Review: Ψ_{nlm} = Orbitals

- For $n=1$, $l=0$, $m=0$, the electron is called to be in 100 state and the wave function corresponding to this electron is ψ_{100}
- The other wave functions possible for $n=2$ are ψ_{200}, ψ_{210}, ψ_{211} and ψ_{21-1}
- All these four states have the same energy i.e. $-R_H/4$
- The other way of representing the wave function is a orbital…the orbital is actually the wave-function
- If l=0, s; l=1, p; l=2, d
- So all ψ_{210}, ψ_{211} and ψ_{21-1} would be called 2p.

What does Ψ_{nlm} mean?

$$\Psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\,Y_{\ell m}(\theta,\phi)$$

TABLE 2.1 Hydrogenlike Wavefunctions* (Atomic Orbitals), $\psi = RY$

(a) Radial wavefunctions

n	l	$R_{nl}(r)$
1	0	$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
2	1	$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$
3	0	$\frac{2}{9\sqrt{3}}\left(\frac{Z}{a_0}\right)^{3/2}\left(3-\frac{2Zr}{a_0}+\frac{2Z^2r^2}{9a_0^2}\right)e^{-Zr/3a_0}$
3	1	$\frac{2}{9\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{3a_0}\right)e^{-Zr/3a_0}$
3	2	$\frac{4}{81\sqrt{30}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

(b) Angular wavefunctions

l	"m_l"†	$Y_{lm_l}(\theta,\phi)$
0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
1	x	$\left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\cos\phi$
1	y	$\left(\frac{3}{4\pi}\right)^{1/2}\sin\theta\sin\phi$
1	z	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
2	xy	$\left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\sin 2\phi$
2	yz	$\left(\frac{15}{4\pi}\right)^{1/2}\cos\theta\sin\theta\sin\phi$
2	zx	$\left(\frac{15}{4\pi}\right)^{1/2}\cos\theta\sin\theta\cos\phi$
2	x^2-y^2	$\left(\frac{15}{16\pi}\right)^{1/2}\sin^2\theta\cos 2\phi$
2	z^2	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$

*Note: In each case, $a_0 = \varepsilon_0 h^2/\pi m_e e^2$, or close to 52.9 pm; for hydrogen itself, $Z = 1$.

†In all cases except $m_l = 0$, the orbitals are sums and differences of orbitals with specific values of m_l.

$\Psi^2_{nlm}(r,\theta,\varphi)$

- What does the wave function actually mean and how does it actually represent the electron?
- Wave function is just a mathematical function

Max Born: If I take the wave function and I square it, if I interpret that as a probability density then I can interpret all the predictions made in the Schrodinger equation

$\Psi^2_{nlm}(r,\theta,\varphi)$ = probability density or probability/unit volume

H-Atom Complete $\Psi(r,\theta,\phi)$ for n=1,2

e^{-r/a_0} e^{-r/a_0}

$\sigma \rightarrow r/a_0$

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

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

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

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

or the alternate linear combinations

Linear combination Of two solutions is also a solution (Real wavefunctions)

$$\psi_{2p_x} = \quad = \frac{1}{\sqrt{2}}\left(\psi_{21+1} + \psi_{21-1}\right)$$

$$\psi_{2p_y} = \quad = \frac{1}{\sqrt{2i}}\left(\psi_{21+1} - \psi_{21-1}\right)$$

S-Orbitals (l=0,m_l=0)" R_{nl} and R_{nl}^2

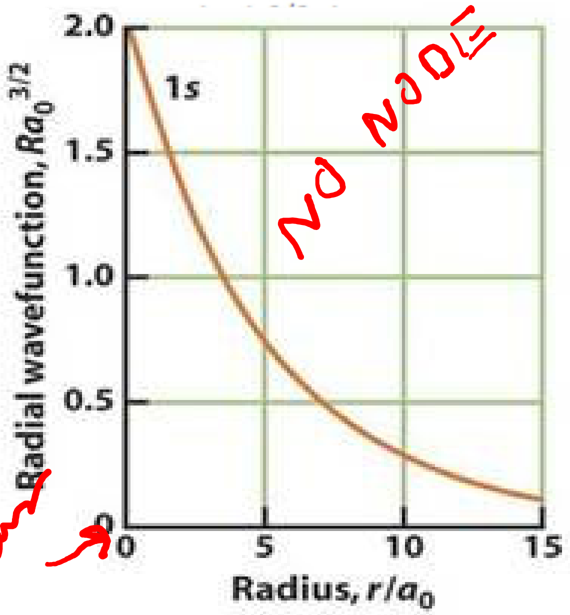
value of ψ

$$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

Z=1

$$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$

$$\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$



NO NODE

nucleus

ONE NODE

$r/a_0 = 2$

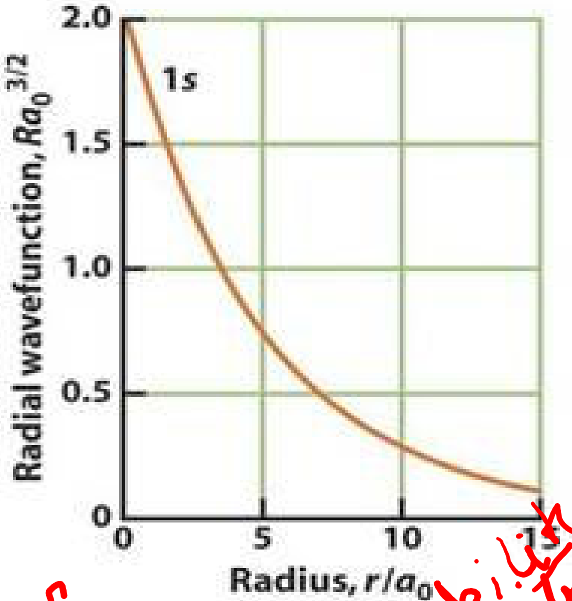
TWO NODES

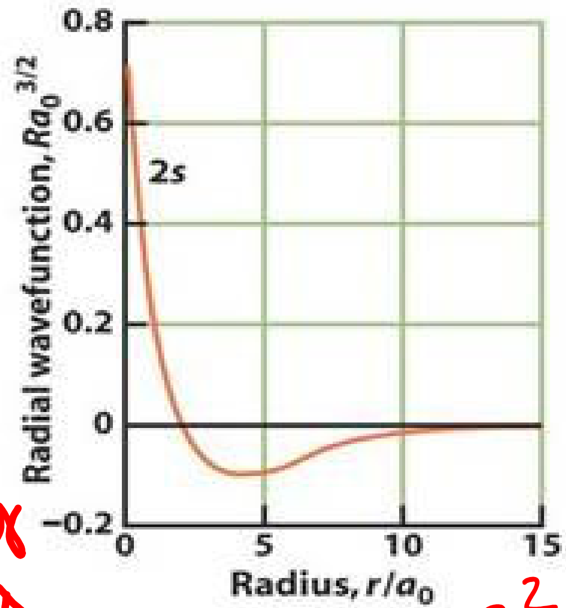
S-Orbitals (l=0,m_l=0)" R_{nl} and R_{nl}^2

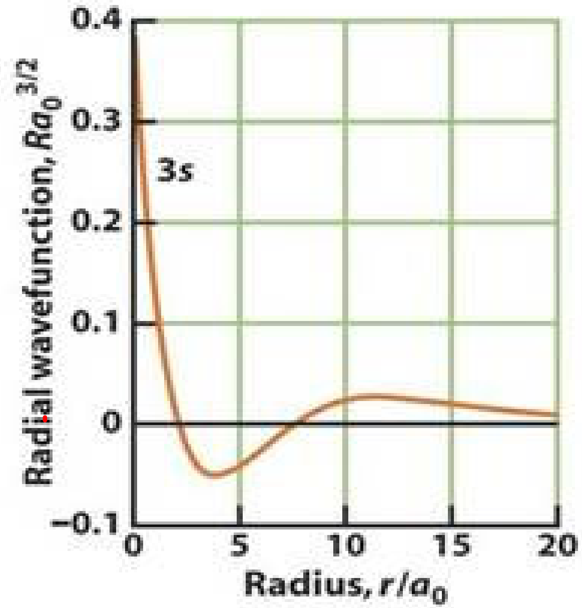
$$2\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

$$\frac{1}{2\sqrt{2}}\left(\frac{Z}{a_0}\right)^{3/2}\left(2-\frac{Zr}{a_0}\right)e^{-Zr/2a_0}$$

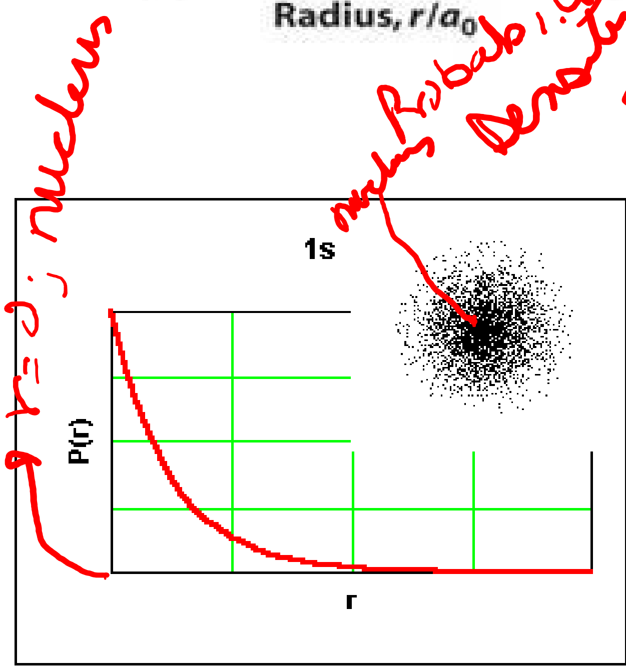
$$\cancel{\frac{1}{2\sqrt{6}}\left(\frac{Z}{a_0}\right)^{3/2}\left(\frac{Zr}{a_0}\right)}e^{-Zr/2a_0}$$

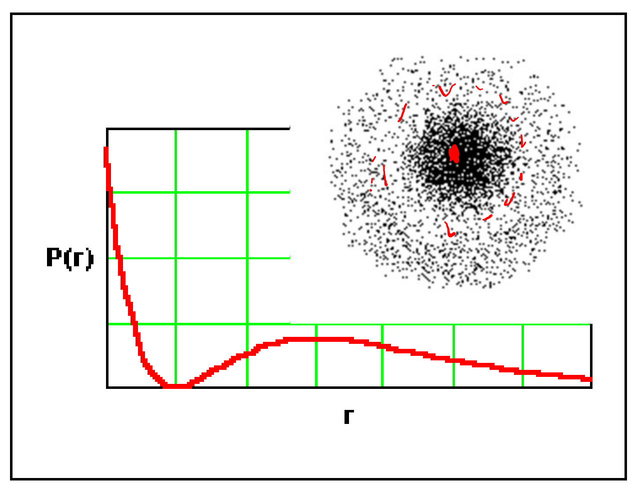


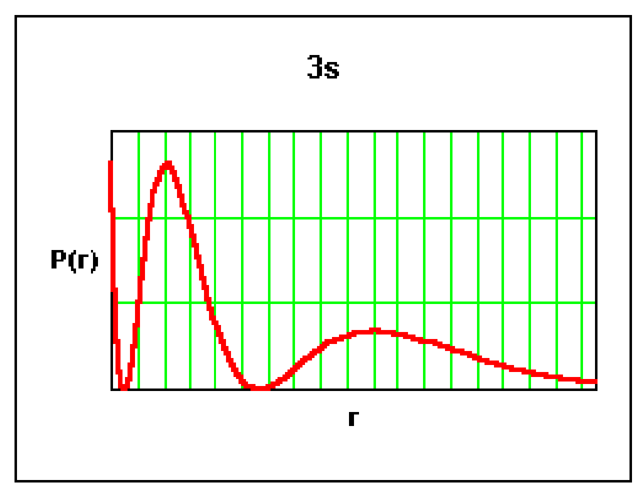




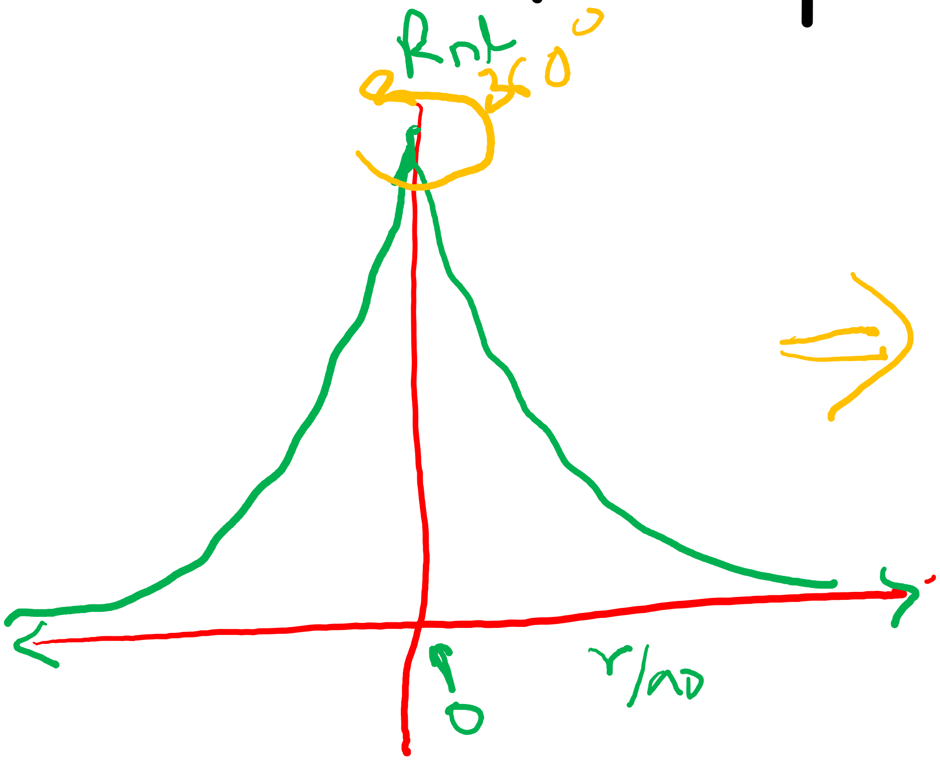
Probability Density $\Leftarrow P(r) = R_{nl}^2$

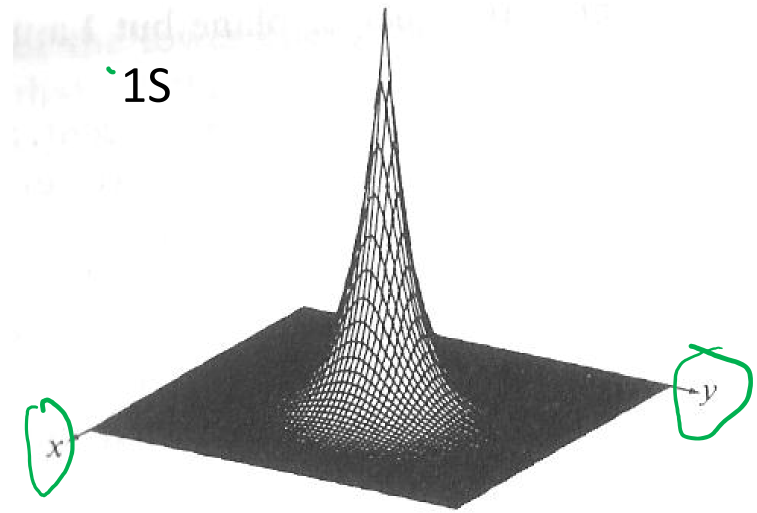


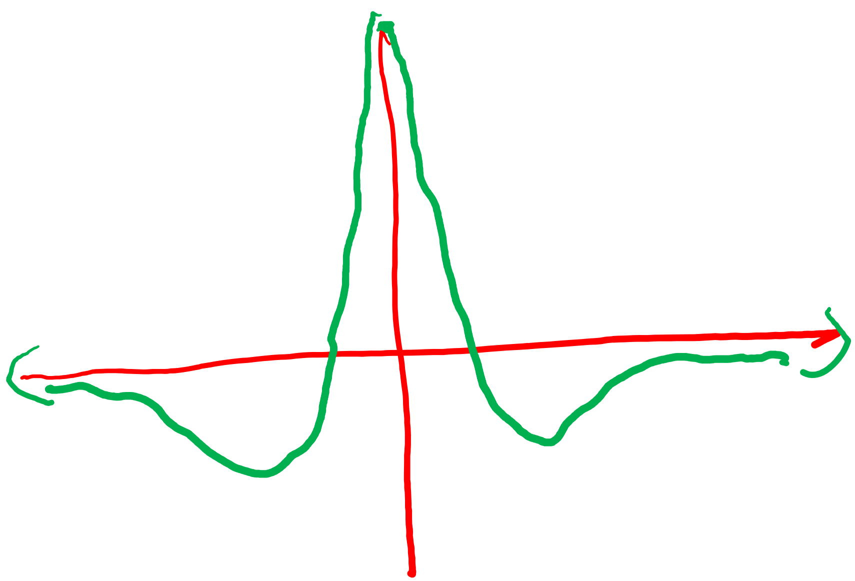


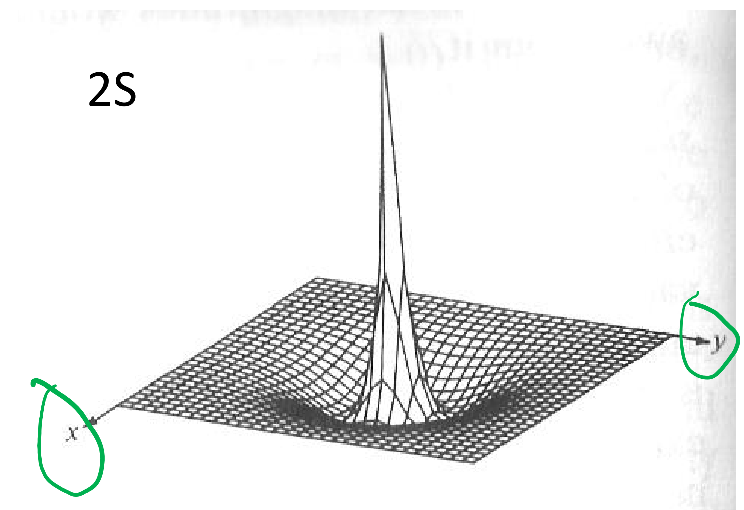


Surface plot of Ψ for S

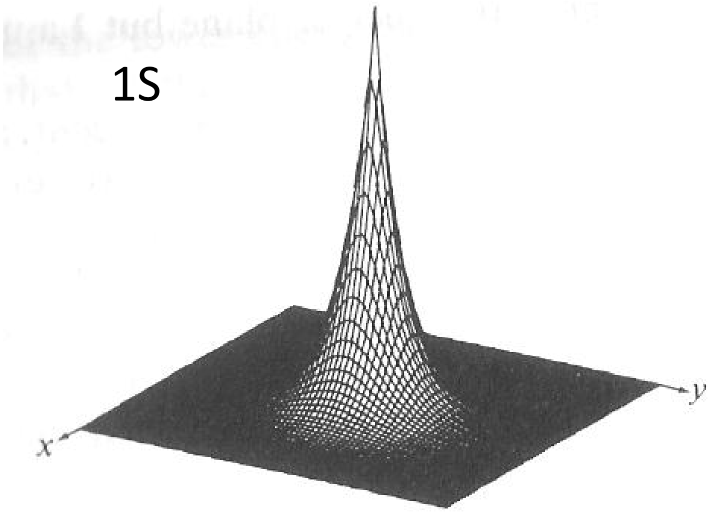


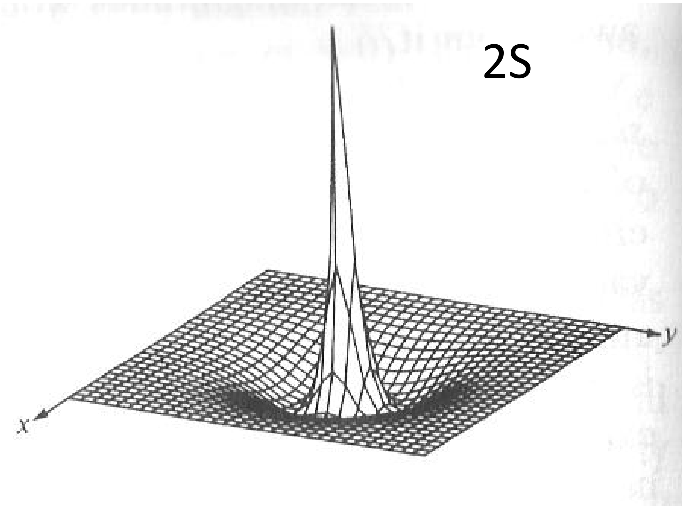


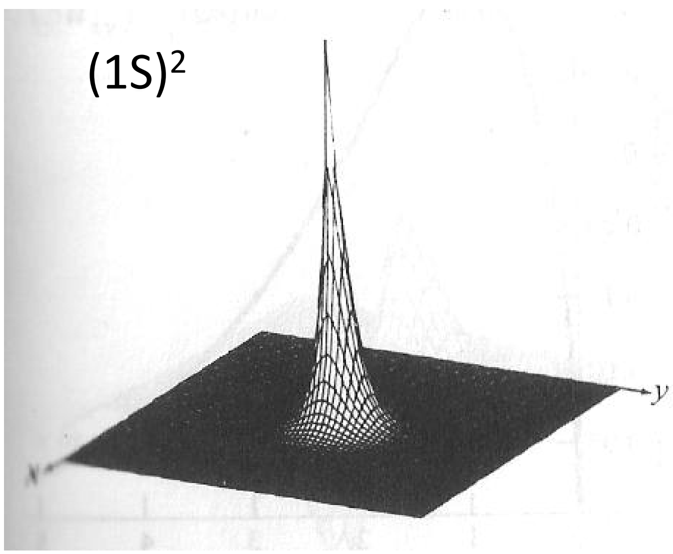


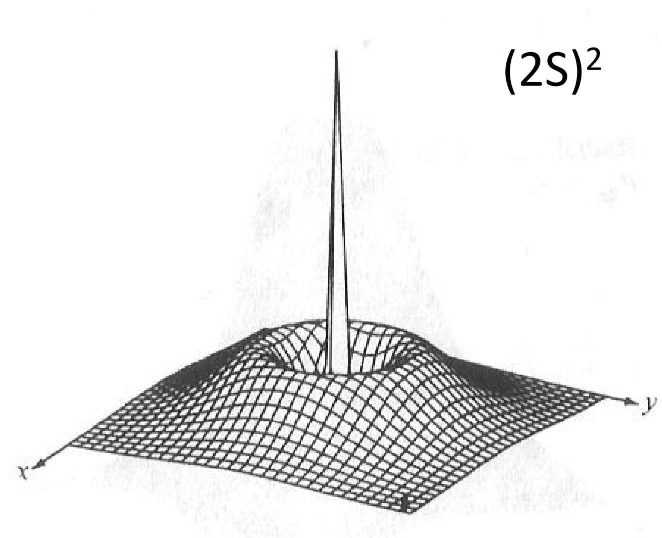


Surface plot of Ψ^2 for S









Maximum probability of finding the electron?