Honors Physics IIIa

Lecture 13:
Spin-orbital coupling, Anomalous Zeeman effect, Pauli Exclusion Principle

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Recap: Electron Spin Angular Momentum

- Relativistic quantum theory needed.
- Dirac equation (1928) was the answer.
- Electron must have a spin (or intrinsic) angular momentum.

\[ S = \sqrt{s(s + 1)} \hbar \quad \text{where} \quad s = \frac{1}{2} \]

So \[ S = \sqrt{(\frac{1}{2})(\frac{3}{2})} \hbar = \frac{\sqrt{3}}{2} \hbar \]

Then \[ S_z = m_s \hbar \quad \text{where} \quad m_s = -s, -s + 1, ..., +s \]

\[ \begin{align*}
&= -\frac{1}{2} \quad \text{or} \quad +\frac{1}{2}
\end{align*} \]
Consequences of Electron Spin

- Electron spin creates a spin magnetic moment.
- Electron’s orbital motion creates an internal magnetic field in an atom → spin-orbit coupling
- The two interact to cause a splitting of energy levels even if $B_{\text{external}} = 0$

\[ \vec{\mu}_L = -g \frac{e}{2m} \vec{L} \quad \text{with} \quad g = 1 \]

\[ \vec{\mu}_S = -g \frac{e}{2m} \vec{S} \quad \text{with} \quad g = 2 \quad \text{(because of relativity)} \]

(Predicted by relativistic QM [Dirac equation])
Letter convention

- Upper: operators, expectation values, …
  - H, L, L_z, S, S_z
- Lower: quantum #’s
  - n, l, m_l, s, m_s, …
Spin-orbit coupling (SOC)

- SOC is dipolar interaction between orbital magnetic moment ($\mu_L$) and spin magnetic moment ($\mu_S$).

- SOC is expressed in form of

$$H_{so} = \lambda_{so} \vec{L} \cdot \vec{S}$$

- It can be “derived” from a semi-classical picture, i.e. Zeeman energy due to magnetic field generated by circular motion of nucleus in electron’s rest frame.

- SOC is an relativistic effect (due to spin!)
SOC in H-atom (a semi-classical picture)

In the electron’s rest frame:

\[ B = \frac{\mu_0 I}{2r}, \quad I = \frac{ev}{2\pi r} \]

The magnetic field \( \Rightarrow B = \frac{\mu_0}{2r} \frac{ev}{2\pi r} = \frac{\mu_0 e}{4\pi r^3 m_e} L \)

The Coulomb potential of H-atom:

\[ U(r) = -\frac{1}{4\pi \varepsilon_0} \frac{e^2}{r} \Rightarrow \frac{\partial U(r)}{\partial r} = \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r^2} \]

\[ \Rightarrow B = \frac{\mu_0 e}{4\pi r^3 m_e} L = \frac{\mu_0 \varepsilon_0}{rm_e e} \left( \frac{1}{4\pi \varepsilon_0} \frac{e^2}{r^2} \right) L = \frac{1}{m_e c^2 \varepsilon_0} \frac{1}{r} \frac{\partial U(r)}{\partial r} L \]

\[ \Rightarrow H_{so} = -\frac{\mu}{\hbar} \cdot \vec{B} = g_s \mu_B \frac{\vec{S}}{\hbar} \cdot \vec{B} = \lambda_{so} \vec{S} \cdot \vec{L} \quad \lambda_{so} = \frac{g_s \mu_B}{m_e c^2 \varepsilon_0} \frac{1}{r} \frac{\partial U(r)}{\partial r} L \]

Although the picture is incorrect, the result is almost correct (except a factor of \( \frac{1}{2} \)).
Spin-Orbit Coupling

- Recall: \( \vec{\mu}_L = -g_L \mu_B \frac{\vec{L}}{\hbar} \) with \( g_L = 1 \)
  \[
  \mu_B = \frac{e \hbar}{2m_e}
  \]
  \( \vec{\mu}_S = -g_S \mu_B \frac{\vec{S}}{\hbar} \) with \( g_S = 2 \)

- Interaction of \( \mu_L \) and \( \mu_S \) causes a fine-structure splitting of energy levels, even if \( B_{\text{external}} = 0 \).

- Total angular momentum: \( \vec{J} = \vec{L} + \vec{S} \)
  \[
  J = |\vec{J}| = \sqrt{j(j + 1)\hbar}
  \]
  \( J_z = m_j \hbar \)
  \[
  j = |\ell - s|, |\ell - s| + 1, ..., (\ell + s)
  \]
  \( m_j = -j, -j + 1, ..., +j \)

- Dirac theory: use \( n, \ell, j, m_j \) instead of \( n, \ell, m_\ell, m_s \)
Total Angular Momentum

No external magnetic field:

\[ \vec{J} = \vec{L} + \vec{S} \]

(We’ll talk about what happens in a B field next time.)
Hydrogen Fine-Structure (SOC)

\[ j = |\ell - s|, |\ell - s| + 1, \ldots, (\ell + s) \]

- Only one electron, so \( s = 1/2 \)

so \( j = (\ell - \frac{1}{2}) \) or \( j = (\ell + \frac{1}{2}) \)

- Most of the Schrödinger energy levels in hydrogen should split into two levels.

- Exception: for \( \ell = 0 \), note that \( j = 1/2 \) only, i.e. no splitting.

where the fine structure constant is:

\[
E_{\text{Bohr}} = -\frac{1}{2} mc^2 \frac{\alpha^2}{n^2}
\]

\[
\alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c} = \frac{1}{137}
\]

\[
E_{\text{fine}} = E_{\text{Bohr}} \left[ 1 + \frac{\alpha^2}{n} \left( \frac{1}{j + 1/2} - \frac{3}{4n} \right) \right]
\]

- In the Dirac theory, levels of same \( n \) and \( j \) are degenerate.

- Fine structure splitting is \( \sim 10^{-5} \) eV
Spectroscopic Notation

- Useful to use spectroscopic notation: $n^{2s+1} L_j$
- and remember that $j = |\ell - s|$, $\ldots$, $(\ell + s)$.

- Since $s = 1/2$ in Hydrogen, $2s + 1 = 2$ always.

- Example:
  - $n = 4$, $\ell = 1$, $j = 3/2$
  - We write this as $4^2P_{3/2}$
  - Called “four doublet P three-halves”
Energy Level Diagram Revisited

Energy-level diagram for hydrogen in the Dirac theory of H-atom with zero external magnetic field (B=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!
Total Angular Momentum

With an external magnetic field:

- $\vec{J}$ precesses about $\vec{B}_{ext}$.
- $\vec{L}$ and $\vec{S}$ precess about $\vec{J}$
- Same for $\vec{\mu}_L$ and $\vec{\mu}_S$
Anomalous Zeeman Effect

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

- Again, the magnetic moments are:

  $$\vec{\mu}_L = -g_L \mu_B \frac{\vec{L}}{\hbar} \text{ with } g_L = 1$$

  $$\vec{\mu}_S = -g_S \mu_B \frac{\vec{S}}{\hbar} \text{ with } g_S = 2$$

- Let’s draw all the vectors ....
\( \vec{\mu}_L \) is antiparallel to \( \vec{L} \)

\( \vec{\mu}_S \) is antiparallel to \( \vec{S} \)

\[ \vec{\mu}_J = \vec{\mu}_L + \vec{\mu}_S \] is not on the axis of \( \vec{J} = \vec{L} + \vec{S} \).

However, due to Wigner-Eckart theorem, the expectation value \( \langle \vec{\mu}_J \rangle \) does effectively lie on the direction of \( \vec{J} \). Thus, we can define Lande g-factor \( g_J \) as \( \langle \vec{\mu}_J \rangle = -g_J \mu_B \langle \vec{J} \rangle / \hbar \). For convenience, we drop \( \langle \langle \rangle \) in following discussion.
\[ \vec{\mu}_J = -g_J \mu_B \vec{J} / \hbar \quad \Rightarrow \quad \vec{\mu}_J \cdot \vec{J} = -g_J \mu_B \vec{J}^2 / \hbar \]

\[ \vec{\mu}_J = \vec{\mu}_L + \vec{\mu}_S \quad \vec{\mu}_L = -g_L \mu_B \frac{\vec{L}}{\hbar} \quad \text{with} \quad g_L = 1 \quad \vec{L}^2 = j(j+1)\hbar^2 \]

\[ \vec{\mu}_S = -g_S \mu_B \frac{\vec{S}}{\hbar} \quad \text{with} \quad g_S = 2 \quad \vec{S}^2 = s(s+1)\hbar^2 \]

\[ \Rightarrow -\left( g_L \mu_B \vec{L} + g_S \mu_B \vec{S} \right) \cdot \left( \vec{L} + \vec{S} \right) = -g_J \mu_B \vec{J}^2 \]

\[ \Rightarrow g_J = \frac{g_L \vec{L}^2 + g_S \vec{S}^2 + (g_L + g_S) \vec{L} \cdot \vec{S}}{\vec{J}^2} \]

\[ \vec{J}^2 = (\vec{L} + \vec{S})^2 = \vec{L}^2 + \vec{S}^2 + 2\vec{L} \cdot \vec{S} \quad \Rightarrow \quad \vec{L} \cdot \vec{S} = \frac{\vec{J}^2 - \vec{L}^2 - \vec{S}^2}{2} \]

\[ \Rightarrow g_J = \frac{3\vec{J}^2 - \vec{L}^2 + \vec{S}^2}{2\vec{J}^2} \quad \Rightarrow \quad g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \]
This is called the Landé g-factor

\[ g_J = 1 + \frac{j(j+1) + s(s+1) - l(l+1)}{2j(j+1)} \]

Alternatively:

\[ g_J = \frac{3}{2} + \frac{s(s+1) - l(l+1)}{2j(j+1)} \]

\[ |\vec{J}| = \sqrt{j(j+1)\hbar} \]

\[ \vec{\mu}_J = -g \frac{e}{2m} \vec{J} \]

This is “the” magnetic moment

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

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

\[ \Rightarrow \Delta E = g \frac{e}{2m} B J_z = g \frac{e}{2m} B m_j \hbar = m_j g \mu_B B \]
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:

\[
E = E_{B=0} + m_j g \mu_B B
\]
\[ 3P_{\frac{1}{2}} : \quad \ell = 1, s = \frac{1}{2}, j = \frac{1}{2} \]

\[ g = 1 + \frac{(\frac{1}{2})(\frac{1}{2} + 1) + (\frac{1}{2})(\frac{1}{2} + 1) - (1)(2)}{(2)(\frac{1}{2})(\frac{1}{2} + 1)} = \frac{2}{3} \]

\[ 3S_{\frac{1}{2}} : \quad \ell = 0, s = \frac{1}{2}, j = \frac{1}{2} \]

\[ g = 1 + \frac{(\frac{1}{2})(\frac{3}{2}) + (\frac{1}{2})(\frac{3}{2}) - (0)(1)}{(2)(\frac{1}{2})(\frac{3}{2})} = 2 \]

Not surprising since \( \ell = 0 \), there is only spin.

Values of \( m_j \)
H-atom in External Field B

\[ E = E_{\text{Dirac}, B=0} + \Delta E \]

\[ \Delta E = m_j g \mu_B B \quad \text{and} \quad \mu_B = \frac{e\hbar}{2m} \]

- Each Dirac level splits into \((2j+1)\) sublevels.
- Each sublevel has a different value of \(m_j\).
- Let’s look at this effect for the \(n=3\) energy levels in the H atom in an external B field (figure on right)
Question 1

- Which of the following statements are true about the H atom fine-structure in no external magnetic field.
  A. $3P_{3/2}$ is degenerate with $3D_{3/2}$ but not with $3P_{1/2}$
  B. $3P_{3/2}$ is degenerate with $3P_{1/2}$ but not with $3D_{3/2}$
  C. $3P_{3/2}$ is degenerate with $3D_{3/2}$ as well as $3P_{1/2}$
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B. $3P_{3/2}$ is degenerate with $3P_{1/2}$ but not with $3D_{3/2}$

C. $3P_{3/2}$ is degenerate with $3D_{3/2}$ as well as $3P_{1/2}$

For fine-structure without an external field, $n$ and $j$ are degenerate.

For $3P_{3/2}$, $n=3$, $j=3/2$
Summary of H-Atom (single $e^-$)

Bohr’s model

<table>
<thead>
<tr>
<th>$n$</th>
<th>$E$ (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\infty$</td>
<td>0.00</td>
</tr>
<tr>
<td>4</td>
<td>-0.85</td>
</tr>
<tr>
<td>3</td>
<td>-1.51</td>
</tr>
<tr>
<td>2</td>
<td>-3.40</td>
</tr>
</tbody>
</table>

Energy Levels:

- $E_{Bohr} = -\frac{1}{2} mc^2 \frac{\alpha^2}{n^2}$
- $E_{fine} = E_{Bohr} \left[ 1 + \frac{\alpha^2}{n} \left( \frac{1}{j + 1/2} - \frac{3}{4n} \right) \right]$

Non-Rel. Sch. Eq.

<table>
<thead>
<tr>
<th>$\ell$</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n$</td>
<td>$\infty$</td>
<td>0</td>
<td>4</td>
<td>3</td>
<td>2</td>
</tr>
</tbody>
</table>

$S$ series:
- $-13.6$ (1s)

$P$ series:
- $-3.4$ (2p)

$D$ series:
- $-1.51$ (3d)

$F$ series:
- $-0.85$ (4f)

Dirac Eq. (SOC)

$\ell = 0$
- $4^2\text{S}_{1/2}$

$\ell = 1$
- $4^2\text{P}_{1/2}$
- $4^2\text{P}_{3/2}$

$\ell = 2$
- $4^2\text{D}_{5/2}$
- $4^2\text{D}_{3/2}$

$\ell = 3$
- $4^2\text{F}_{7/2}$
- $4^2\text{F}_{5/2}$
- $4^2\text{F}_{3/2}$
SOC in condensed matter physics

- Magnetocrystalline anisotropy (hard magnets)
- Rashba interaction (spintronics)
- Band inversion
  - Topological insulators
  - Dirac/Weyl semi-metals
- Dzyaloshinskii-Moriya interaction
  - Non-collinear spin orders
  - Skyrmions