Late 1800s/early 1900s - People studying interactions between light and matter

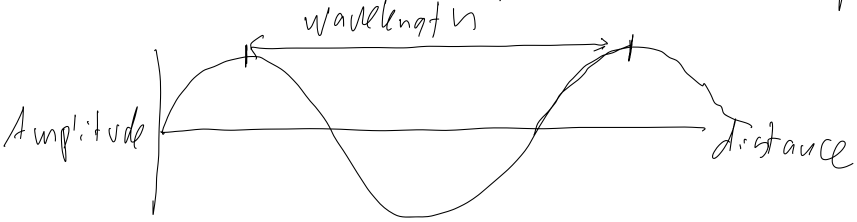
light = radiation

wavelength (λ) units of distance

frequency (ν) units of $\frac{1}{\text{time}}$

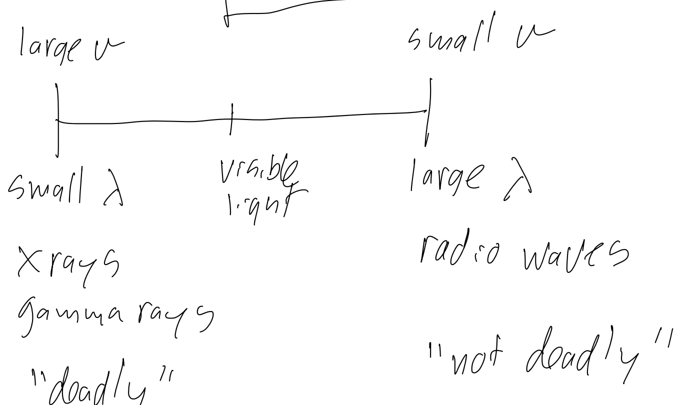
velocity (c) units of $\frac{\text{distance}}{\text{time}}$

For now, consider light as wave propagating thru space

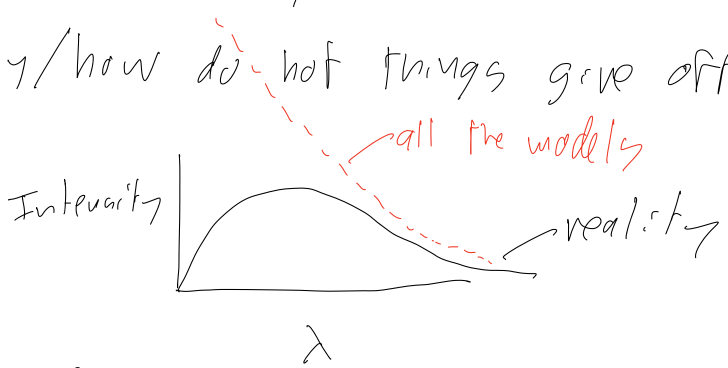


velocity always 3×10^8 m/sec

$$\boxed{c = \lambda \nu}$$



why/how do hot things give off light?



Max Planck — came up with good model

- hot atoms/molecule vibrate and give off light

* But only some vibrational frequencies were possible so only some wavelengths of light can be given off

* Frequency of light related to energy

* only certain energies possible

Energy of radiation is "quantized" - only certain values are possible

$$E = n h \nu$$

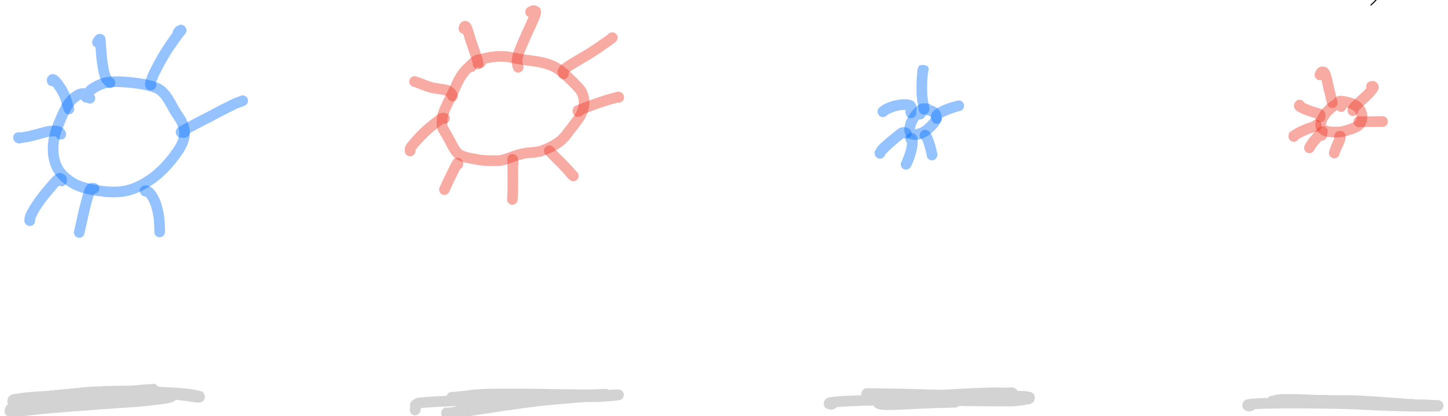
n = integer # of "pieces" of radiation

ν = frequency in sec^{-1}

h = Planck's constant 6.626×10^{-34} J·sec

E = energy of radiation

Photoelectric effect - shining light on metal makes electricity flow



lots of electricity | no electricity | some electricity | no electricity

Einstein - light is a massless particle → photon

$E_{photon} = h\nu$ ← for 1 "particle" of light

"wave-particle duality"

400 nm | 550 nm | 700 nm

Blue | Green | Red

Blue	Red
big ν	smaller ν
small λ	big λ
higher E photons	lower E photons

Blue light with $\lambda = 450$ nm

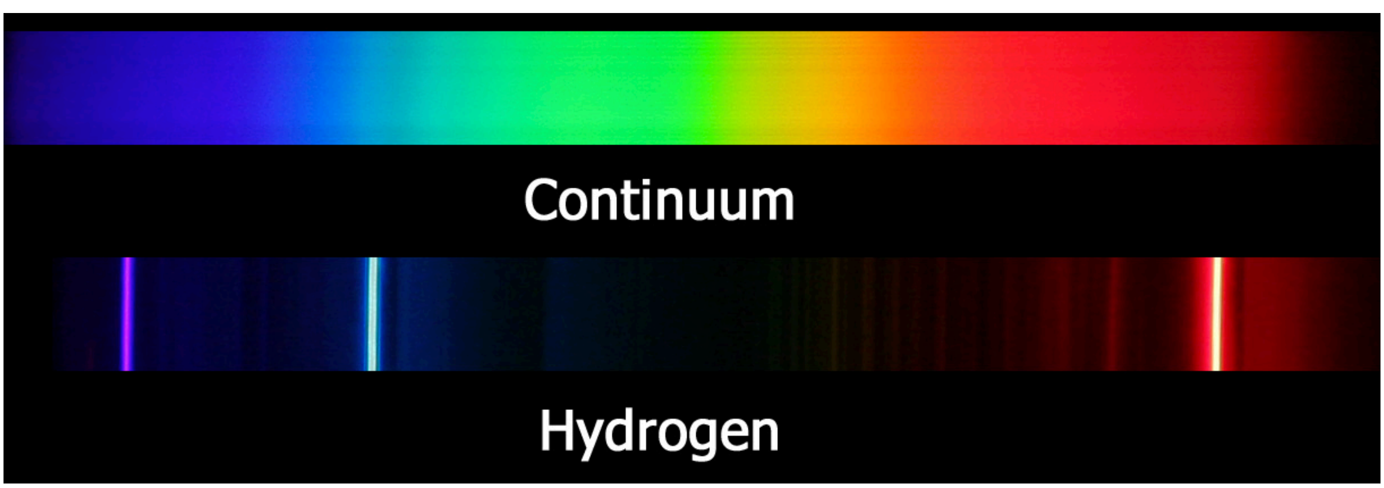
$E_{photon} = h\nu$

$c = \lambda\nu$

$$\rightarrow E_{photon} = \frac{hc}{\lambda} = \frac{(6.626\times10^{-34}\ J\cdot \cancel{sec})(3\times10^{8}\ \cancel{m}/\cancel{sec})}{450\times10^{-9}\ \cancel{m}} = 4.4\times10^{-19}\ J$$

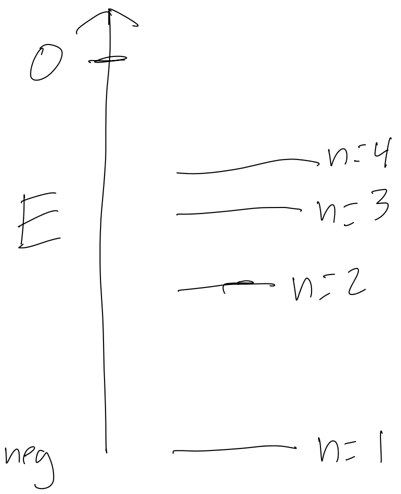
Atomic Line Spectrum from Hydrogen Discharge Lamp

- tube filled w/ H_2
- electrodes in top+bottom
- high voltage electricity splits H_2 in H atoms and then it glows



light from lamp made up of 3 different "lines"
only 3 types of photons emitted by lamp

H atom has 1 e^- - can live at several different energies
adding energy makes e^- go to higher level
going from higher level → lower level requires energy to be emitted → as a photon



Ryberg constant $1.097 \times 10^7\ m^{-1}$

Planck

$$E_n = -\frac{Rhc}{n^2}$$

speed of light

level

low → high requires input of energy
high → low energy given off as photon

under certain circumstances particles with mass can exhibit wave-like properties

$$\lambda_{\text{particle with mass}} = \frac{h}{mv}$$

velocity of particle

mass of particle

De Broglie wavelength

Quantum mechanics is how we will describe electrons

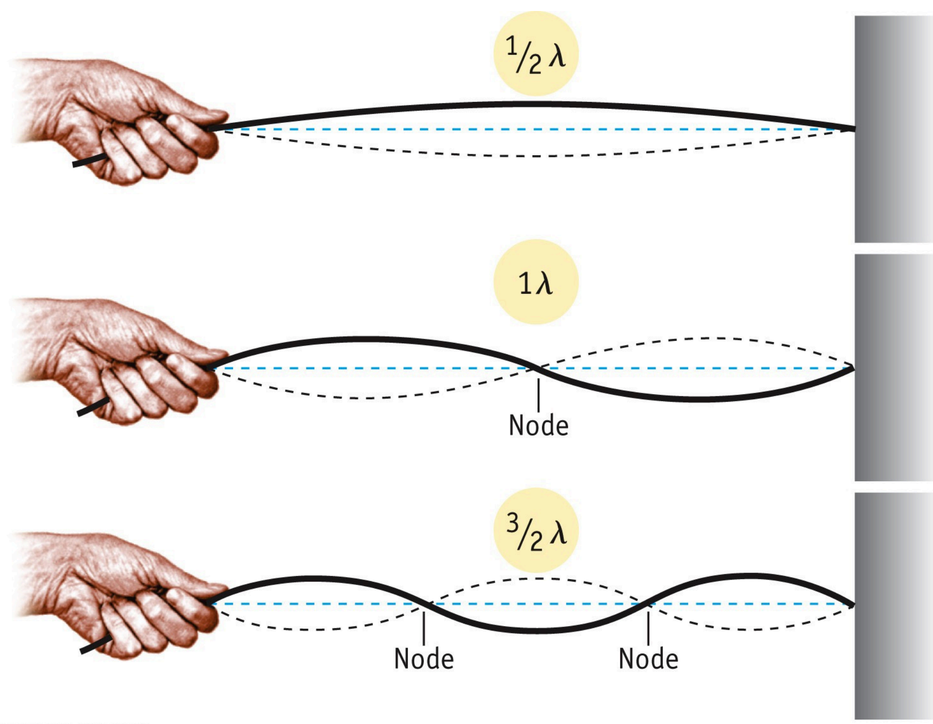
standing wave - has limited possible wavelengths

$\rightarrow$ has limited possible values of energy

$\rightarrow$ this idea will be how we describe electrons

Electrons $\rightarrow$ 3D standing wave

Ψ = wavefunction = equation that describes 3D standing wave



Wave motion: wave length and nodes
"Quantization" in a standing wave

$\Psi = 42x^4 + 13y^{3/2} - 7z^8$ — if you plug in x, y, z values you calculate a value of Ψ = amplitude of wavefunction

$\Psi^2 \rightarrow$ probability of e^- being located at that point in space

Electron exists only as probability density quantum numbers are a shorthand to describe wavefunctions

n = principal quantum # "shell"

$n = 1, 2, 3, 4 \ldots\ldots$

describes energy

describes ~~exten~~ spatial extent of probability distribution with respect to nucleus ~~of~~ of atom

l = orbital angular momentum quantum # "subshell"

$l = 0, 1, 2, n-1$

describes shape

$l = 0 \rightarrow s$
$l = 1 \rightarrow p$
$l = 2 \rightarrow d$
$l = 3 \rightarrow f$

m_l = magnetic quantum #

$m_l = -l \ldots 0 \ldots +l$ (integers)

~~desc~~ describes orientation in 3-D space

If $n=1$ then l must $=0$ and $m_l=0$

only 1 ψ with $n=1$ $\rightarrow$ $n=1$ $l=0$ $m_l=0$

If $n=2$ then $l=0$ or $l=1$

$l=0 \downarrow m_l=0$

$l=1 \downarrow m_l=-1,0,1$

4 ψ with $n=2$

$n=2$ $l=0$ $m_l=0$
$n=2$ $l=1$ $m_l=-1$
$n=2$ $l=1$ $m_l=0$
$n=2$ $l=1$ $m_l=+1$

If $n=3$ $l=0$ or $l=1$ or $l=2$

$l=0 \downarrow m_l=0$

$l=1 \downarrow m_l=-1,0,1$

$l=2 \downarrow m_l=-2,-1,0,1,2$

9 ψ when $n=3$

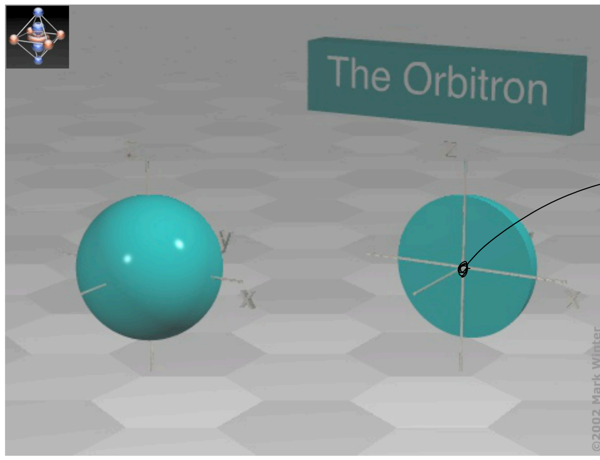
n	l	m_l
3	0	0
3	1	-1
3	1	0
3	1	+1
3	2	-2
3	2	-1
3	2	0
3	2	+1
3	2	+2

* Wavefunction = orbital

1s orbital

$n=1$
$l=0$
$m_l=0$

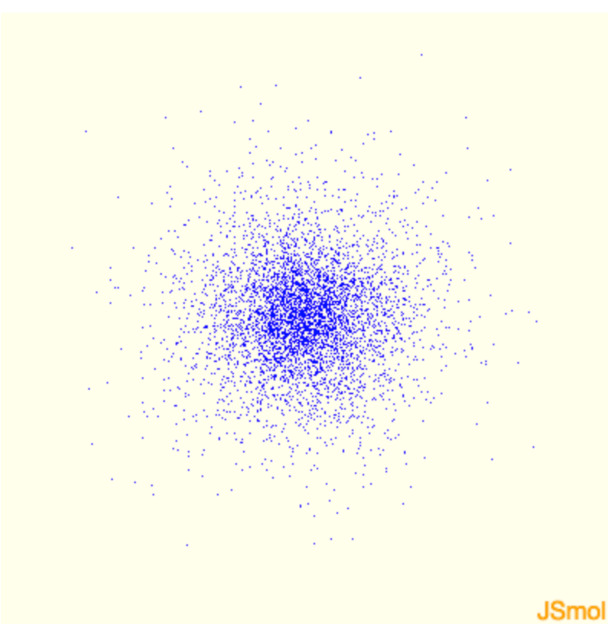
Atomic orbitals: 1s



The shape of the 1s orbital.

For any atom there is just one 1s orbital. Consider the shape on the left. The surface of

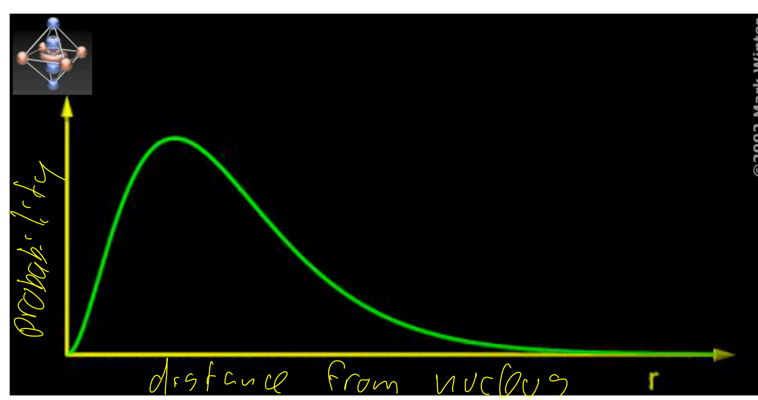
Atomic orbitals: 1s electron density



"Dot-density" plot of the 1s electron density function ψ_{1s}^2.

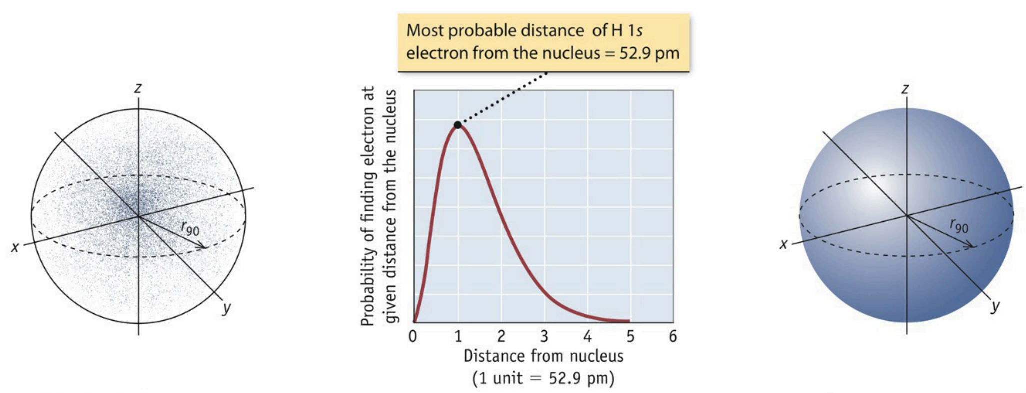
probability of finding e- at a certain distance from nucleus

Atomic orbitals: 1s radial distribution function



Schematic plot of the 1s radial distribution function $4\pi r^2\psi_{1s}^2$

s-Orbitals

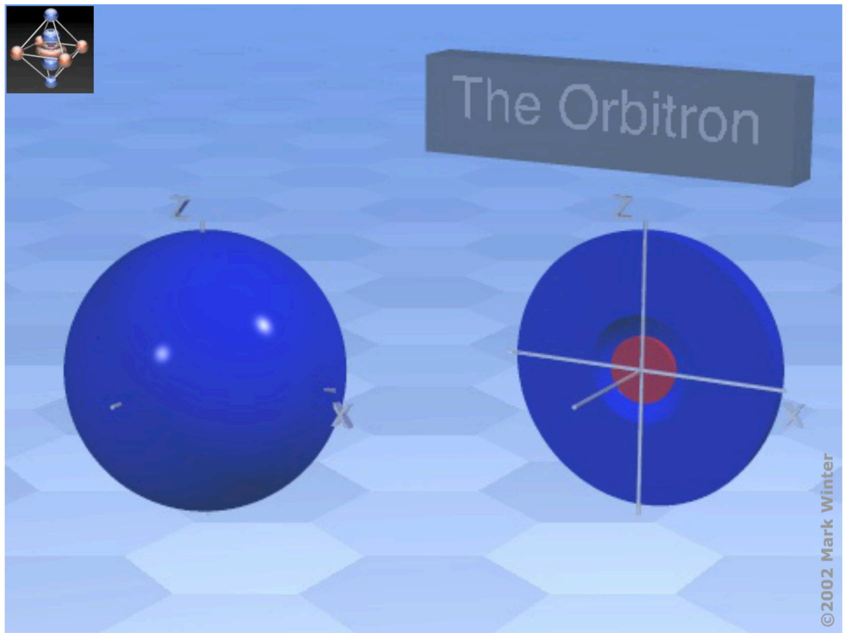


- $l = 0$, $m_l = 0$
- $2l+1 = 1$
- one *s*-orbital that extends in a radial manner from the nucleus forming a spherical shape.

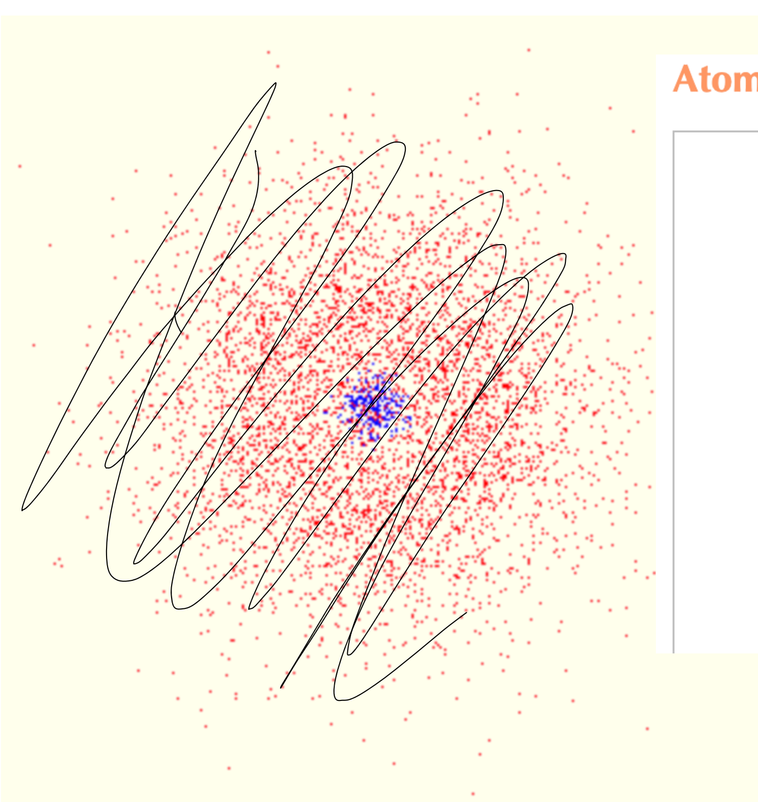
2s orbital

$n=2$
$\ell=0$
$m_\ell=0$

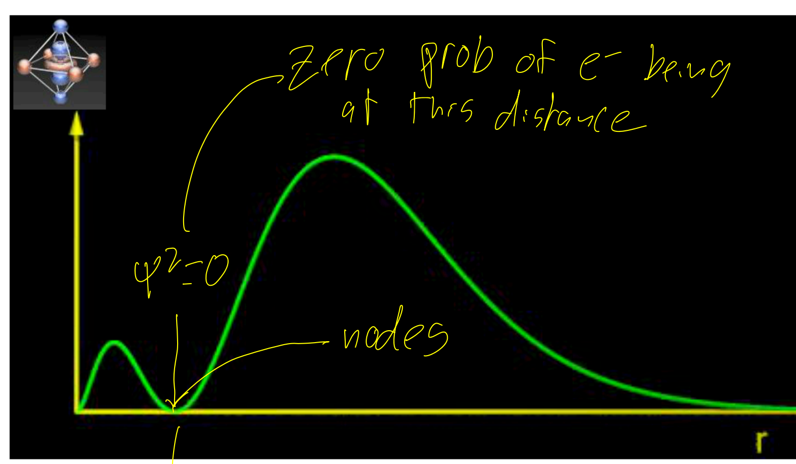
Atomic orbitals: 2*s*



The shape of the 2s orbital. *The blue zone is where the wave function has negative values while the red zone is where values are positive.*



Atomic orbitals: 2*s* radial distribution function



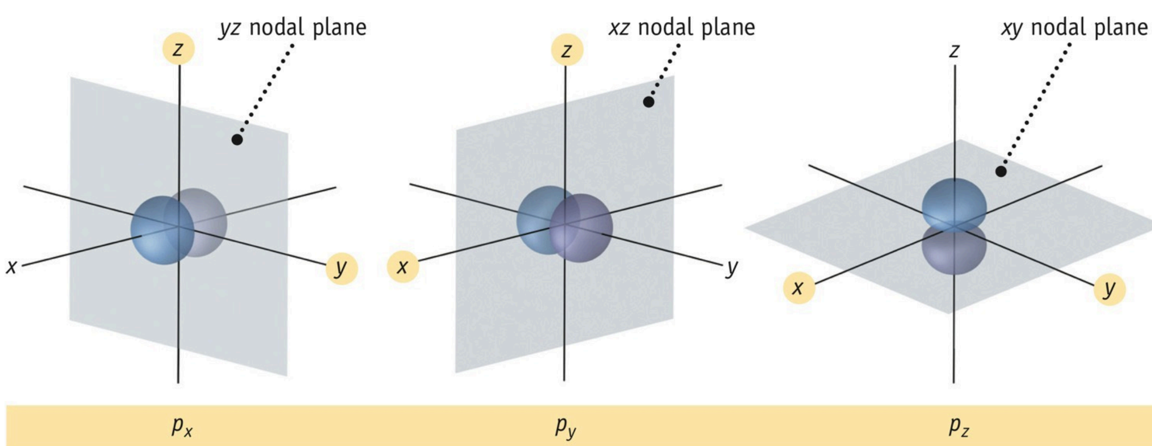
zero prob of e⁻ being at this distance

$\psi^2=0$

nodes

spherical node/nodal surface

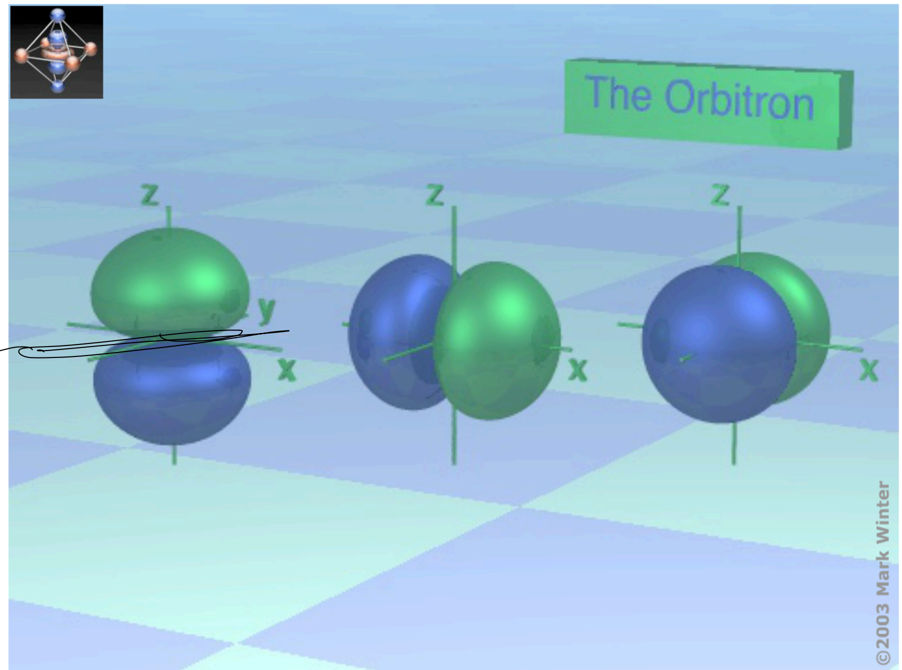
p-Orbitals



The three degenerate *p*-orbitals spread out on the x, y & z axis, 90° apart in space.

2p orbital

n=2
l=1
ml=-1, 0 or 1

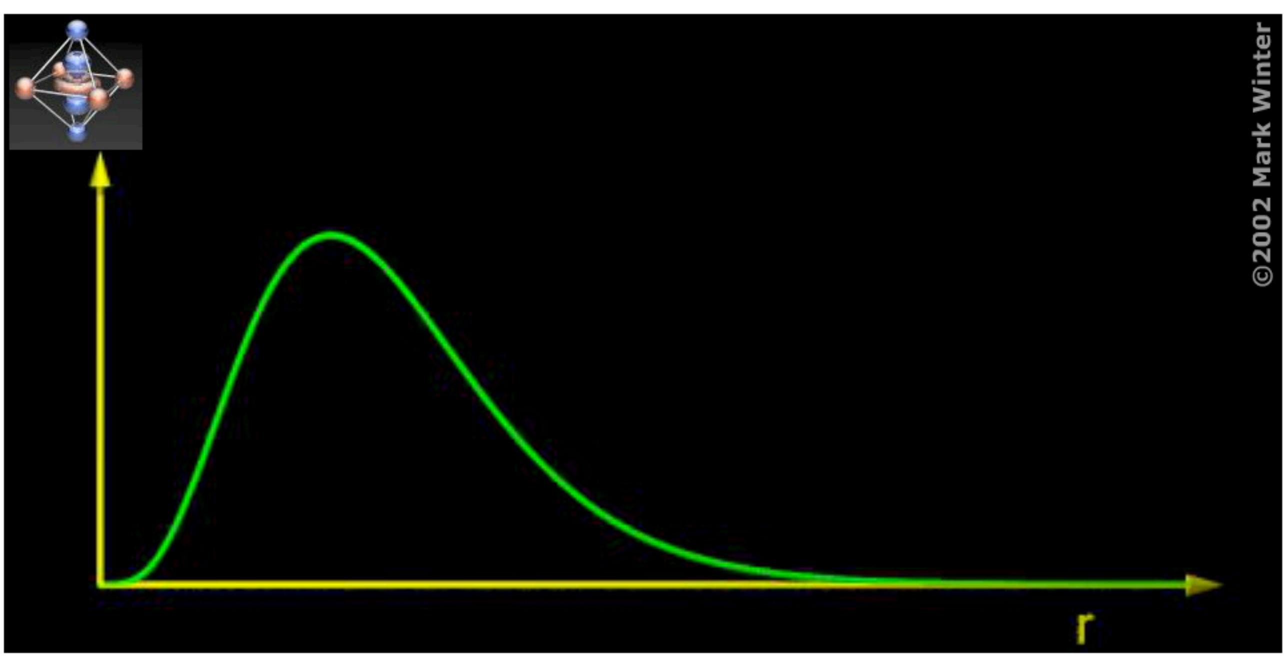


nodal plane

The shape of the three 2p orbitals. *From left to right: $2p_z$, $2p_x$, and $2p_y$. For each, the blue zones are where the wave functions have negative values and the green zones denote positive values.*

Atomic orbitals: 2*p* radial distribution function

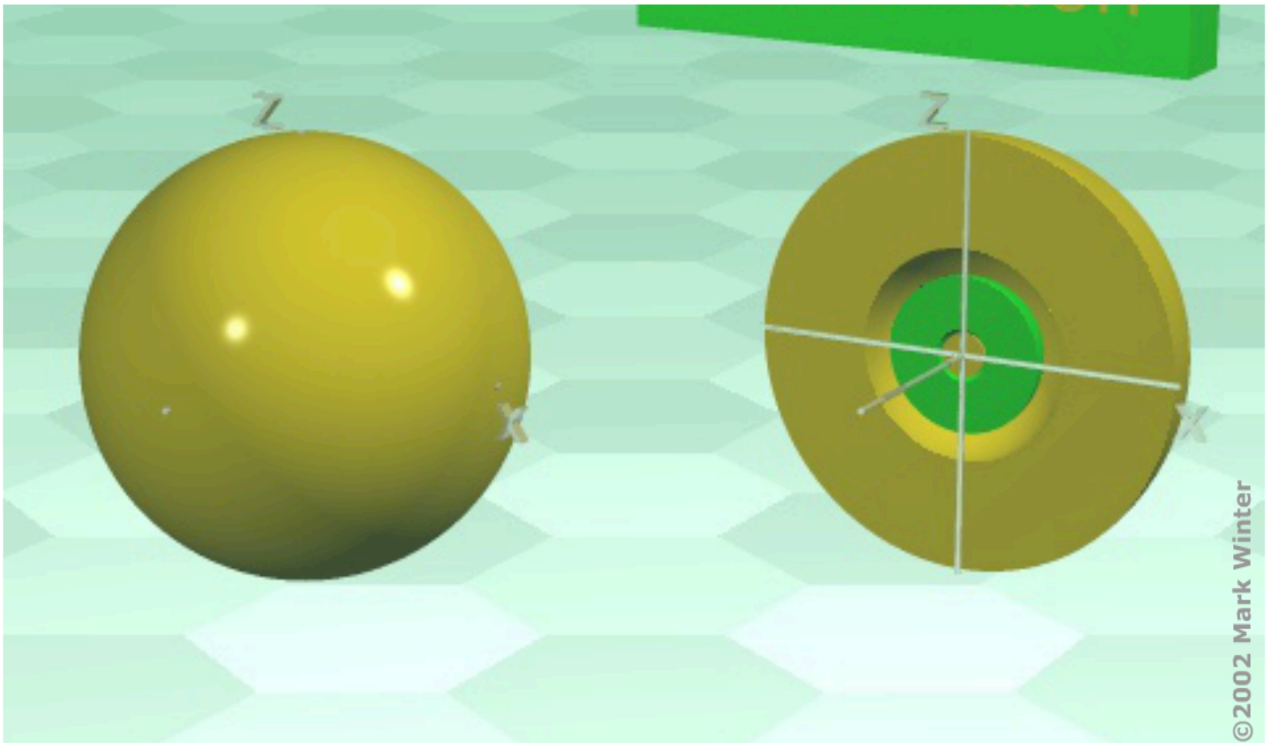
– for all 3 p orbitals together



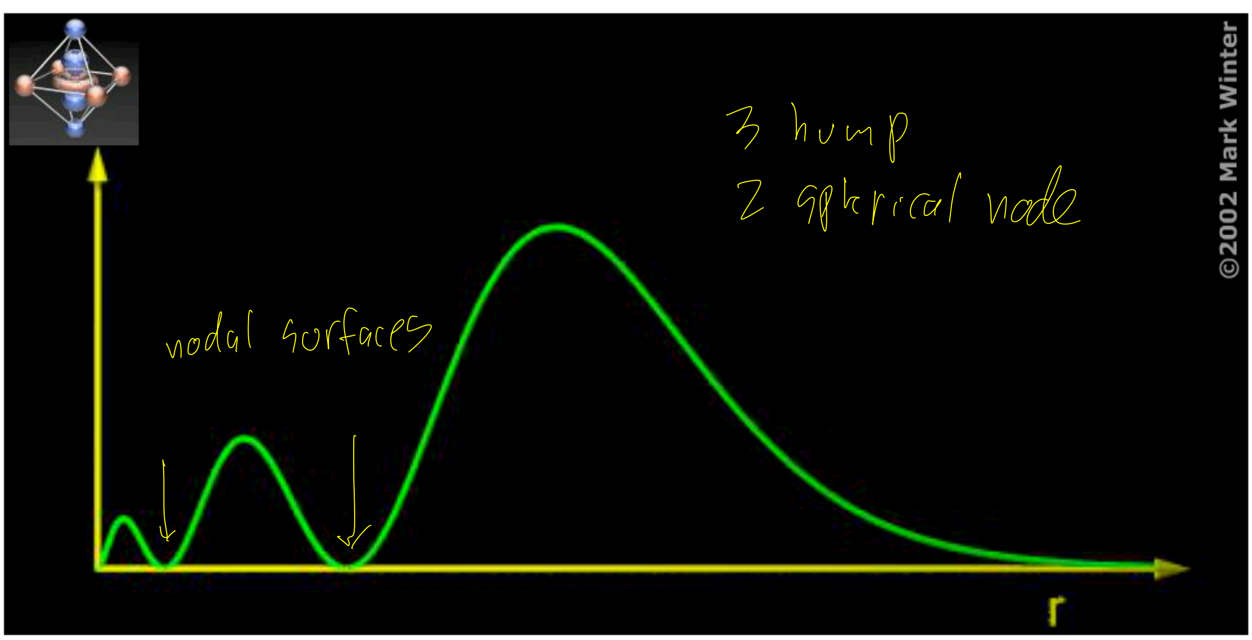
Schematic plot of the 2p radial distribution function $r^2R_{2p}^2$ *(R_{2p} = radial wave function).*

3s orbital

$n=3$
$\ell=0$
$m_\ell=0$



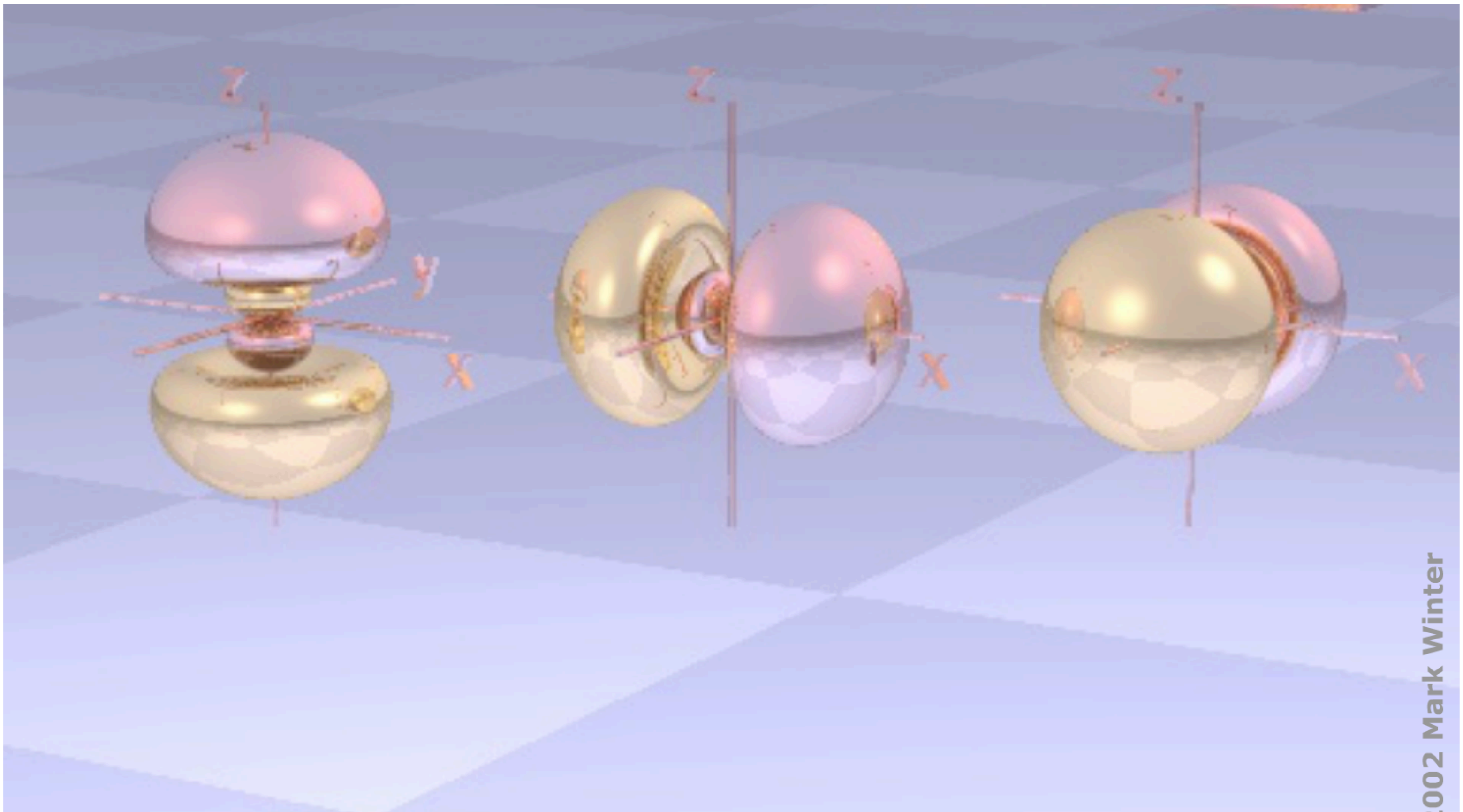
Atomic orbitals: 3*s* radial distribution function

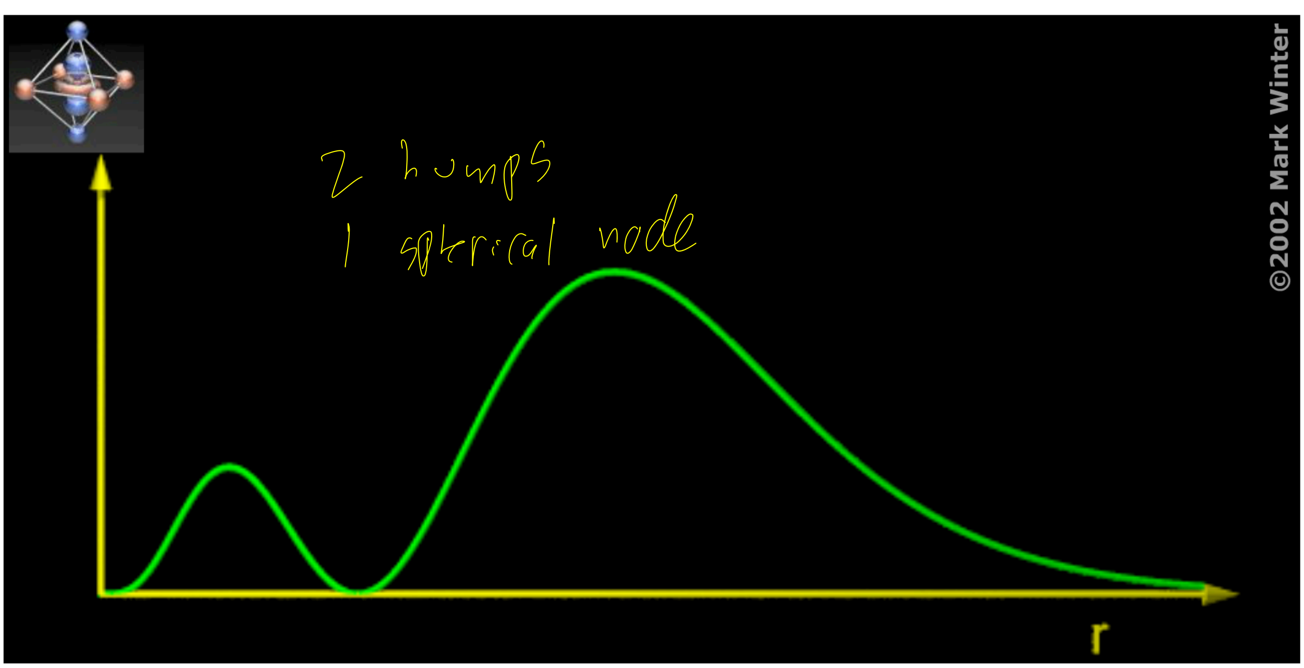


Schematic plot of the 3s radial distribution function $4\pi r^2\psi_{3s}^2$. *Blue represents regions within which the wave function is negative and red represents regions where the wave function is positive.*

3p orbital

n = 3
ℓ = 1
m_ℓ = -1, 0 or 1



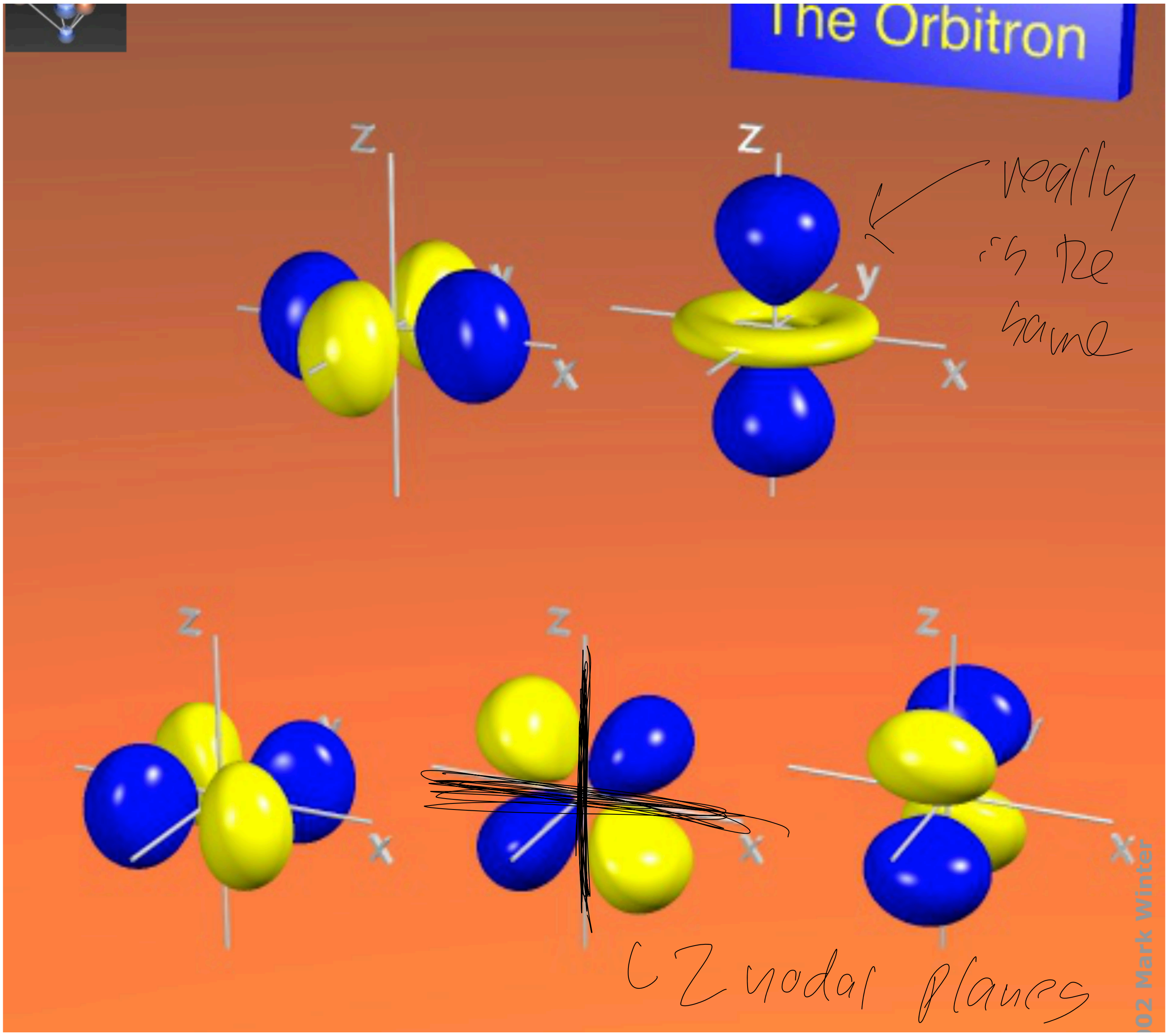


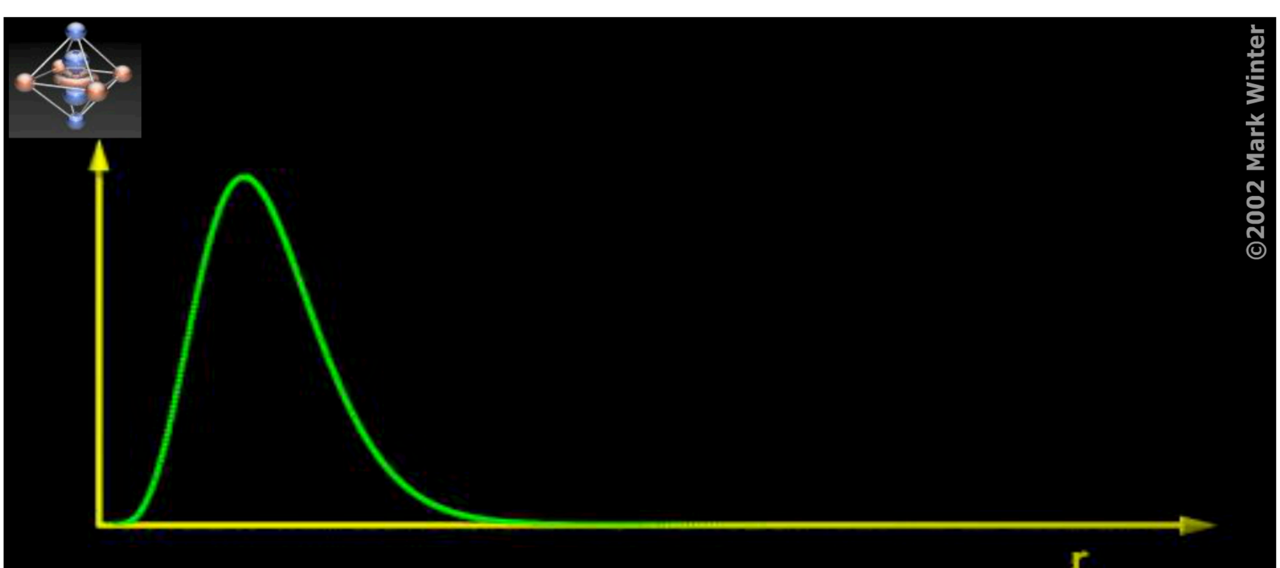
Schematic plot of the 3p radial distribution function $r^2R_{3p}^2$ *(R_{3p} = radial wave function).*

3d orbital

n=3
l=2

m_l=-2,-1
0,1,2



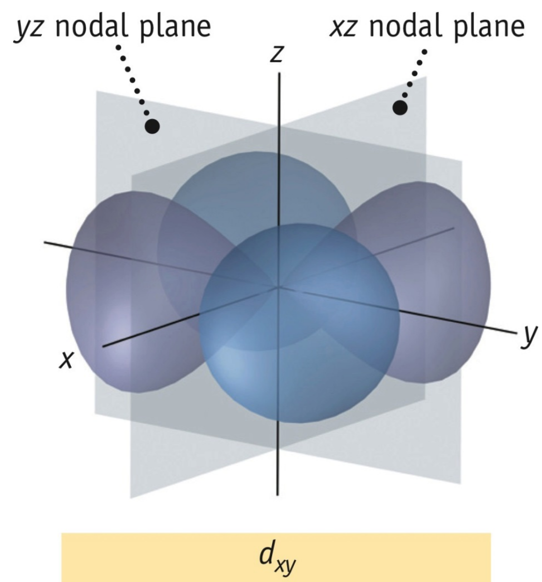


d-Orbitals

s-orbitals have no nodal planes ($l = 0$)

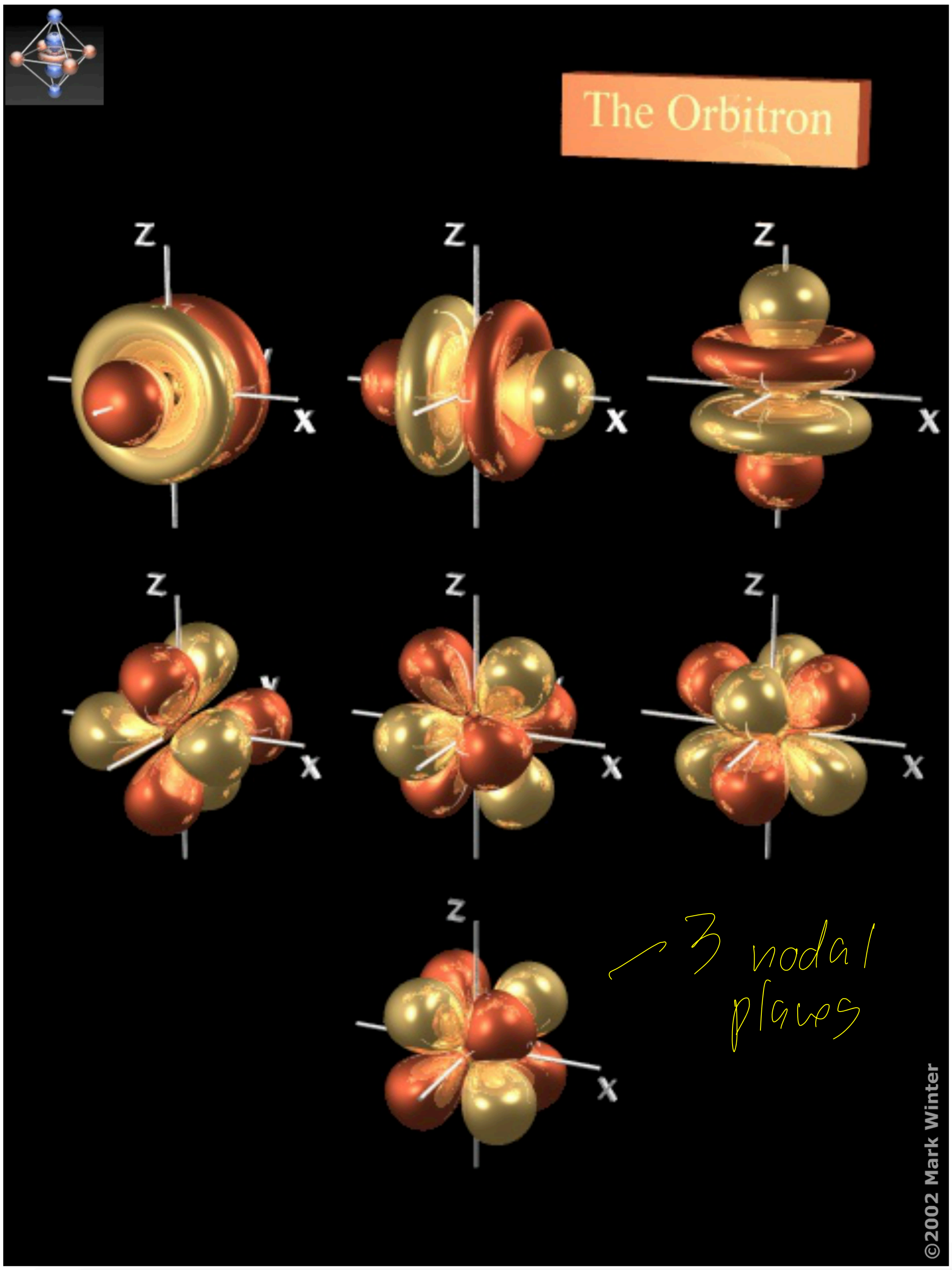
p-orbitals have one nodal plane ($l = 1$)

d-orbitals therefore have two nodal planes ($l = 2$)

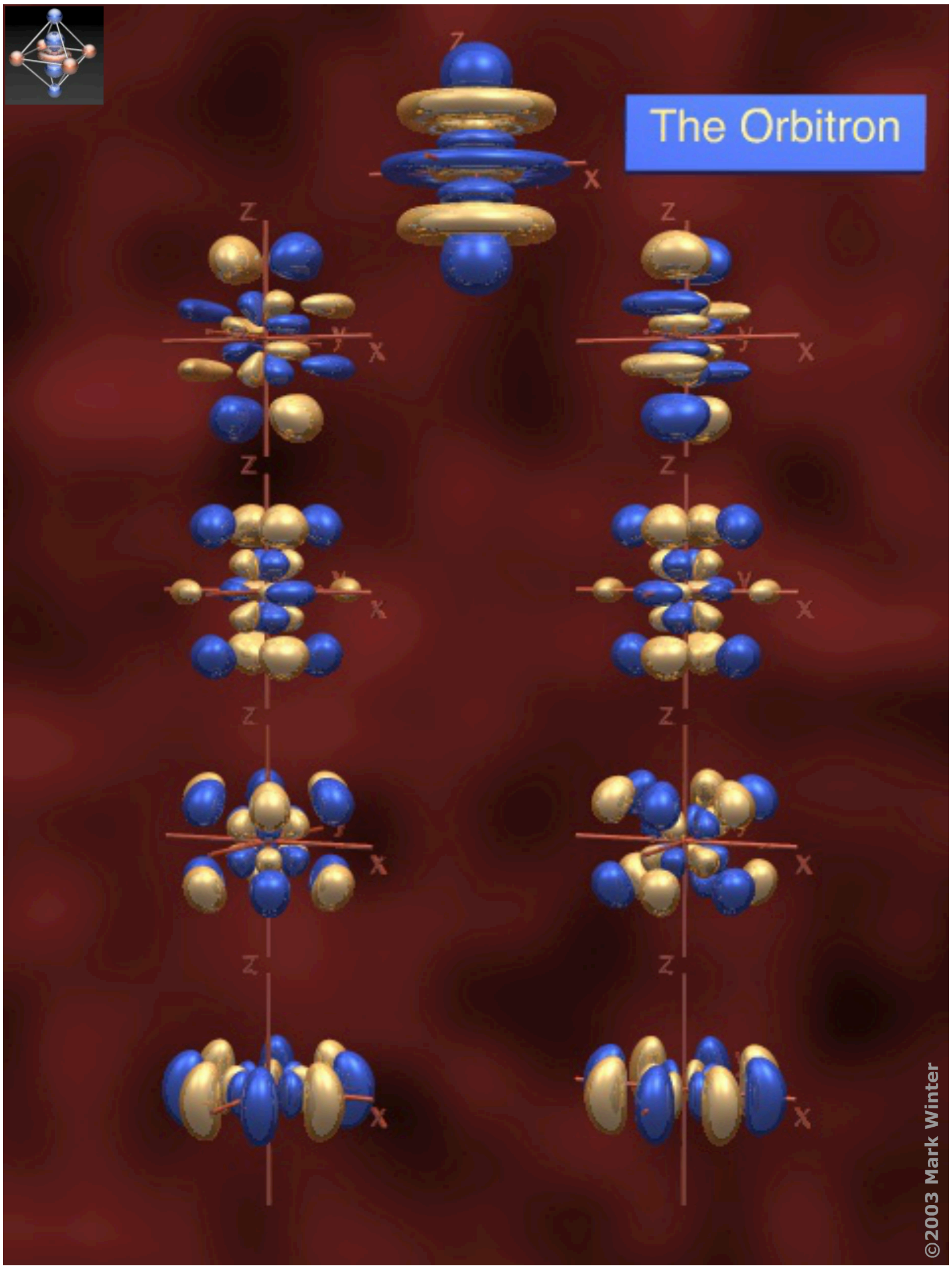


Crazy orbital (4f)

n = 4
l = 3
ml = -3, -2, -1, 0, 1, 2, 3



Bananas orbital (6g)



4^{th} quantum # m_s electron spin quantum #

$m_s = +\frac{1}{2}$ or $-\frac{1}{2}$

* Each electron in an atom must have a unique set of 4 quantum numbers

n	ℓ	m_ℓ	m_s
2	0	0	$+\frac{1}{2}$
2	1	-1	$+\frac{1}{2}$
2	1	0	$+\frac{1}{2}$
2	1	+1	$+\frac{1}{2}$
2	0	0	$-\frac{1}{2}$
2	1	-1	$-\frac{1}{2}$
2	1	0	$-\frac{1}{2}$
2	1	+1	$-\frac{1}{2}$

atom where $\Sigma m_s = 0$
is diamagnetic - not attracted to magnet

atom where $\Sigma m_s \neq 0$
is paramagnetic - yes attracted to magnet

$90s^+ \rightarrow 37$ Avg 92.3
$<90 \rightarrow 15$ Med 94.5