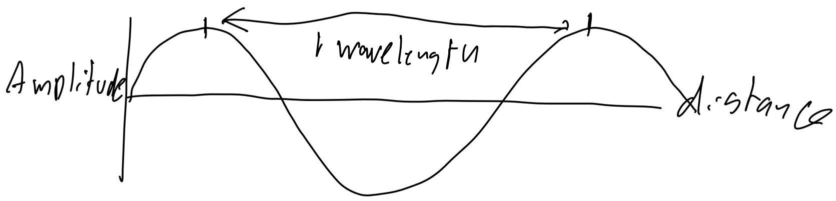
Late 1800s/early 1900s – Interaction btw light + matter was under investigation

light = radiation

wavelength	(λ)	distance
frequency	(ν)	1/time
velocity	(c)	dist/time

For the moment light behaves like a wave

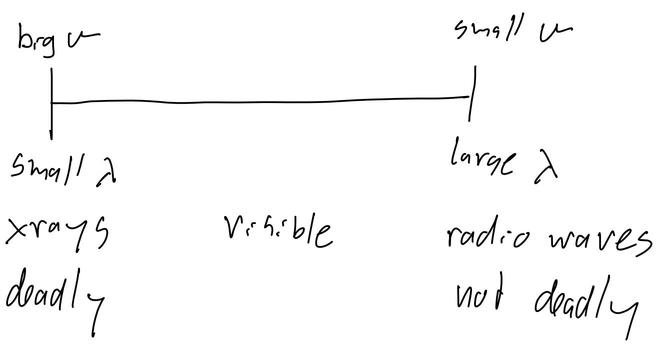


frequency = # of wavelengths per unit time

All light moves at same velocity

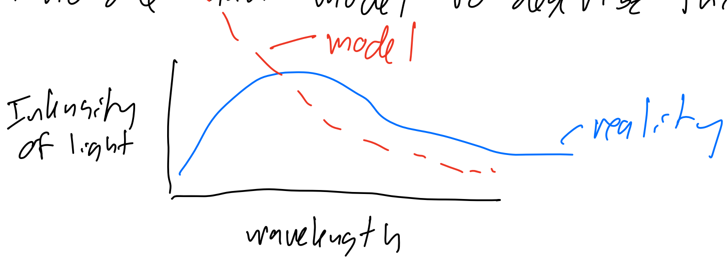
C = speed of light is constant 3×10^8 m/sec

$C = \lambda \nu$



Exptl observation – hot things give off light (ie glow)

Problem – no one had model to describe this



Max Planck's model – when atoms/molecules heated, they vibrate and give off light waves

* only some vibrational frequencies are possible

Consequence is that only certain frequencies of light waves given off

* frequency of light is related to its energy

* only some values of energy are possible

Energy of radiation is "quantized"

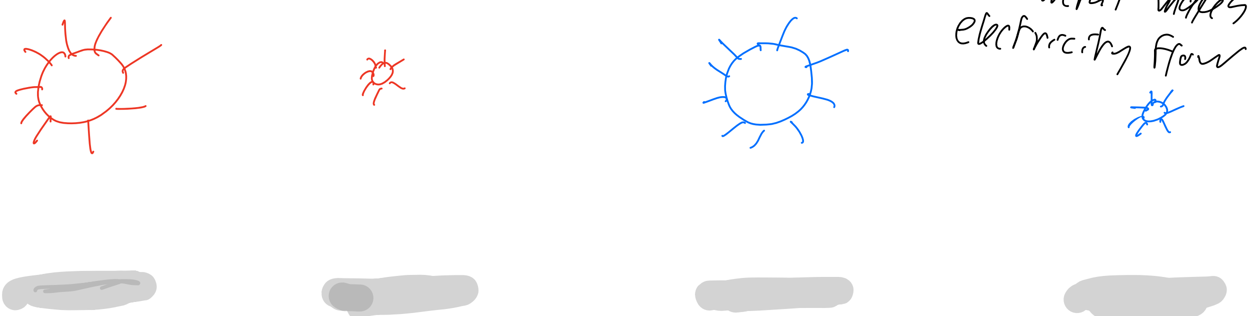
$$E_{\text{of radiation}} = nh\nu$$

ν – frequency (in $Hz = sec^{-1}$)

h – Planck's constant $= 6.626 \times 10^{-34}$ J·sec

n – integer – how many "pieces" of radiation you have

Einstein looked at photoelectric effect – shining light on metal makes electricity flow



no electricity | no electricity | lots of electricity | a bit of electricity

Einstein proposed to think of light as not a wave but as massless particles "photons"

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

"wave particle duality"

400nm — 550nm — 700nm
blue — green — red

Blue light w/ 450 nm

E of photon of 450nm light $= \frac{hc}{\lambda}$

$$\boxed{\begin{aligned} E &= h\nu \\ c &= \lambda\nu \\ \frac{c}{\lambda} &= \nu \end{aligned}}$$

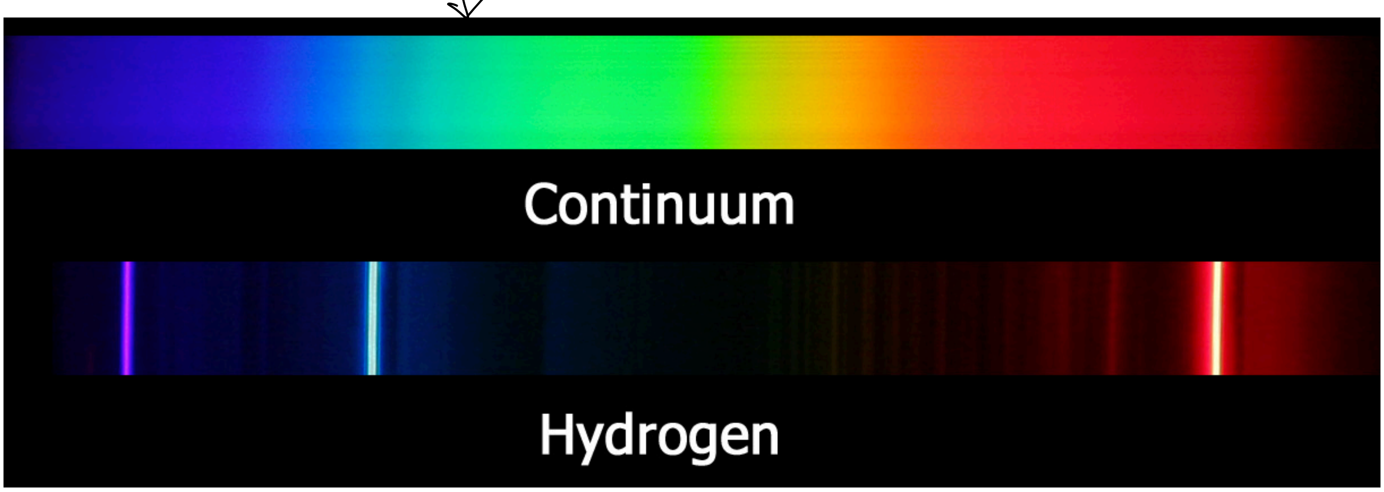
$$E = \frac{(6.626\times10^{-34}\,J\cdot sec)(3\times10^{8}\,m/sec)}{450\times10^{-9}\,m} = 4.42\times10^{-19}\,J$$

$E = \frac{hc}{\lambda}$

Atomic Line Spectrum from Hydrogen Discharge Lamp

- Tube filled w/ hydrogen
- apply high voltage and H_2 splits into 2 H atoms
- H atoms give off light

white light



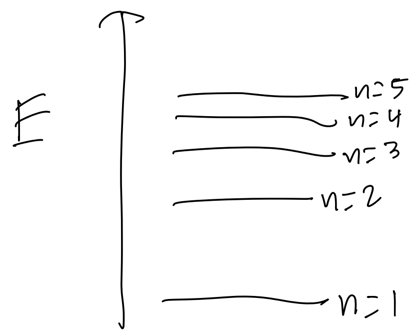
3 discrete "lines" ~~mean~~ means 3 different types (wavelengths) of photons → 3 diff energies

H atom giving off light — imagine there are energy levels at which the electron in H atom can "live"

- when electron moves btw energy

levels either energy given off
or energy is taken in

When e⁻ goes from higher energy level to lower one
it gives off light



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

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

Wave particle duality part 2

- particles with mass can show wave-like behavior

$$\lambda_{particle} = \frac{h}{m\,V}$$

m: mass
V: velocity

bowling ball - 4 kg moving at 30 kph

30 kph → 10 m/sec

$$\lambda_{bowling\ ball} = \frac{6.626 \times 10^{-34}\ J\,sec}{(4\ kg)(10\ \frac{m}{sec})} = 1.66 \times 10^{-35}\ m$$

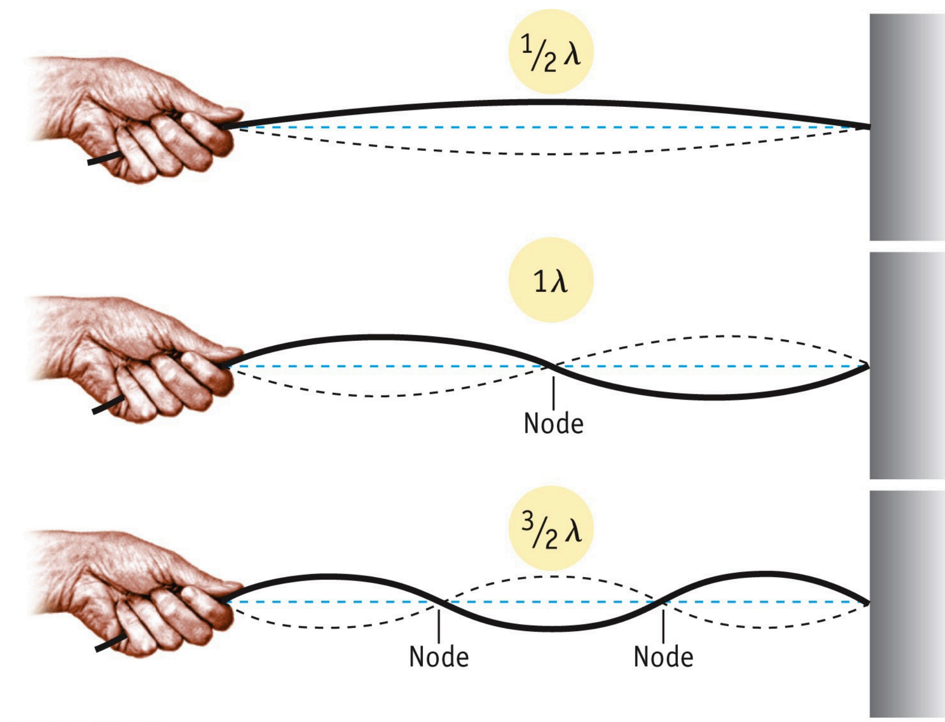
$J = \frac{kg\,m^2}{sec^2}$

$$\frac{\frac{kg\,m^2}{sec^2} \times sec}{kg\ \frac{m}{sec}}$$

but mass of electron is 9.1×10^{-31} kg
so it will have appreciable λ

Quantum mechanics - how we describe electrons
- mostly math

Concept: standing wave (tie rope to pole + shake it)
only certain wavelengths possible
so only certain energies possible



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

describe electrons w/ ~~a~~ 3-D standing wave

Ψ = wavefunction → equation that describes shape of 3-D standing wave

$\Psi = 42x^4 + 13y^2 + 1.5z^{3/2}$

there is a value of Ψ for each x, y, z coordinate trio
"amplitude"

ψ^2 is the probability of an electron being at particular place in 3-D space

Electrons are not anywhere in particular - "location" of electron is described by probabilities that come from ψ^2

Can describe wavefunctions using shorthand of "quantum numbers" (3 or 4)

n = principal quantum # "shells"

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

describes "extent" or "size" of probability distribution

describes energy

ℓ = orbital angular momentum # "subshell"

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

describes shape of wavefunction

$\ell = 0 \rightarrow s$

$\ell = 1 \rightarrow p$

$\ell = 2 \rightarrow d$

$\ell = 3 \rightarrow f$

m_ℓ = magnetic #

$m_\ell = -\ell \ldots 0 \ldots +\ell$

describes orientation in space of wavefunction

If $n=1$ ℓ must $=0$ and $m_\ell=0$

only 1 ψ exists for $n=1$ $\longrightarrow$ $n=1$ $\ell=0$ $m_\ell=0$

If $n=2$ ℓ could be 0 or 1

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

n	ℓ	m_ℓ
2	0	0
2	1	−1
2	1	0
2	1	+1

4 different ψ when $n=2$

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

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

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 ψ when $n=3$

orbital = wavefunction

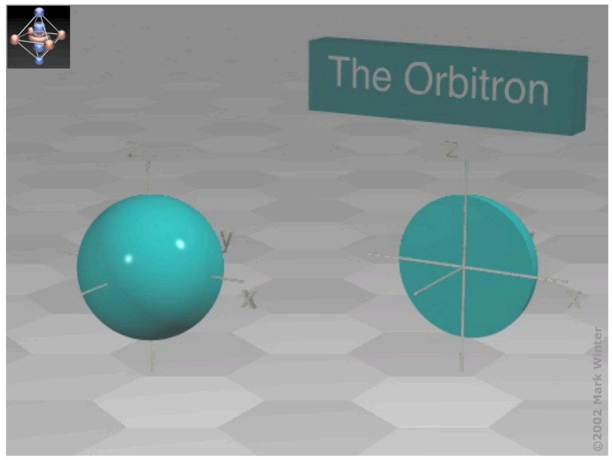
1s orbital

n=1

l=0

n=1
l=0
m_l=0

Atomic orbitals: 1s

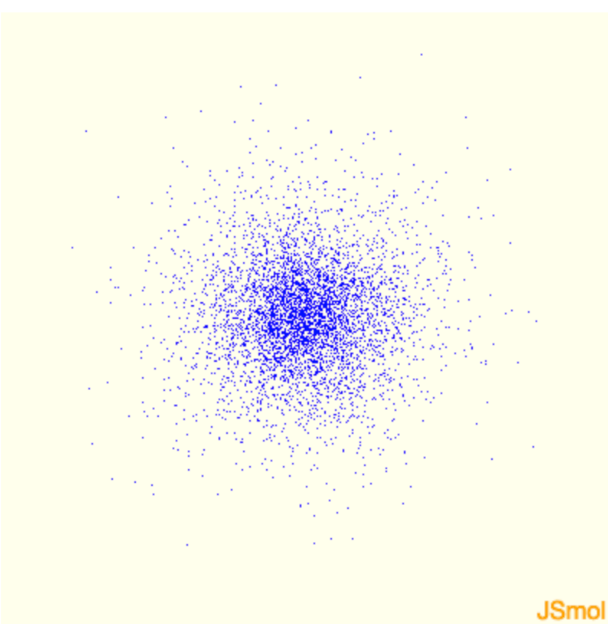


The shape of the 1s orbital.

shape = spherical

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

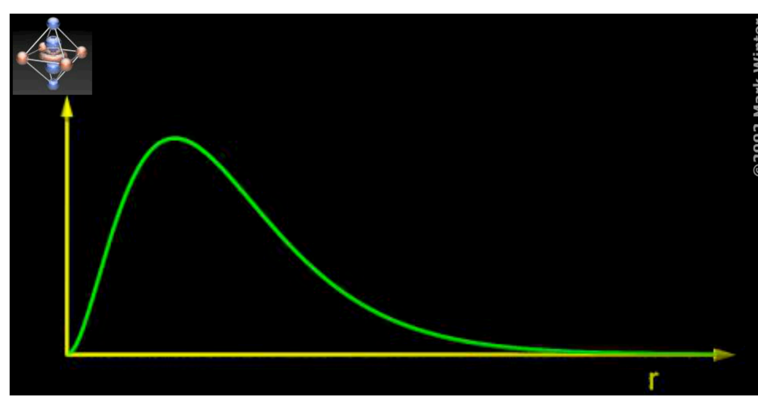
Atomic orbitals: 1s electron density



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

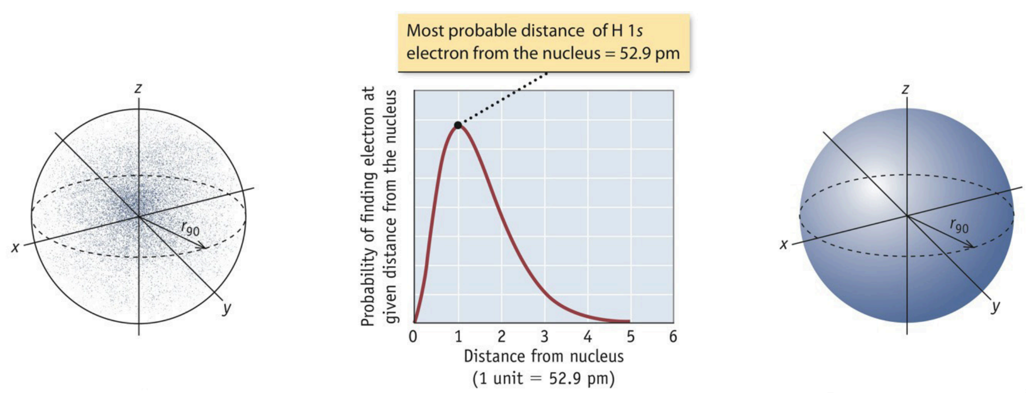
probability of finding
e⁻ at particular distance
from nucleus

Atomic orbitals: 1s radial distribution function



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

s-Orbitals

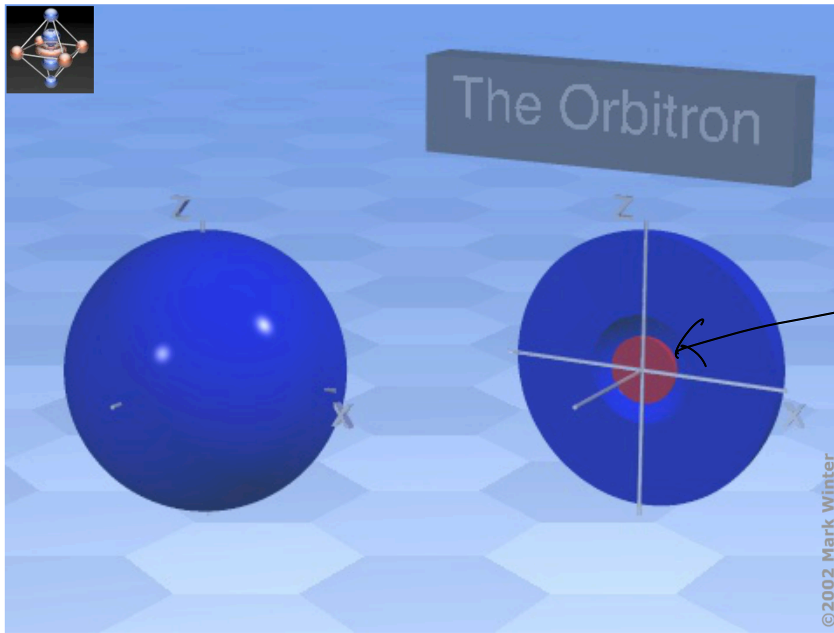


- $l = 0$, $m_l = 0$
- $2l+1 = 1$
- one *s*-orbital that extends in a radial manner from the nucleus forming a spherical shape.

2s orbital

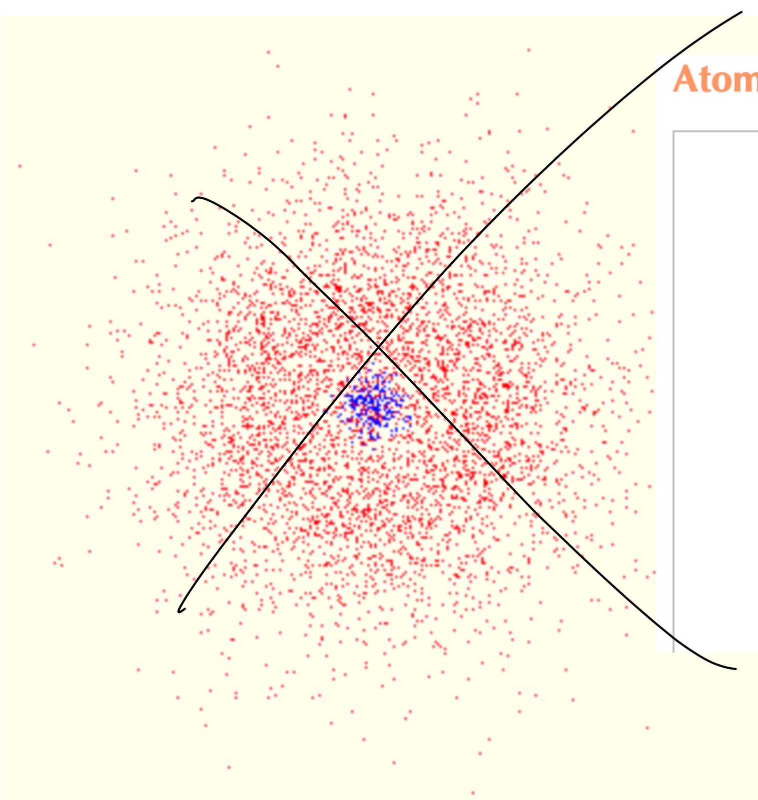
$n=2$
$\ell=0$
$m_\ell=0$

Atomic orbitals: 2*s*

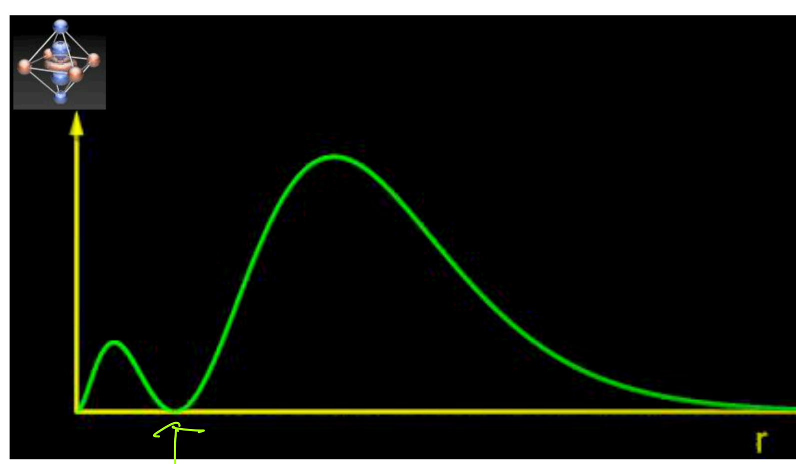


The shape of the 2s orbital. *The blue zone is where the wave function has negative values while the red zone is where values are positive.*

nodal surface or a spherical node separating red yolk from blue "white"



Atomic orbitals: 2*s* radial distribution function

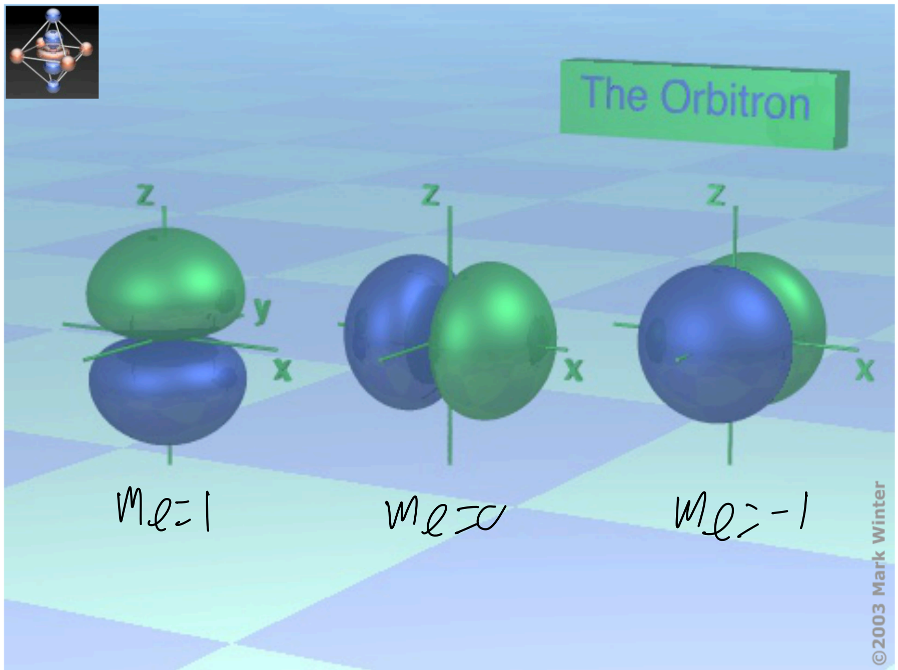


at this distance probab of finding e- = 0

this is a node (zero electron density)

2p orbital

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



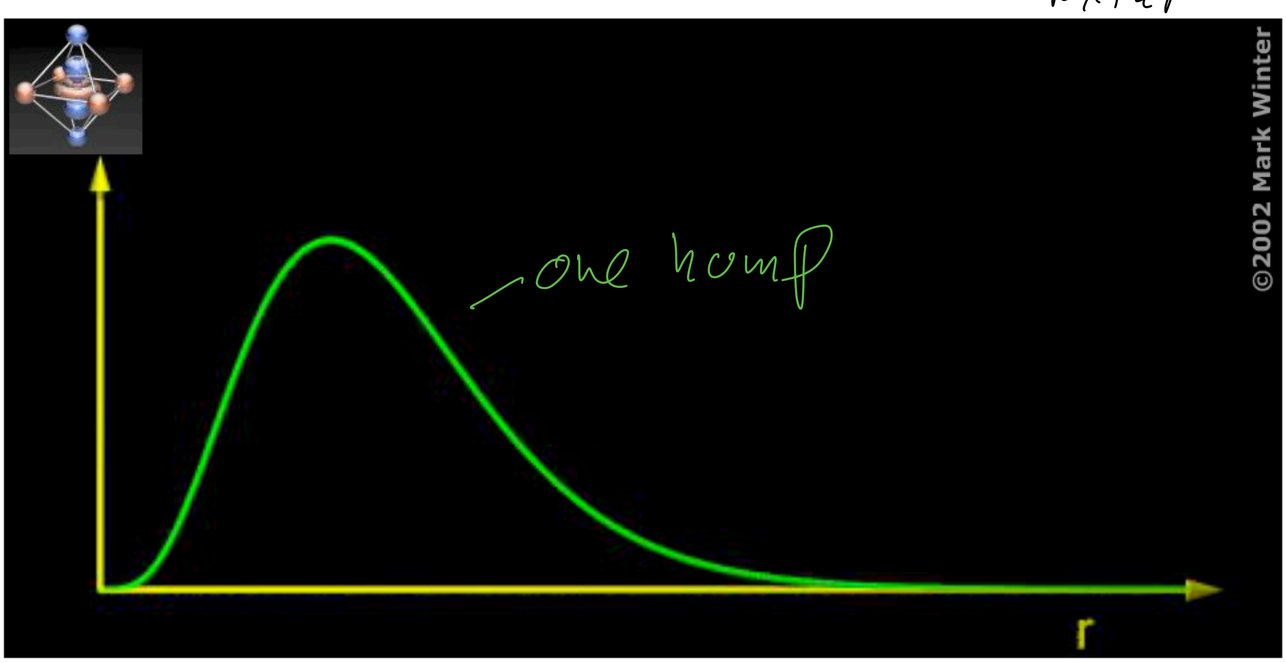
no nodal surface or spherical node

yes nodal plane between 2 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.*

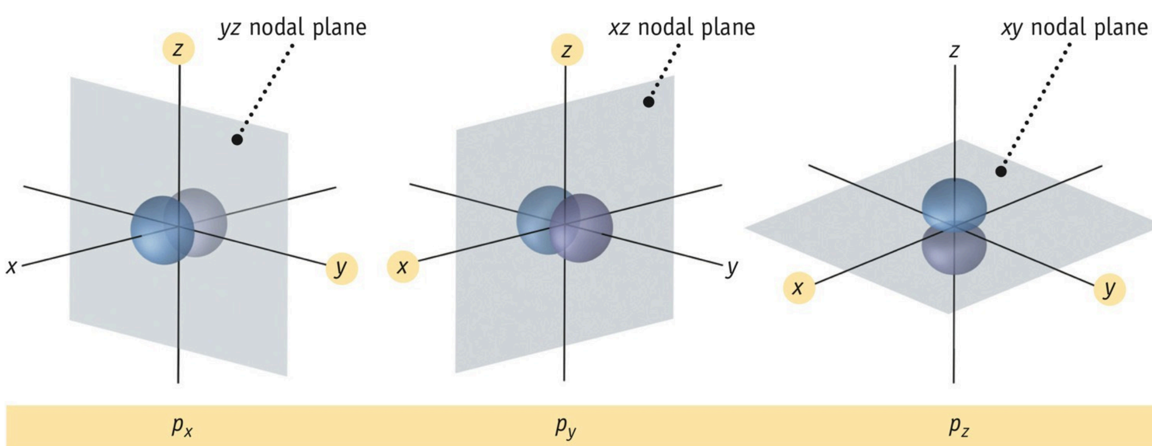
Atomic orbitals: 2*p* radial distribution function

— for all 3 of the orbitals mashed together



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

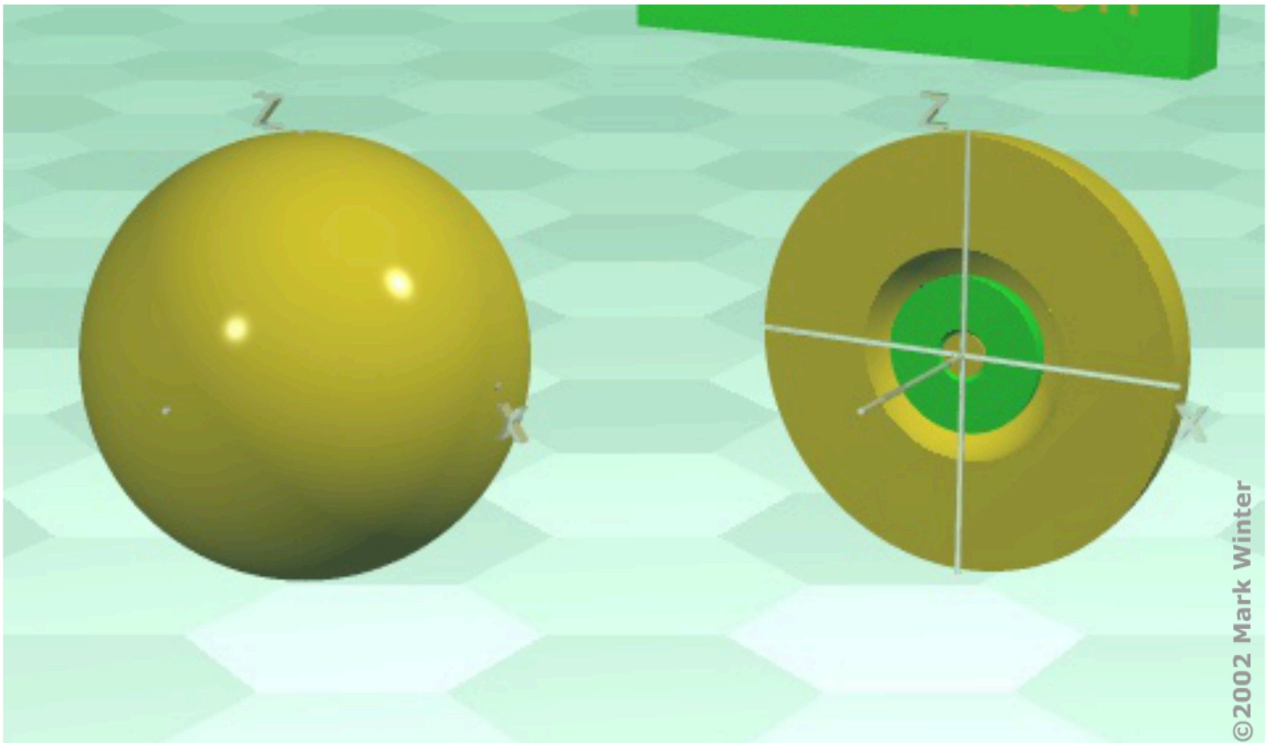
p-Orbitals



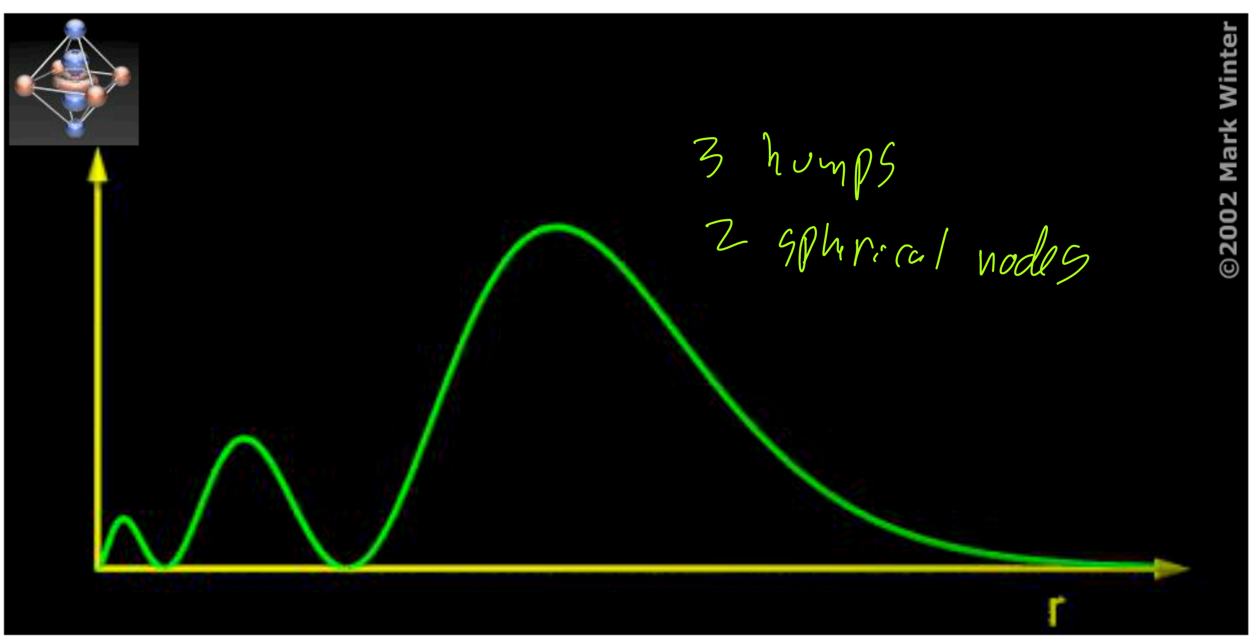
The three degenerate *p*-orbitals spread out on the x, y & z axis, 90° apart in space.

3s orbital

n=3
l=0
m_l=0



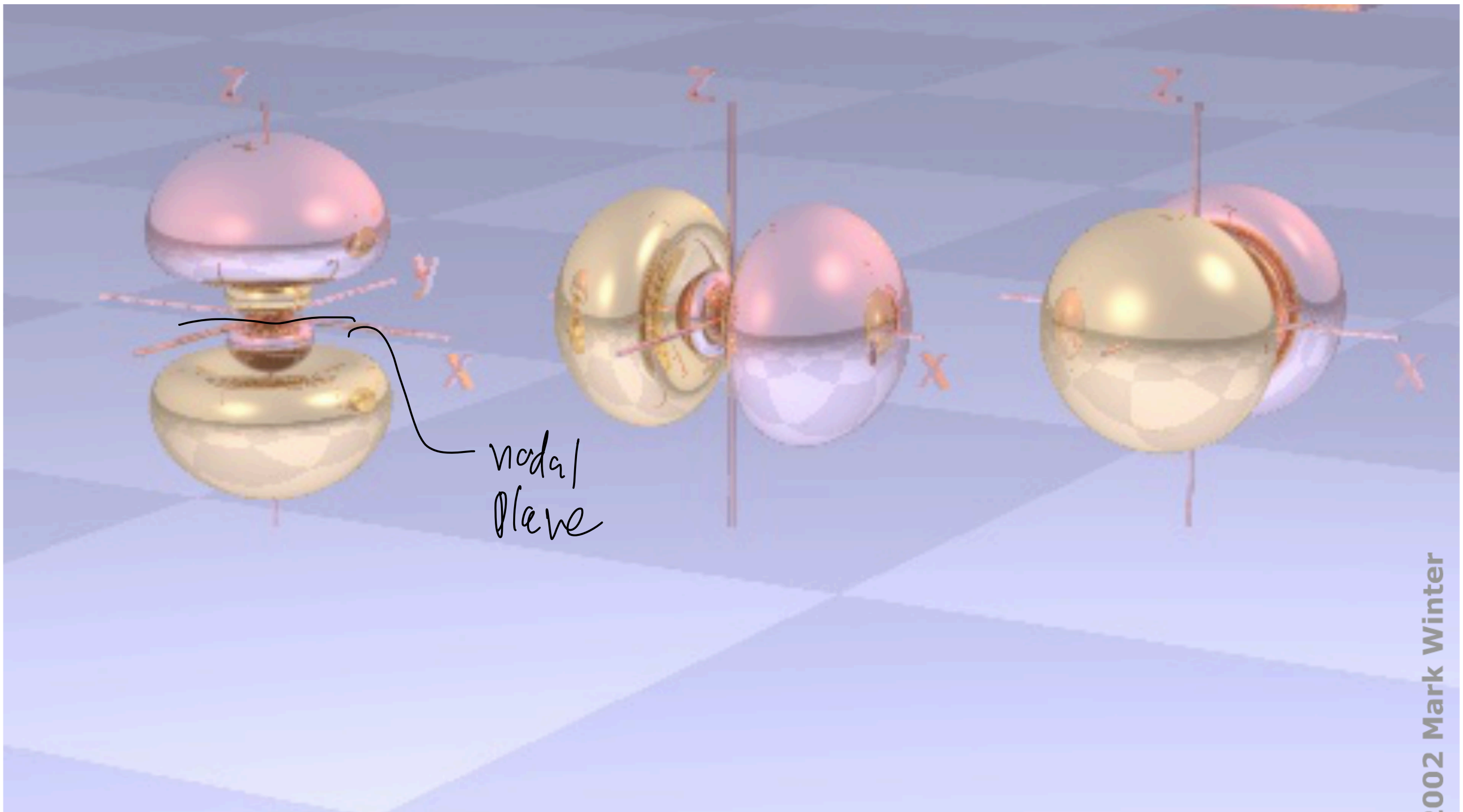
Atomic orbitals: 3*s* radial distribution function

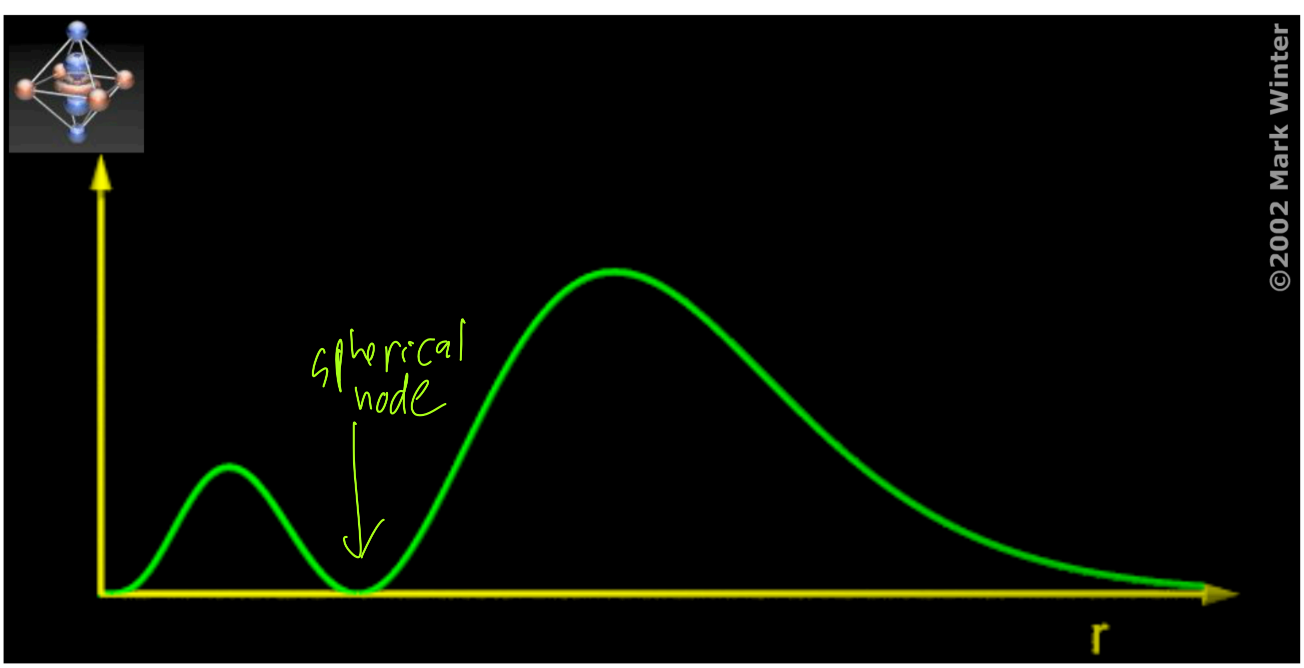


Schematic plot of the 3s radial distribution function $4\pi r^2\psi_{3s}^2$. *Blue represents regions within which the wave function is negative and red represents regions where the wave function is positive.*

3p orbital

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

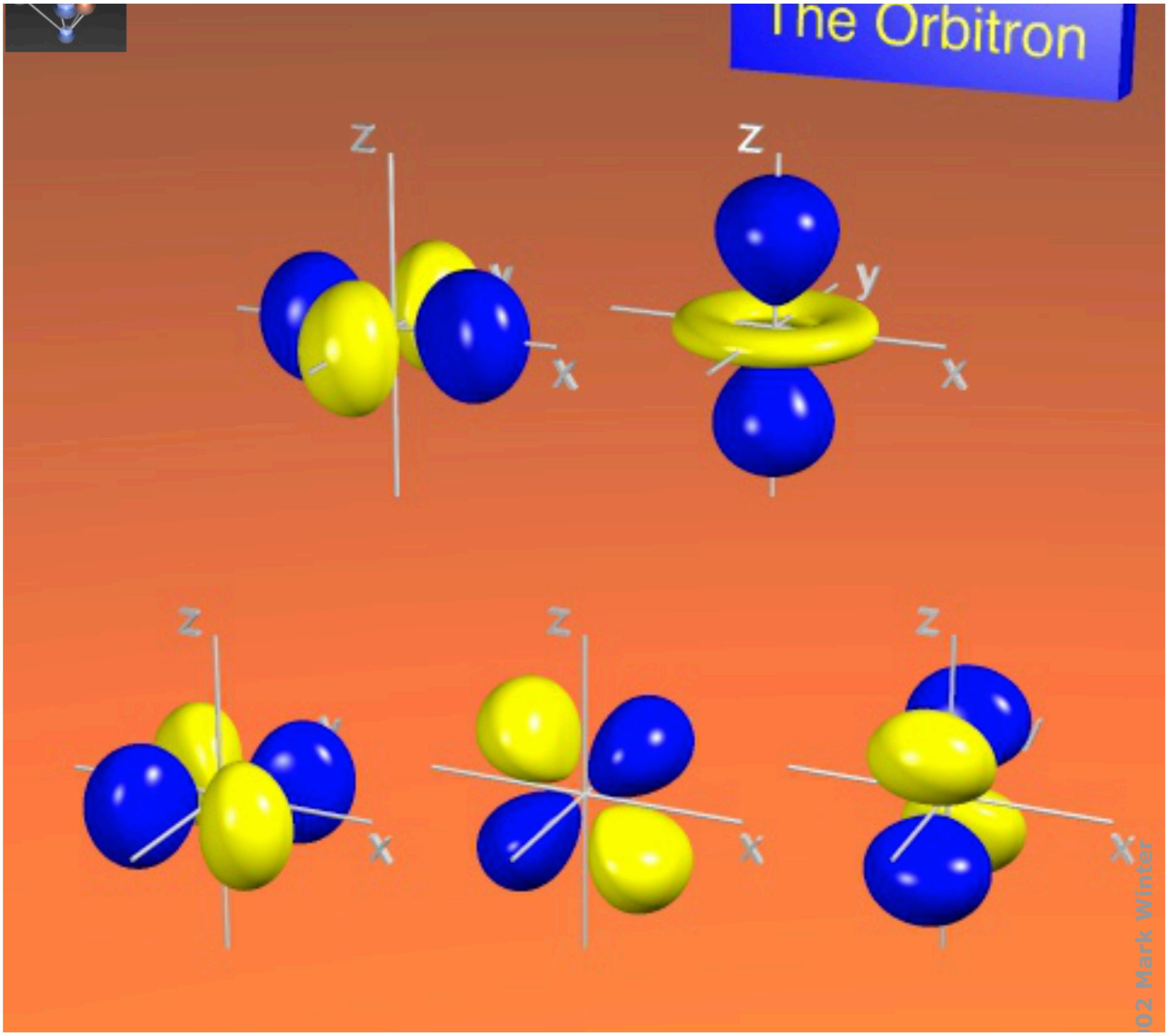


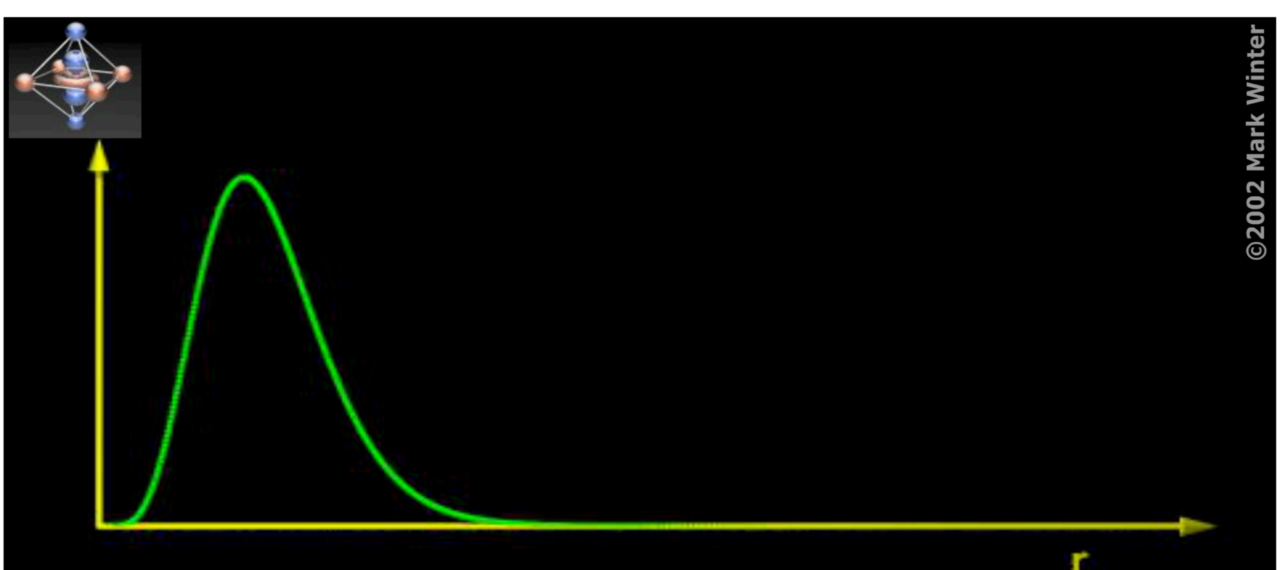


***Schematic plot of the 3p radial distribution function $r^2R_{3p}^2$** (R_{3p} = radial wave function).*

3d orbital

$n=3$
$l=2$
$m_l=-2,-1,0,1,2$



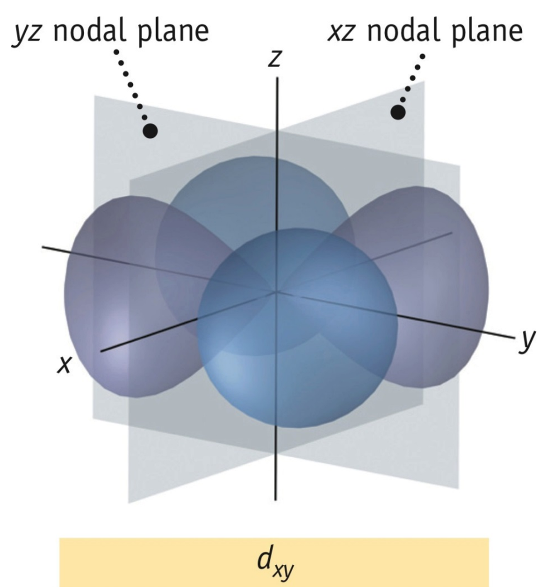


d-Orbitals

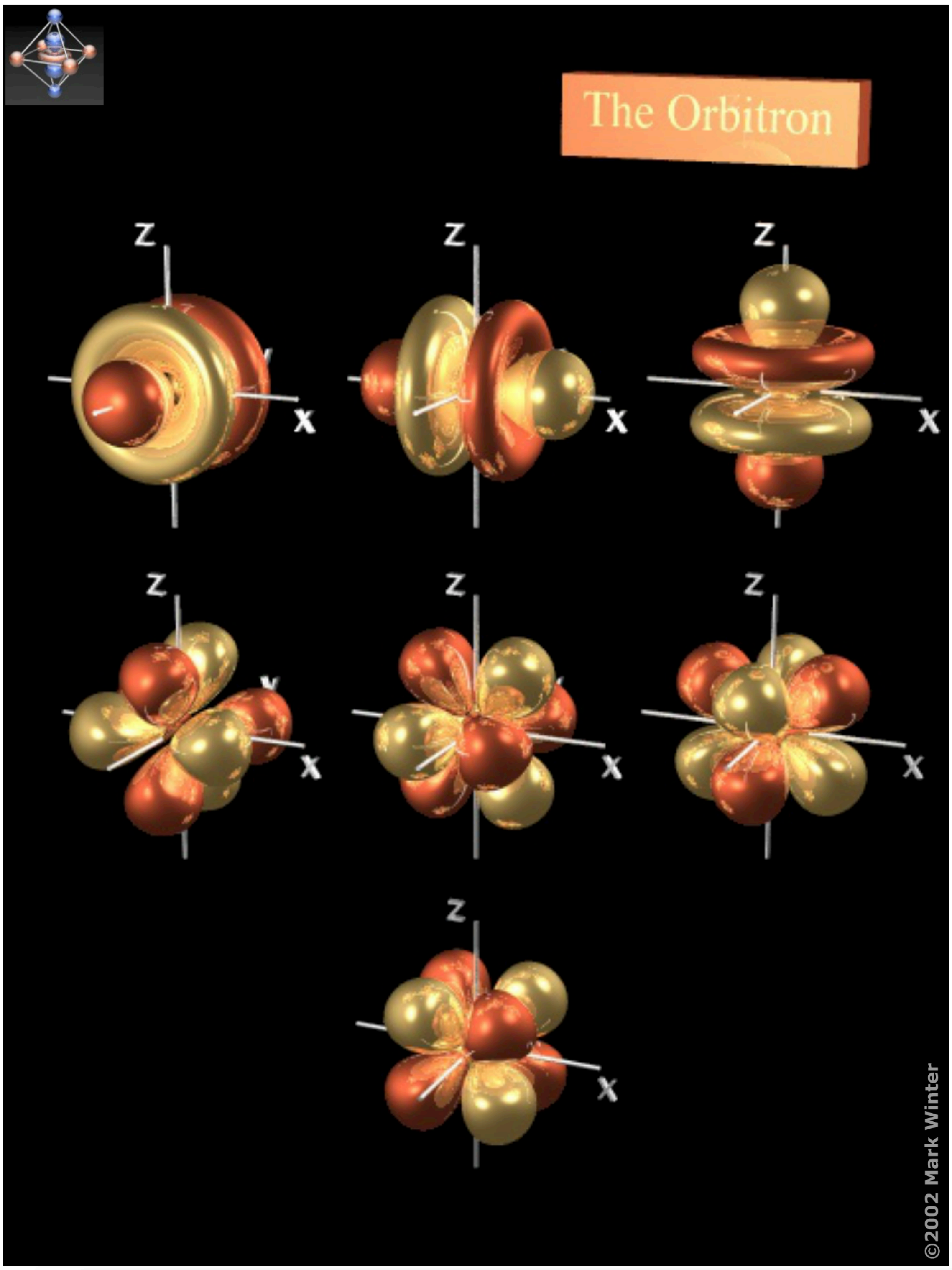
s-orbitals have no nodal planes (l = 0)

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

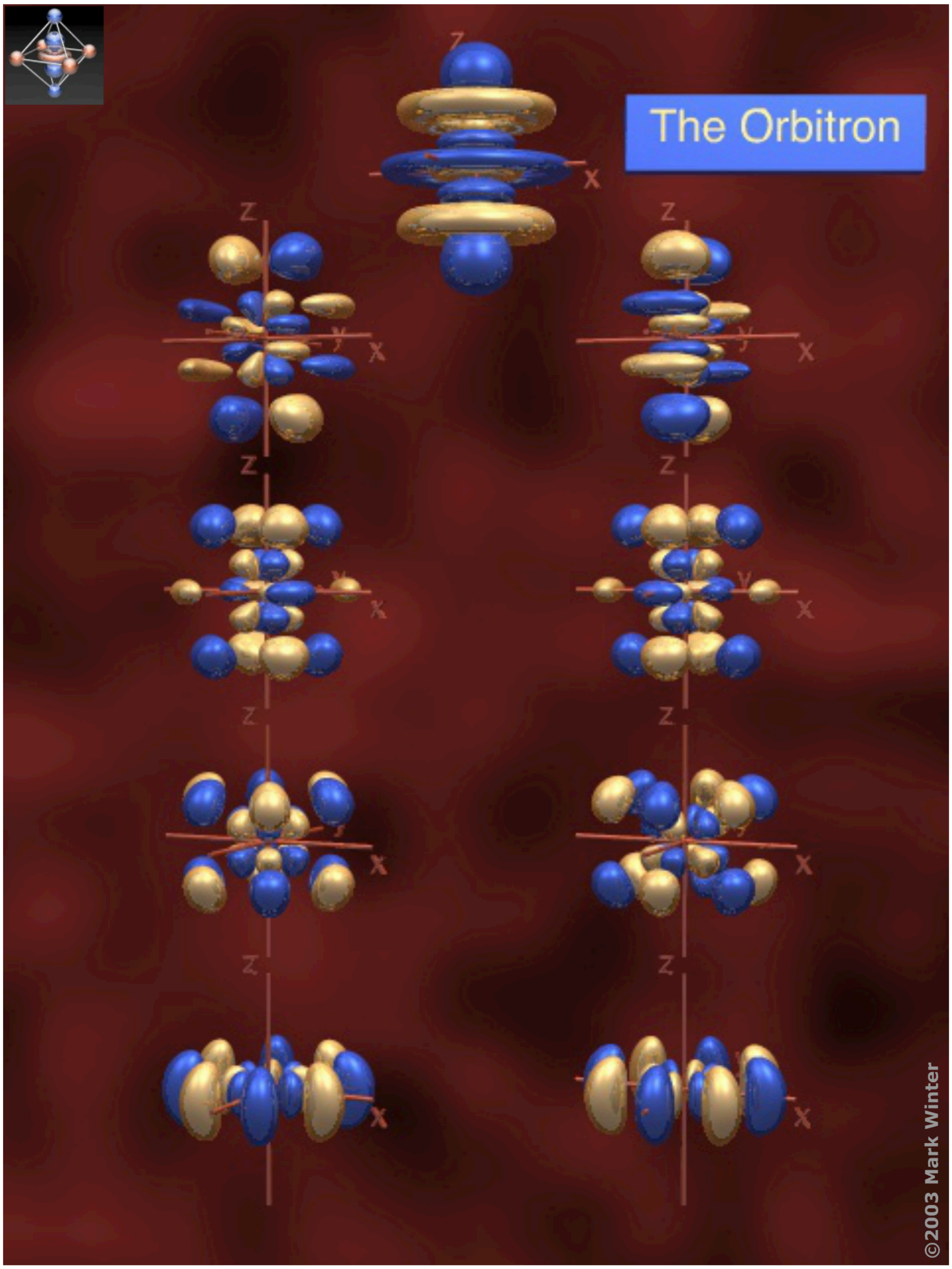
d-orbitals therefore have two nodal planes (l = 2)



Crazy orbital (4f)



Bananas orbital (6g)



There is a 4^{th} quantum #

m_s electron spin #

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

An electron must have a unique set of 4 quantum numbers

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

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

If $\sum m_s$ in atom $= 0$ diamagnetic — not attracted to mag. field

$\sum m_s \neq 0$ Paramagnetic — attracted to mag field

Avg 91

median 95

90+ — 37

80s — 9

below 80 — 7