UNIVERSITAT POLITÈCNICA DE CATALUNYA

Titulació: EFiS

Assignatura: QPHYS – SEC. IV (.3-.4)

Cognoms

Nom

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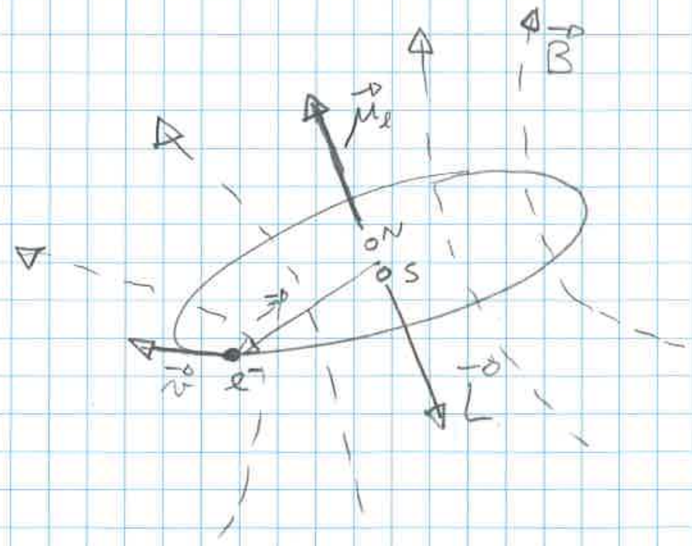
Pàgina 1 de

MAGNETIC DIPOLES, SPIN AND SPIN-ORBIT COUPLING

- Now that we've set the formalism to quantify orbital angular momentum in Schrödinger's one-e^- atom, we're gonna see how to measure it.
- Because (in some states) the e^- can be regarded as a moving charge, it will produce an ELECTRIC CURRENT and an associated MAGNETIC FIELD.
- So the quantity that we can use to measure angular momentum indirectly is the: $\boxed{\text{MAGNETIC DIPOLE MOMENT} \Leftrightarrow \text{ANGULAR MOMENTUM}}$
- We'll use a semi-classical approach: A MIX OF $\Rightarrow$ { Bohr-like orbits, electromagnetic theory, quantum mechanics }

  But the results agree with those obtained from a full Q-MEC treatment.
- We'll find a "surprise" along the way: e^- HAVE INTRINSIC ANGULAR MOMENTUM (CALLED 'SPIN', NOT ORBITAL) AND AN ASSOCIATED MAGNETIC DIPOLE MOMENT.

An e^- with mass m and charge $-e$ moving with velocity $\vec{v}$ in a circular orbit of radius r.



This creates a loop of current $\left(\frac{\text{charge}}{\text{unit time}}\right)$:

$$i = \frac{e}{T} = \frac{e v}{2\pi r}$$ where T is the 'orbital' period of the e^-.

- Recall that a charge produces an electric field $(\vec{E})$ and a moving charge produces a magnetic field $(\propto \vec{v} \times \vec{E})$
- Next semester in electromagnetism (EMAG-Q4-2B, TOPIC 3), if you haven't yet, you'll see that A LOOP OF CURRENT i AND AREA A PRODUCES A MAGNETIC FIELD EQUIVALENT TO THAT OF A MAGNETIC DIPOLE MOMENT OF MAGNITUDE:

$$\boxed{\mu_e = i A} \quad (\text{VI}.1)$$

And the direction of the magnetic dipole moment vector is $\propto q\, \vec{v} \times \vec{r}$ (shown in the figure, opposite to $\vec{L}$ since e^- has negative charge q).

This is often represented with the two poles N & S of the magnetic dipole, and μ_e gives the strength of this dipole and of the associated magnetic field.

$\vec{\mu}_e$ is thus antiparallel to the orbital angular momentum, with magnitude given by

$$\boxed{L = m v r} \quad (\text{VI}.2)$$

(in the semi-classical approach we're taking we will introduce L quantization later)

so $$\boxed{\mu_e = \frac{e v}{2\pi r} \cdot \pi r^2 = \frac{e v r}{2}} \quad (\text{VI}.3)$$

or in terms of L: $$\boxed{\frac{\mu_e}{L} = \frac{e v r}{2 m v r} = \frac{e}{2m}} \quad (\text{VI}.4)$$

This ratio is usually written as:

$$\boxed{\frac{\mu_\ell}{L} = \frac{g_\ell \mu_B}{\hbar}}$$

→ UNITS OF MAGNETIC DIPOLE MOMENT (charge · area/time)

RECALL UNITS OF ANGULAR MOMENTUM

where $\begin{cases} \mu_B = \dfrac{e\hbar}{2m} \quad (= 0{,}93\cdot 10^{-23}\, A\text{-}m^2) \\ g_\ell = 1 \quad \text{(we'll see why we use this :)} \end{cases}$

- μ_B is the "Bohr magneton": $\begin{cases}\text{unit of magnetic dipole moment} \\ \text{typical m.d.m of an atom}\end{cases}$
- g_ℓ is the "orbital g factor", a dimensionless parameter introduced to compare with other ang. mom.

SO THE ORBITAL MAGNETIC DIPOLE MOMENT VECTOR IS GIVEN BY:

$$\boxed{\vec{\mu}_\ell = -\frac{g_\ell \mu_B}{\hbar} \vec{L}} \quad \text{(VI.5)}$$

Note the ratio $\frac{\mu_\ell}{L}$ does not depend on the details of the orbit (r, T), AND it turns out that calculating μ_ℓ/L properly (Q-MEC) also gives $\frac{g_\ell \mu_B}{\hbar}$ (VI.5)

So if we use our quantization relations for L and L_z (V.1) we get:

$$\text{(VI.6)} \quad \boxed{\mu_\ell = \frac{g_\ell \mu_B}{\hbar}\sqrt{\ell(\ell+1)}\,\hbar = g_\ell \mu_B \sqrt{\ell(\ell+1)}}$$

MAGNITUDE/MODULUS OF ORBITAL MAGNETIC DIPOLE MOMENT

and:

'MINUS' BECAUSE THEY'RE ANTIPARALLEL (negative charge)

$$\text{(VI.7)} \quad \boxed{\mu_{\ell_z} = -\frac{g_\ell \mu_B}{\hbar} L_z = -\frac{g_\ell \mu_B}{\hbar} m_\ell \hbar = -g_\ell \mu_B m_\ell}$$

Z COMPONENT OF $\vec{\mu}_\ell$

THEREFORE: BECAUSE $\vec{L}$ IS QUANTIZED, SO IS $\vec{\mu}_\ell$!

$\Rightarrow$ ORBITAL (AND ANY OTHER) ANGULAR MOMENTUM PRODUCES A CURRENT AND A MAGNETIC DIPOLE MOMENT, WHICH IS ALSO QUANTIZED AND WHICH WE CAN MEASURE EXPERIMENTALLY.

HOW? ADD AN EXTERNAL (OR 'INTERNAL'*) MAGNETIC FIELD! ASSOCIATED TO $\vec{\mu}$, $\vec{B}$:

• **ENERGY**: A magnetic dipole of moment $\vec{\mu}_\ell$ placed in an external magnetic field $\vec{B}$ experiences a torque, which tends to align it with $\vec{B}$, and associated with this torque there is a

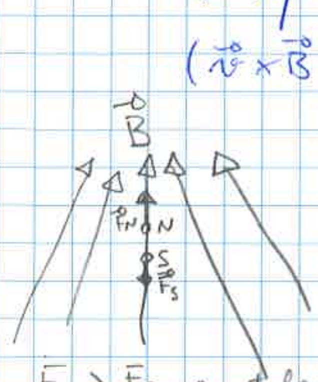
POTENTIAL ENERGY OF ORIENTATION

$$\boxed{\Delta E = -\vec{\mu}_\ell \cdot \vec{B}} \qquad \text{(VI.8)}$$

Thus turning the magnetic dipole from a parallel ($-\mu_\ell B$) to an antiparallel ($+\mu_\ell B$) orientation with respect to the external field $\vec{B}$ will change its energy by $2\mu_\ell B$

$$\Delta E = -\mu_\ell B \cos\alpha \quad \begin{cases} \alpha = 0^\circ, \text{ parallel}: -\mu_\ell B & \text{(stable equil.)} \\ \alpha = 180^\circ, \text{ antiparall.}: +\mu_\ell B & \text{(unstable equil.)} \end{cases}$$

• **FORCE**: If the dipole is placed in a NON-UNIFORM B FIELD there will be a net TRANSLATIONAL FORCE acting on the dipole (in addition to the torque acting to turn it). This is ultimately a consequence of the fact that a moving charge in a $\vec{B}$ field experiences a force ($\vec{v} \times \vec{B}$). For details see Figs 8.3 & 8.4 in E&R and EM6 next semester!



$F_N > F_S \Rightarrow$ net force

$$\boxed{F_z = \frac{\partial B_z}{\partial z} \mu_{\ell z}} \qquad \text{(VI.9)}$$

(ALIGN z

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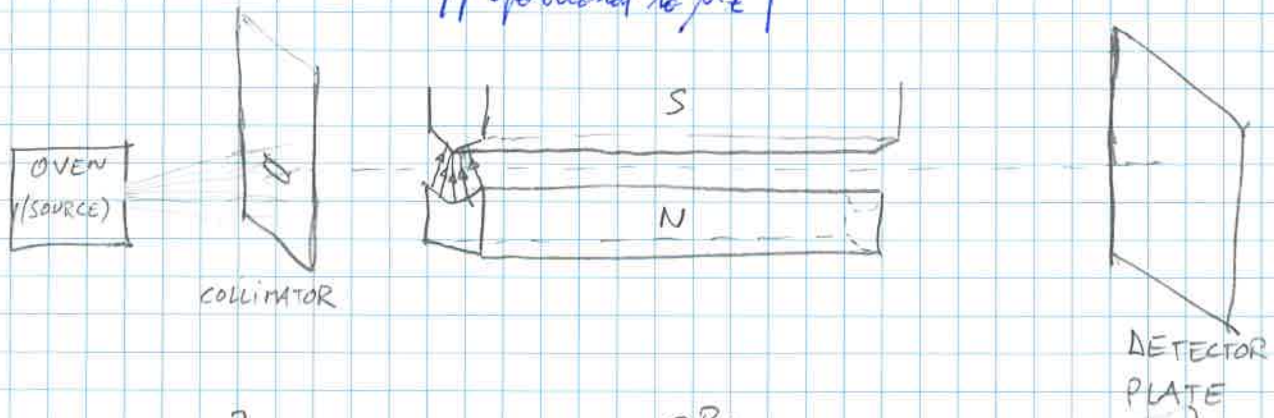
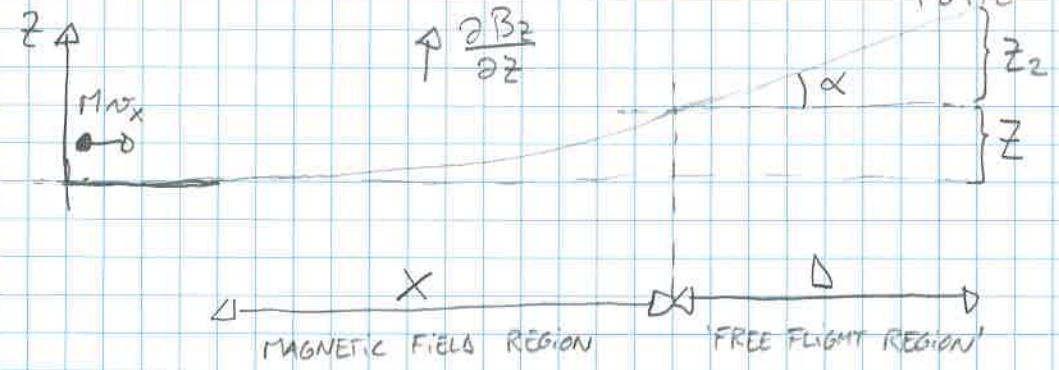
and this takes us to the $\boxed{\text{STERN-GERLACH EXPERIMENT}}$ (1922)

BEAM of {neutral silver atoms collimated} enters a MAGNET {with a non-uniform B field increasing in the z direction} where it is DEFLECTED ...

... where it is DEFLECTED {by the net force F_z (IV.9) due to the interaction between $\vec{B}$ and $\vec{\mu}$, which is proportional to μ_z} and when it leaves the magnet it is ANALYZED {by means of a metallic plate where atoms collide, condense and leave a trace}





When going through the region of non-uniform B field, the atoms are deflected, by an amount which is proportional to F_z $\left(z = \frac{1}{2} a_z t^2 \right) = \frac{1}{2}\frac{F_z}{M} t^2$

AND THEREFORE DEFLECTED BY AN AMOUNT PROPORTIONAL TO μ_z.

- CLASSICALLY : $\vec{\mu}_\ell$ ($\vec{L}$) CAN HAVE ANY ORIENTATION, THUS $\mu_{\ell z}$ CAN HAVE ANY VALUE (between $+\mu_\ell$ and $-\mu_\ell$)

- QUANTUM-MECHANICS PREDICTION :

$$\mu_{\ell z} = -g_\ell \mu_b m_\ell \qquad (m_\ell = -\ell, -\ell+1, \dots \ell-1, \ell)$$

Thus: Q-MEC predicts that the beam is split into several discrete components.

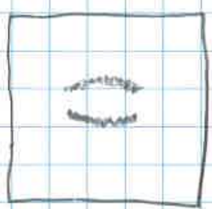
(The same happens if we rotate the magnet by 90°: our measuring apparatus defines the direction of the z axis, breaks the spherical symmetry of Coulomb's potential and the degeneracy with m (m_ℓ).)

WHAT STERN & GERLACH FOUND (after some struggle) WAS NOT

THE CLASSICAL PREDICTION

X

BUT RATHER THIS :



!

⟹ CONFIRMING THE (SPACE) QUANTIZATION OF μ_z AND THUS L_z !

- HOWEVER, SCHROEDINGER'S THEORY OF THE ORBITAL ANGULAR MOMENTUM PREDICTS $2\ell+1$ COMPONENTS (e.g. for $\ell=1$: $m_\ell=+1$, $m_\ell=0$, $m_\ell=-1$)

BUT THEY FOUND THE BEAM WAS SPLIT IN ONLY TWO COMPONENTS.

WRONG? INCOMPLETE?

One could think there's ambiguity in Ag atoms as to the exact value of ℓ, but Phipps & Taylor repeated the experiment with H atoms in the $n=1$ ($\ell=0$) state and found:

THE SAME TWO SPOTS WITH H ATOMS IN $n=1$, $\ell=0$ STATE!

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Assignatura: QPhys - Sec. IV

Pàgina 4 de

Cognoms / DNI:

NOTE: on silver atoms and Stern-Gerlach: Ag: $Z=47$; $A=108$; $[Kr]\,4d^{10}\,5s^1$

THEN: trial & error, misinterpreted as $m=\pm 1$ in Bohr's atomic model.

NOW: we know they have 'closed shell' (no magn. dipole) AND a $5s^1$ electron ($\ell=0$) so that they act as a "heavy electron" without orbital ang. moment.

$4d^{10}$: $\ell=2$, $2\cdot(2\ell+1)=10$

⟹ THUS THERE MUST BE SOME ADDITIONAL MAGNETIC DIPOLE MOMENT IN THE ATOM.

SUGGESTED HOMEWORK (PROBLEM 9)

- The measured size of the splitting (SEE EXAMPLE 8.2 & PROBLEMS) was consistent with $\mu \sim \mu_B = \frac{e\hbar}{2m}$ and therefore with being originated by the electron (NOT with the nucleus which has a magnetic dipole moment $\sim \frac{e\hbar}{2M} \sim 2000$ times smaller).

This led to the conclusion* that: (* after some debate.)

$$\boxed{\text{THE } e^- \text{ HAS AN INTRINSIC MAGNETIC DIPOLE MOMENT } \vec{\mu}_S \text{ CAUSED BY AN INTRINSIC ANGULAR MOMENTUM } \vec{S} \text{ CALLED "SPIN".}^{(*)}}$$

By analogy with $\vec{L}$ one can then make the following assumptions:

- SAME QUANTIZATION RELATIONS APPLY TO THE SPIN ANGULAR MOMENTUM $\vec{S}$:

$$\boxed{\begin{aligned} S &= \sqrt{s(s+1)}\,\hbar \\ S_z &= m_s\,\hbar \end{aligned}} \qquad \text{VI.10} \qquad (\text{cf. VI.1})$$

- SAME RELATION WITH SPIN MAGNETIC DIPOLE MOMENT $\vec{\mu}_S$:

$$\boxed{\vec{\mu}_S = -\frac{g_s \mu_B}{\hbar}\vec{S}} \qquad \text{VI.11} \qquad (\text{cf. VI.5})$$

$$\boxed{\mu_{S_z} = -g_s \mu_B m_s} \qquad \text{VI.12} \qquad (\text{cf. VI.7})$$

where g_s is the "spin g factor"

(*): $\vec{S}$ can be imagined as a 'spin' or rotation around axis in a classical image. BUT it does not mean that image is right!

- The beam in the Stern-Gerlach experiment was split into two beams, both deflected, one up / one down.
- If we assume these correspond to $m_s = +1$ AND $m_s = -1$, and that m_s changes in steps of 1 (just like m_ℓ), then we are led to these values for the new quantum numbers:

Uhlenbeck & Goudsmit (1925)

$$\boxed{\begin{aligned} m_s &= -\tfrac{1}{2}, +\tfrac{1}{2} \\ s &= \tfrac{1}{2} \end{aligned}} \qquad \text{VI.13}$$

NOTE SAME ℓ, m_ℓ FORMALISM BUT NOW $s = \frac{1}{2}$ ONLY POSSIBLE VALUE.

- By measuring the size of the splitting Z we can know the force $F_z = -\frac{\partial B_z}{\partial z} \mu_B g_s m_s$ (cf. VI.9 & VI.7)

and that's how they measured that the product

$$g_s m_s = \pm 1$$

- Since we concluded that $m_s = \pm\frac{1}{2} \Rightarrow \boxed{g_s = 2}$

Recall that $\frac{\mu_\ell}{L} = g_\ell \frac{\mu_B}{\hbar}$ with $g_\ell = 1$

UNITS OF MAGN. DIP. MOM.

UNITS OF ANG. MOM.

So $g_s = 2$ implies that the spin magnetic dipole is 2x STRONGER, relative to S, than μ_ℓ is relative to L.

- THE ZEEMAN EFFECT CONFIRMS THESE CONCLUSIONS (supports assumptions) SPLITTING OF ENERGY LEVELS (VIA MEASUREMENTS OF SPECTRAL LINES) WHEN A UNIFORM, STRONG, EXTERNAL MAGNETIC FIELD IS APPLIED.

$$\boxed{\Delta E = -\vec{\mu}_s \cdot \vec{B} = -\mu_{sz} B = g_s \mu_B m_s B = \pm \frac{g_s \mu_B B}{2}}$$

'SPIN-RECAP'

- Hence besides the three quantum numbers that we have found from Schrödinger's theory of the H atom:
  n, l, m_l (ASSOCIATED TO THE 3 SPATIAL COORDS. OR 'DEGREES OF FREEDOM')

WE NEED A FOURTH QUANTUM NUMBER TO DESCRIBE THE ELECTRON: m_s, which can take the values $+1/2$ and $-1/2$.
(an additional "degree of freedom")

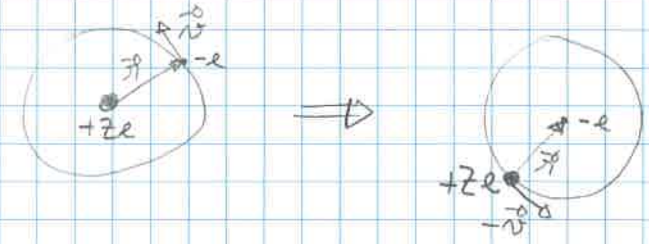
- m_s DESCRIBES THE SPACE ORIENTATION (Z COMPONENT) OF THE e^-'s SPIN:
  $\Rightarrow$ TWO POSSIBLE m_s STATES COMMONLY CALLED "SPIN UP & DOWN".
- Classical image of a spinning 'ball' is tempting BUT e^- spin is a NON-classical phenomenon! NOT even with classical limit (like we did for $l \to \infty$ e.g.), since note that s can only take $s = \frac{1}{2}$.
  (There's also physical inconsistencies if we try to reconcile the size, charge and mass/energy of the e^- with such classical image.)
- e^- SPIN IS NOT PREDICTED BY SCHROEDINGER's theory, but it can be added 'a posteriori', as a separate postulate.
- Dirac's relativistic theory of quantum mechanics (1929+) does explain the intrinsic $s = \frac{1}{2}$ angular momentum of the e^-, so it "needs" both quantum mechanics and relativity.
  (not for this course though)

SPIN-ORBIT INTERACTION

- e^- spin is subtle and it took a while to discover, but it certainly has noticeable and measurable consequences.
- e.g. it doubles the number of possible states ($2n^2$ instead of n^2) that can be populated according to Pauli's exclusion principle.
- SPIN also CHANGES THE ENERGY LEVELS WHEN THE SPIN MAGNETIC DIPOLE MOMENT OF THE e^- INTERACTS WITH A MAGNETIC FIELD
  - EXTERNAL B FIELD $\Rightarrow$ ZEEMAN EFFECT.
  - INTERNAL B FIELD $\Rightarrow$ SPIN-ORBIT COUPLING/INTERACTION.

An e^- moving around the nucleus 'sees' the nucleus moving.
$\rightarrow$ a $+Ze$ moving charge $\rightarrow$ an effective 'atomic'/'internal' magnetic field.

REF. FRAME nucl. $\Rightarrow e^-$



In the ref. frame of the e^-, the nucleus produces a loop of current:

$$\vec{j} = -Ze\vec{v}$$

& the corresponding $\vec{B}$ field at the e^-'s location is (Ampere's law):

$$\vec{B} = \frac{\mu_0}{4\pi}\frac{\vec{j}\times\vec{r}}{r^3} = -\frac{Ze\mu_0}{4\pi}\frac{\vec{v}\times\vec{r}}{r^3}$$

In terms of the electric field acting on the e^-, $\vec{\mathcal{E}} = \frac{Ze}{4\pi\varepsilon_0}\frac{\vec{r}}{r^3}$:

$$\text{VI.14} \quad \boxed{\vec{B} = -\frac{1}{c^2}\vec{v}\times\vec{\mathcal{E}}} \quad \text{where } c = \frac{1}{\sqrt{\mu_0\varepsilon_0}}$$

So while the e^- moves around the nucleus through the electric field $\vec{\mathcal{E}}$ that this produces, it also feels a magnetic field $\vec{B}$.

- The e^- (ITS INTRINSIC/SPIN MAGNETIC DIPOLE MOMENT) can have different orientations with respect to this internal $\vec{B}$ field of the atom. The corresponding ORIENTATION POTENTIAL ENERGY is:

$$\Delta E = -\vec{\mu}_s \cdot \vec{B} \qquad \text{(analogous to VI.8)}$$

since $\vec{\mu}_s = -\frac{g_s \mu_B}{\hbar}\vec{S}$ (from VI.11)

$$\Delta E = \frac{g_s \mu_B}{\hbar} \vec{S} \cdot \vec{B}$$

We've found this ΔE in the e^- ref. frame (e^- at rest); going back to the reference frame where the nucleus is at rest reduces ΔE by a factor 2 (Appendix O):

$$\boxed{\Delta E = \frac{1}{2} \frac{g_s \mu_B}{\hbar} \vec{S} \cdot \vec{B}} \qquad \text{VI.15}$$

- Now we want to express the internal magnetic field $\vec{B}$ as a function of the orbital angular momentum, so that we can have the interaction energy as a function of $\vec{S}$ and $\vec{L}$.
- For that, recall that:

$$-e\vec{\mathcal{E}} = \vec{F} \qquad \text{(by definition of electric field: FORCE/charge)}$$

and:

$$\vec{F} = -\frac{dV(r)}{dr}\frac{\vec{r}}{r} \qquad \frac{\vec{r}}{r} = \hat{r} \qquad \text{(by definition of potential energy)}$$

to $\vec{B}$ (VI.14) can be written as:

$$\vec{B} = -\frac{1}{ec^2}\frac{1}{r}\frac{dV(r)}{dr}\,\vec{v}\times\vec{r}$$

since the orbital angular momentum is $\vec{L} = \vec{r}\times m\vec{v}$

(cross product anti-commutative) $= -m\,\vec{v}\times\vec{r}$

$$\Longrightarrow \boxed{\vec{B} = \frac{1}{emc^2}\frac{1}{r}\frac{dV(r)}{dr}\vec{L}} \quad \text{(VI.16)} \; (*)$$

Plugging this into the expression for ΔE (VI.15)

$$\Delta E = \frac{g_s \mu_B}{2emc^2\hbar}\frac{1}{r}\frac{dV(r)}{dr}\,\vec{S}\cdot\vec{L}$$

which using $g_s = 2$ and $\mu_B = \frac{e\hbar}{2m}$ turns into:

$$\boxed{\Delta E = \frac{1}{2m^2c^2}\frac{1}{r}\frac{dV(r)}{dr}\,\vec{S}\cdot\vec{L}} \quad \text{(VI.17)}$$

SPIN-ORBIT INTERACTION ENERGY

→ SUGGESTED HOMEWORK: { APPLY THIS TO { $n=2, l=1$ (EXAMPLE 8.3) & ESTIMATE ΔE

• IMPORTANT EQUATION GIVING THE ~~SIZE~~ STRENGTH OF THE SPIN-ORBIT INTERACTION, DIRAC's relativistic Q-Mec treatment gives exactly the same.

(*) NOTE: this field is strong, of the order ~ 1 T (10^4 G)

(MRI scans use ~ 1,5 T typically)

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- Eq's VI.16 and VI.17 reflect a COUPLING between the spin and orbital angular momentum of the electron: SPIN-ORBIT COUPLING
  - The e^- feels a strong magnetic field in the atom, with strength and orientation set by its own orbital angular momentum $\vec{L}$,
  - and this $\vec{B}$ induces a torque $(\vec{\mu}_s \times \vec{B})$ on the spin magnetic dipole moment, with strength and orientation set by its own spin angular momentum $\vec{S}$.

⇒ This coupling implies that $\vec{L}$ and $\vec{S}$ are not free to point anywhere (besides their respective quantization conditions), BUT THE ORIENTATION OF ONE DEPENDS ON THE OTHER.

⇒ In particular, $\vec{L}$ and $\vec{S}$ precess around their sum:

$$\boxed{\vec{J} = \vec{L} + \vec{S}} \qquad \text{VI.18}$$

THE TOTAL ANGULAR MOMENTUM VECTOR

⇒ So in the presence of spin-orbit coupling L_z and S_z are not well defined anymore, they don't have fixed values ($\vec{L}$ and $\vec{S}$ are not in cones around the z axis, but they precess around $\vec{J}$).

⇒ SO IT IS THE TOTAL ANGULAR MOMENTUM $\vec{J} = \vec{S} + \vec{L}$ WHAT HAS A "SIMPLE" BEHAVIOR NOW, WITH FIXED, KNOWN AND QUANTIZED J & J_z.

• One can show (we won't) that the MAGNITUDE AND Z COMPONENT of the TOTAL ANGULAR MOMENTUM obey the usual QUANTIZATION CONDITIONS:

$$\boxed{J = \sqrt{j(j+1)}\,\hbar} \quad \text{VI.19}$$

$$\boxed{J_z = m_j\,\hbar} \quad \text{VI.20}$$

with $\boxed{m_j = -j, -j+1, \ldots, j-1, j}$ VI.21

OPTIONAL: derive possible j values

The maximum value for m_j is:

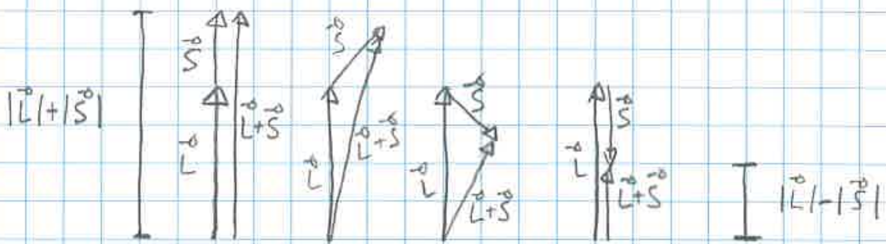
$$(m_j)_{max} = \underbrace{l}_{\text{MAXIMUM VALUE for } m_l} + \underbrace{\frac{1}{2}}_{\text{MAX. VAL for } m_s}$$

(NOT PROVING THIS, BUT INTUITIVELY: "$\vec{L}$ and $\vec{S}$ aligned")

And this is also the max. value for j (VI.21)

So j will decrease in steps of 1 starting from $l+\frac{1}{2}$:

$j = l+\frac{1}{2}, l-\frac{1}{2}, \ldots$



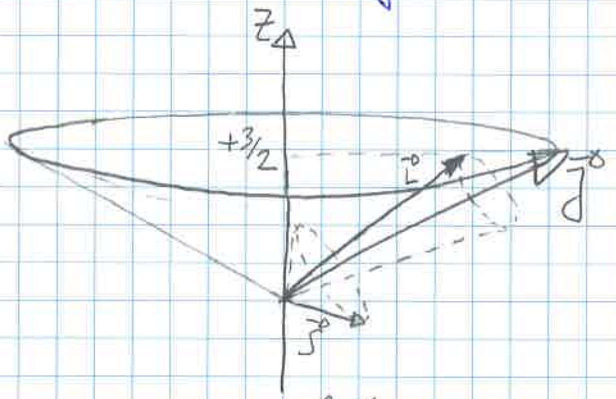
$$|\vec{L}+\vec{S}| = |\vec{J}| \geq \big||\vec{L}|-|\vec{S}|\big|$$

$$\sqrt{j(j+1)} \geq \left|\sqrt{l(l+1)} - \sqrt{s(s+1)}\right| \Rightarrow \text{ONLY TRUE FOR } j = l+\tfrac{1}{2}, l-\tfrac{1}{2}$$

↑ OPTIONAL: derive possible j values

• AND WITH $\boxed{\begin{array}{ll} j = l+\frac{1}{2}, l-\frac{1}{2} & (\text{if } l>0) \\ j = \frac{1}{2} & (\text{if } l=0) \end{array}}$ VI.22

- This interplay between $\vec{L}$, $\vec{S}$ and $\vec{J}$ is also often represented in terms of VECTOR DIAGRAMS:



$l=2,\ j=\frac{5}{2},\ m_j=+\frac{3}{2}$

"It's now $\vec{J}$ the vector that's well behaved and well defined, and $\vec{L}$ and $\vec{S}$ precess around it so we can't say anything about their z components."

THIS IS THE CASE $j=l+\frac{1}{2}$:
$\vec{L}$ and $\vec{S}$ "aligned" (NOT strictly, pointing towards the same direct.)

- In other words: INSTEAD OF THE QUANTUM NUMBERS n, l, m_l, m_s
(E, L, L_z, S_z)

IN THE PRESENCE OF SPIN-ORBIT COUPLING WE DESCRIBE THE SYSTEM WITH THE QUANTUM NUMBERS n, l, j, m_j
(E, L, J, J_z)

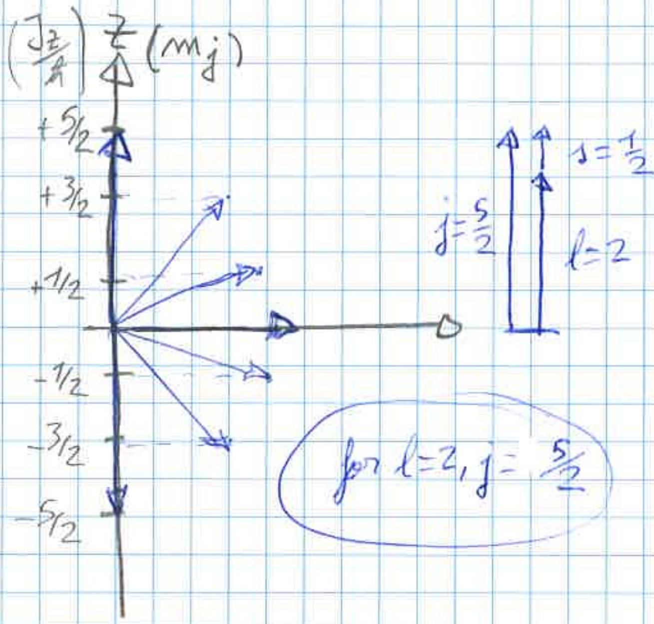
(because now J and J_z are well defined instead of L_z and S_z)

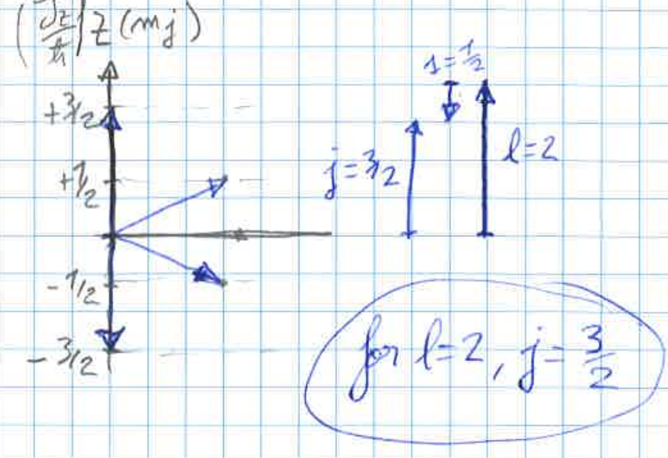
- The total number of states is still $2n^2$:

$$\sum_{l=0}^{n-1}(2j_+ +1)+\sum_{l=1}^{n-1}(2j_- +1)=\dots=2n^2 \qquad \begin{pmatrix} j_+=l+\frac{1}{2} \\ j_-=l-\frac{1}{2}\end{pmatrix}$$

e.g. $n=2\begin{cases} l=0;\ j=\frac{1}{2};\ m_j=\begin{cases}+1/2\\-1/2\end{cases} \\ l=1\begin{cases} j=\frac{3}{2},\ m_j=\begin{cases}+3/2\\+1/2\\-1/2\\-3/2\end{cases} \\ j=1/2,\ m_j=\begin{cases}+1/2\\-1/2\end{cases}\end{cases}\end{cases}$ $[8=2\cdot 2^2]$

And the VECTOR DIAGRAMS LOOK LIKE THIS:





$\Rightarrow$ NOTE THAT THESE DIAGRAMS DO NOT REPRESENT THE RIGHT MAGNITUDE

$J=\sqrt{j(j+1)}\,\hbar$ (for instance it should be $\frac{J}{\hbar}=2{,}96$ on the left diagram, and not $\frac{J}{\hbar}=2.5$)

AND THEREFORE THEY DO NOT REPRESENT THE RIGHT WAY OF ADDING $\vec{L}$ AND $\vec{S}$ (that's more complex, see previous multi-cone Figure)

$\Rightarrow$ THEY ONLY REPRESENT 'VISUALLY' THE RULES FOR ADDING THE QUANTUM NUMBERS l, s TO GET THE POSSIBLE VALUES OF THE QUANTUM NUMBERS j, m_e (i.e. they represent VI.20–VI.22 but NOT VI.19)

Now that we know how $\vec{S}$ and $\vec{L}$ interact, we can obtain a more practical expression for the SPIN-ORBIT INTERACTION ENERGY (VI.17)

$$\vec{J} = \vec{L} + \vec{S} \Rightarrow \vec{J}\cdot\vec{J} = \vec{L}\cdot\vec{L} + \vec{S}\cdot\vec{S} + 2\,\vec{S}\cdot\vec{L}$$

$$\Rightarrow \boxed{\vec{S}\cdot\vec{L} = \frac{J^2 - L^2 - S^2}{2} = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - s(s+1)\right]}$$

in the quantum state l, s, j

So ΔE (VI.17) becomes:

$$\Delta E = \frac{\hbar^2}{4m^2c^2}\left[j(j+1) - l(l+1) - s(s+1)\right]\frac{1}{r}\frac{dV(r)}{dr}$$

So the energy change due to spin-orbit interaction is the expectation value of this:

$$\boxed{\overline{\Delta E} = \underbrace{\frac{\hbar^2}{4m^2c^2}}_{\text{Energy Constant}}\underbrace{\left[j(j+1) - l(l+1) - s(s+1)\right]}_{\text{This part from quantum numbers only}}\underbrace{\overline{\frac{1}{r}\frac{dV(r)}{dr}}}_{\text{This part from } P_r(r)\,\propto\, r^2|R_{nl}^2|}} \quad \text{(VI.23)}$$

$$\boxed{+\ V(r) = \frac{-Ze^2}{4\pi\varepsilon_0 r}}$$

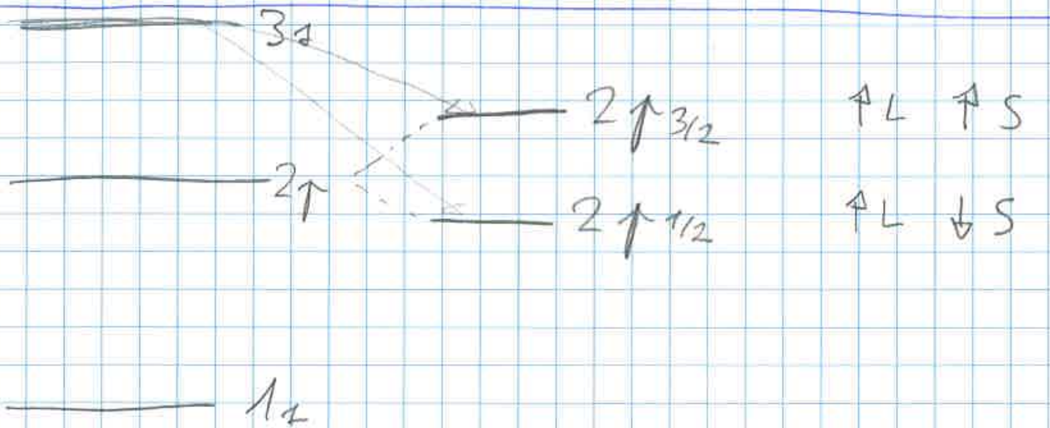
- $\frac{\Delta E}{E}$ 'UP' by 10^{-4} IF $\vec{S}$ and $\vec{L}$ are ~parallel $\left(j = l + \frac{1}{2}\right)$
- $\frac{\Delta E}{E}$ 'DOWN' by 10^{-4} IF $\vec{S}$ & $\vec{L}$ are ~antipar. $\left(j = l - \frac{1}{2}\right)$
- $\frac{\Delta E}{E} = 0$ IF $L = 0$ $\left(j = \frac{1}{2}\right)$

From EXAMPLE 8.3 (SUGGEST HOMEW.!) and Problems

- $\widetilde{\Delta E}$ splits the energy levels that have $l>0$ and gives rise to the FINE STRUCTURE.

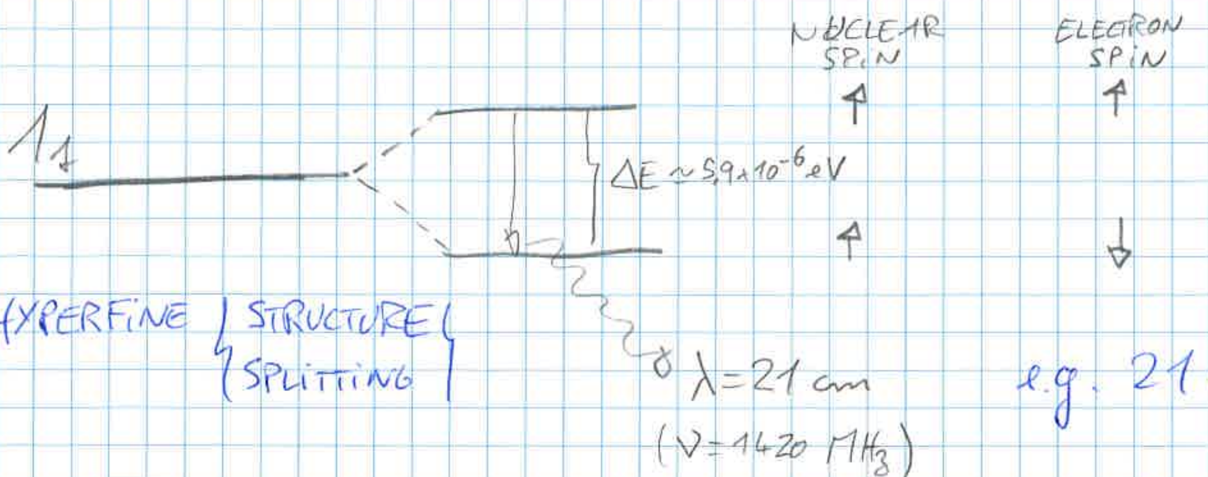
- For a precise comparison with atomic spectral data (lines), other effects have to be taken into account:
  - Relativistic effects ($m = m(v)$) shift all levels down by $\Delta E / E \sim 10^{-4}$ (depending on level, e.g. H $n=1$ E_1 decreases by 1.8×10^{-4} eV)
  - But these become even smaller for heavier atoms, so we don't study this correction in this course.

- Other type of spin couplings exists: WITH THE MAGNETIC DIPOLE MOMENT OF THE NUCLEUS: HYPERFINE STRUCTURE



FINE {STRUCTURE / SPLITTING}, e.g. $H\alpha$, $\lambda = 6564.7$ Å

$\Delta\lambda \simeq 0.16$ Å $(j = 3/2, 1/2)$



HYPERFINE {STRUCTURE / SPLITTING}

e.g. 21 cm H line