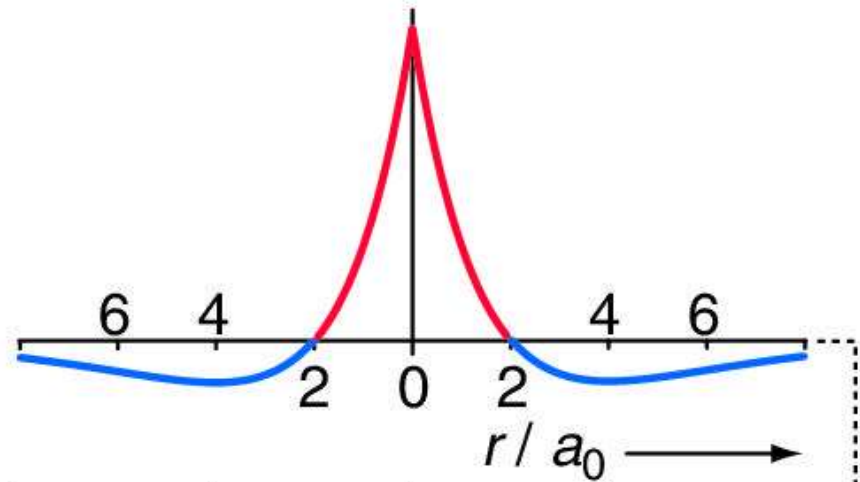
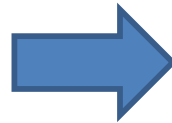
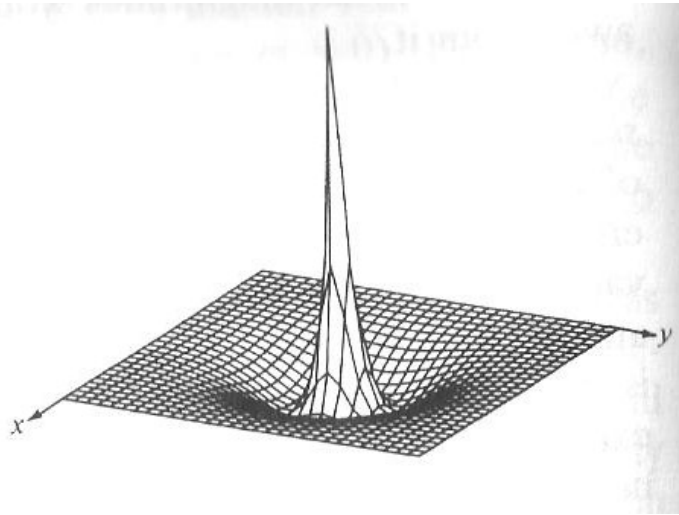
Equal Probability Iso-surface



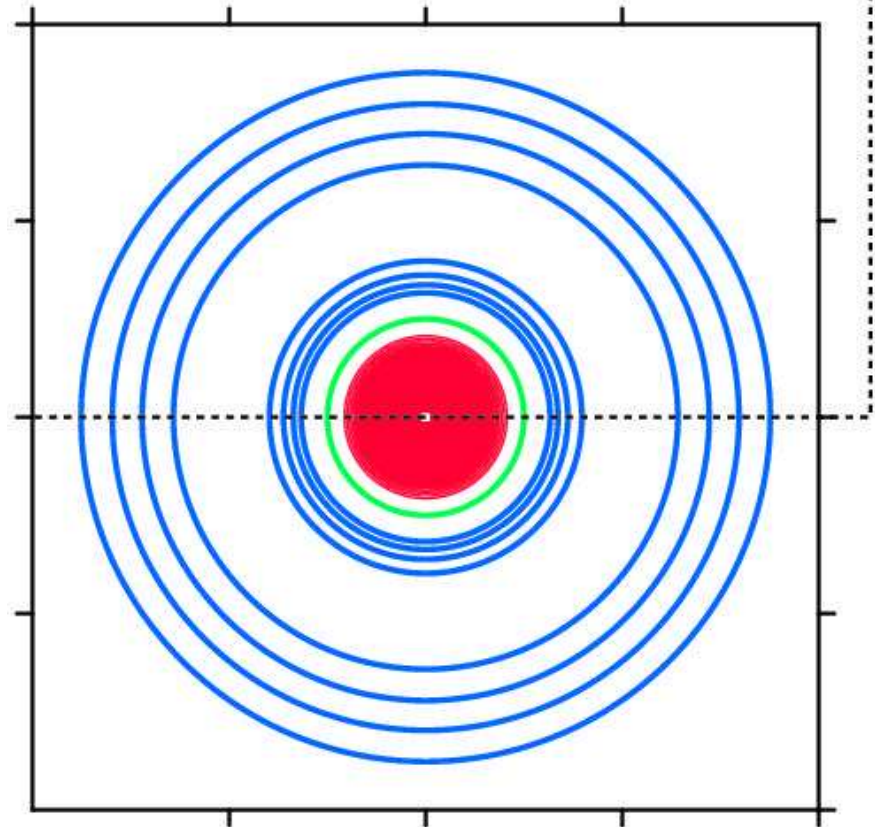
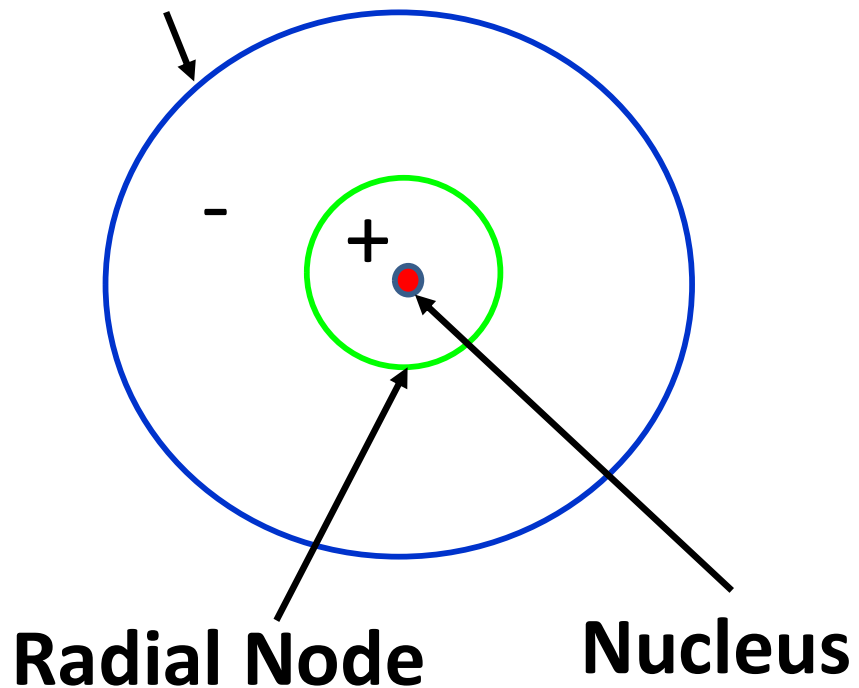
Nucleus



# Surface plot of 2s



**Equal Probability Iso-surface**





**P ORBITALS:** wavefunctions

Not spherically symmetric: depend on  $\theta, \phi$

“Shapes” of orbitals depend on Orbital quantum number  $l$  and Magnetic quantum no.  $m_l$

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

$\psi_{2p_z}$  independent of  $\phi$  symmetric about z axis

No  $\phi$  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?

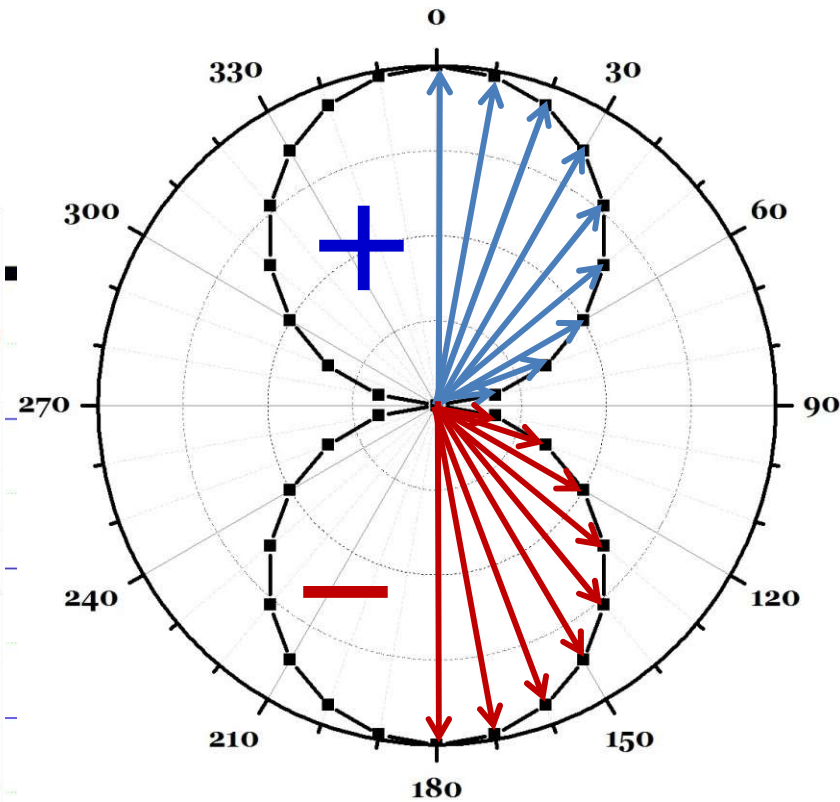
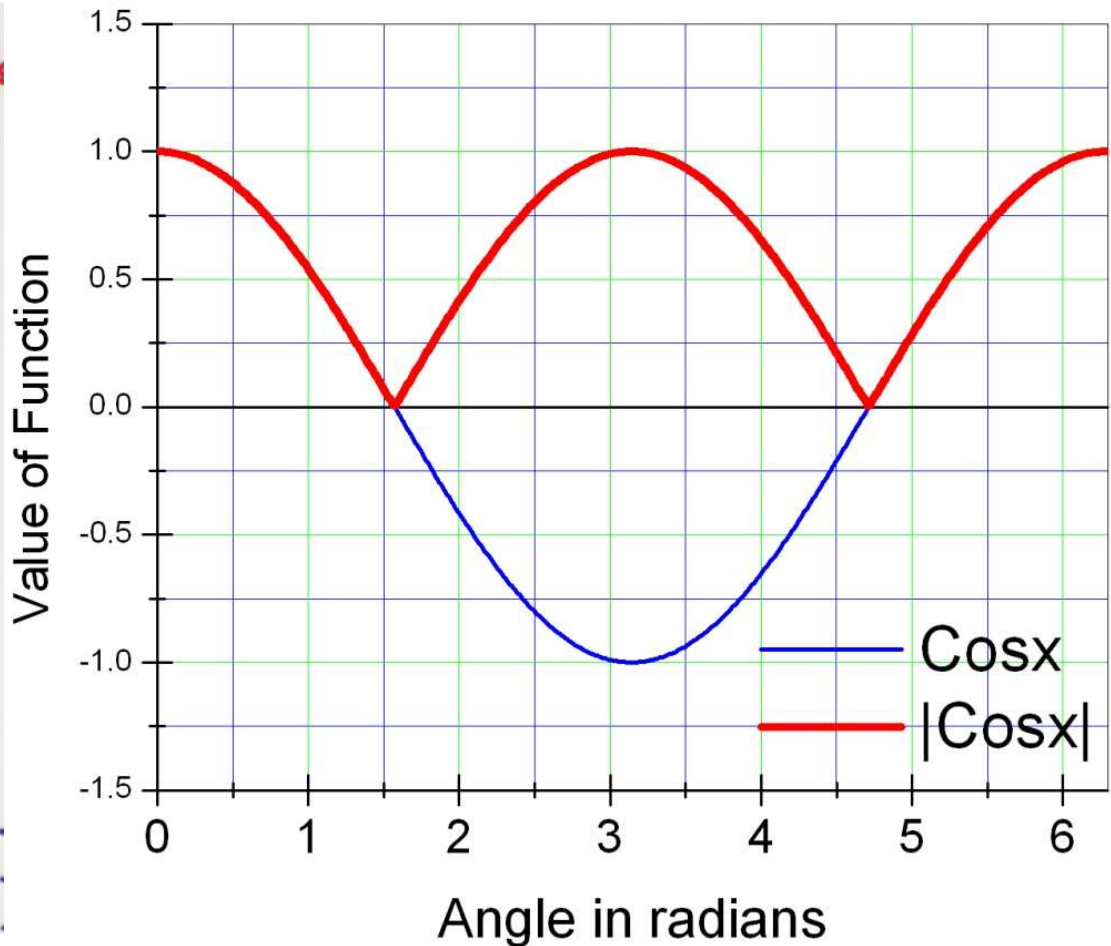
$$\Psi_{2pz} = (re^{-r}) \times (\cos\theta)$$

# Angular part of Wave Functions

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

$\psi_{2p_z}$  independent of  $\phi$       symmetric about z axis       $\Psi_{210}(2p_z) = N \rho e^{-\rho/2} \cdot \cos \theta$

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



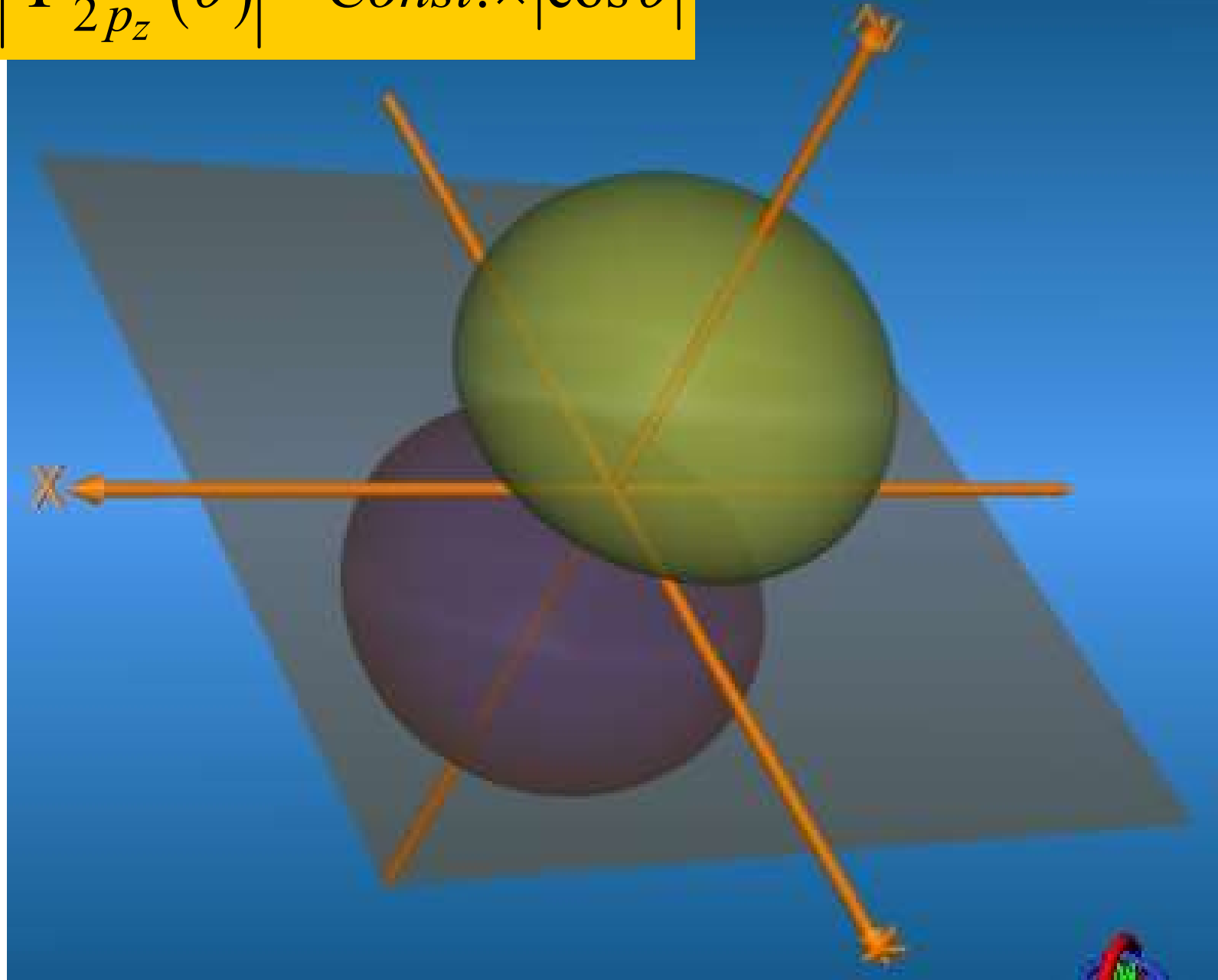
Same logic for  $p_x$  and  $p_y$

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

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

# Is this a "p" orbital?

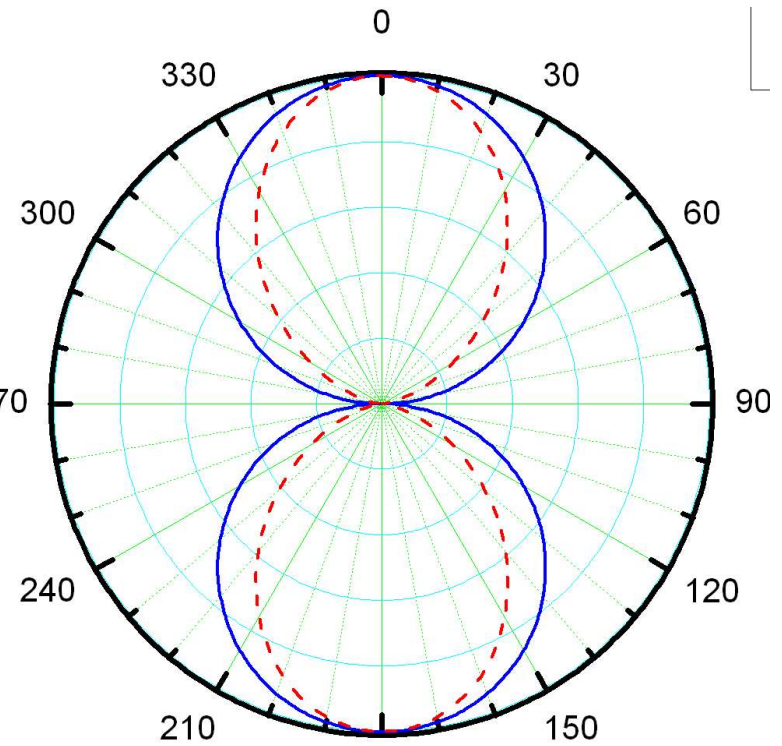
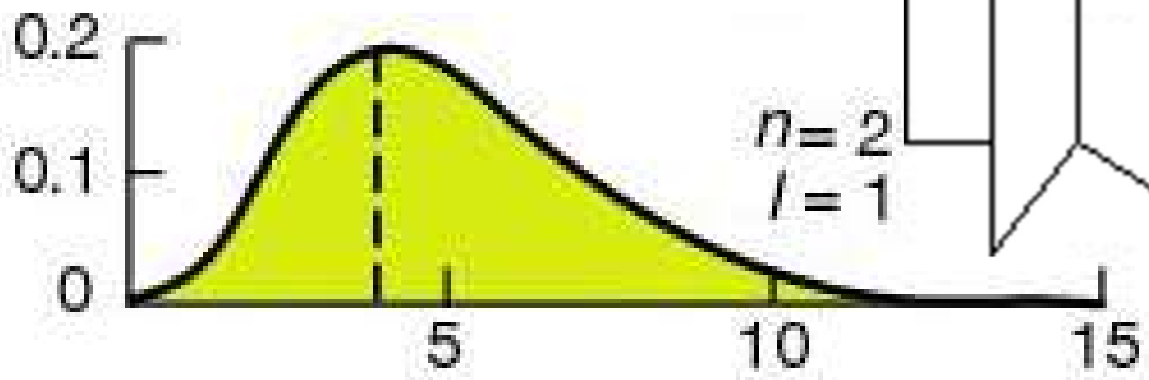
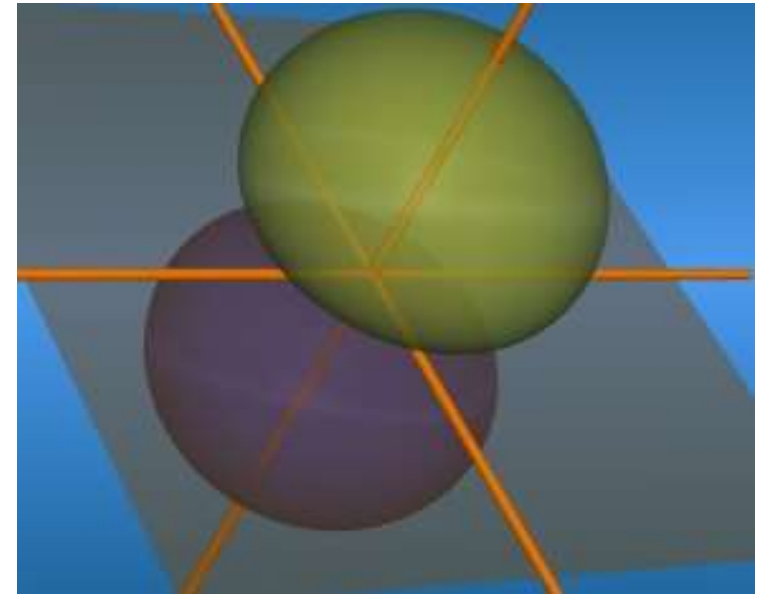
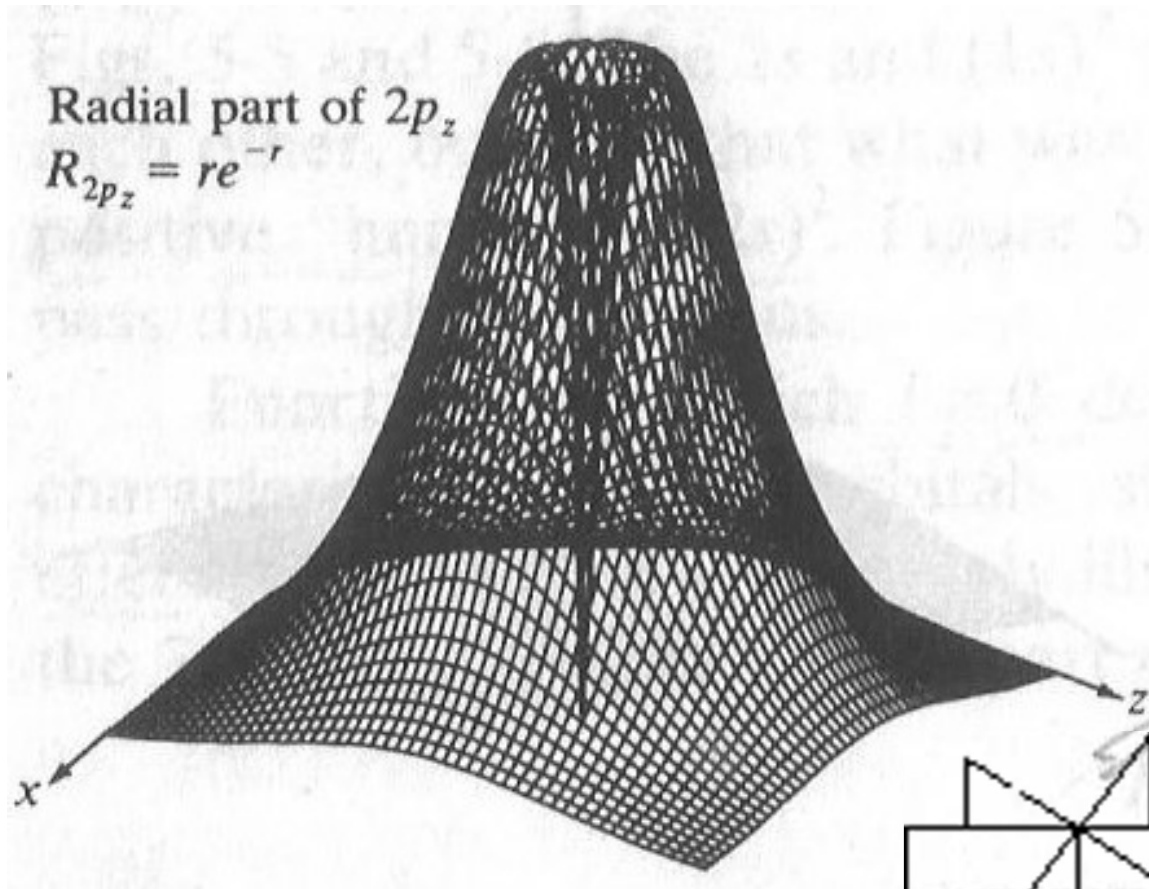
$$|\Psi_{2p_z}(\theta)| = \text{Const.} \times |\cos \theta|$$



What are we up to?

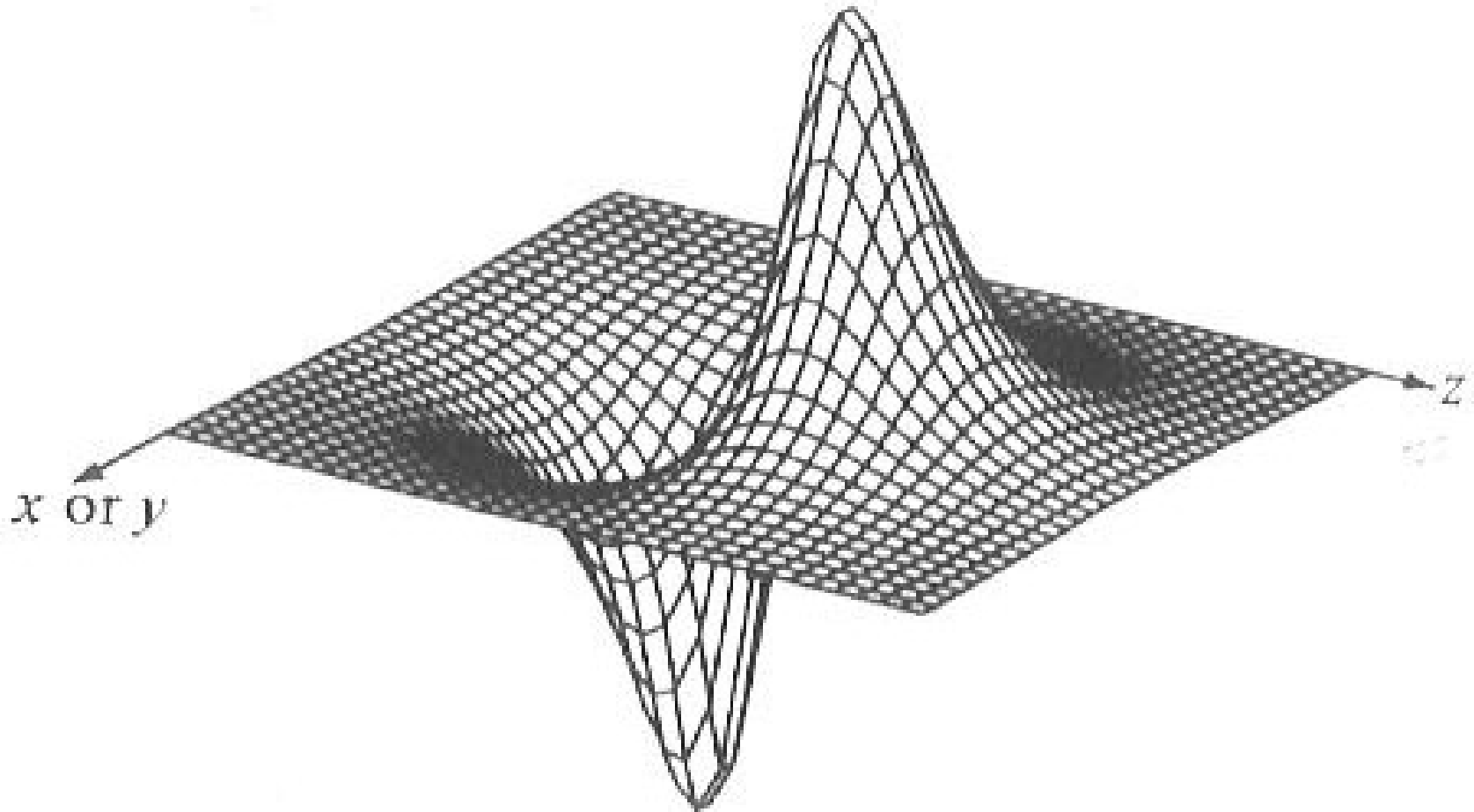
$$\Psi_{2pz} = (re^{-r}) \times (\cos\theta)$$

# Surface plot of $re^{-r}$ & $\cos\theta$ for all $\Phi$

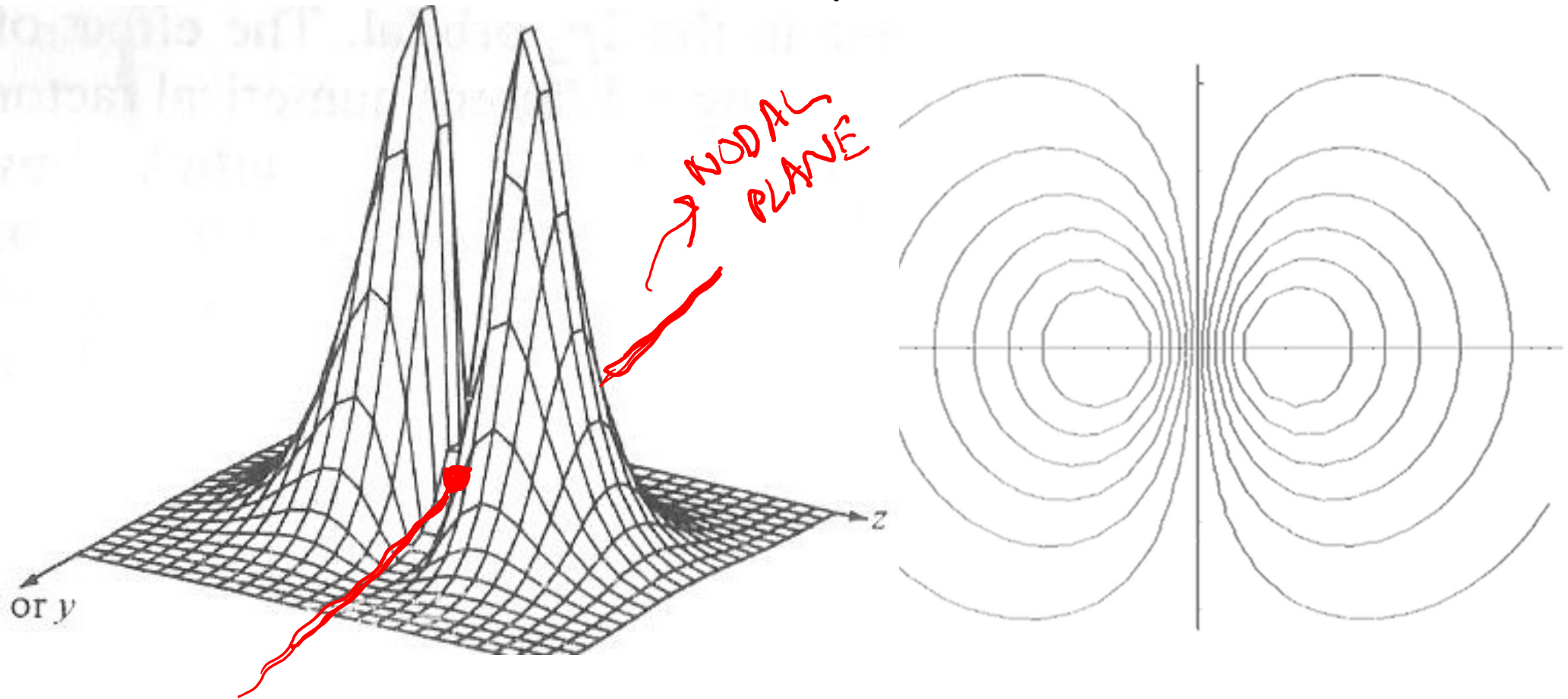




Surface plot of  $\Psi_{2pz} = (re^{-r})x(\cos\theta)$

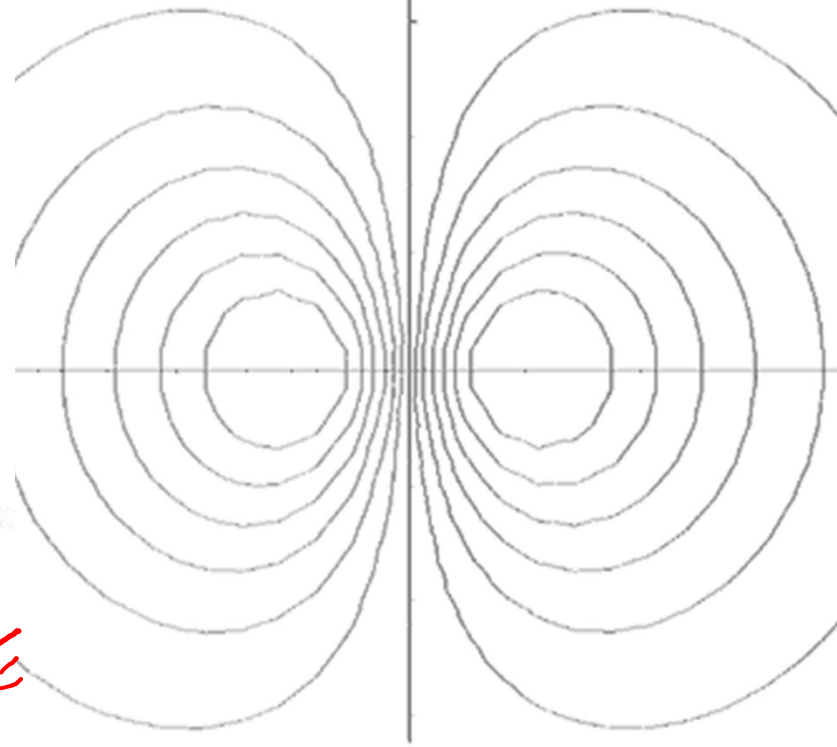
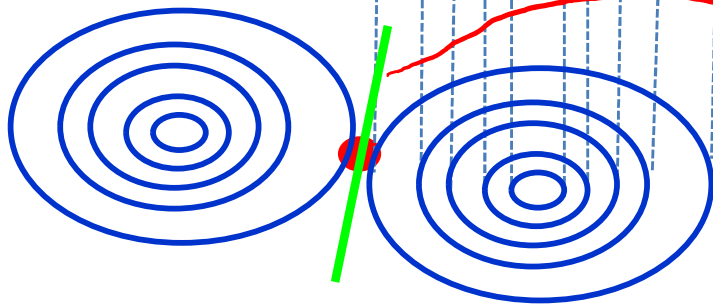
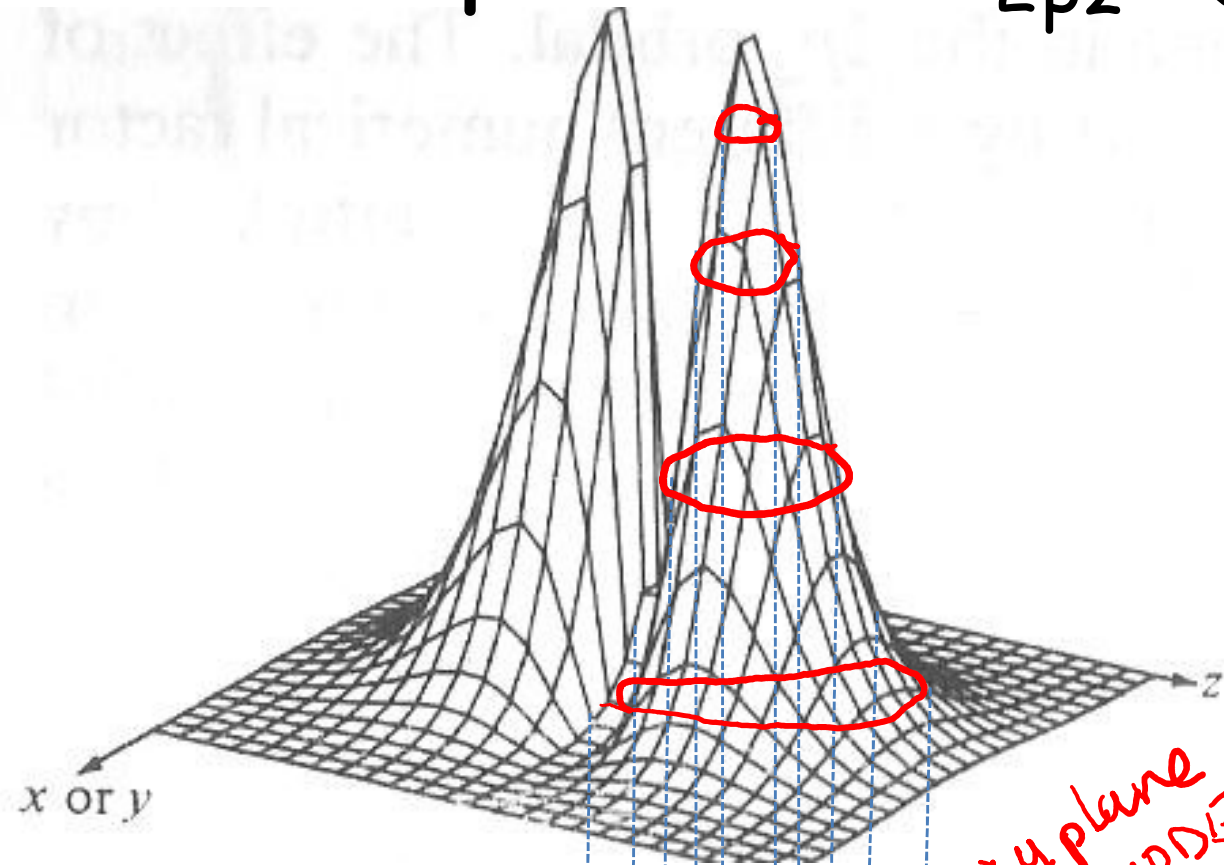


# Surface plot of $\Psi^2_{2p_z} \sim (r^2 e^{-2r}) x (\cos^2 \theta)$



In books, or in class, one of the low valued probability density contour are shows as "Orbitals"

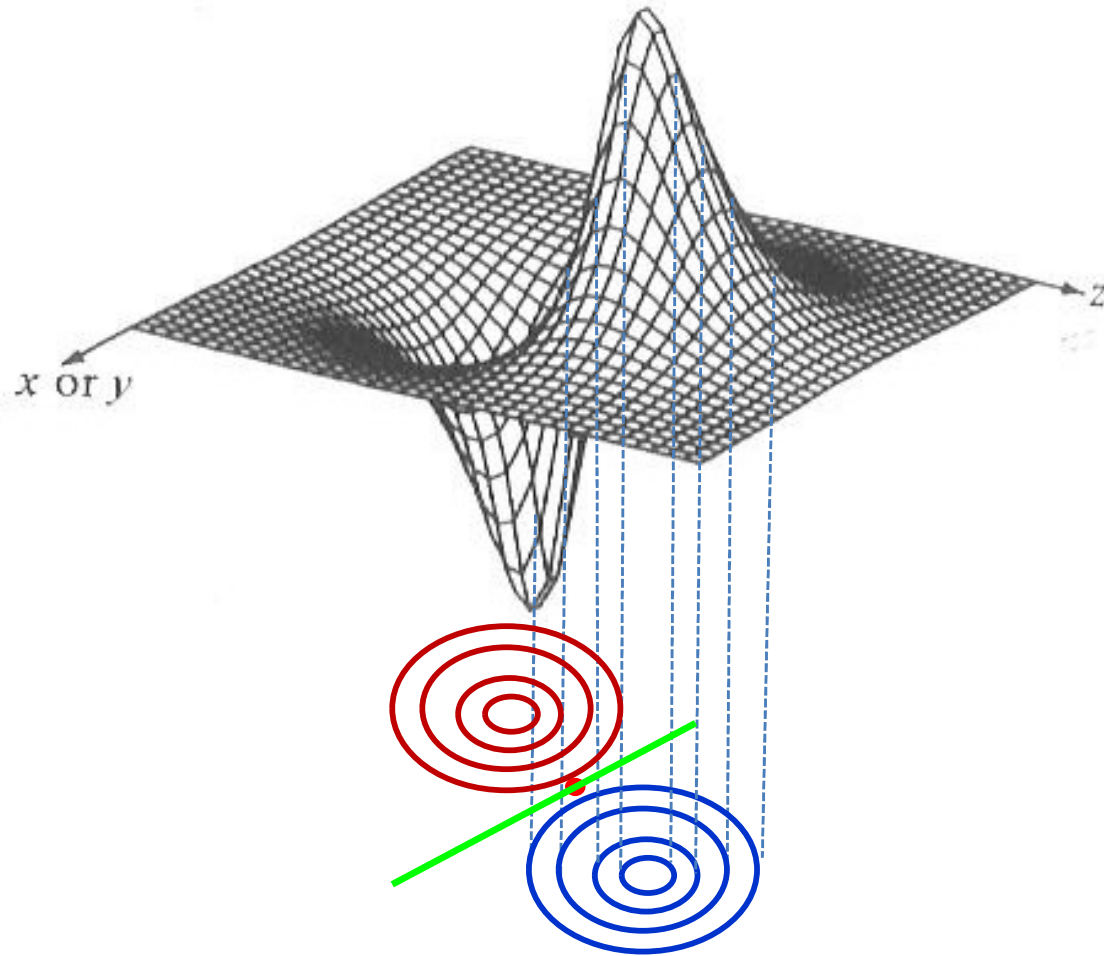
Surface plot of  $\Psi^2_{2p_z} \sim (r^2 e^{-2r}) x (\cos^2 \theta)$



xy plane node  
z-axis



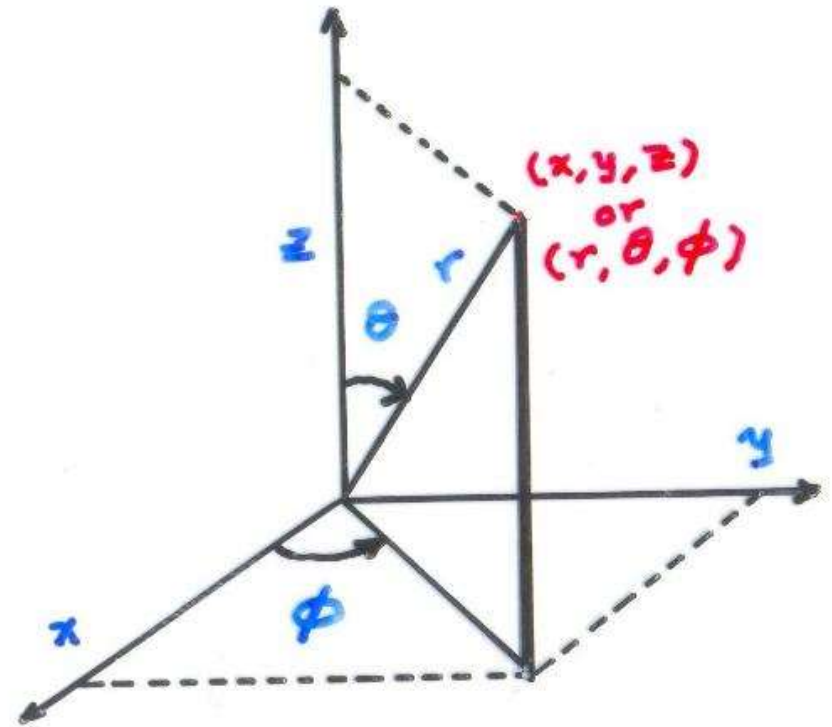
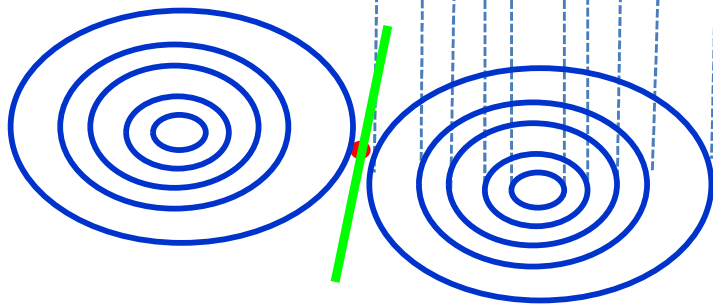
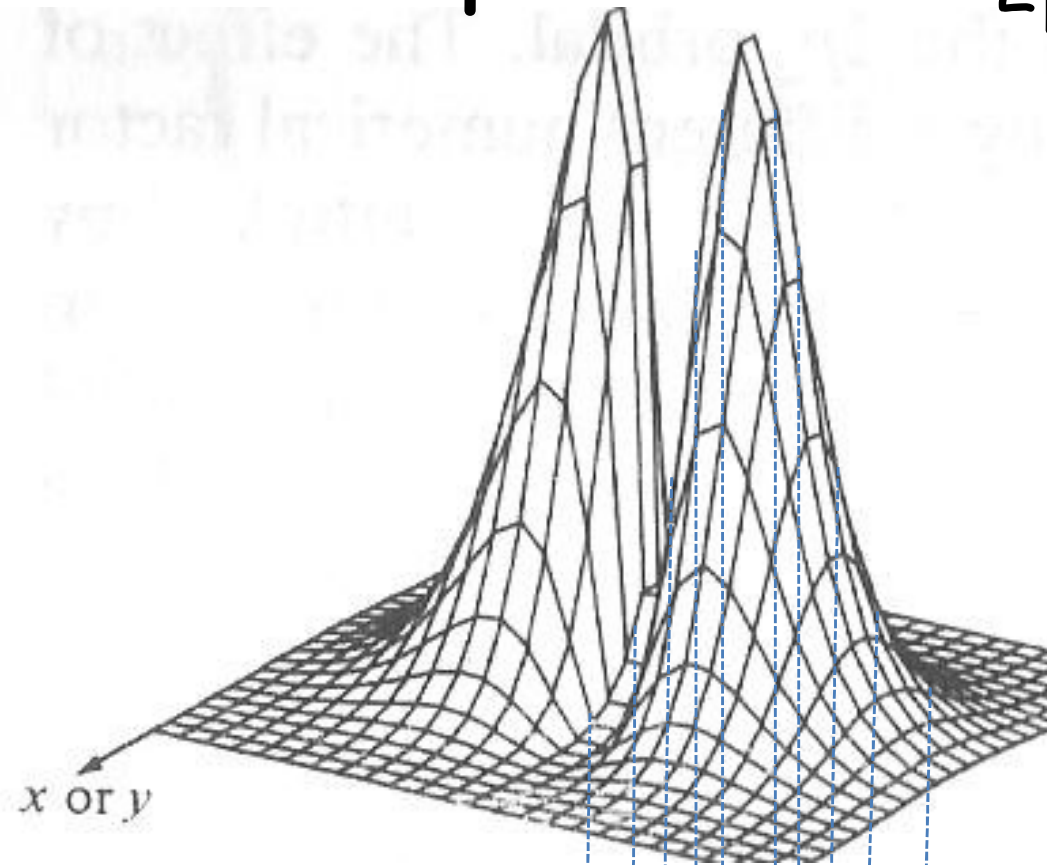
Review: Surface plot of  $\Psi_{2pz} = (re^{-r})x(\cos\theta)$



Nodal Plane is represented by a line in 2D plot

Radial node is represented by circle in 2D plot

Surface plot of  $\Psi^2_{2p_z} \sim (r^2 e^{-2r}) x (\cos^2 \theta)$

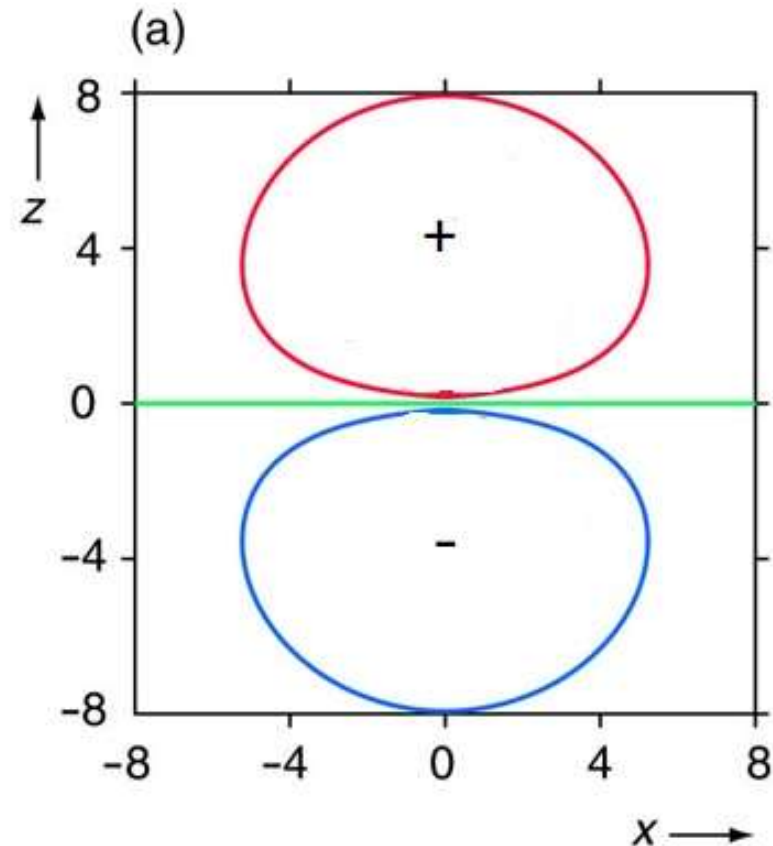
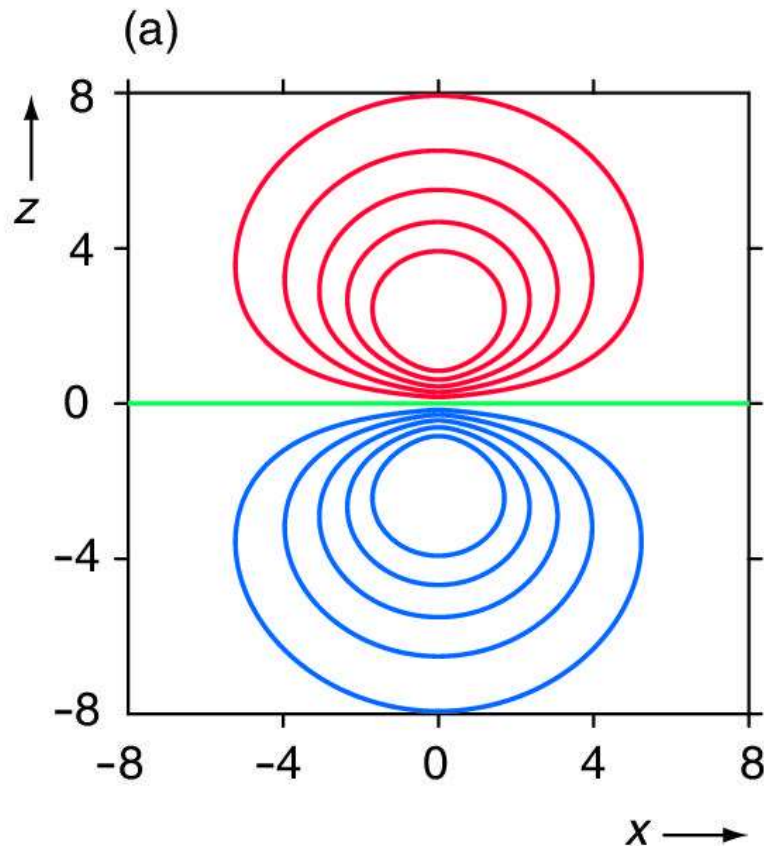


$$r \propto \cos \theta$$

$$\theta = \frac{\pi}{2}$$

At  $\theta = \pi/2$  we are in the xy plane regardless of the values of  $r$  and  $\phi$ , so  $\theta = \pi/2$  describes the nodal plane in the  $2p_z$  orbital

# Wavefunction/ Probability-density contours for $2p_z$

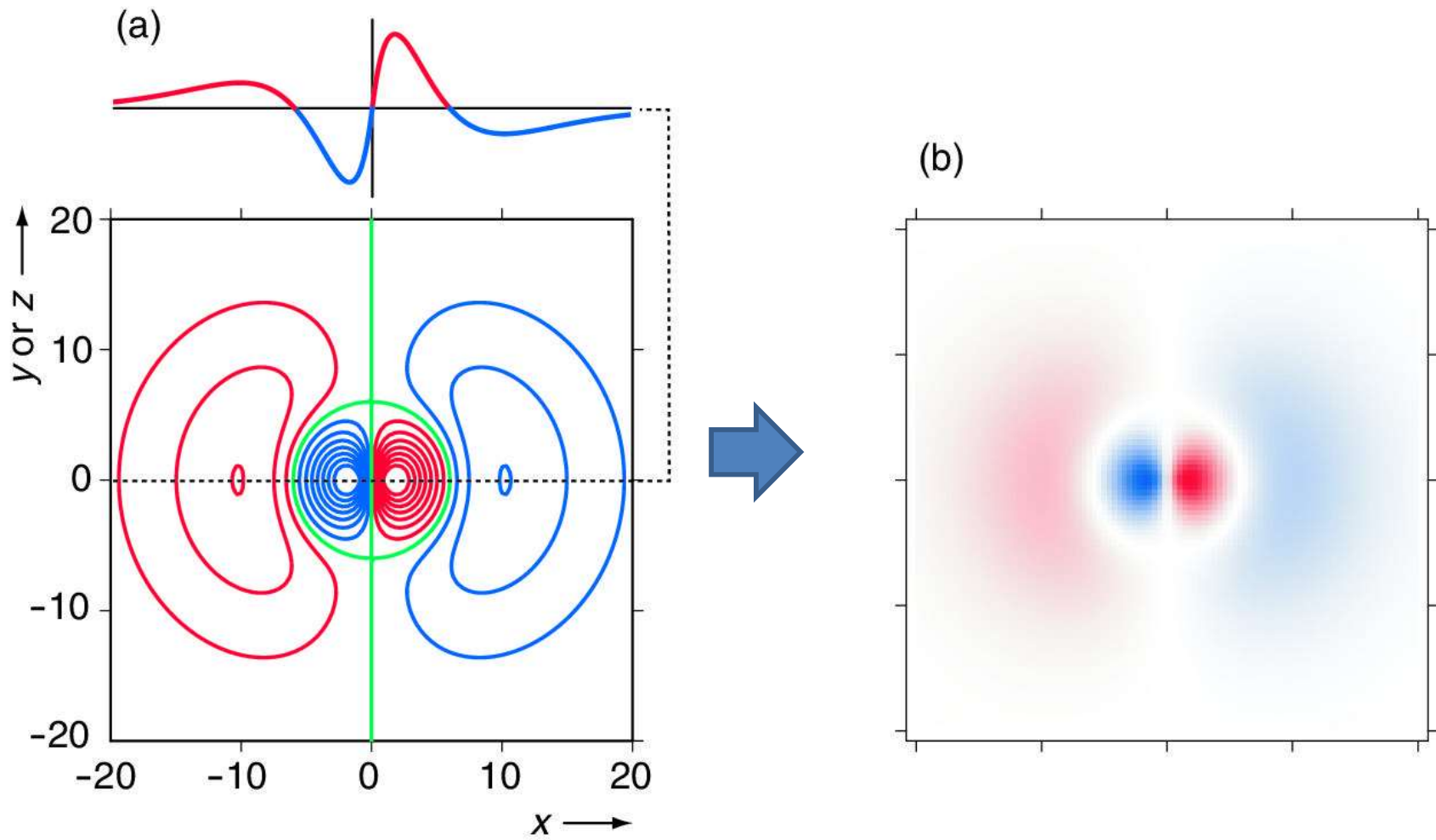


Each contour line is called “equal probability iso-surface”

A low probability contour is what is shown in your textbook as a “p” orbital



# Wavefunction/Probability-density contours for $3p_x$



# Probability-density contours for

$3p_x$

