Lecture 6 Zeemann Effects ICPY471 AMP, Second Trimester 2020-21

Udom Robkob, Physics-MUSC

Wednesday 27, 2021

Udom Robkob, Physics-MUSC

Lecture 6 Zeemann Effects

▶ ▲ ≧ ▶ ▲ ≧ ▶ ≧ ∽ Q (? Wednesday 27, 2021 1 / 15

The Zeemann effect.

- Pieter Zeeman in 1896 discovered that a magnetic field broadened the yellow D lines produced when sodium is placed in a flame. This is known as *normal Zeemann effect*.
- In 1897, Thomas Preston reported a similar effect to Zeeman but with more complicated results, it is known as *anomalous Zeemann effect*.
- The line splitting results from the effect of the magnetic field on the atomic energy levels. The magnetic interaction of atomic electron produces an amount of energy

$$U_B = -\vec{\mu}_e \cdot \vec{B},\tag{1}$$

$$\vec{\mu}_e = \frac{-e}{2m_e}(\vec{L} + g\vec{S}), \quad g = 2$$
 (2)

• For a uniform magnetic in z-direction, $\vec{B} = B\hat{z}$, we will have

$$U_B = \frac{e}{2m_e}(L_z + 2S_z)B = \frac{\mu_B B}{\hbar}(L_z + 2S_z)$$
(3)

where $\mu_B = \frac{e\hbar}{2m_e} = 5.788 \times 10^{-5} eV/T$ is Bohr magneton.

Weak-field Zeemann effect

• The weak-field Zeemann effect can be *normal* when the electron spin magnetic moment dose not have any contribution to the magnetic interaction, or it can be *anomalous* when the electron spin magnetic moment have contribution in magnetic interaction.

Weak-field Zeemann effect

- The weak-field Zeemann effect can be *normal* when the electron spin magnetic moment dose not have any contribution to the magnetic interaction, or it can be *anomalous* when the electron spin magnetic moment have contribution in magnetic interaction.
- Normal Zeeman effect is determined from the magnetic interaction energy

$$U_B = \frac{\mu_B B}{\hbar} L_z \tag{4}$$

Takes this as the perturbation to the hydrogen energy level, when apply with perturbation theory using the unperturbed atomic state $|nlm\rangle$, we will have perturbed atomic energy, at the first order, as

$$\Delta E_{nlm}^{(1)} = < nlm | U_B | nlm > = m\mu_B B \tag{5}$$

$$E_n \to E_{nlm}^{(1)} = E_n^{(0)} + m\mu_B B$$
 (6)



3

イロト イヨト イヨト イヨト



• Anomalous Zeemann effect is determined from the magnetic interaction energy

$$U_B = \frac{\mu_B B}{\hbar} (L_z + gS_z), \ g = 2 \tag{7}$$

Takes this as the perturbation of atomic energy level. In the weak field limit, the magnetic interaction energy is comparable to the spin-orbit coupling energy, so that we have to determine it from the total angular momentum state $|nljm_j >$.

Udom Robkob, Physics-MUSC

Lecture 6 Zeemann Effects

• Let us determine the total angular momentum

The projection of \vec{S} onto the direction of \vec{J} is written as

$$\vec{S}_J = \frac{\vec{S} \cdot \vec{J}}{J^2} \vec{J}$$
(9)

It will be used to evaluate the quantum expectation value from the state $|nljm_j >$.

• (Cont.) We can evaluate $\vec{S} \cdot \vec{J}$ from the fact that

$$\vec{L} = \vec{J} - \vec{S} \to L^2 = J^2 + S^2 - 2\vec{S} \cdot \vec{J}$$
(10)

$$\rightarrow \vec{S} \cdot \vec{J} = \frac{1}{2} (J^2 - L^2 - S^2)$$
 (11)

• (Cont.) We can evaluate $\vec{S} \cdot \vec{J}$ from the fact that

$$\vec{L} = \vec{J} - \vec{S} \to L^2 = J^2 + S^2 - 2\vec{S} \cdot \vec{J}$$
 (10)

$$\rightarrow \vec{S} \cdot \vec{J} = \frac{1}{2} (J^2 - L^2 - S^2)$$
 (11)

It follows that

$$\langle nljm_j | (L_z + gS_z) | nljm_j \rangle = \left\langle nljm_j \left| \left(1 + (g-1)\frac{\vec{S} \cdot \vec{J}}{J^2} \right) J_z \right| nljm_j \right\rangle$$
$$= \hbar m_j \left(1 + \frac{(g-1)}{2} \frac{j(j+1) - l(l+1) + s(s+1)}{j(j+1)} \right) = \hbar g_J m_j (12)$$

where we have defined Lande g-factor

$$g_J = 1 + \frac{g - 1}{2} \frac{j(j+1) - l(l+1) + s(s+1)}{j(j+1)}$$
(13)

Udom Robkob, Physics-MUSC

< 47 ▶

Lande g-factors for one electron atoms

L	Term	9j	g _j m _j
0	² S _{1/2}	2	± 1
1	² P _{1/2}	2/3	±1/3
	² P _{3/2}	4/3	±2/3, ±6/3
2	² D _{1/2}	4/5	±2/5, ±6/5
	² D _{3/2}	6/5	±3/5, ±9/5, ±15/5
3	² F _{1/2}	6/7	±3/7, ±9/7, ±15/7
	² F _{3/2}	8/7	±4/7, ±12/7, ±20/7, ±28/7

- 2

イロト イポト イヨト イヨト

Lande g-factors for one electron atoms

L	Term	9j	g _j m _j
0	² S _{1/2}	2	± 1
1	² P _{1/2}	2/3	±1/3
	² P _{3/2}	4/3	±2/3, ±6/3
2	² D _{1/2}	4/5	±2/5, ±6/5
	² D _{3/2}	6/5	±3/5, ±9/5, ±15/5
3	² F _{1/2}	6/7	±3/7, ±9/7, ±15/7
	² F _{3/2}	8/7	±4/7, ±12/7, ±20/7, ±28/7

• From (7) we have the perturbed energy, at the first order level, equal to

$$\Delta E_{nljm_j}^{(1)} = g_J m_j \mu_B B \tag{14}$$

< □ > < □ > < □ > < □ > < □ > < □ >

3



We have no transitions 2S
ightarrow 1S, according to the *selection rules*.

3

A D N A B N A B N A B N

Strong-field Zeemann effect

- In the strong field limit, the magnetic interaction energy become greater than the spin-orbit coupling energy, so the we may think of the magnetic interaction independently with orbital and spin magnetic moments.
- Takes this interaction as the perturbation of the atomic levels, and the first order perturbation energy will be determined form the atomic state $|nlm_lsm_s>$

Strong-field Zeemann effect

- In the strong field limit, the magnetic interaction energy become greater than the spin-orbit coupling energy, so the we may think of the magnetic interaction independently with orbital and spin magnetic moments.
- Takes this interaction as the perturbation of the atomic levels, and the first order perturbation energy will be determined form the atomic state $|nlm_lsm_s>$
- Then we have

$$\Delta E_{nlm_lm_s}^{(1)} = \left\langle nlm_l sm_s \left| \frac{\mu_B B}{\hbar} (L_z + gS_z) \right| nlm_l sm_s \right\rangle$$
$$= (m_l + gm_s) \mu_B B \tag{15}$$

It is known as the Paschen-Back effect.



** Magnetic interaction effects to the atomic energy levels splitting in the same order of atomic fine structures.

Udom Robkob, Physics-MUSC

Lecture 6 Zeemann Effects

Wednesday 27, 2021 10 / 15

Intermediate-field Zeemann effect

- We do not have asymptotic connection between the weak and strong field Zeemann effects, since they use different sets of atomic state.
- One way we can do this is by rewriting one atomic state in term of the other.

Intermediate-field Zeemann effect

- We do not have asymptotic connection between the weak and strong field Zeemann effects, since they use different sets of atomic state.
- One way we can do this is by rewriting one atomic state in term of the other.
- We choose |ls; m_lm_s > as a good set of atomic state, and will do the expansion of the other set |ls; jm_j > on this set as

$$|ls; jm_j \rangle = \sum_{m_l, m_s} C_{m_l m_s m_j}^{lsj} |ls; m_l m_s \rangle$$
(16)

$$C_{m_l m_s m_j}^{lsj} = < ls; m_l m_s | ls; jm_j > \rightarrow CG - coefficient$$
 (17)

where we have ignored the independent *n*-quantum number.

Intermediate-field Zeemann effect

- We do not have asymptotic connection between the weak and strong field Zeemann effects, since they use different sets of atomic state.
- One way we can do this is by rewriting one atomic state in term of the other.
- We choose |ls; m_lm_s > as a good set of atomic state, and will do the expansion of the other set |ls; jm_j > on this set as

$$|ls; jm_j \rangle = \sum_{m_l, m_s} C_{m_l m_s m_j}^{lsj} |ls; m_l m_s \rangle$$
(16)

$$C_{m_l m_s m_j}^{lsj} = < ls; m_l m_s | ls; jm_j > \rightarrow CG - coefficient$$
 (17)

where we have ignored the independent *n*-quantum number.

• For I = 0, we have $\psi_{I,i} = |jm_j >, i = 1, ..., 2j + 1$ as

$$\psi_{0,1} = |1/2, +1/2 \rangle = |0, 1/2; 0, +1/2 \rangle$$
(18)

$$\psi_{0,2} = |1/2, -1/2 \rangle = |0, 1/2; 0, = 1/2 \rangle$$
(19)



• For l = 1, we will have

$$\begin{split} \psi_{1,1} &= |\frac{3}{2}, +\frac{3}{2} >= |1, \frac{1}{2}; +1, +\frac{1}{2} > \tag{20} \\ \psi_{1,2} &= |\frac{3}{2}, -\frac{3}{2} >= |1, \frac{1}{2}; -1, -\frac{1}{2} > \tag{21} \\ \psi_{1,3} &= |\frac{3}{2}, +\frac{1}{2} >= \sqrt{\frac{1}{3}} |1, \frac{1}{2}; 1, -\frac{1}{2} > +\sqrt{\frac{2}{3}} |1, \frac{1}{2}; 0, +\frac{1}{2} > (22) \\ \psi_{1,4} &= |\frac{1}{2}, +\frac{1}{2} >= \sqrt{\frac{2}{3}} |1, \frac{1}{2}; +1, -\frac{1}{2} > -\sqrt{\frac{1}{3}} |1, \frac{1}{2}; 0, +\frac{1}{2} > (23) \end{split}$$

Udom Robkob, Physics-MUSC

Wednesday 27, 2021 12 / 15

э

イロト イヨト イヨト イヨト

• For l = 1, cont.

$$\begin{split} \psi_{1,5} &= |\frac{3}{2}, -\frac{1}{2} >= \sqrt{\frac{2}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} > +\sqrt{\frac{1}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} > (24) \\ \psi_{1,6} &= |\frac{1}{2}, -\frac{1}{2} >= \sqrt{\frac{1}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} > -\sqrt{\frac{2}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} > (25) \end{split}$$

- 2

• For l = 1, cont.

$$\begin{split} \psi_{1,5} &= |\frac{3}{2}, -\frac{1}{2} >= \sqrt{\frac{2}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} > +\sqrt{\frac{1}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} > (24) \\ \psi_{1,6} &= |\frac{1}{2}, -\frac{1}{2} >= \sqrt{\frac{1}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} > -\sqrt{\frac{2}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} > (25) \end{split}$$

• The weak-field Zeemann effect will be calculated in term of the matrix elements as

$$W_{I,ij} = \mu_B B \langle \psi_i | (m_I + gm_s) | \psi_j \rangle$$
(26)

Image: A matrix

• For l = 1, cont.

$$\psi_{1,5} = |\frac{3}{2}, -\frac{1}{2} \rangle = \sqrt{\frac{2}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} \rangle + \sqrt{\frac{1}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} \rangle (24)$$

$$\psi_{1,6} = |\frac{1}{2}, -\frac{1}{2} \rangle = \sqrt{\frac{1}{3}} |1, \frac{1}{2}; 0, -\frac{1}{2} \rangle - \sqrt{\frac{2}{3}} |1, \frac{1}{2}; -1, +\frac{1}{2} \rangle (25)$$

• The weak-field Zeemann effect will be calculated in term of the matrix elements as

$$W_{I,ij} = \mu_B B \langle \psi_i | (m_I + gm_s) | \psi_j \rangle$$
(26)

• For l = 0

$$W_{0,ij} = \mu_B B \left(\begin{array}{cc} 1 & 0 \\ 0 & -1 \end{array} \right) \tag{27}$$

Image: A matrix

• For l = 1

$$W_{1,ij} = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2/3 & -\sqrt{2}/3 & 0 & 0 \\ 0 & 0 & -\sqrt{2}/3 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2/3 & -\sqrt{2}/3 \\ 0 & 0 & 0 & 0 & -\sqrt{2}/3 & -1/3 \end{pmatrix}$$
(28)

- 2

• For *l* = 1

$$W_{1,ij} = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2/3 & -\sqrt{2}/3 & 0 & 0 \\ 0 & 0 & -\sqrt{2}/3 & 1/3 & 0 & 0 \\ 0 & 0 & 0 & 0 & -2/3 & -\sqrt{2}/3 \\ 0 & 0 & 0 & 0 & -\sqrt{2}/3 & -1/3 \end{pmatrix}$$
(28)

• The following sub matrices need diagonalization

$$W_{1,(34)_{ij}} = \begin{pmatrix} 2/3 & -\sqrt{2}/3 \\ -\sqrt{2}/3 & 1/3 \end{pmatrix}$$
(29)
$$W_{1,(56)_{ij}} = \begin{pmatrix} -2/3 & -\sqrt{2}/3 \\ -\sqrt{2}/3 & -1/3 \end{pmatrix}$$
(30)

Image: A match a ma

Conclusions

- ▶ In the weak field limit, $|n|; jm_j >$ is a good quantum state
- In the strong field limit, |nls; m₁m₅ > is a good quantum state, and related to |nl; jm_j >, as appear in (18-25).

• The diagonalization process will be posted in Mathematica Code later!