PHYS-3301

Lecture 18

Oct. 24, 2024

Chapter. 7
QM in 3-dims & Hydrogen Atom

Outline:

- The Schrödinger Eq. in 3-Dimensions
- The 3D Infinite Well
- Energy Quantization & Spectral Lines in Hydrogen
- The Schrödinger Eq. for a Central Force
- Angular Behavior in a Central Force
- The Hydrogen Atom
- Radial Probability
- Hydrogen-like Atoms

Now, we can discuss where hydrogen's e might be found

Traditional naming scheme

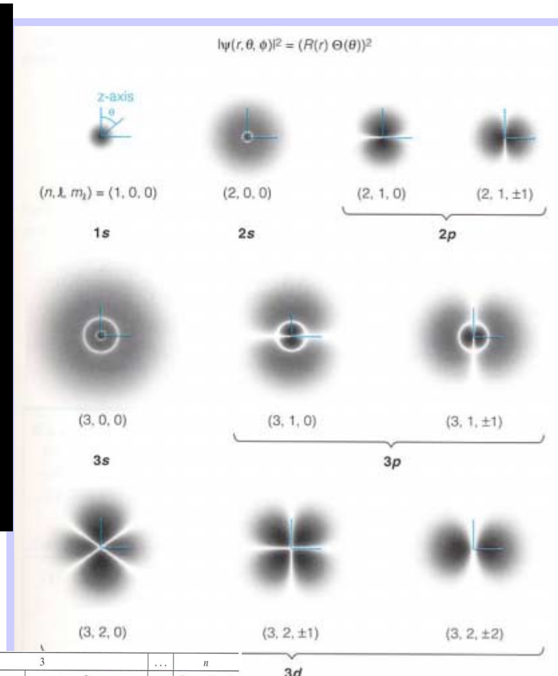
Spectroscopic notation

Letter	s	p	d	f	g	h
Value of ℓ	0	1	2	3	4	5

s: sharp, p: principle, d: diffuse, f: fundamental…
3d state: n=3 & l = 2
2p state: n=2 & l = 1

Electron Prob. Densities in the Hydrogen atom, through n = 3

State are labeled using spectroscopic notation; n, l



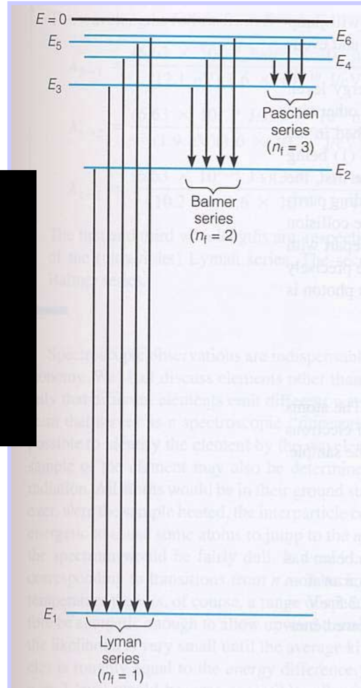
n	1	2				3									…	n
ℓ	0	0	1			0	1			2					…	$0, \ldots, n-1$
m_ℓ	0	0	−1	0	+1	0	−1	0	+1	−2	−1	0	+1	+2	…	$-\ell, \ldots, +\ell$

2d state is possible? -- No!! Because, here, n=2, d =2; Remember n > d

Spectral Lines

Hydrogen' energies & spectral lines;

A photon is emitted when the electron jumps downward.



$$E = -\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n^2} \qquad (n = 1, 2, 3, \ldots)$$

$$|L| = \sqrt{\ell(\ell+1)}\,\hbar \qquad (\ell = 0, 1, 2, \ldots, n-1)$$

$$L_z = m_\ell \hbar \qquad (m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell)$$

$$E = E_i - E_f$$

$$= \left[-\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n_i^2}\right] - \left[-\frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\frac{1}{n_f^2}\right]$$

$$= \frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

For a photon, $E = hf = hc/\lambda$. Therefore,

$$\frac{hc}{\lambda} = \frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

or

$$\frac{1}{\lambda} = \frac{me^4}{2(4\pi\epsilon_0)^2\hbar^2 hc}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

$$= 1.097 \times 10^7\ \text{m}^{-1}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

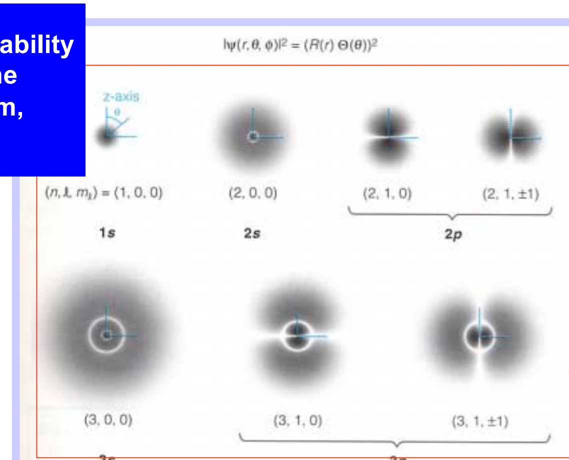
Chapter. 8
Spin & Atomic Physics

Outline:

- Evidence of Angular Momentum Quantization
- Identical Particles
- The Exclusion Principle
- Multi-electron Atoms & the Periodic Table
- Characteristic X-Rays

It's open said that in Q.M. there're only 3 bound-state problems solvable (w/o numerical approximation tech.)
1. Infinite well, 2. Harmonic oscillation, 3. hydrogen atom – all 1-particle problem.
Most real application: multiple system. so, let's start an atom with multiple electrons

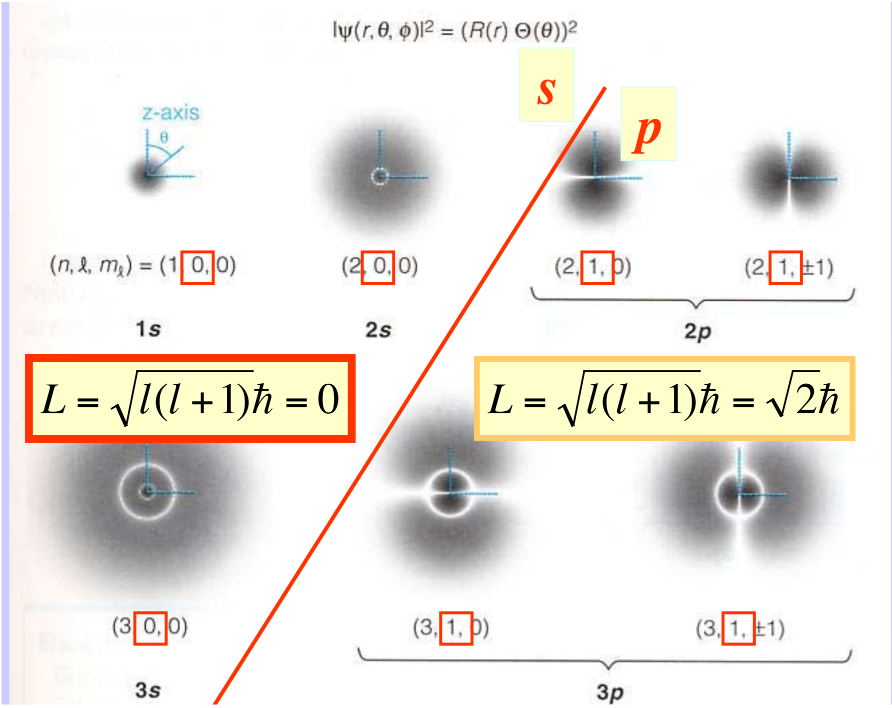
Electron Probability densities in the hydrogen atom, through n = 3



Spectroscopic notation

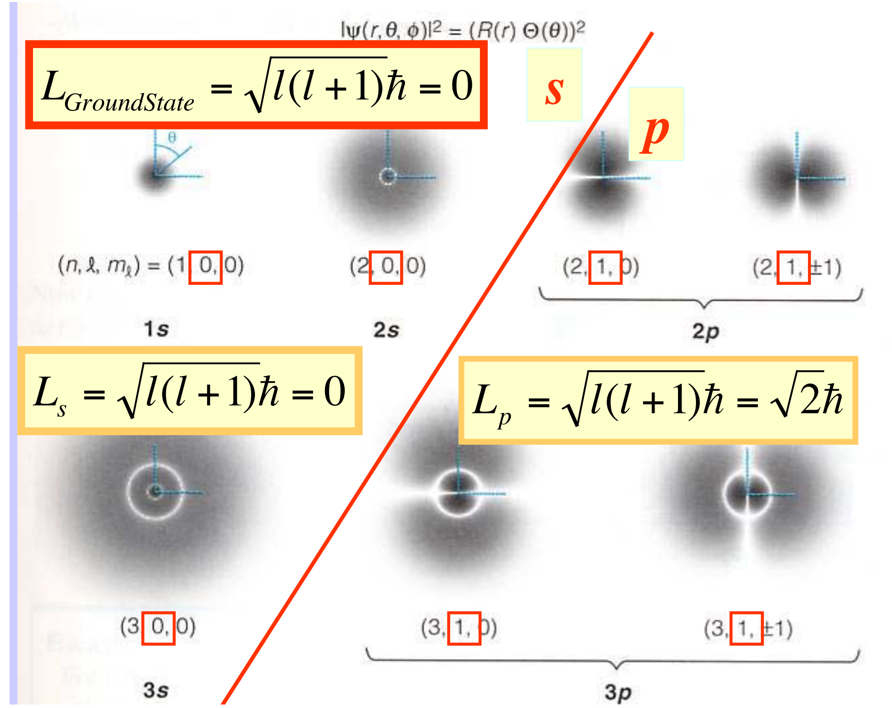
Letter	s	p	d	f	g	h
Value of ℓ	0	1	2	3	4	5

n	1	2				3								…	n
ℓ	0	0	1			0	1			2				…	$0, \ldots, n-1$
m_ℓ	0	0	−1	0	+1	0	−1	0	+1	−2	−1	0	+1	+2	…	$-\ell, \ldots, +\ell$



$$L = \sqrt{l(l+1)}\hbar = 0$$

$$L = \sqrt{l(l+1)}\hbar = \sqrt{2}\hbar$$



$$L_{GroundState} = \sqrt{l(l+1)}\hbar = 0$$

$$L_s = \sqrt{l(l+1)}\hbar = 0$$

$$L_p = \sqrt{l(l+1)}\hbar = \sqrt{2}\hbar$$

$$L_{GroundState} = \sqrt{l(l+1)}\hbar = 0$$

Ground State:

The Electron is NOT Orbiting around the proton

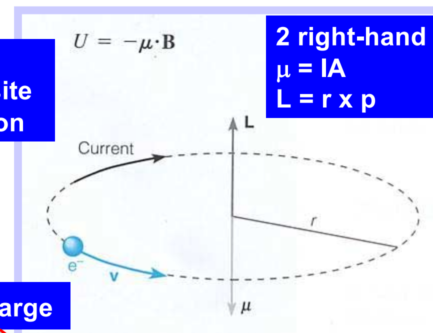
Classical Physics:

The Electron is Orbiting around the Proton

Orbiting in Classical Physics

Conventional current is opposite to electron motion

2 right-hand rules:
μ = IA
L = r x p



A charge with angular m/m has a magnetic dipole moment

fundamental charge

$$\mu = IA = \frac{e}{T}\pi r^2 = \frac{e}{2\pi r/v}\pi r^2 = \frac{e}{2}vr = \frac{e}{2m_e}(m_e vr)$$

L

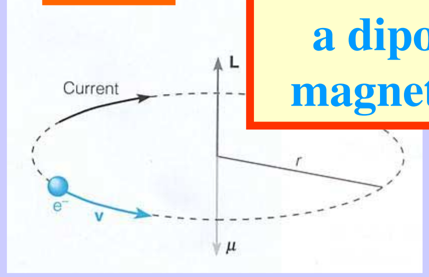
period of revolution

$$\mu_L = -\frac{e}{2m_e}\mathbf{L}$$

Magnetic Dipole Moment

Orbiting in Classical Physics

$U = -\boldsymbol{\mu}\cdot\mathbf{B}$



Potential energy of a dipole μ in a magnetic field B

$$\mu = IA = \frac{e}{T}\pi r^2 = \frac{e}{2\pi r/v}\pi r^2 = \frac{e}{2}vr = \frac{e}{2m_e}(m_e vr)$$

$$\boldsymbol{\mu}_{\mathbf{L}} = -\frac{e}{2m_e}\mathbf{L}$$

Magnetic Dipole Moment

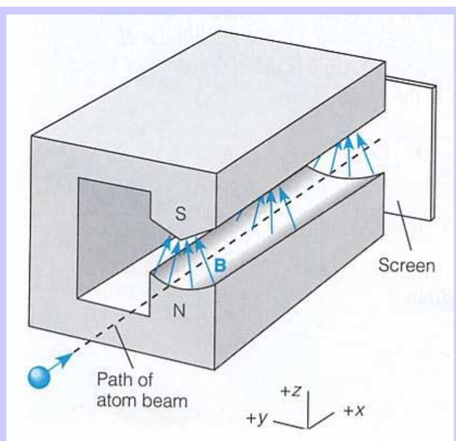
Magnetic force on a system with dipole moment μ

$$\mathbf{F} = -\nabla(\underbrace{-\boldsymbol{\mu}\cdot\mathbf{B}}_{U}) = \nabla(\mu_x B_x + \mu_y B_y + \mu_z B_z)$$

F = negative gradient of potential energy

F can be measured

The Stern-Gerlach Experiment



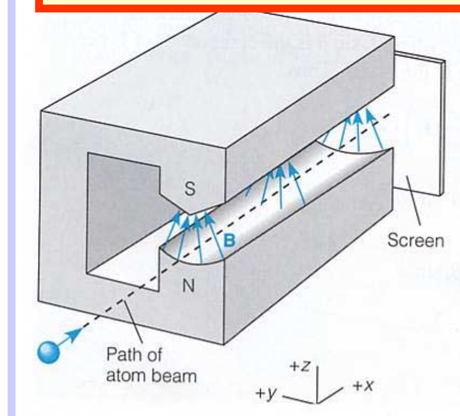
An atom with a magnetic dipole moment passing through a non-uniform B-field

The Stern-Gerlach Experiment

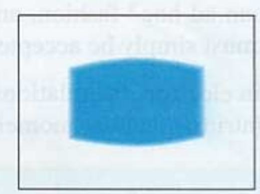
Classical Expectation

$$\mathbf{F} = \mu_z \frac{\partial B_z}{\partial z}\hat{\mathbf{z}}$$

$$\mathbf{F} = \left(-\frac{e}{2m_e}L_z\right)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}}$$



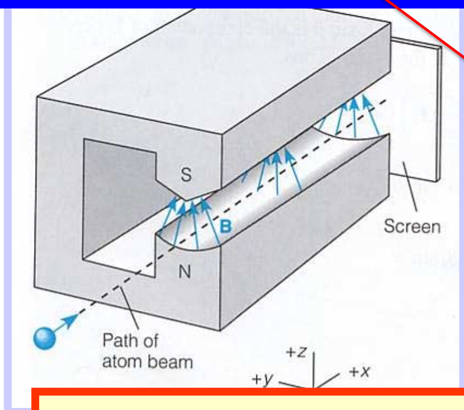
$$\mathbf{F} = -\nabla(-\boldsymbol{\mu}\cdot\mathbf{B}) = \nabla(\mu_x B_x + \mu_y B_y + \mu_z B_z)$$



Classical expectation ($L \neq 0$)

Quantum Theory Expectation

important factor governing the effect of B-field; so, magnetic quantum #



$$\mathbf{F} = \mu_z \frac{\partial B_z}{\partial z}\hat{\mathbf{z}}$$

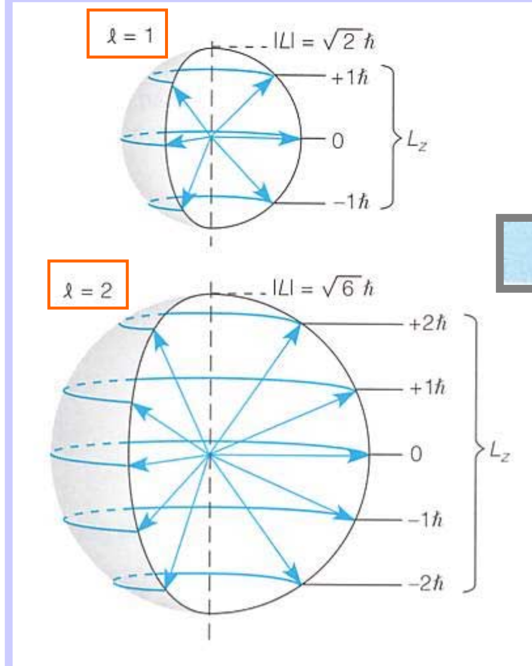
$$\mathbf{F} = \left(-\frac{e}{2m_e}L_z\right)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}}$$

$L_z = m_\ell \hbar$ $(m_\ell = 0, \pm 1, \pm 2, \ldots, \pm \ell)$

$$\mathbf{F} = -\frac{e}{2m_e}(m_\ell \hbar)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}}$$

$$(m_\ell = -\ell, \ldots, +\ell)$$

Ground State -> *l = 0* -> *L = 0* -> *F = 0*



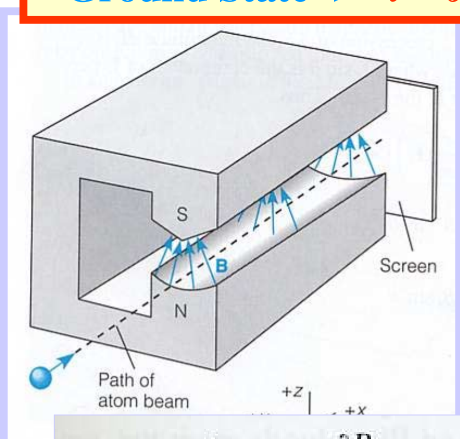
Angular Momentum Quantization

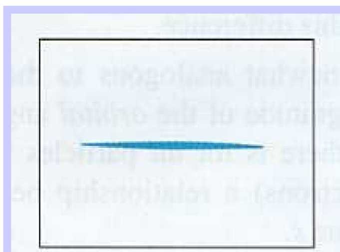
$$|L| = \sqrt{L^2} = \sqrt{\ell(\ell+1)}\hbar$$

$$L_z = m_\ell \hbar$$

Quantum Theory Expectation

Ground State -> *l = 0* -> *L = 0* -> *F = 0*



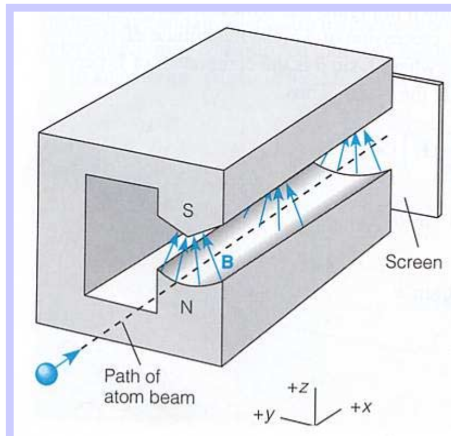


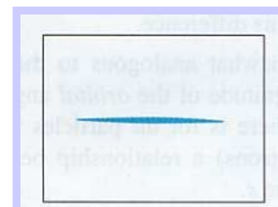
ℓ = 0 prediction

$$\mathbf{F} = -\frac{e}{2m_e}(m_\ell \hbar)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}} \qquad (m_\ell = -\ell, \ldots, +\ell)$$

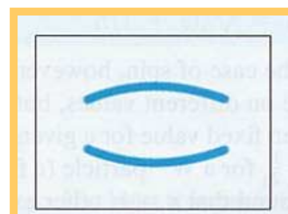
Surprise: Real Experimental Result

Ground State -> *l = 0* -> *L = 0* -> *F = 0 (???)*





ℓ = 0 prediction



ℓ = 0 observation

Oops!

The Solution:

INTRINSIC MAGNETIC MOMENT and ANGULAR MOMENTUM called

"SPIN"

is "carried" by every electron

SPIN

$\mu_L = -\frac{e}{2m_e}\mathbf{L}$

Magnetic Dipole Moment

related to intrinsic angular m/m, S

gyromagnetic ratio

$$\mu_S = -g_e \frac{e}{2m_e}\mathbf{S} \qquad (g_e \cong 2)$$

Like for *L*: $L = \sqrt{\ell(\ell+1)}\hbar$

Intrinsic angular momentum:

$$S = \sqrt{s(s+1)}\hbar$$

***s* – the quantum number of SPIN**

Intrinsic property of a particle

For and electron: *s = 1/2*

Intrinsic angular momentum:

$$S = \sqrt{s(s+1)}\hbar$$

$$S = \sqrt{\tfrac{1}{2}(\tfrac{1}{2}+1)}\hbar = \tfrac{\sqrt{3}}{2}\hbar.$$

e.g. for proton s = 1/2, for W s = 1,
see Table 8.1 (p295)

Stern-Gerlach Experiment?

Intrinsic angular momentum:

$$S = \sqrt{s(s+1)}\hbar$$

$$S_z = m_s\hbar \qquad (m_s = -s, -s+1, \ldots, s-1, s)$$

spin quantum number: allowed values are from –s to +s in integral steps

$$\mathbf{F} = \left(-2\frac{e}{2m_e}S_z\right)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}} = -\frac{e}{m_e}(m_s\hbar)\frac{\partial B_z}{\partial z}\hat{\mathbf{z}} \quad (m_s = -s, \ldots, +s)$$

Now let us return to the Stern-Gerlach experiment. For l =0, the orbital magnetic moment $\mu_L = 0$, so it shouldn't be subject to a force, but there should still be a force on the intrinsic magnetic dipole moment.

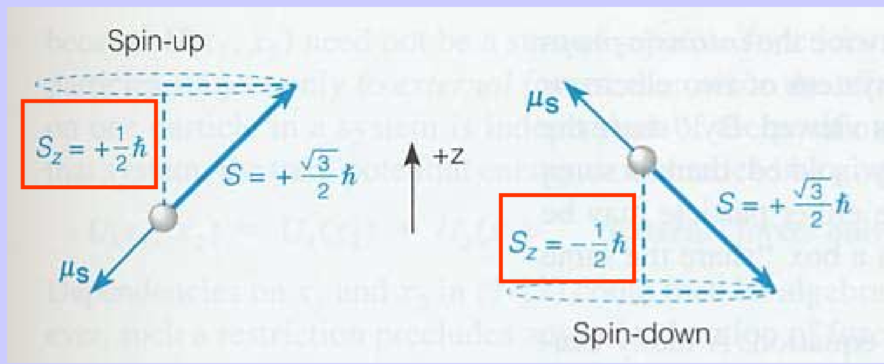
$$S_z = \pm\frac{1}{2}\hbar$$

for electrons

spin quantum #: +- 1/2

Spin Orientation

2 possible spin states of an electron



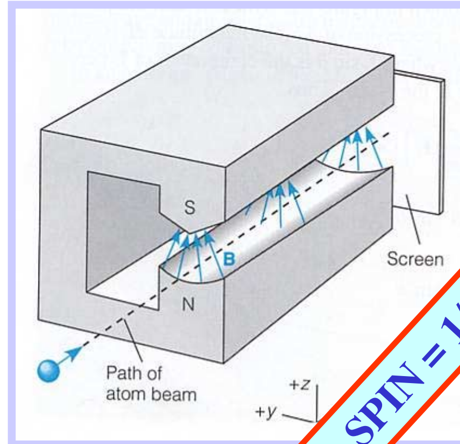
$$\Psi_{n,l,m_l,m_s} = \Psi_{n,l,m_l}(r,\theta,\phi)\ m_s$$

$$\Psi_{n,l,m_l,+1/2} = \Psi_{n,l,m_l}(r,\theta,\phi)\ \textit{up}$$

$$\Psi_{n,l,m_l,-1/2} = \Psi_{n,l,m_l}(r,\theta,\phi)\ \textit{down}$$

→ **spin**

The Stern-Gerlach Experiment



$$S_z = \pm\frac{1}{2}\hbar$$

$$F = \pm F_0$$

SPIN = 1/2

2 lines corresponding to m_s = +1/2 & -1/2