Wavefunctions of Hydrogen Atom

$$\psi_{n,l,m}(r,\theta,\phi) = R_{n,l}(r)\cdot Y_l^m(\theta,\phi)$$

$$\psi_{1,0,0} = \psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2} \boxed{e^{-r/a_o}} \qquad f(r)$$

$$\psi_{2,0,0} = \psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{3/2} \boxed{\left(2-\frac{r}{a_o}\right)e^{-r/2a_o}} \qquad f(r)$$

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{3/2} \boxed{\left(\frac{r}{a_o}\right)e^{-r/2a_o}}\boxed{\cos\theta} \qquad f(r,\theta)$$

$$\psi_{2,1,+1} = \psi_{2p_{+1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2} \boxed{\left(\frac{r}{a_o}\right)e^{-r/2a_o}}\boxed{\sin\theta}\boxed{e^{i\phi}} \qquad f(r,\theta,\phi)$$

$$\psi_{2,1,-1} = \psi_{2p_{-1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2} \boxed{\left(\frac{r}{a_o}\right)e^{-r/2a_o}}\boxed{\sin\theta}\boxed{e^{-i\phi}} \qquad f(r,\theta,\phi)$$

1s and 2s Orbitals

$$\psi_{1,0,0} = \psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2} e^{-r/a_o}$$

$$\psi_{2,0,0} = \psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/2a_o}$$

Functions of only '*r*'

2p Orbitals

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\cos\theta$$

$$\psi_{2,1,+1} = \psi_{2p_{+1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\, e^{i\phi}$$

$$\psi_{2,1,-1} = \psi_{2p_{-1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\, e^{-i\phi}$$

Functions of 'r', 'θ' and 'ϕ'

2p Orbitals

$$\psi_{2,1,0} = \psi_{2p_z} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\cos\theta$$

$$\psi_{2,1,+1} = \psi_{2p_{+1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\, e^{i\phi}$$

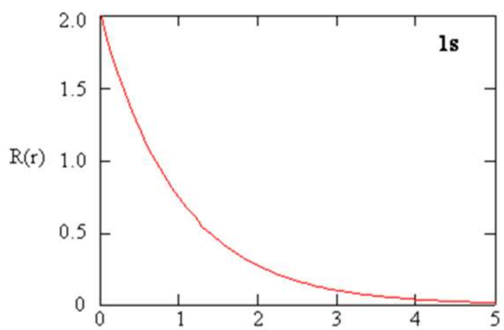
$$\psi_{2,1,-1} = \psi_{2p_{-1}} = \frac{1}{8\sqrt{\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\, e^{-i\phi}$$

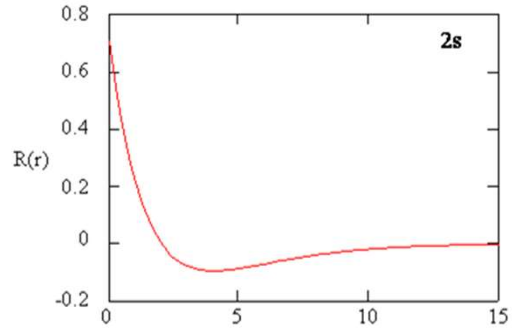
Linear combination

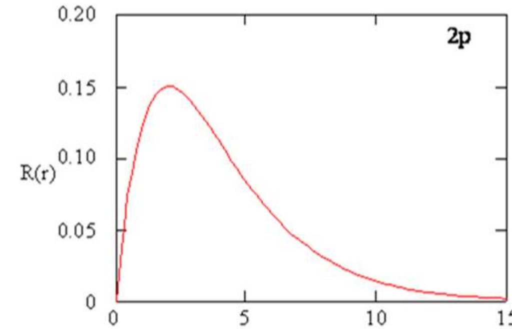
$$\psi_{2p_x} = \frac{1}{\sqrt{32\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\cos\phi = \frac{1}{\sqrt{2}}\left(\psi_{2,1,+1} + \psi_{2,1,-1}\right)$$

$$\psi_{2p_y} = \frac{1}{\sqrt{32\pi}}\left(\frac{1}{a_o}\right)^{3/2}\left(\frac{r}{a_o}\right)e^{-r/2a_o}\sin\theta\sin\phi = \frac{1}{\sqrt{2}i}\left(\psi_{2,1,+1} - \psi_{2,1,-1}\right)$$

Radial functions

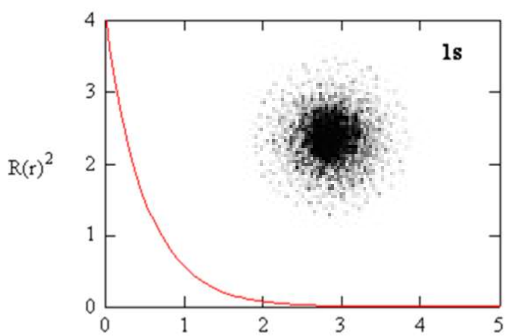


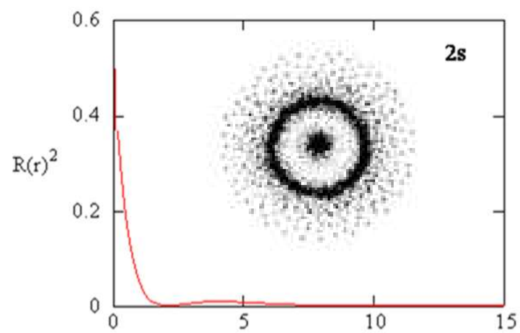


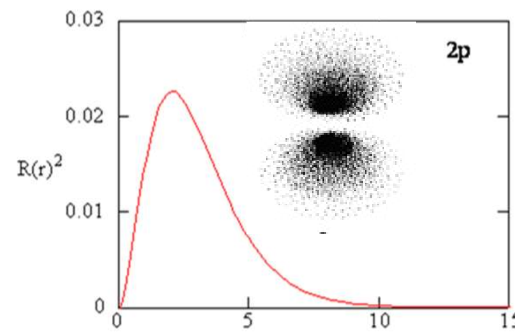


$$\rho = \frac{r}{a_o}$$

$$\psi_{1s}^{100} = N' e^{-\rho} \qquad \psi_{2s}^{200} = N''(2-\rho)e^{-\rho/2} \qquad \psi_{2p_z}^{210} = N''' \rho e^{-\rho/2} \cos\theta$$



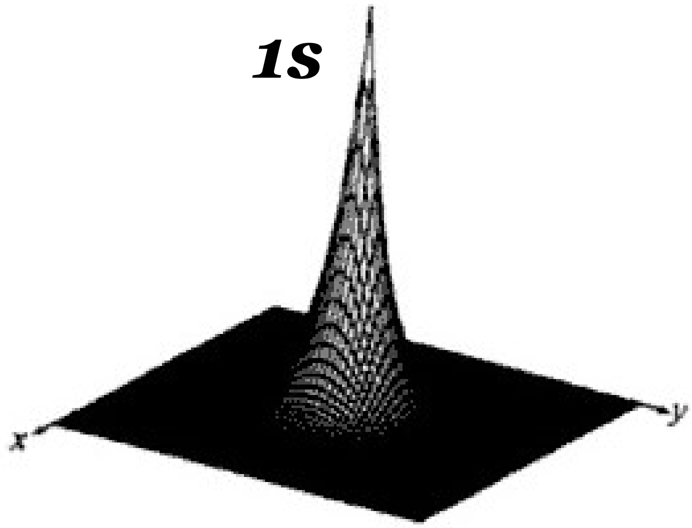




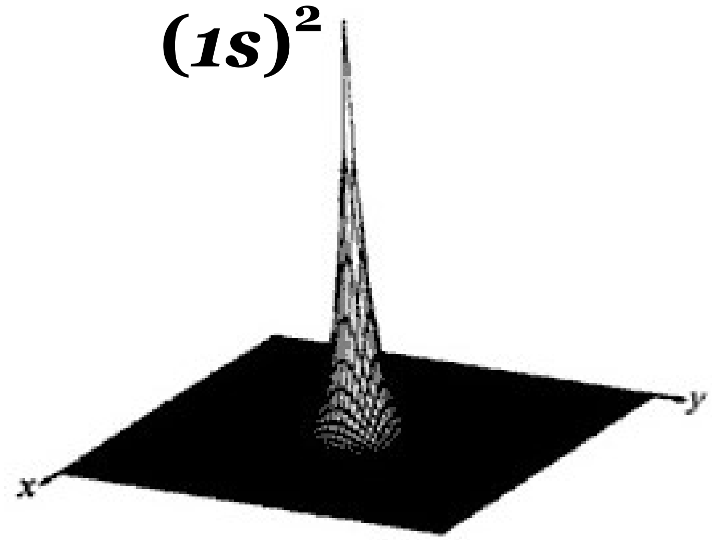
For s-Orbitals the maximum probability denisty of finding the electron is on the nucleus

For s-Orbitals the probability of finding the electron on the nucleus zero

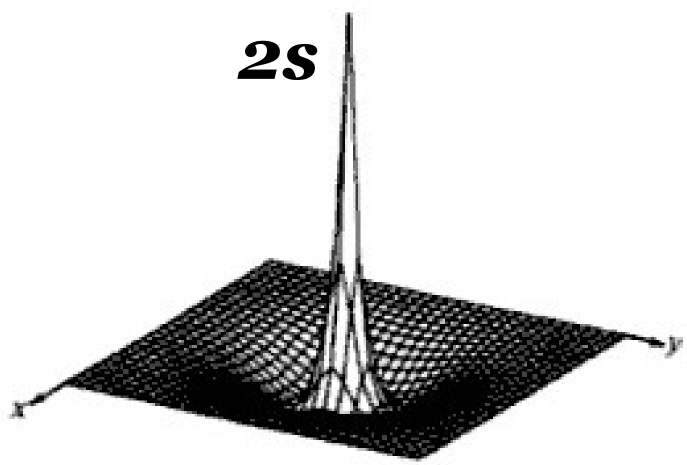
Surface plots



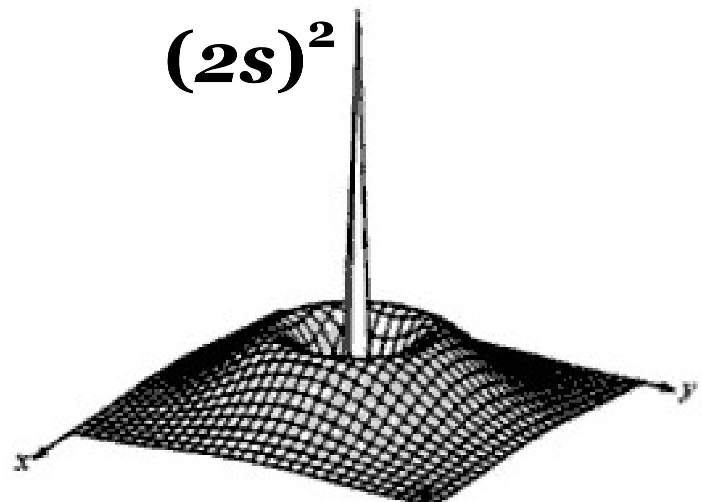
Surface plot of the 1s wavefunction (orbital) of the hydrogen atom. The height of any point on the surface above the *xy* plane (the nuclear plane) represents the magnitude of the Ψ_{1s} function at the at point (*x*,*y*) in the nuclear plane. The nucleus is located in the *xy* place immediately below the 'peak'



Surface plot of the $|\Psi_{1s}|^2$; the probability density associated with the 1s wavefunction of the hydrogen atom.



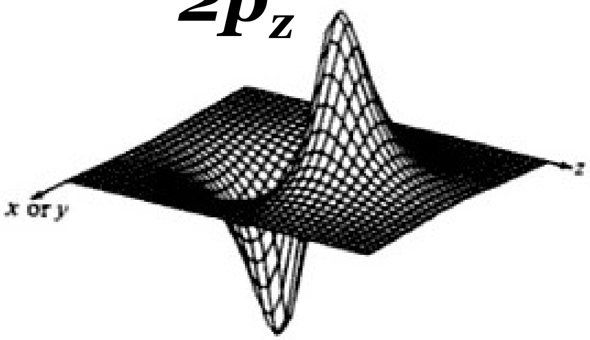
Surface plot of the Ψ_{2s} ; 2s wavefunction (orbital) of the hydrogen atom. The height of any point on the surface above the *xy* plane (the nuclear plane) represents the magnitude of the Ψ_{2s} function at the at point (*x*,*y*) in the nuclear plane. Note that there is a negative region (depression) about the nucleus; the negative region begins at $r=2a_0$ an goes asymptotically to zero at $r=\infty$.



Surface plot of the $|\Psi_{2s}|^2$; the probability density associated with the 1s wavefunction of the hydrogen atom. Note that the negative region of the 2s plot on the left now appears as positive region.

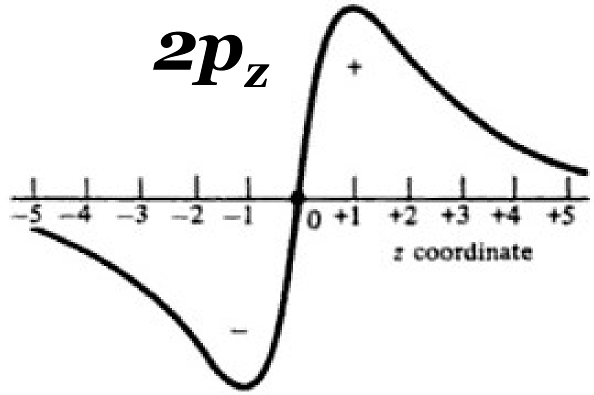
Surface plots

$2p_z$



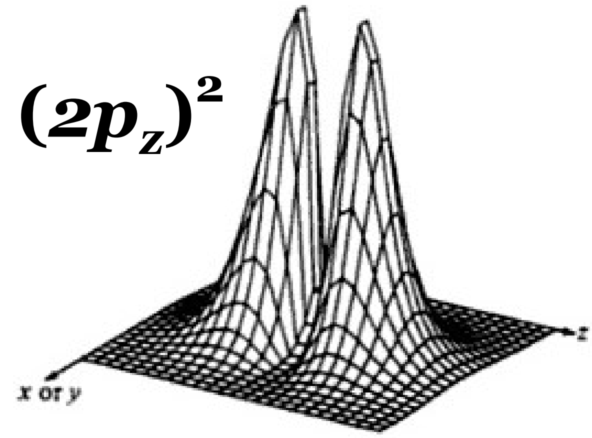
Surface plot of the *$2p_z$* wavefunction (orbital) in the *xz* (or *yz*) plane for the hydrogen atom. The 'pit' represents the negative lobe and the 'hill' the positive lobe of a 2p orbital.

$2p_z$



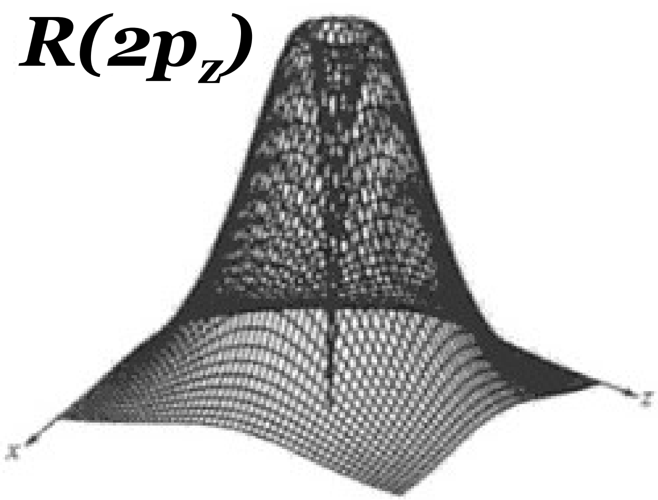
Profile of the $2p_z$ orbital along the z-azis.

$(2p_z)^2$

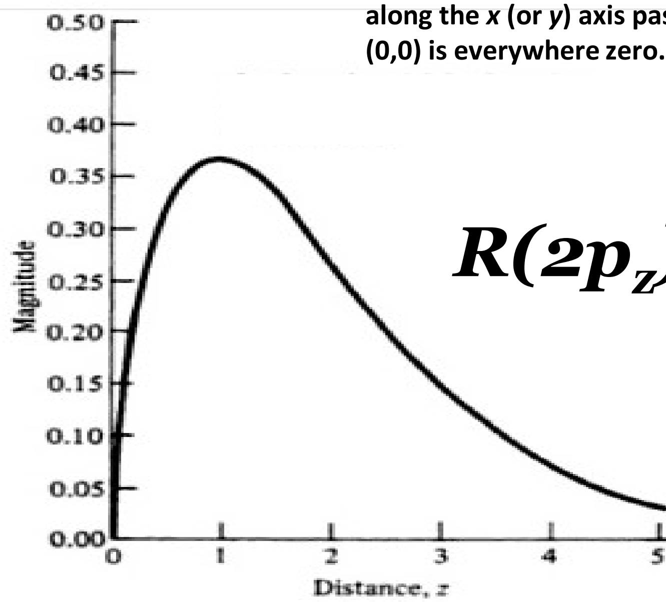


Surface plot of the $(2p_z)^2$; the probability density associated with the *$2p_z$* wavefunction of the hydrogen atom. Each of the hills represents and area in the *xz* (or *yz*) plane where the probability density is the highest, The probability density along the *x* (or *y*) axis passing through the nucleus (0,0) is everywhere zero.

$R(2p_z)$



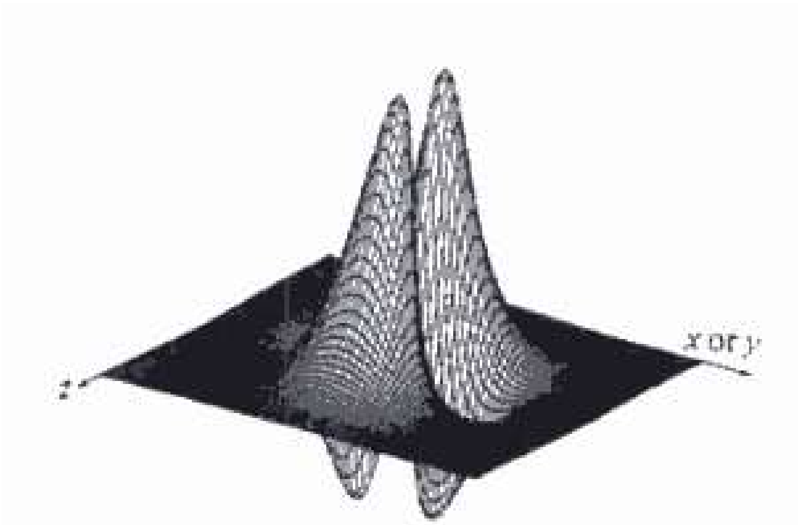
Surface plot of radial portion of a 2p wavefunction of the hydrogen atom. The gird lines have been left transparent so that the inner 'hollow' portion is visible.



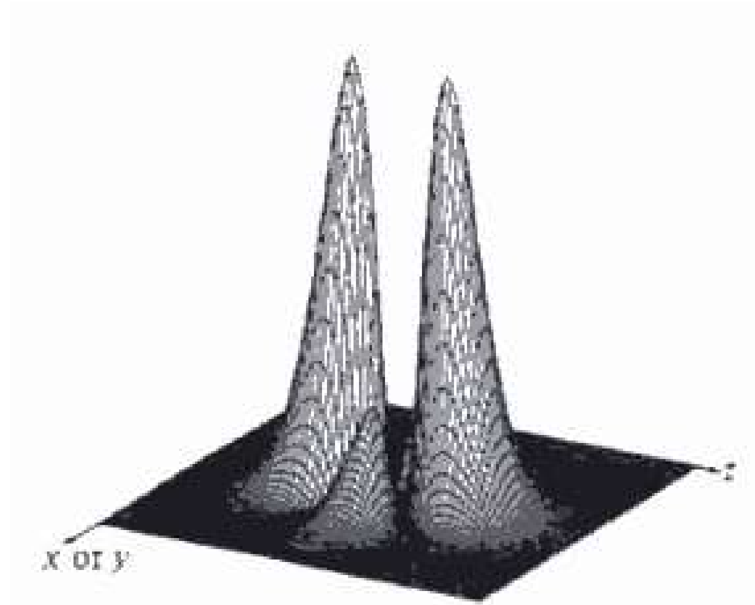
$R(2p_z)$

Profile of the radial portion of a 2p wavefunction of the hydrogen atom.

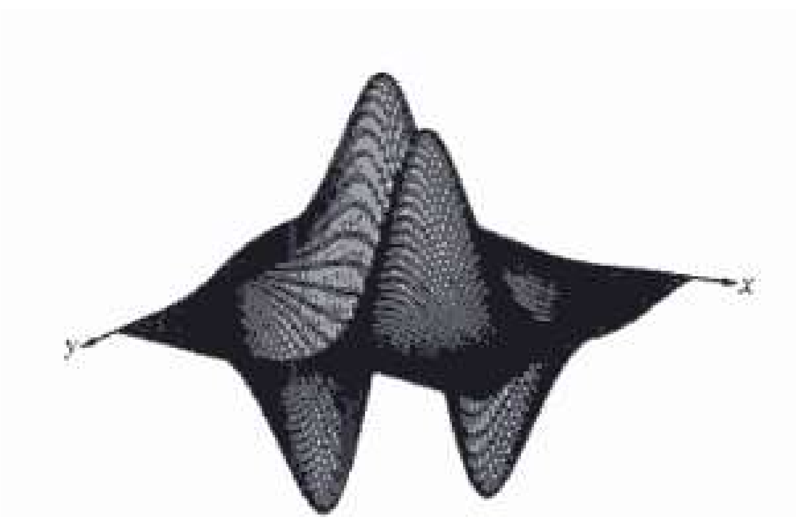
Surface plots



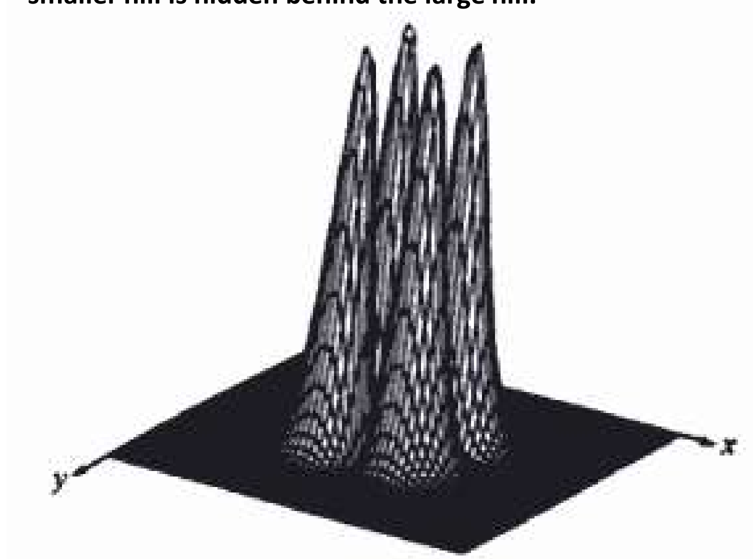
Surface plot of the $3d_{z2}$ wavefunction (orbital) in the *xz* (or *yz*) plane for the hydrogen atom. The large hills correspond to the positive lobes and the small pits correspond to the negative lobes.



Surface plot of the $(3d_{z2})^2$ the probability density associated with the $3d_{z2}$ orbital of the hydrogen atom. This figure is rotated with respect to the figure on the left so that the small hill will be clearly visible. Another smaller hill is hidden behind the large hill.



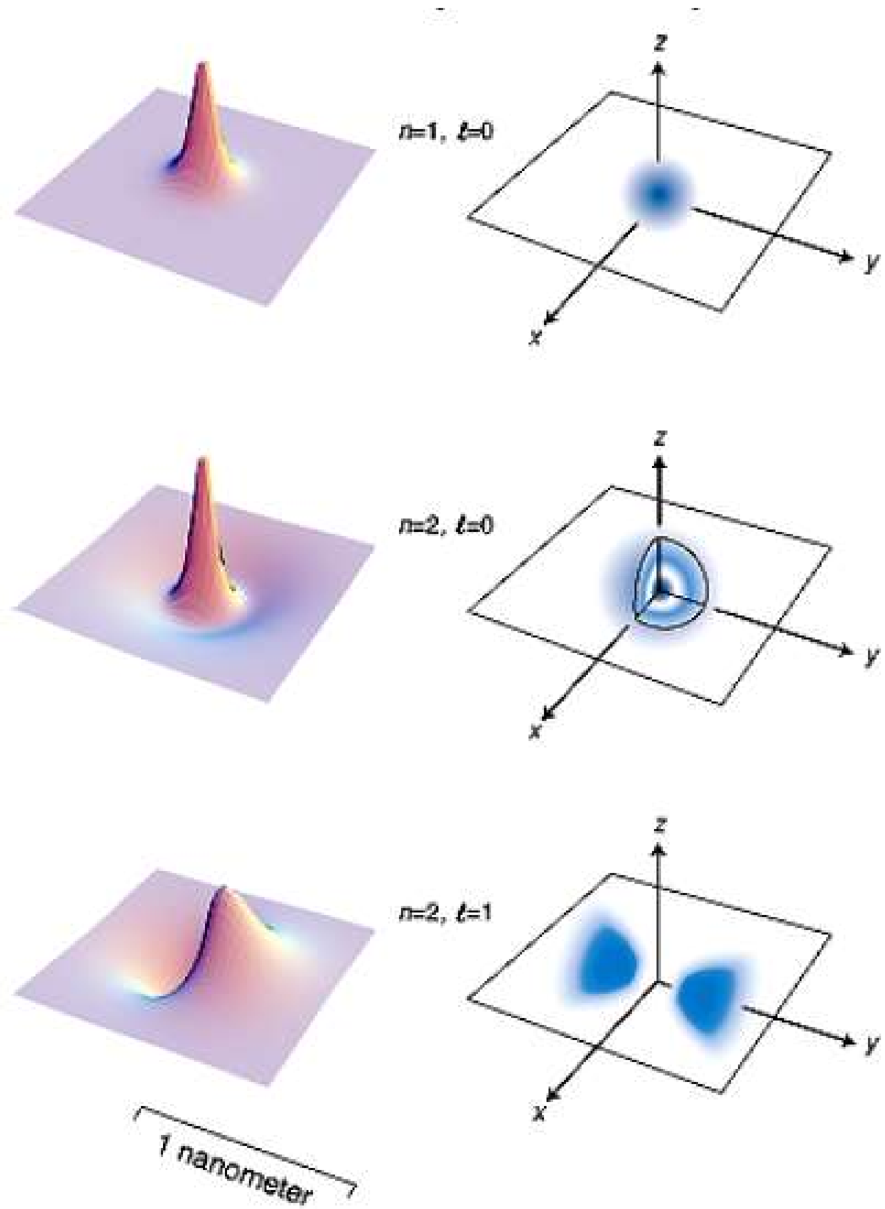
Surface plot of the $3d_{xy}$ wavefunction (orbital) in the *xz* plane for the hydrogen atom. The hills and the pits have same amplitude.

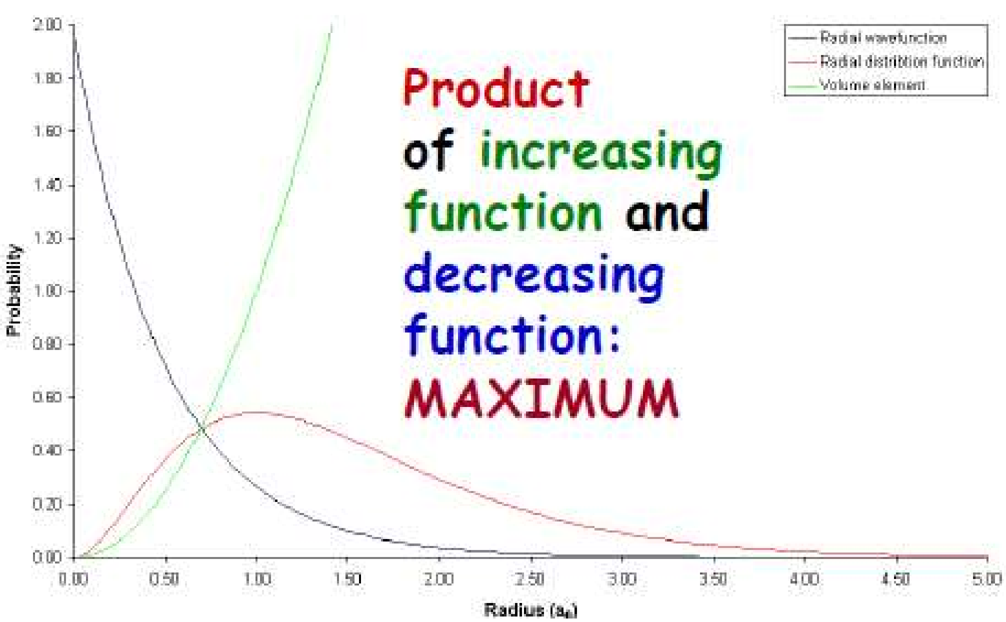


Surface plot of the $(3d_{xy})^2$ the probability density associated with the $3d_{xy}$ orbital of the hydrogen atom. Pits in the figure to the left appear has hills.

Radial and Radial Distribution Functions

Probability of finding the electron anywhere in a shell of thickness dr at radius r is $r^2 R_{nl}^2(r)dr$ (for s)
$r^2 \rightarrow$ increasing function
$r^2 R_{nl}^2(r)dr \rightarrow 0$ as $r^2 dr \rightarrow 0$





Radial Distribution Functions

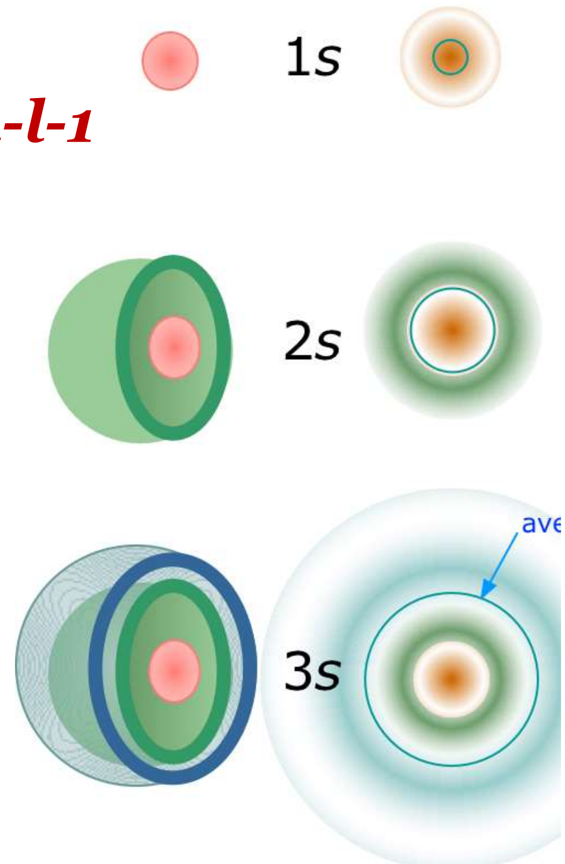
$$4\pi r^2 R_{nl}^2(r)$$

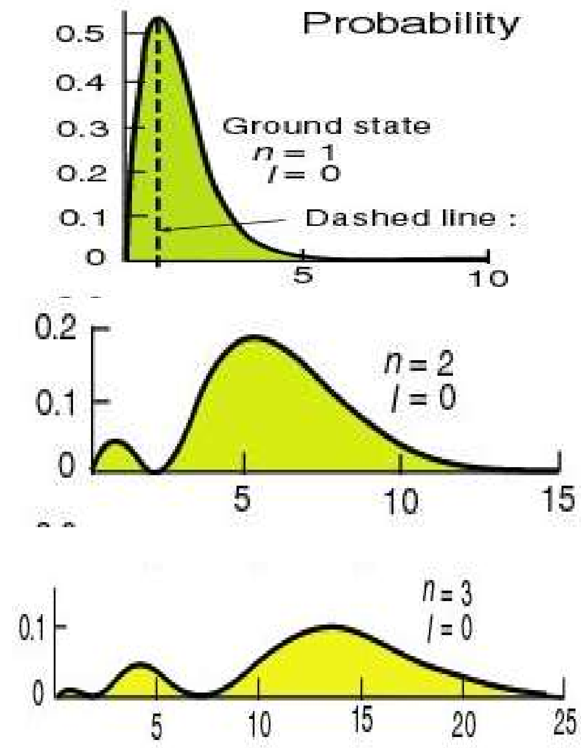
Number of radial nodes = *n-l-1*

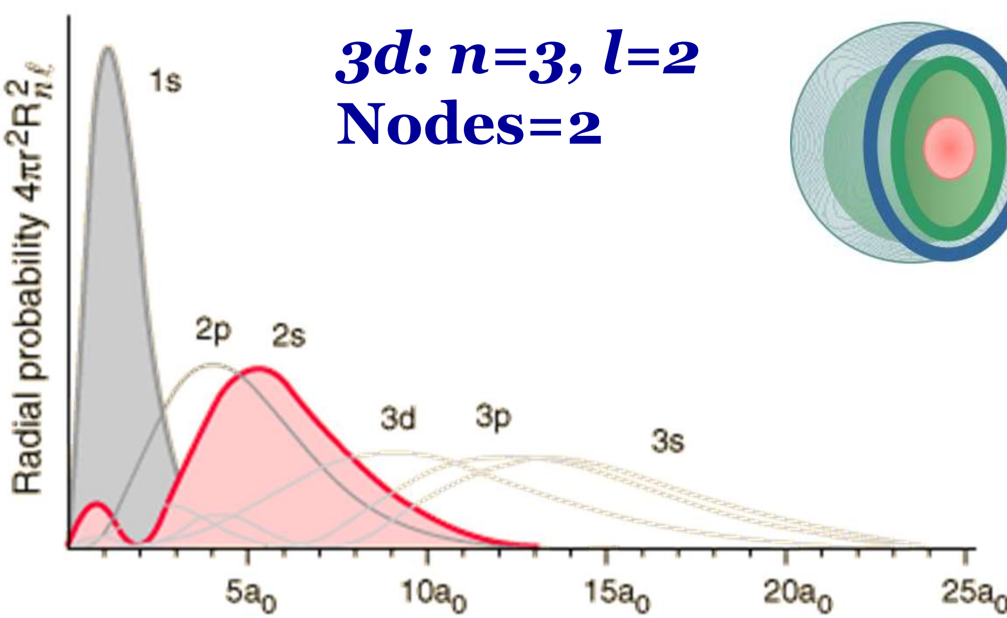
3s: n=3, l=0
Nodes=2

3p: n=3, l=1
Nodes=1

3d: n=3, l=2
Nodes=2







$$\langle r \rangle = \langle \Psi_{ns} | r | \Psi_{ns} \rangle$$