Late 1800s/early 1900s - Interaction btw matter and light was under investigation

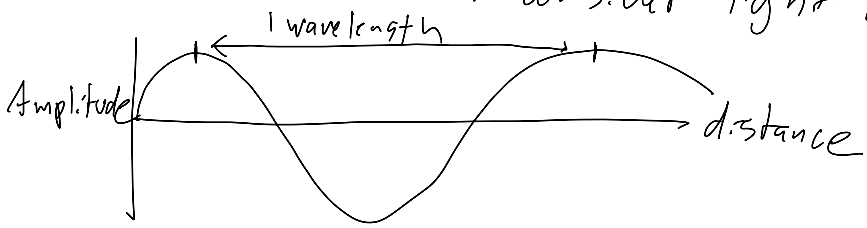
light = radiation

wavelength (λ) distance

frequency (ν) 1/time

velocity (c) dist/time

For the moment lets consider light as a wave



freq = # of wavelengths per time

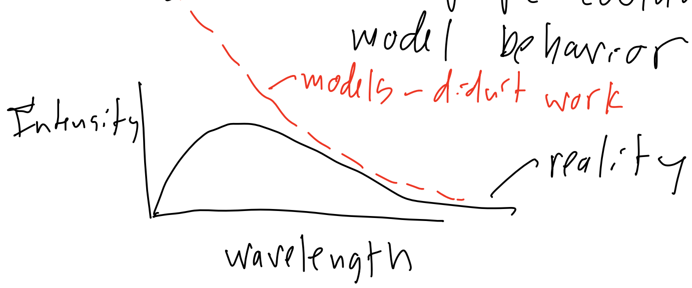
velocity of light is constant

$c = 3 \times 10^8$ m/sec

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

large ν		small ν
small λ	visible light	large λ
x rays gamma rays		radio waves
Deadly		not deadly

Hot things glow - but people couldn't successfully model behavior



Max Planck – new model – that worked

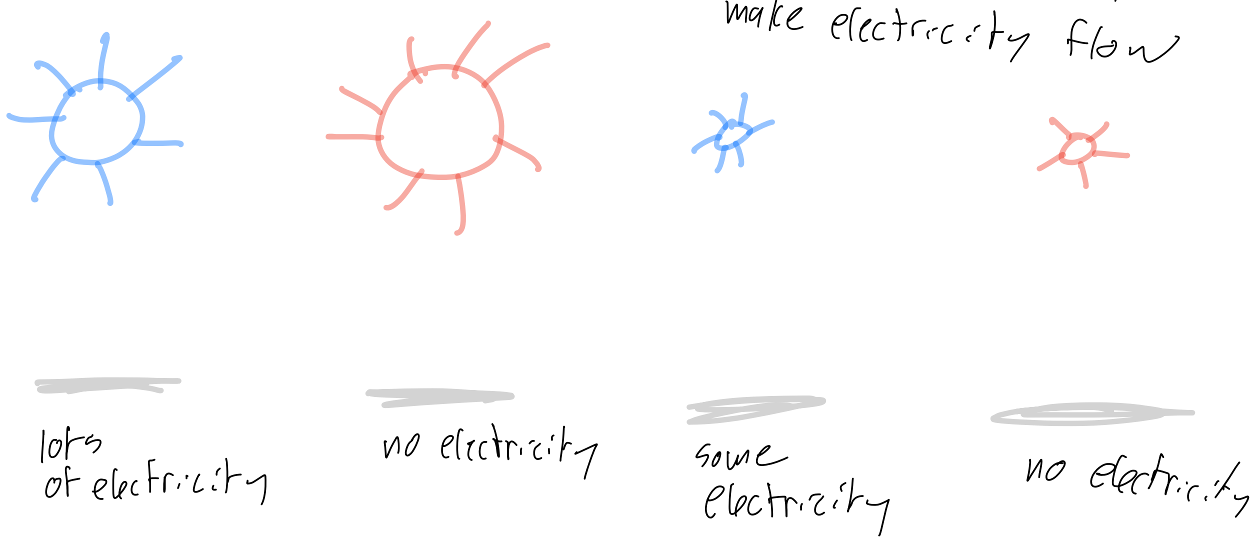
- heated molecules/atoms vibrate and give off light
- only <u>some</u> vibrational frequencies possible
  so only some freq (or wavelengths) of light could be given off
- Frequency (or wavelength) related to energy
- so only certain energies are possible

Energy of radiation is quantized

$$E = nh\nu$$

- 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

Einstein + photoelectric effect – shine light on metal make electricity flow



Einstein – light isn't a wave but is a massless particle → photon

$E_{photon} = h\nu$ or $\frac{hc}{\lambda}$ b/c $c = \lambda\nu$

400nm	550nm	700nm
Blue	Green	Red
larger ν		smaller ν
larger E		smaller E

"wave particle duality"

If we had blue light

w/ $\lambda = 450\,nm$

$E_{photon} = h\nu$

$$3\times10^{8}\,m/sec = (450\times10^{-9}\,m)(\nu)$$

$$\nu = \frac{3\times10^{8}\,m/sec}{450\times10^{-9}\,m} = 6.6\times10^{14}\,sec^{-1}$$

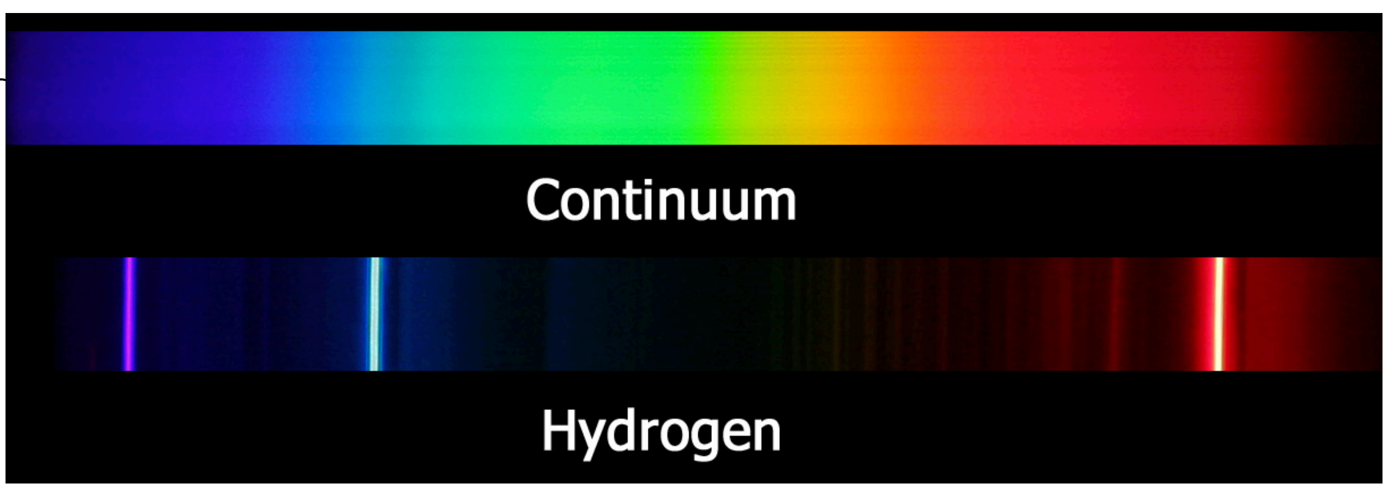
$$E = (6.626\times10^{-34}\,J\cdot sec)(6.6\times10^{14}\,sec^{-1})$$

$$E = 4.4\times10^{-19}\,J$$

Atomic Line Spectrum from Hydrogen Discharge Lamp

- tube filled w/ H_2
- electrodes @ top + bottom
- high voltage
- H_2 split into H atoms
- atoms glow

white light

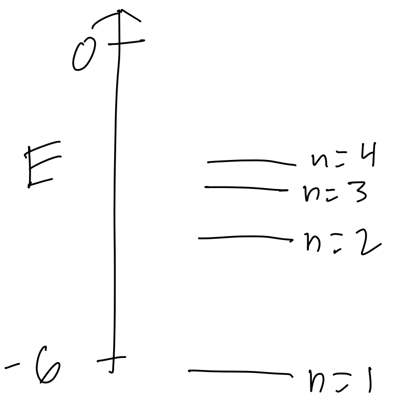


3 lines means light from discharge lamp is made up of 3 different types of photons

Imagine e^- in H atom has different energy levels it can live at

Adding energy causes e^- to go up a level or more

Being at higher energy isn't sustainable so electron eventually falls back down, giving off energy by emitting a photon of light



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

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

energy of n^{th} level

n from n^{th} level

higher → lower   energy given off as photon

lower → higher   energy of photon taken in to allow e^- to move up

Wave particle duality part 2

under certain circumstances particles can be described in wave-like ways

$$\lambda_{particle} = \frac{h}{mv}$$

DeBroglie wavelength

mass of particle

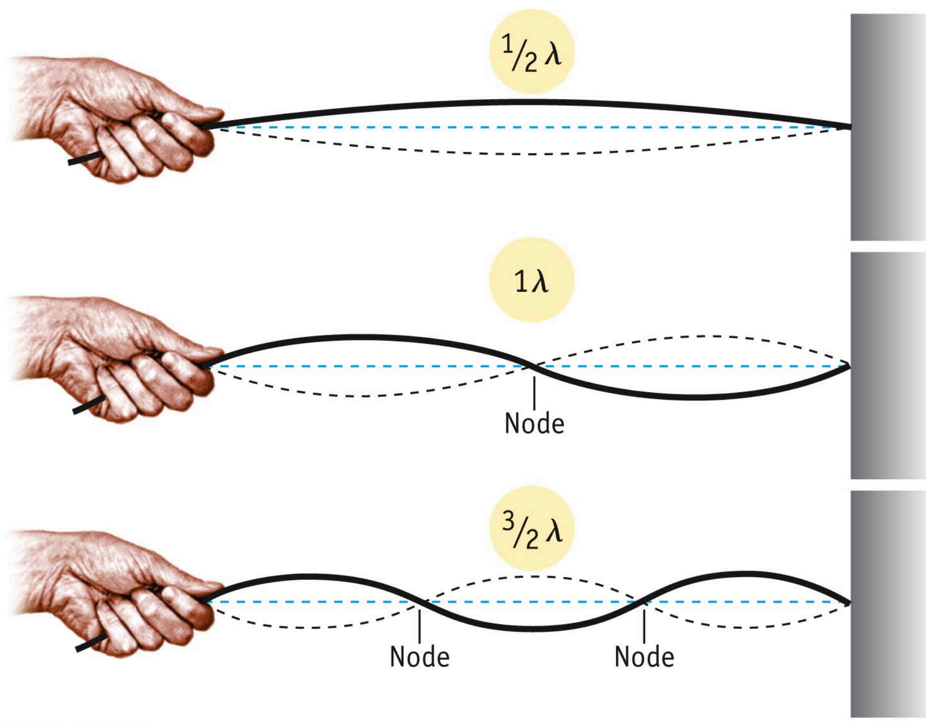
velocity of particle

Quantum mechanics is how we describe electrons

- math but no math

Standing wave is concept to describe electrons → only certain λ possible for a standing wave

→ only certain energies are possible



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

Electrons described as 3-D standing wave

wavefunction (Ψ) is the math equation for the standing wave

$\Psi = 42x^4 + 13y^{3/2} - 7z^8$ for each (x, y, z) point in space Ψ has amplitude

Ψ^2 - tells you probability of electron being at particular place in 3-D space

- electrons only described in terms of probability

use quantum numbers as shorthand to describe wave functions

n = principal quantum # "shell"

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

describes energy

describes extent of spatial probability distribution

ℓ = orbital angular momentum QN "subshell"

$\ell = 0, 1, 2 \ldots n-1$

describes shape

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

m_ℓ = magnetic QN

$m_\ell = -\ell \ldots\ldots +\ell$

describes orientation in 3-D space

If $n=1$ ℓ must $=0$ and m_ℓ must be zero

only 1 ψ when $n=1$ $\rightarrow$ $n=1, \ell=0, m_\ell=0$

If $n=2$ ℓ could be 0 or 1

$0 \downarrow m_\ell=0$

$1 \downarrow m_\ell=-1,0,1$

n	ℓ	m_ℓ
2	0	0
2	1	-1
2	1	0
2	1	1

4 possible ψ when $n=2$

$n=3$ $\ell=0,1,2$

$0 \downarrow m_\ell=0$

$1 \downarrow m_\ell=-1,0,1$

$2 \rightarrow m_\ell=-2,-1,0,1,2$

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

9 possible ψ when $n=3$

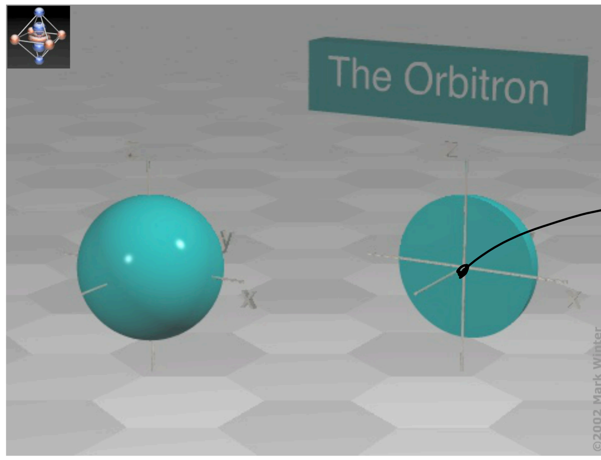
orbital = wavefunction

$1s$ orbital

$l=0$

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

Atomic orbitals: 1s



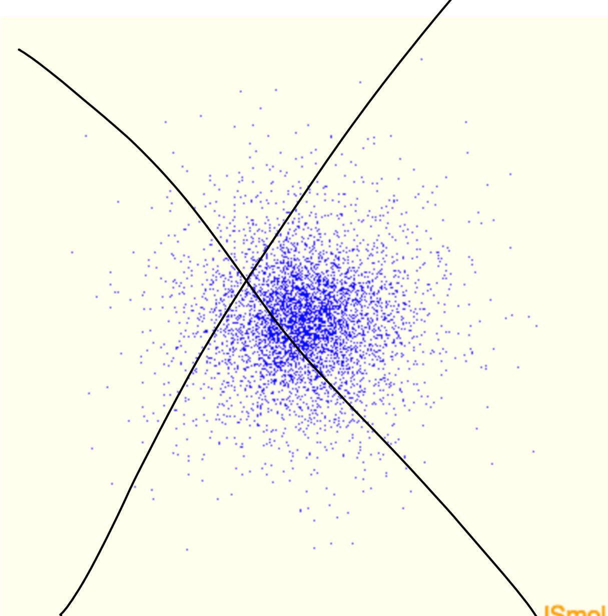
The shape of the 1s orbital.

s → spherical

nucleus

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

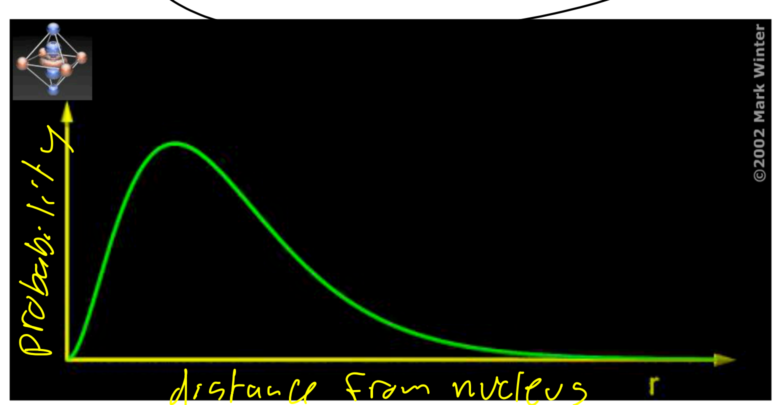
Atomic orbitals: 1s electron density



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

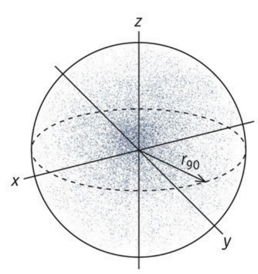
~~probability~~ probability of finding e^- at particular distance from nucleus

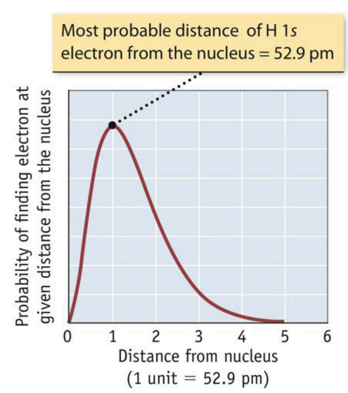
Atomic orbitals: 1s radial distribution function

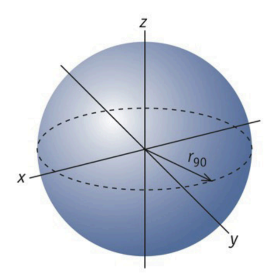


Schematic plot of the 1s radial distribution function $4\pi r^2\psi_{1s}^2$

s-Orbitals





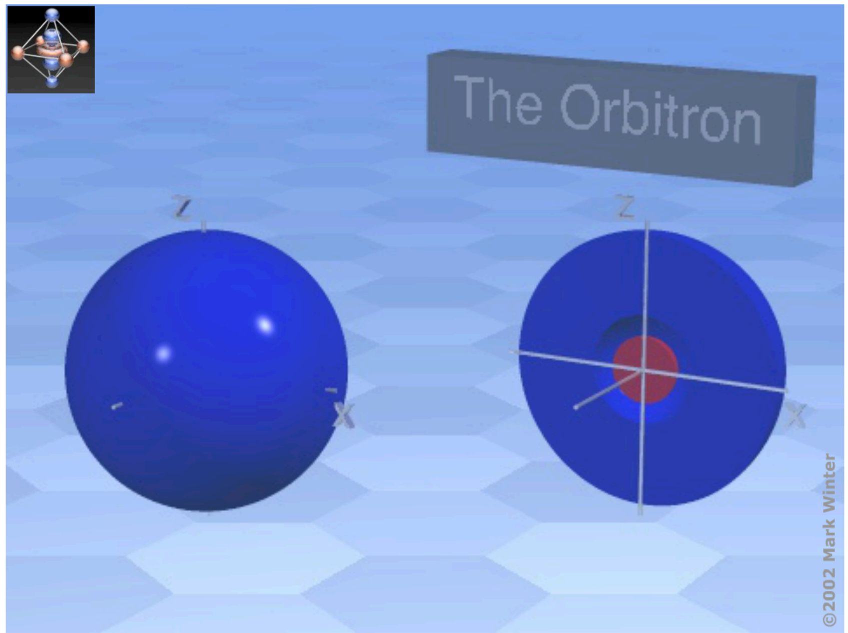


- $l = 0$, $m_l = 0$
- $2l+1 = 1$
- one *s*-orbital that extends in a radial manner from the nucleus forming a spherical shape.

2s orbital

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

Atomic orbitals: 2s

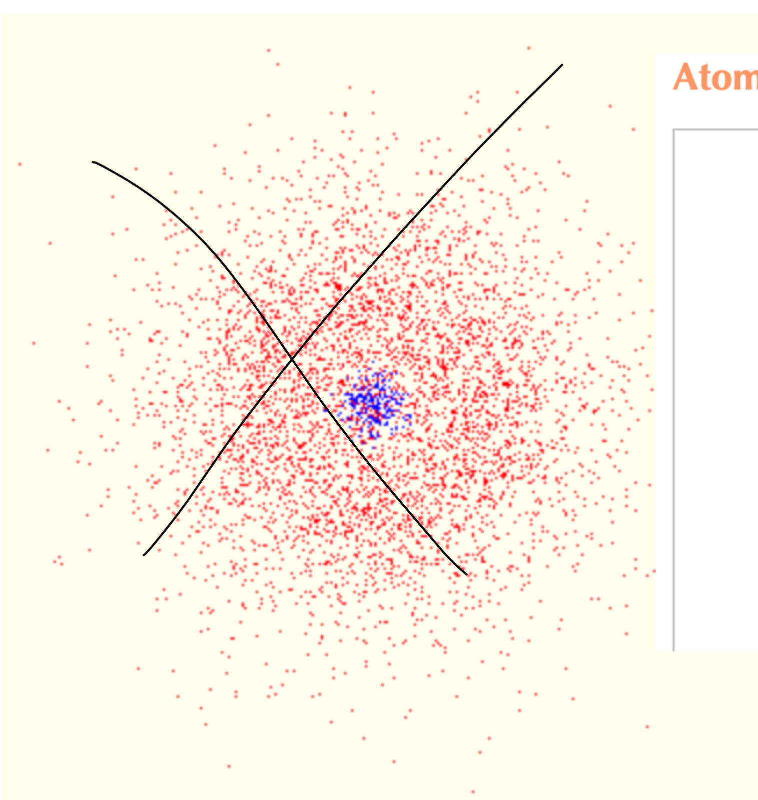


The shape of the 2s orbital. *The blue zone is where the wave function has negative values while the red zone is where values are positive.*

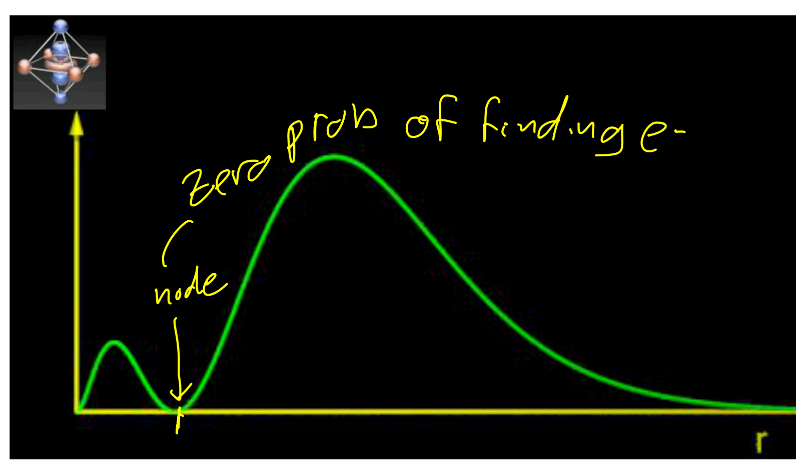
spherical b/c "s"

nodal surface or spherical node in betw spheres

Ø prob of e⁻ at node



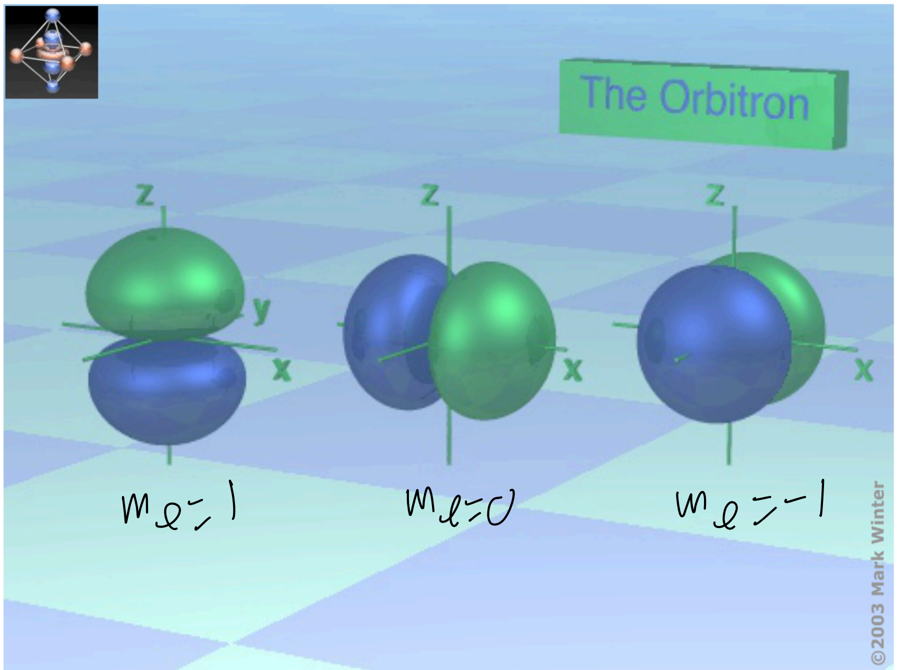
Atomic orbitals: 2s radial distribution function



$\ell = 1$

2p orbital

$n = 2$
$\ell = 1$
$m_\ell = -1, 0, 1$

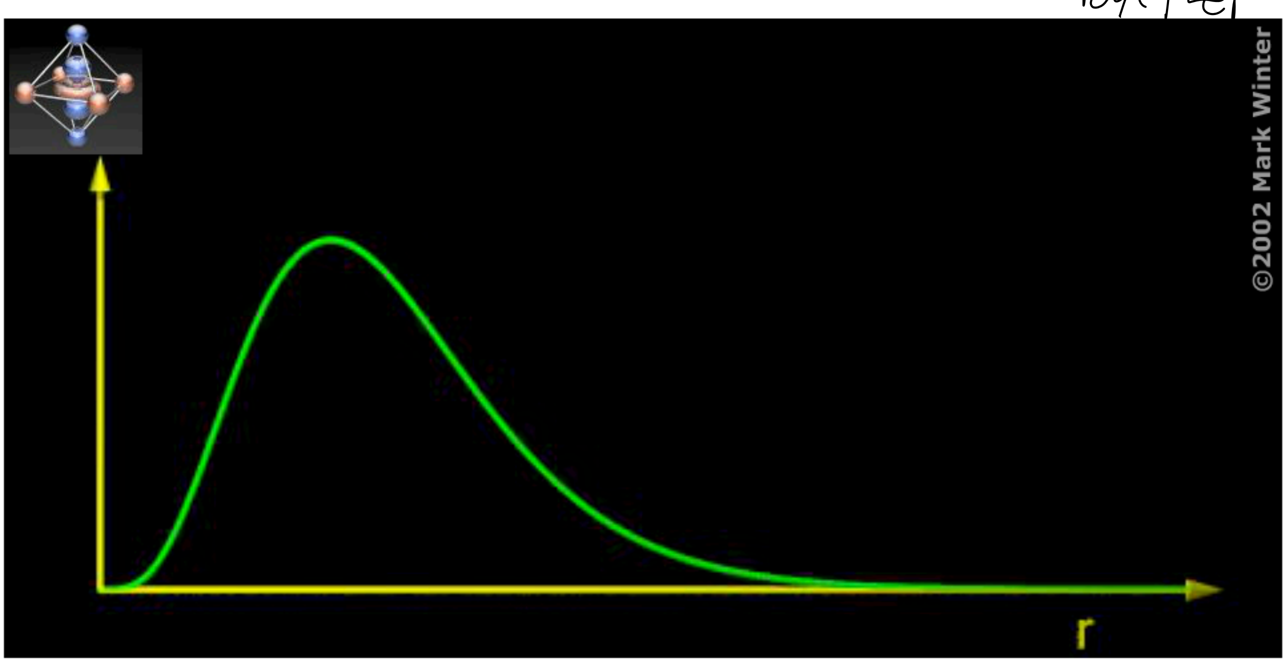


no spherical node
yes nodal plane between mushroom caps

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.*

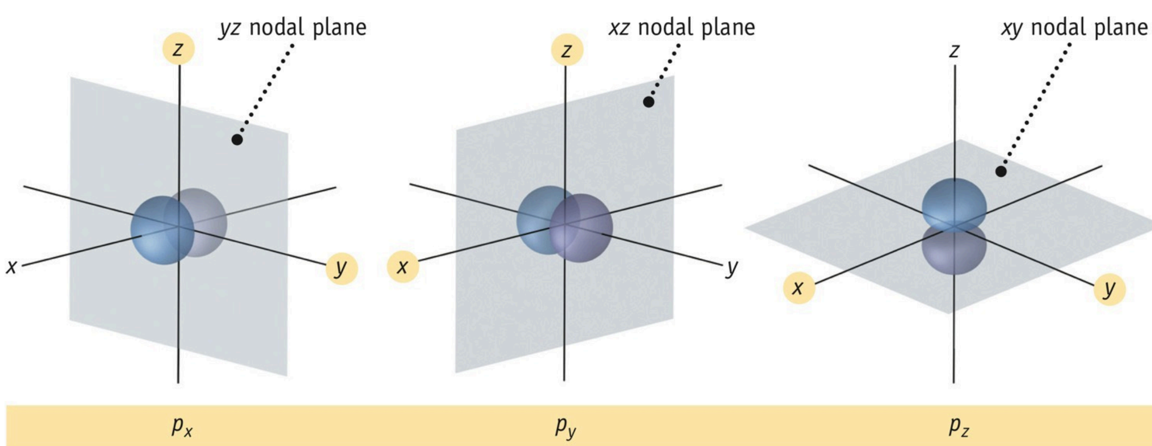
Atomic orbitals: 2*p* radial distribution function

— for all 3 mashed together



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

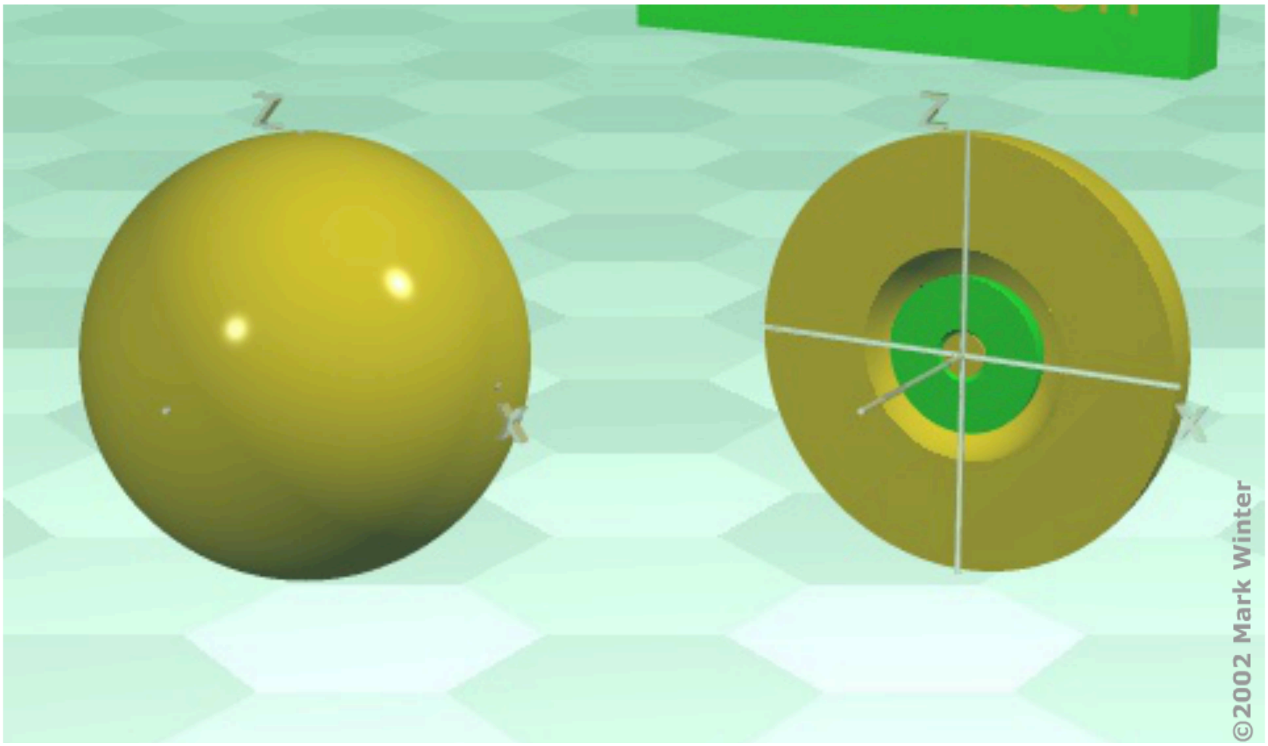
p-Orbitals



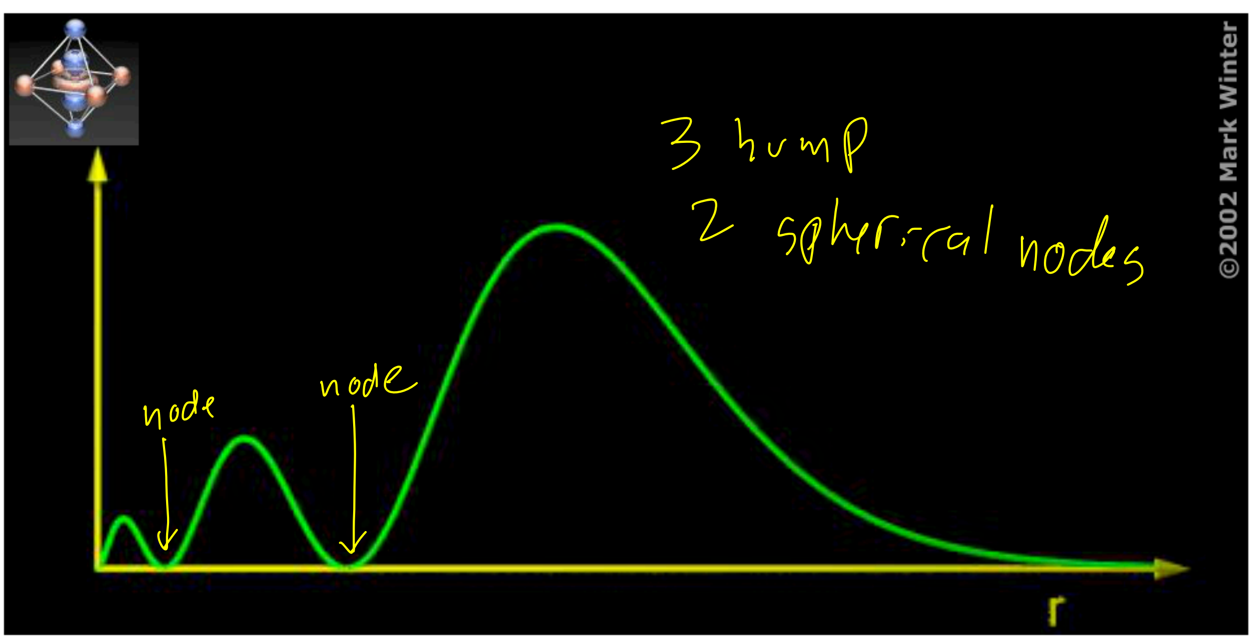
The three degenerate *p*-orbitals spread out on the x, y & z axis, 90° apart in space.

3s orbital

$n=3$
$l=0$
$m_l=0$



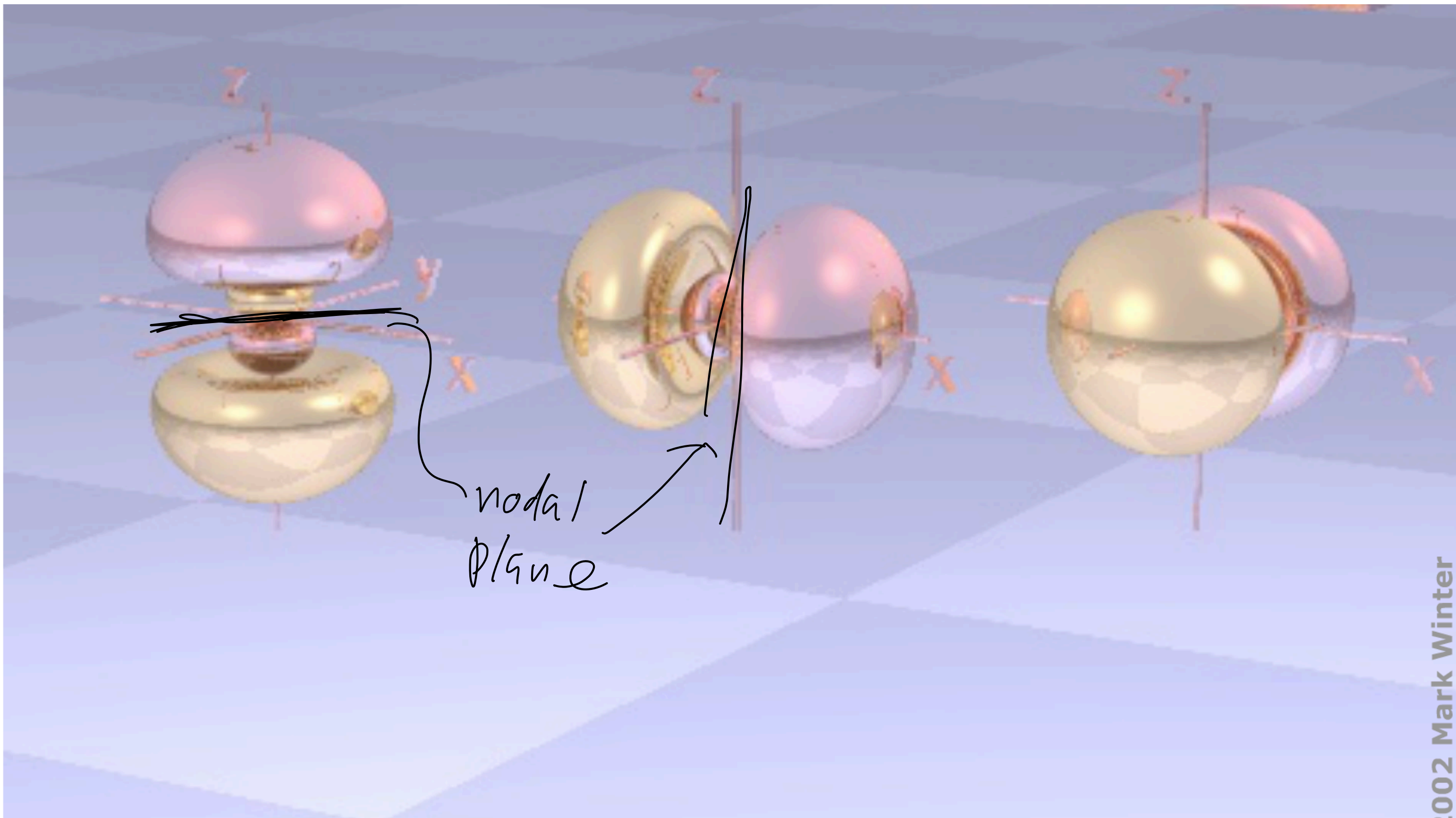
Atomic orbitals: 3*s* radial distribution function

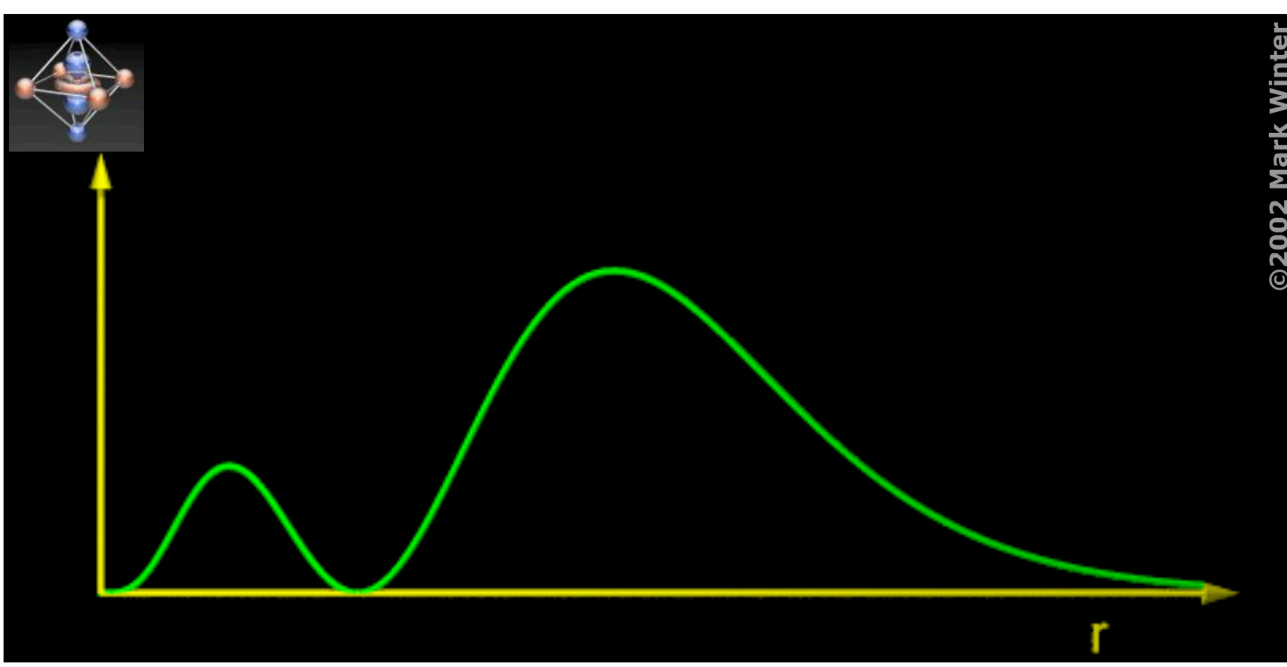


Schematic plot of the 3s radial distribution function $4\pi r^2\psi_{3s}^2$. *Blue represents regions within which the wave function is negative and red represents regions where the wave function is positive.*

3p orbital

$n=3$
$l=1$
$m_l=-1, 0, 1$



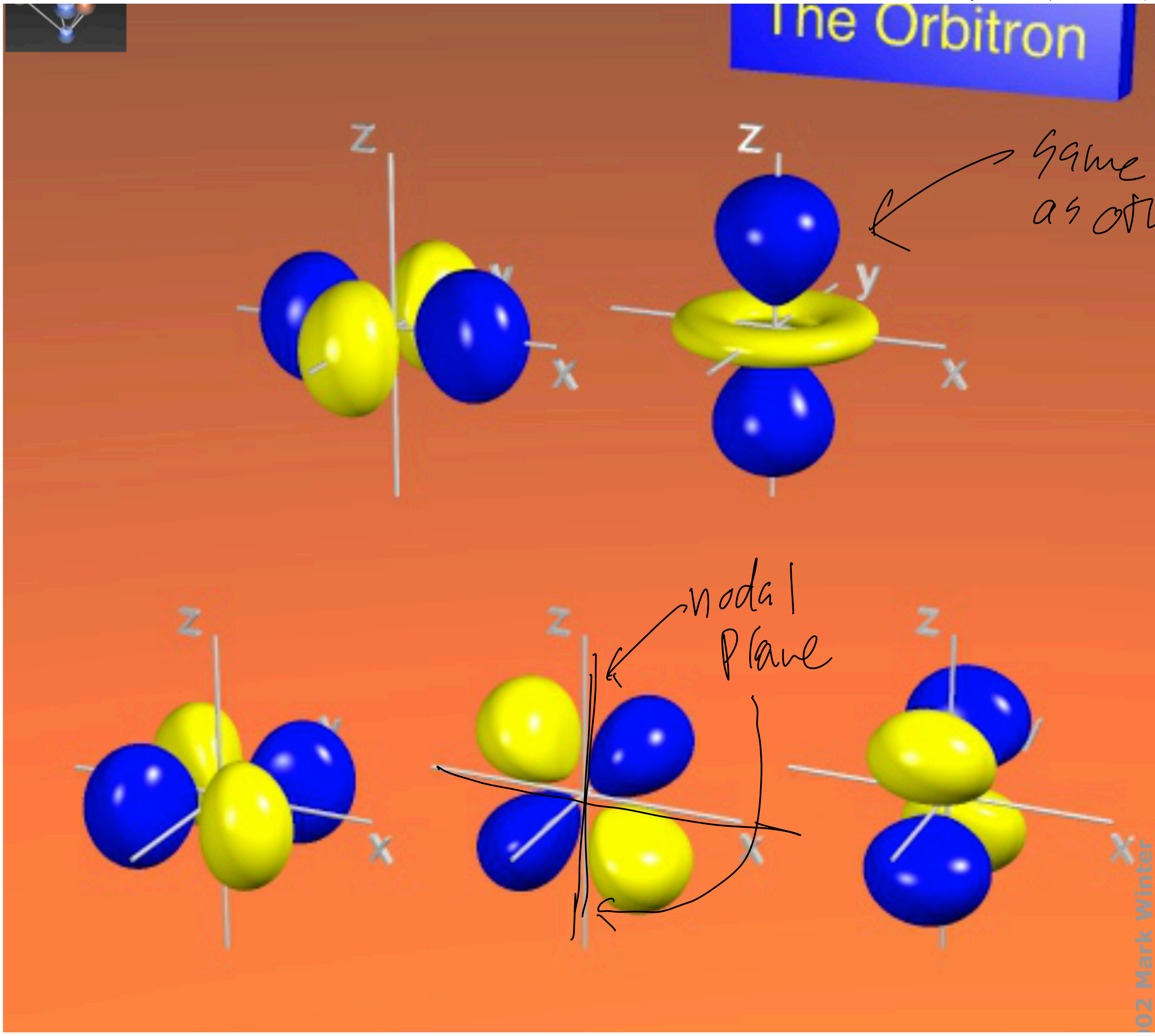


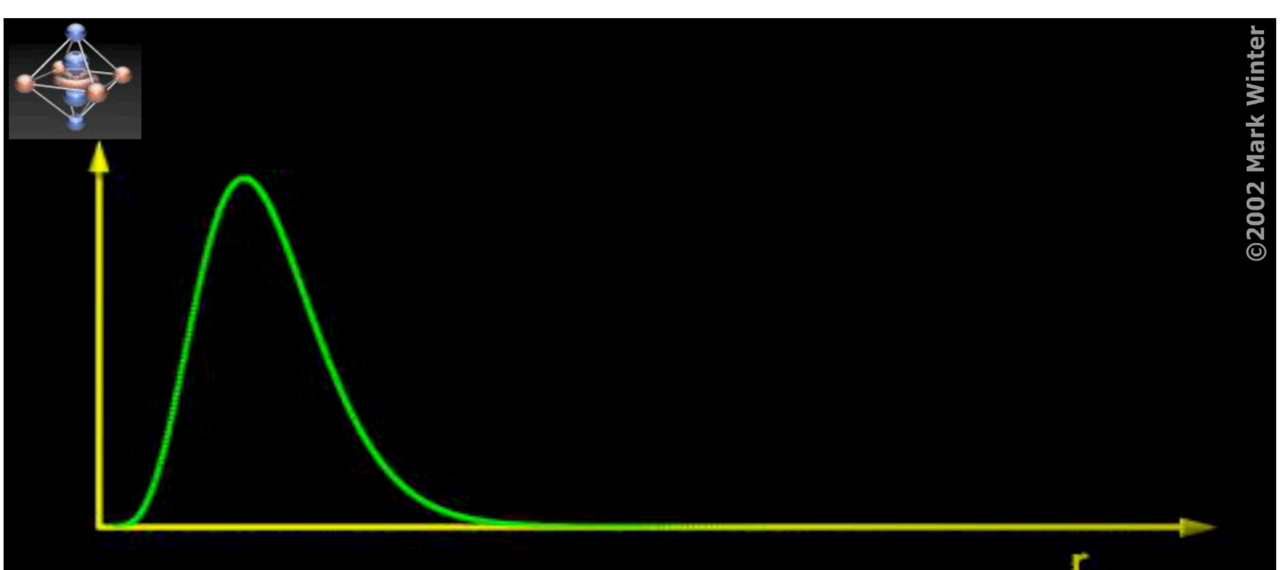
Schematic plot of the 3p radial distribution function $r^2R_{3p}^2$ *(R_{3p} = radial wave function).*

3d orbital

$n=3 \quad \ell=2$

$m_\ell = -2, -1, 0, 1, 2$



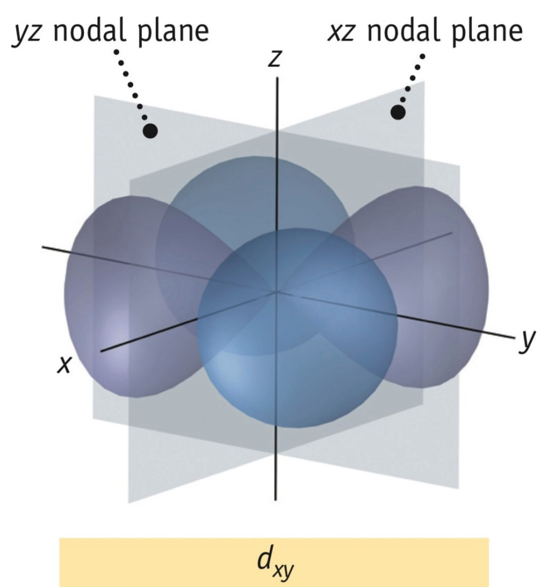


d-Orbitals

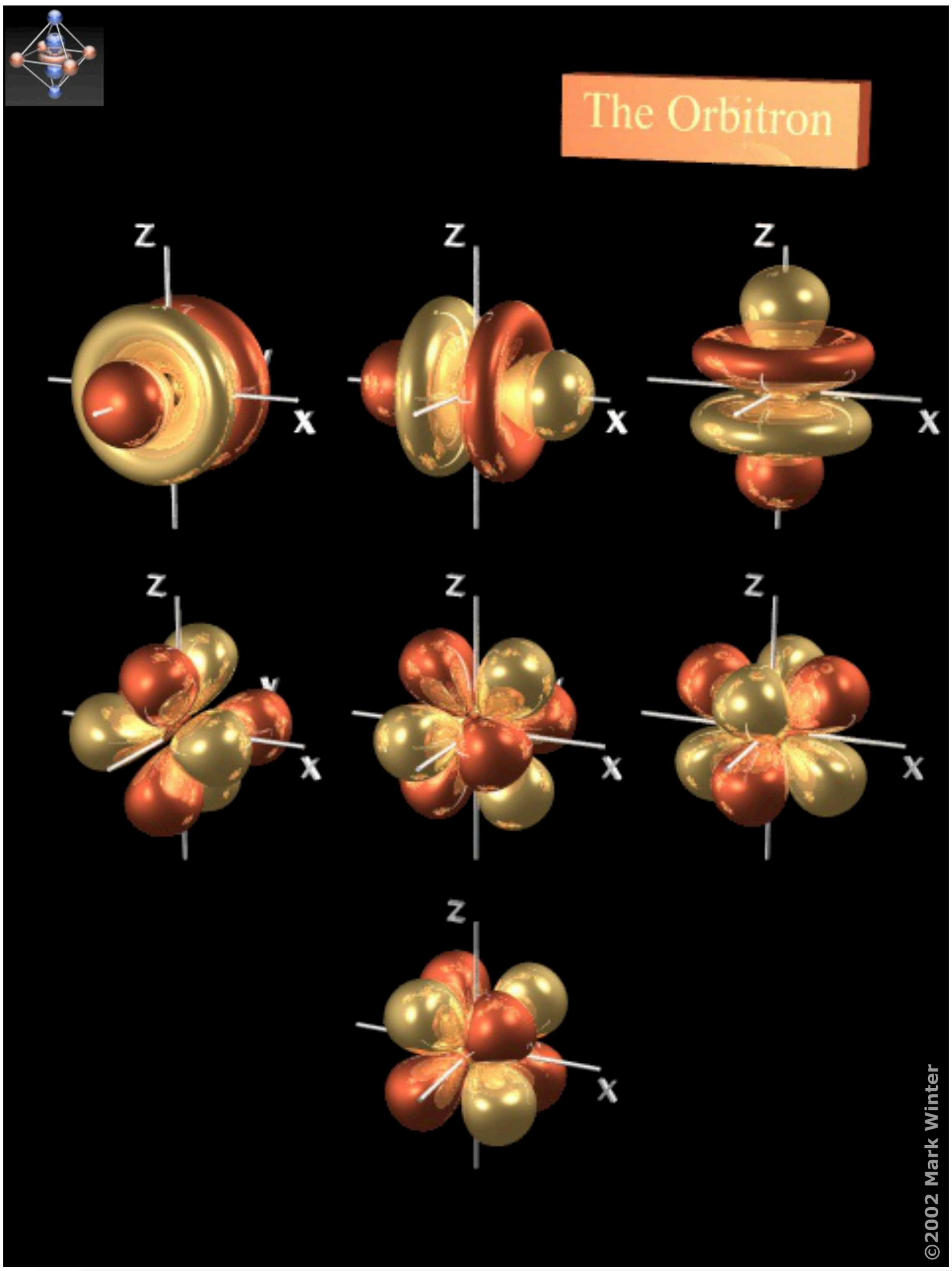
s-orbitals have no nodal planes (*l* = 0)

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

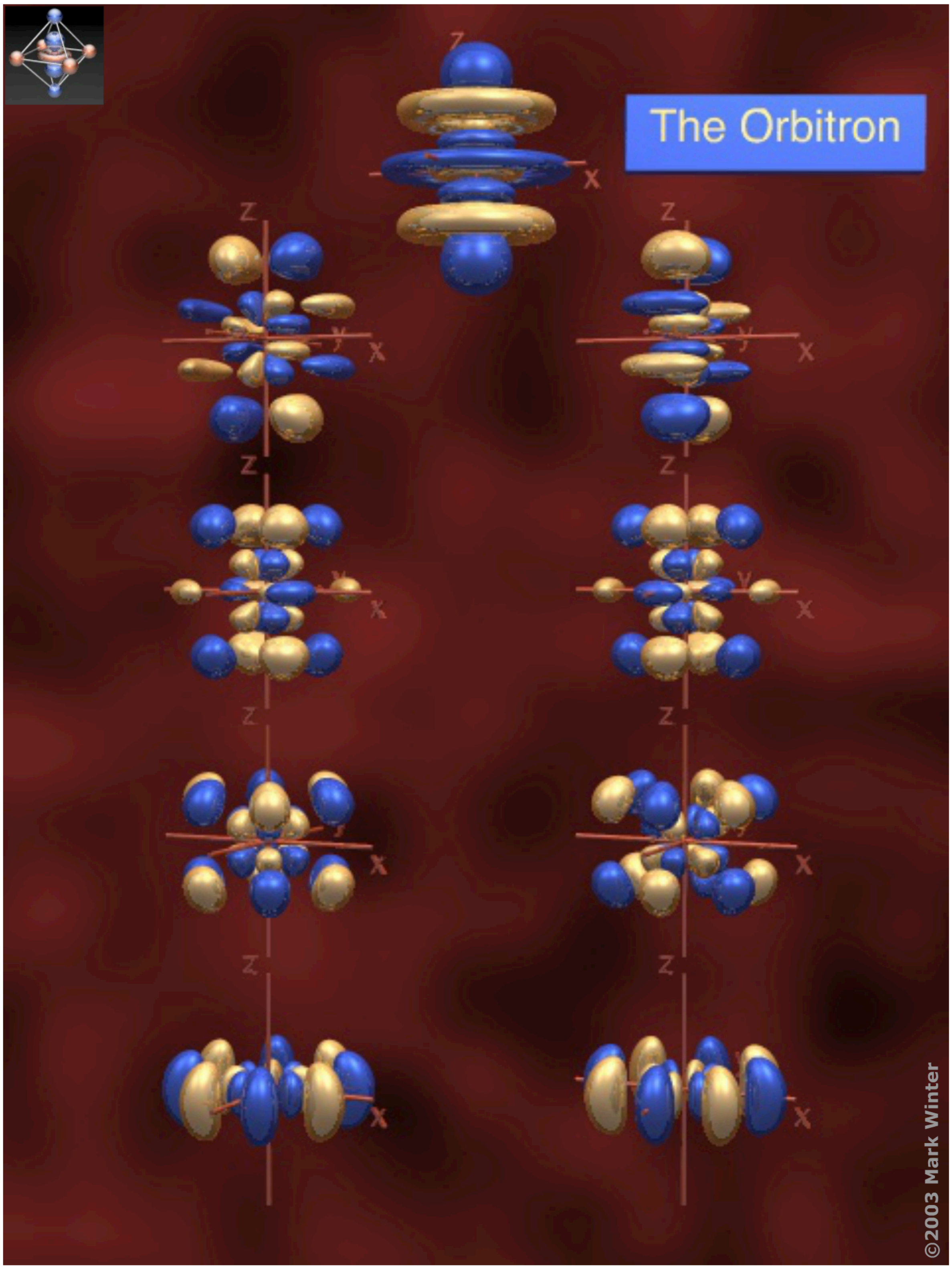
d-orbitals therefore have two nodal planes (*l* = 2)



Crazy orbital (4f)



Bananas orbital (6g)



There is a 4^{th} quantum number

m_s electron spin QN

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

Every electron in an atom must have ~~a~~ its own unique set of 4 quantum numbers

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

not attracted to mag. field

diamagnetic when all m_s of all e^- adds to zero

paramagnetic when all m_s of all e^- doesn't add to zero

will be attracted to mag. field

Avg 89%

Med 97%

100+	-23
90s	-18
80s	-6
<80s	-13