Quantum Mechanics and Atomic Physics

Lecture 21:
Spin-Orbit Coupling & Anomalous Zeeman Effect

http://www.physics.rutgers.edu/ugrad/361

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Last time: Fine-Structure Splitting due to Spin-Orbit Coupling

Now in the Dirac theory with $B_{\text{external}} = 0$

Notes:

1. Clearly this is not to scale!
2. Levels of the same $n$ and $j$ are degenerate
3. S states ($\ell=0$) are labeled “doublet” even though they are not!
Example

- By how much does the $1^2S_{1/2}$ energy differ from the Bohr value of $-13.6$ eV?

\[
\Delta E_{F,8} = E_{\text{Bohr}} \left[ \frac{3}{8n} \left( \frac{1}{j+y_2} - \frac{3}{4n} \right) \right]
\]

\[
= -13.6 \text{ eV} \left[ \left( \frac{1}{137} \right)^2 \left( \frac{1}{1} \right) \left( \frac{1}{y_2+y_2} - \frac{3}{4(1)} \right) \right]
\]

\[
= -13.6 \text{ eV} \left[ \left( \frac{1}{137} \right)^2 \left( \frac{1}{4} \right) \right]
\]

\[
= -13.6 \text{ eV} \left( 1.33 \times 10^{-5} \right)
\]

\[
= 1.81 \times 10^{-4} \text{ eV}
\]

- A little below the Bohr value
  - This is generally true
Example

- **Find the energy separation of** $^2P_{1/2}$ **and** $^2P_{3/2}$

\[ n=2 : \quad E_{\text{Bohr}} = -\frac{13.6 \text{ eV}}{(2)^2} = -3.4 \text{ eV} \]

\[
\Delta E_F (j=1/2) = -(3.4 \text{ eV}) \left( \frac{1}{3 \hbar} \right)^2 \left( \frac{1}{2} \right) \left( \frac{1}{2} \right) \left( \frac{1}{y_2 y_2} - \frac{3}{4.2} \right) \\
= -5.66 \times 10^{-5} \text{ eV}
\]

\[
\Delta E_F (j=3/2) = -(3.4 \text{ eV}) \left( \frac{1}{13 \hbar} \right)^2 \left( \frac{1}{2} \right) \left( \frac{1}{y_2 y_2} - \frac{3}{4.2} \right) \\
= -1.13 \times 10^{-5} \text{ eV}
\]

\[
E(2^2P_{3/2}) - E(2^2P_{1/2}) = +4.53 \times 10^{-5} \text{ eV}
\]

- **This is why it’s called “fine” structure!**
Selection Rules for radiative transitions

Similar to before, we have these selection rules:

\[
\Delta l = \pm 1, \\
\Delta j = 0, \pm 1, \\
\Delta m_j = 0, \pm 1
\]

So, for example:

- Forbidden or allowed?
- \(2 \, S_{1/2} \rightarrow 1 \, S_{1/2}\)
  - is forbidden
- \(2 \, P_{3/2} \rightarrow 1 \, S_{1/2}\)
  - is allowed
- \(2 \, P_{1/2} \rightarrow 1 \, S_{1/2}\)
  - is allowed
Anomalous Zeeman Effect

- Now we will again place the Hydrogen atom in an external B field

- Again, the magnetic moments are:

\[
\begin{align*}
\vec{\mu}_e &= -g \frac{e}{2m} \hat{\imath} \quad \text{with } g=1 \\
\vec{\mu}_s &= -g \frac{e}{2m} \hat{\jmath} \quad \text{with } g=2
\end{align*}
\]

- Let’s draw all the vectors ....
- $\mu_L$ is antiparallel to $L$
- $\mu_S$ is antiparallel to $S$

\[ \vec{\mu}_{\text{tot}} = \vec{\mu}_L + \vec{\mu}_S = -\frac{e}{2m} (\hat{L} + 2\hat{S}) \]

- $\mu_{\text{tot}}$ is not antiparallel to $J$
  - This is because $g \neq 1$ in formula for $\mu_S$
- So we cannot write \[ \vec{\mu}_{\text{tot}} = (\text{const}) \vec{J} \]

- Instead, we can define “the” magnetic moment as the component of $\mu_{\text{tot}}$ along the direction of $J$
- This is called $\mu_J$
The Magnetic Moment

So now we can define:

\[ M_J = \frac{\mu_{\text{Tot}} \cdot J}{J} \]

\[ \mu_{\text{Tot}} = \mu_L + \mu_S = -\frac{e}{2m}(\mathbf{L} + \mathbf{S}) \]

\[ = -\frac{e}{2m}(\mathbf{S} + \mathbf{S}) \]

Since \[ \mathbf{J} = \mathbf{L} + \mathbf{S} \]

\[ \Rightarrow M_J = -\frac{e}{2m} \left( \frac{\mathbf{J} \cdot \mathbf{J} + \mathbf{S} \cdot \mathbf{J}}{\sqrt{J(J+1)} \ h} \right) \]

Used \[ J = \sqrt{J(J+1)} \ h \]

\[ \Rightarrow M_J = -\frac{e}{2m} \left( \frac{1}{\sqrt{J(J+1)} \ h} \left( J(J+1) \ h^2 + \sqrt{s(sth)} \ \sqrt{s(sth)} \ h^2 \cos\theta \right) \right) \]

\[ M_J = -\frac{e \ h}{2m} \left( \sqrt{J(J+1)} + \sqrt{s(sth)} \ \cos\theta \right) \]

\( \theta \) is angle between \( \mathbf{S} \) and \( \mathbf{J} \)
Use the law of cosines

This is called the Landé g-factor

This is “the” magnetic moment
Back to anomalous Zeeman effect

- If the atom is placed in an external $B$ field, the energy levels will split:

\[
\Delta E = -\vec{\mu}_J \cdot \vec{B} = - (g \frac{e}{2m}) J \cdot \vec{B} = g \frac{e}{2m} B J \cos \theta = g \frac{e}{2m} B J y
\]

\[
= g \frac{e}{2m} B m_j \hbar
\]

\[
= \Delta E = m_j g \mu_B B
\]

\[
\mu_B = \frac{e\hbar}{2m} = 5.8 \times 10^{-5} \text{ eV/T}
\]

- Again $\mu_B$ is the Bohr magneton

- And $g$ is the Landé $g$-factor given earlier
Example

- For B=0, $3 \, S_{1/2}$ and $3 \, P_{1/2}$ are degenerate because they have the same n and j. What happens when $B \neq 0$?

- Since $j=1/2$, they split into $2j+1$ states, which in this case is 2 states

- With $m_j = -1/2$ and $m_j = +1/2$

- And energies:

$$E = E_{B=0} + m_j g \mu_B B$$
It should not be a surprise that $g=2$ for the $3S_{1/2}$ state. It means that since $\ell=0$ there is only spin!
Anomalous Zeeman Effect

- In an external B field, each Dirac level splits into \((2j+1)\) sublevels (“magnetic substates”)
- Each sublevel has a different value of \(m_j\)
- And the energy splitting is:

\[
E = E_{\text{Dirac}} + \Delta E
\]
\[
\Delta E = m_j g \mu_B B
\]
Anomalous Zeeman Effect

Let’s look at this effect for the n=3 energy levels in the H atom in an external B field:

\[
\begin{align*}
\frac{\hbar}{2} & \quad \frac{3\hbar}{2} \\
\frac{1\hbar}{2} & \quad \frac{3\hbar}{3} \\
\frac{-1\hbar}{2} & \quad \frac{2\hbar}{3} \\
\frac{-3\hbar}{2} & \quad \frac{4\hbar}{3}
\end{align*}
\]
Radiative transitions

- Let’s consider the $n=3 \rightarrow n=2$ transition.

- If $B=0$, then the energy of the radiated photon is the Bohr energy:

  $$E_\gamma = -\frac{13.6\text{eV}}{(3)^2} - (-\frac{13.6\text{eV}}{(2)^2}) = 1.9\text{eV}$$

- The $g$ factors are:

  $$g(2s_{1/2}) = 2, \quad g(3p_x) = \frac{\sqrt{3}}{2}, \quad g(3p_{3/2}) = \frac{\sqrt{3}}{2}$$

- And, if $B \neq 0$, $\Delta E = m_j g \mu_B B$

- The selection rules are:

  $$\Delta \ell = \pm 1, \quad \Delta j = 0, \pm 1, \quad \Delta m_j = 0, \pm 1$$
So the difference in the photon energy spectral lines will be (the total energy will be $E_{\text{Dirac}} + \Delta E \approx E_{\text{Bohr}} + \Delta E$):

$$\Delta E = \Delta E_i - \Delta E_f = [(m_j)_i - (m_j)_f] \mu eB$$

So the photon line splits into 4
So the photon line splits into six equally spaced lines.

Recall the normal Zeeman effect predicted 3 equally spaced lines.
Zeeman Effect in Sodium

- The sodium spectrum has a bright doublet at 588.9950 and 589.5924 nm.
- These lines are emitted in a transition from the 3p to the 3s levels.
- The sodium doublet is further split by the application of an external magnetic field.

Zeeman Effect
Animation

- [Website Link](https://web.phys.ksu.edu/vqm/software/online/vqm/html/zeemanspec.html)
Hyperfine Structure

- Proton and neutrons are also spin 1/2 particles

- So **nuclear** spin angular momentum can interact with the **electron’s** $\mu_J$ to split each Dirac energy level into two!

- But ... it’s a very tiny effect
  - Because $m_{\text{proton}} >> m_{\text{electron}}$

- This has only been observed for a few states of a few atoms

- Hyperfine splitting is $\sim 10^{-6} - 10^{-7}$ eV
In Hydrogen the hyperfine structure of the ground state has been observed only in astronomic measurements, not in labs!

- The electron and proton spins can be parallel and antiparallel
  - The antiparallel has slightly lower energy: \( \Delta E \sim 6 \times 10^{-6} \text{ eV} \)

- A spin flip transition can occur, emitting a photon of \( \lambda = 21 \text{ cm} \), \( \nu = 1420 \text{ MHz} \)
  - This is highly forbidden!

- The 21 cm line has been very useful for radio astronomy (e.g. measure the Doppler shift of the line to obtain the rotation speed of hydrogen in galaxy as a function of distance from the galactic center).

- Also used by SETI!
There’s even more to the story

- In 1947, Willis Lamb discovered that the $2P_{1/2}$ state is slightly lower than the $2S_{1/2}$ state resulting in a slight shift of the corresponding spectral line.
  - This is called the Lamb shift.

```
2s_{1/2} (l=0)  
|  4.372 \times 10^{-6} \text{ eV}  |
2p_{1/2} (l=1)
```

- One would think that such a tiny effect would be considered insignificant.
- But later Hans Bethe was the first to explain the Lamb shift in the hydrogen spectrum.
- Beginning of the modern development of quantum electrodynamics!
Summary/Announcements

- **Next time:** Multi-electron atoms
- **Next homework due on Monday Nov 25.**
- **Quiz next Monday, Nov. 25 on Chapter 7.**
- **Next Wednesday, November 27 we have no class**
  - *Wednesday ➔ Friday classes*