PHY127 FS2023

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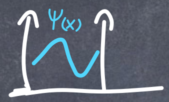
Lecture 7
April 21st, 2023

Today: quantum levels of hydrogen atom.
spherical potential in 3-D.

Review from recent lectures:

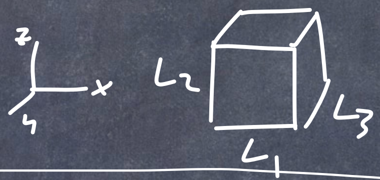
Particle trapped in $\boxed{\text{1-D box}}$ has a wave function like a standing wave



$$E_n = \frac{n^2 h^2}{8 m L^2}, \quad n = 1, 2, 3, \ldots$$

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \text{for } n = 1, 2, 3, \ldots$$

Particle trapped in $\boxed{\text{3-D box}}$:



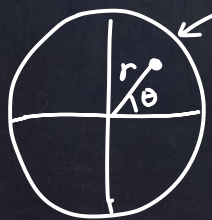
$$E_{n_1, n_2, n_3} = \frac{\hbar^2 \pi^2}{2m}\left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}\right)$$

for $n_1 = 1, 2, \ldots$
$n_2 = 1, 2, \ldots$
$n_3 = 1, 2, \ldots$

$$\boxed{\psi(x, y, z) = A(\sin k_1 x)(\sin k_2 y)(\sin k_3 z)}$$

$$k_1 = \frac{n_1 \pi}{L_1}, \quad k_2 = \frac{n_2 \pi}{L_2}, \quad k_3 = \frac{n_3 \pi}{L_3}$$

Standing waves on a $\boxed{\text{2-D drum}}$

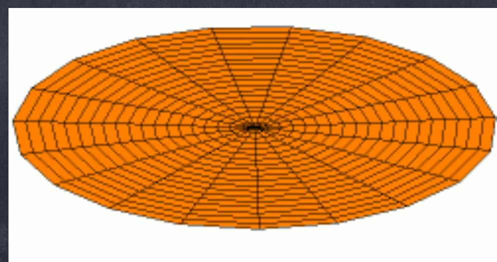


border is fixed.

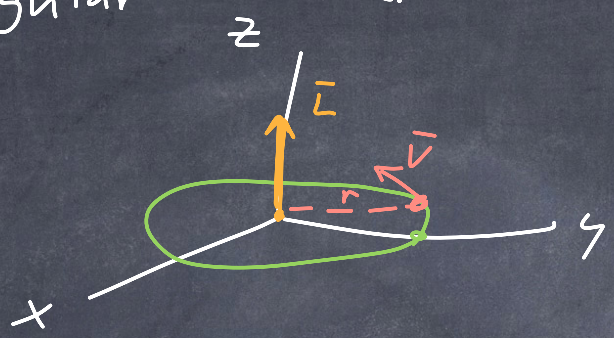
solutions to 2D circle: Bessel functions

$$\psi(r, \theta) = \psi(r)\, \psi(\theta)$$

2 "quantum" numbers
$m = 0, 1, 2, \ldots$
$n = 0, 1, 2, \ldots$



Angular momentum review (see script 1)



A particle moving in a circle in the x-y plane with a velocity $\bar{v}$. Its speed $|\bar{v}|$ is constant.

Use the right-hand rule to get the angular momentum vector.

$$\bar{L} = \bar{r} \times \bar{p} = \bar{r} \times (m\bar{v})$$

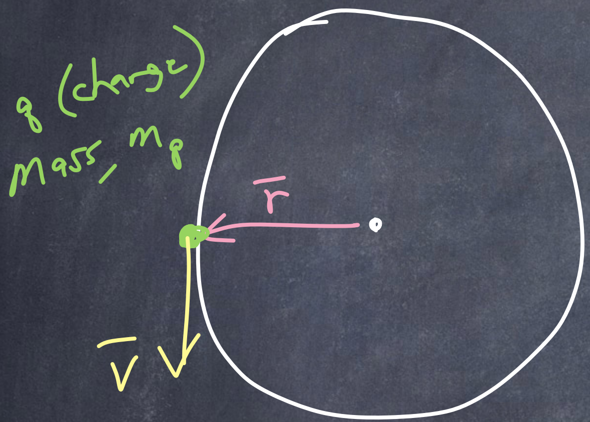
(In our example, $\bar{L}$ points in z-direction)

If the particle has electric charge, we know that a moving electric charge generates a magnetic field.* Electric charge moving in a circle generates a magnetic moment. The magnetic moment vector $\bar{\mu}$ points in the same direction as the angular momentum $\bar{L}$ (if charge is positive)

The magnetic moment μ is the product of the area (A) of the circle and the electric current (I)

$$\mu = IA$$

$$I = \frac{\text{charge}}{\text{time}} = \frac{q}{t}$$



q : charge
m_q : mass
V: velocity
r : radius

The angular momentum is $\boxed{L = m_q V r}$ (1)

$\bar{a} \times \bar{b} = |a||b| \sin\theta$
$\theta = 90°$

The magnetic moment is $\mu = IA = I(\pi r^2)$

The current is $I = \frac{q}{T}$ where T is the time it takes the particle to move in a circle.

$$\text{velocity} = \frac{\text{distance}}{\text{time}} = \frac{2\pi r}{T} \quad \text{so} \quad T = \frac{2\pi r}{v}$$

so the current is $I = \frac{q}{t} = \frac{qv}{2\pi r}$

Then the magnetic moment is

$$\mu = IA = \frac{qv}{2\pi r} \cdot \pi r^2 = \frac{1}{2} q v r$$

Using ① to get $\boxed{\bar{\mu} = \frac{q}{2m_q} \bar{L}}$ ②

magnetic moment of a charged particle depends on its angular momentum, charge, & its mass.

It is conventional to write ② as

$$\bar{\mu} = \frac{q\hbar}{2m_q}\left(\frac{\bar{L}}{\hbar}\right)$$

For an electron, $m_q = m_e$ and $q = -e$

so $\bar{\mu} = \frac{-e\hbar}{2m_e} \frac{\bar{L}}{\hbar}$

we define a constant $\mu_B = \frac{e\hbar}{2m_e} = 9.27\text{E-}24 \ A \cdot m^2$

μ_B : Bohr magneton

Then the magnetic moment of an atom is

$$\boxed{\bar{\mu} = -\mu_B \frac{\bar{L}}{\hbar}} \quad ⓐ$$

(Negative because electrons are negatively charged)

Last time :

Hydrogen atom

$$\boxed{E_0 = \frac{k^2 e^4 m}{2\hbar^2} \approx 13.6\,eV}$$

ground state energy constant

$$\boxed{E_n = -\frac{Z^2}{n^2} E_0}$$

These are the allowed energy levels of the hydrogen atom $(Z=1)$

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

Negative because electrons are bound to atom

so lowest energy state is $n=1 \Rightarrow -13.6\,eV$

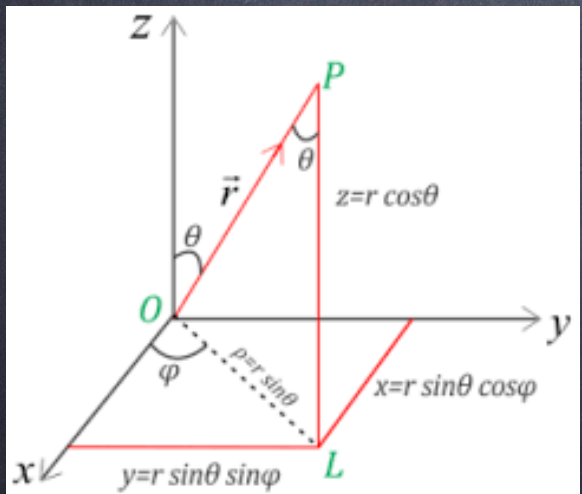
We consider an electron stuck in an atom.
The atom is 3-D. The potential $U = -\frac{kZe^2}{r}$
(This is a spherical potential)

Schroedinger wave equation in 3-D

$$\boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+U\Psi=E\Psi} \quad (1)$$

$$\Psi=\Psi(x,y,z)=\Psi(x)\,\Psi(y)\,\Psi(z)$$

But U is a spherical potential. we need to write (1) in spherical coordinates. (r,θ,ϕ)



$$x=r\sin\theta\cos\phi$$
$$y=r\sin\theta\sin\phi$$
$$z=r\cos\theta$$

In spherical coordinates, the Schroedinger wave equation becomes:

$$\boxed{-\frac{\hbar^2}{2m}\left[\frac{\partial}{\partial r}r^2\frac{\partial\Psi}{\partial r}-\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Psi}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2\Psi}{\partial\phi^2}\right]+U\Psi=E\Psi}$$

Looks complicated, but like the particle in a 3D box, we get solutions that factorize

$$\Psi(r,\theta,\phi) = \Psi_r(r)\,\Psi_\theta(\theta)\,\Psi_\phi(\phi)$$

As in the case of the 3-D box, we will get 3 quantum numbers, but they ~~ar~~ are interdependent.

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

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

$$m = -\ell, -\ell+1, \ldots, +\ell$$

m has $2\ell+1$ options

So n is an integer, and ℓ + m depend on it.

If $n=1$, then the allowed quantum numbers are $n=1, l=0, m=0$

If $n=2$, $\begin{cases} l=0, & m=0 \\ l=1, & m=-1,0,+1 \end{cases}$

If $n=3$, $\begin{cases} l=0, & m=0 \\ l=1, & m=-1,0, \text{ or } 1 \\ l=2, & m=-2,-1,0,+1,2 \end{cases}$

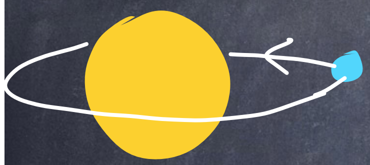
n: principle quantum number, has to do with $\psi_n(r)$, wave function that describes the amplitude as a function of distance in r of the electron moving in a circle

$$E_n = \frac{-Z^2 E_0}{n^2} \qquad n=1,2,3,\ldots$$

The quantum numbers ℓ + m have to do with angular momentum of the electron, and the angular dependence of the probability of finding the electron.

ℓ: orbital quantum number

analogy:

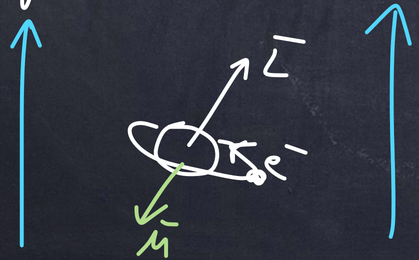


The orbital angular momentum of the electron is $L = \sqrt{\ell(\ell+1)}\,\hbar$

From ⓐ, we see that $\mu = -\mu_B \dfrac{\bar{L}}{\hbar}$

so $\mu = -\sqrt{\ell(\ell+1)}\,\mu_B$ is also quantized.

If we put the atom in a magnetic field,



$\bar{B}$ in z-direction

The L_z component of ~~the~~ $\bar{L}$ points along the magnetic field direction

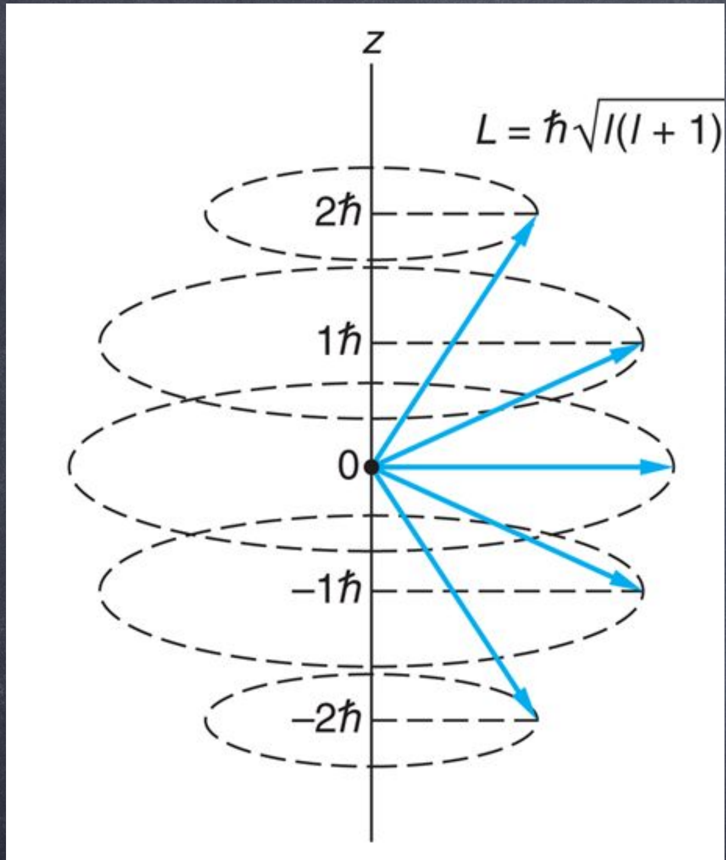
L_z can also only take on integer values.

$$L_z = m\hbar$$

sketch is for the case of $\ell = 2$:

$$L = \hbar\sqrt{\ell(\ell+1)} = \hbar\sqrt{6}$$

$\bar{B}$



$L_z = 2\hbar$

$L_z = 1\hbar$

$L_z = 0$

$L_z = -1\hbar$

$L_z = -2\hbar$

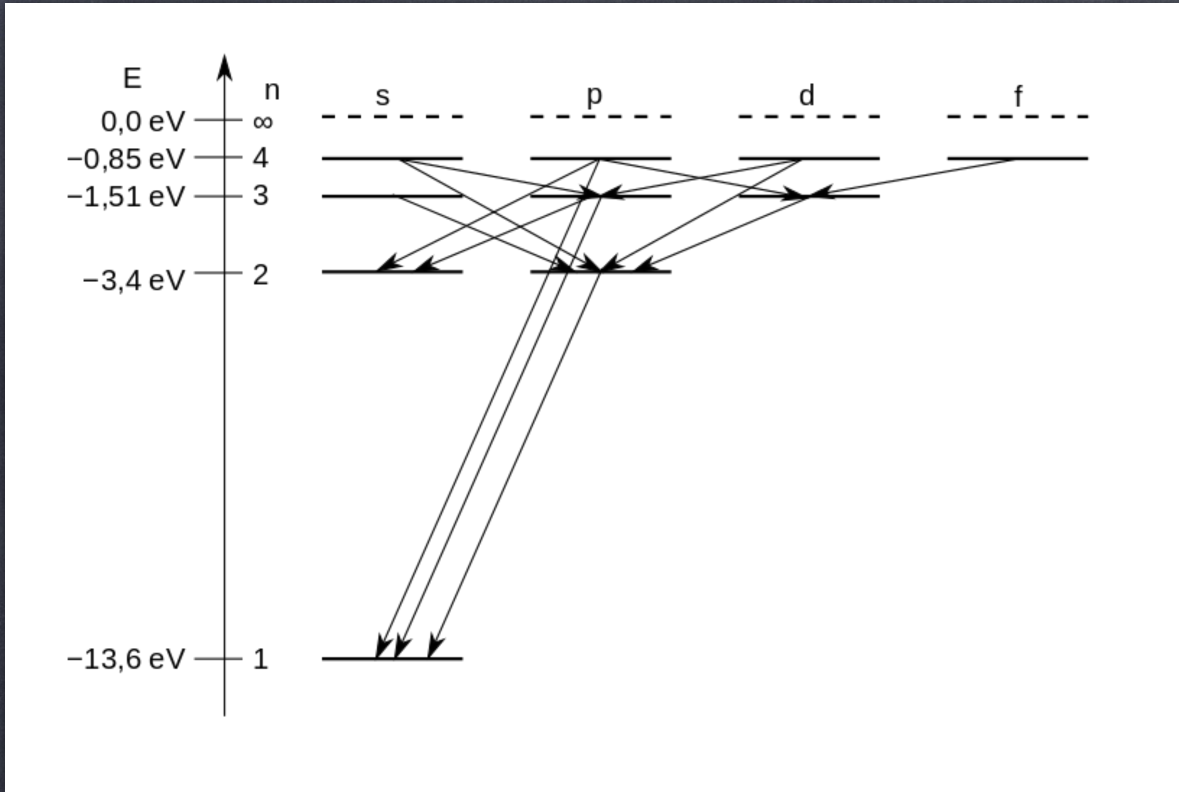
m : is known as the magnetic quantum number

$$\mu_z = \frac{\mu_B L_z}{\hbar} = -m\mu_B$$

$$E_n = \frac{-Z^2 E_0}{n^2} \qquad n = 1, 2, 3, \ldots$$

The fact that the energy doesn't depend on l is only true for the hydrogen atom. For more complicated atoms with multiple electrons, E can depend on l.

The energy doesn't depend on m unless the atom is in a magnetic field.



$\ell = 0 \Rightarrow$ s-level

$\ell = 1 \Rightarrow$ p-level

$\ell = 2 \rightarrow$ d level

$\ell = 3 \rightarrow$ f level

Transitions of the electron obey selection rules:

$\Delta m = 0, \pm 1$

$\Delta \ell = \pm 1$

when we absorb or emit a photon, it has an angular momentum of $\pm \hbar$.

These photons have an energy released that is $\epsilon = h\nu = \frac{hc}{\lambda}$

The energy transitions $\epsilon_f - \epsilon_i = h\nu = \frac{hc}{\lambda}$

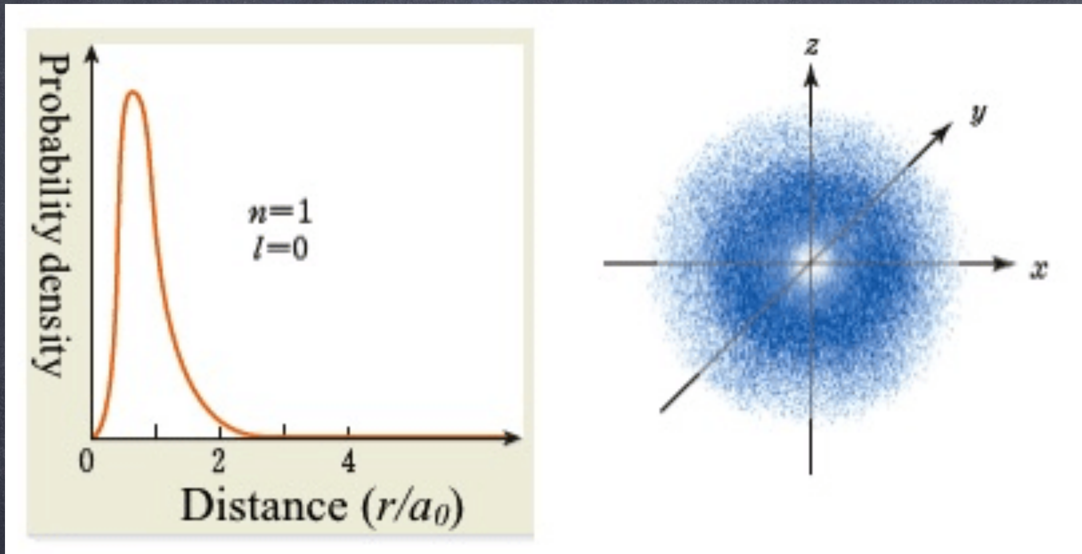
Where is the electron in our 3-D atom?
(spherical electric potential)

Probability $= \Psi^2(r)$
of the electron to be
at a distance r

$$\Psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

$\begin{pmatrix} n=1 \\ \ell=0 \\ m=0 \end{pmatrix}$

$\Psi^2(r)$

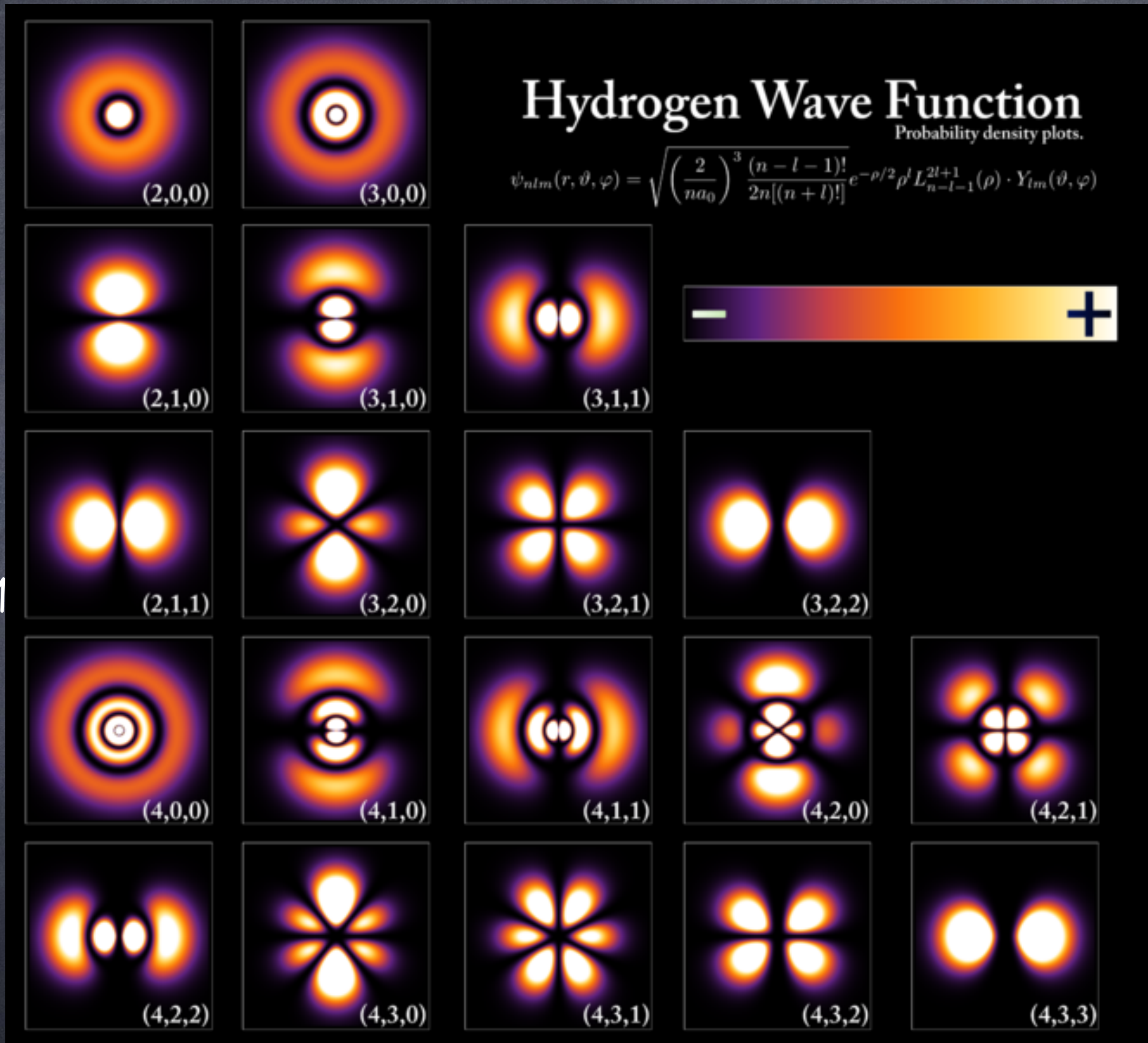


The probability of
finding the electron
depends only on r
(for $n=1, \ell=0, m=0$)

Here, we see the quantized electron standing waves in a hydrogen atom that come from the 3-D Coulomb potential and have 3 quantum numbers: n, ℓ, m

$\psi^2(r,\theta,\phi)$

Depends on $n, \ell, + m$ and probability depends on r, θ and ϕ



(n,ℓ,m)

Probability of finding electrons is given by brightness

Experiment : Chladni plate
2D

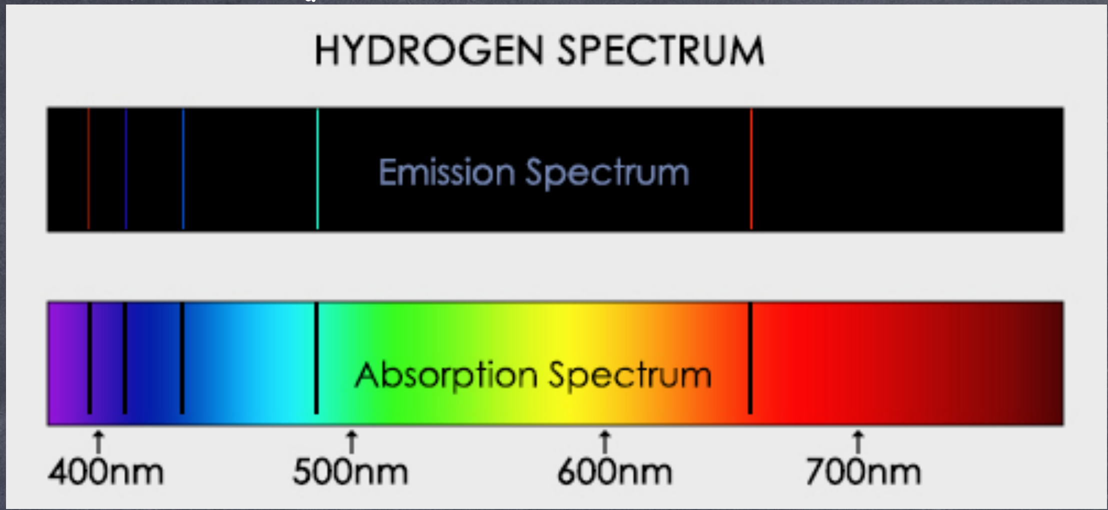
interesting frequencies

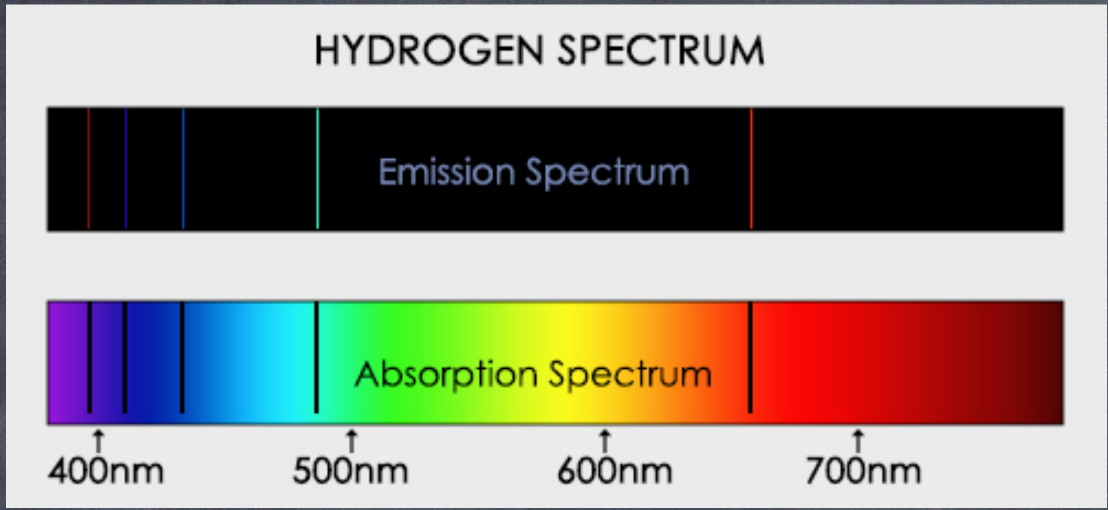
150.0 Hz
206.0
313.6
482.3
815.0
979.9
3428
4978

rich pattern of standing waves
dependent on frequency

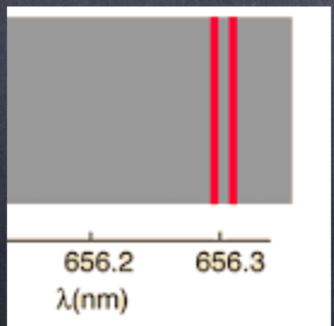
These are 2-D
standing waves
described by
~~the~~ two
"quantum number"

Balmer series



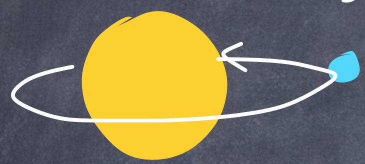

HYDROGEN SPECTRUM
Emission Spectrum
Absorption Spectrum
400nm
500nm
600nm
700nm

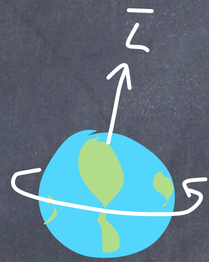
2 lines here


656.2
656.3
λ(nm)

The electron has something called spin.
Spin is intrinsic angular momentum.

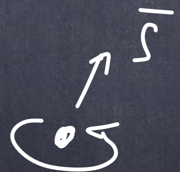
The earth has orbital angular momentum.





The earth also has spin.

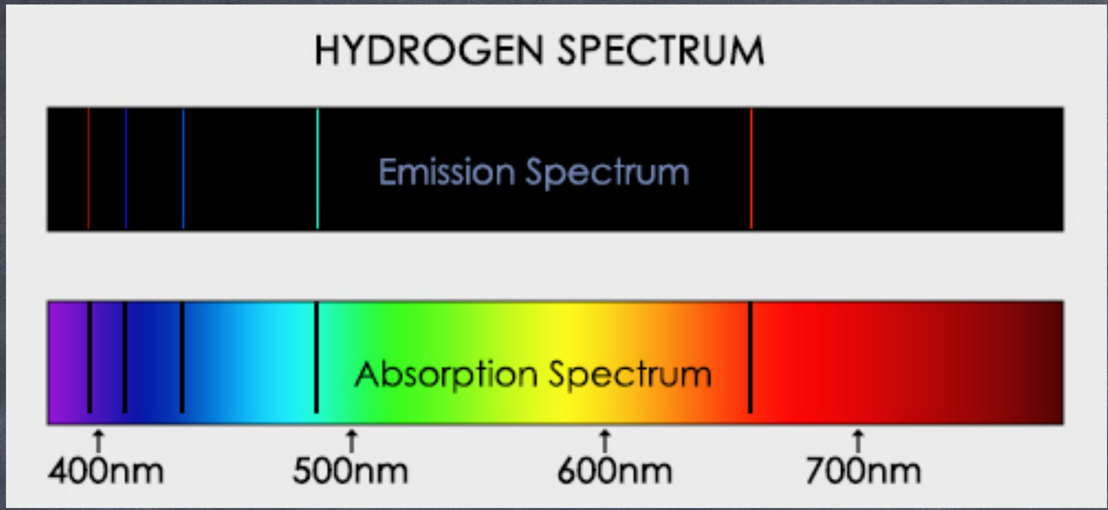
Similarly, the electron has spin.



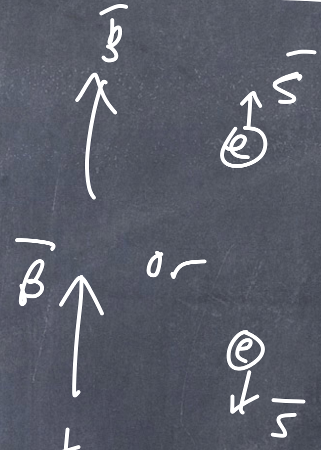
$S = \frac{1}{2}\hbar$ has values $-\frac{1}{2}\hbar$ or $+\frac{1}{2}\hbar$

~~The~~ In addition to n, ℓ, m, the atom has an additional quantum number to describe the electron spin $m_s = \frac{1}{2}$ or $-\frac{1}{2}$

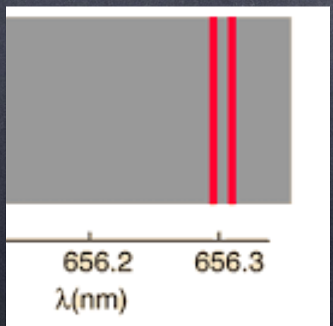
Fine structure is 4 th quantum number, m_s



from spin of electron when atom is in a magnetic field.



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



$2p$ line is actually split into two energy levels

Fine ~~str~~ structure