

Spin in magnetic field

$$\vec{S} = S_x \hat{x} + S_y \hat{y} + S_z \hat{z} = \frac{\hbar}{2} (\sigma_x \hat{x} + \sigma_y \hat{y} + \sigma_z \hat{z}), \quad \langle S^2 \rangle = \hbar^2 s(s+1), \quad s = \frac{1}{2}$$

σ 's are 2×2 Pauli matrices. $\langle S_z \rangle = m_s \hbar \quad m_s = \pm \frac{1}{2}$

Hamiltonian: $H = 2 \frac{\mu_B}{\hbar} \vec{S} \cdot \vec{B} = \mu_B \sigma_z B_z \quad (\vec{B} = B_z \hat{z})$

↑
"Lorentz boost" → "Thomas factor"
"electron g-factor"

$$H = \begin{bmatrix} \mu_B B_z & 0 \\ 0 & -\mu_B B_z \end{bmatrix} \xrightarrow[\text{eigenvectors}]{\text{eigenvalues}}$$

$$E = +\mu_B B_z, \quad \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{"up"} = |\uparrow\rangle$$

$$E = -\mu_B B_z, \quad \begin{bmatrix} 0 \\ 1 \end{bmatrix} \quad \text{"down"} = |\downarrow\rangle$$

$$= \overset{2}{\downarrow} g \mu_B B_z m_s$$

State evolution

Example: $|\psi(0)\rangle$ is eigenvector of $S_x = \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \Rightarrow +\frac{\hbar}{2}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = |+\rangle$
 $-\frac{\hbar}{2}, \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = |-\rangle$

Now, apply $\vec{B} = B_z \hat{z}$

$$|+\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} : \frac{1}{\sqrt{2}} \left(\begin{bmatrix} 1 \\ 0 \end{bmatrix} e^{-i \frac{\mu_B B_z t}{\hbar}} + \begin{bmatrix} 0 \\ 1 \end{bmatrix} e^{+i \frac{\mu_B B_z t}{\hbar}} \right)$$

What is $\langle S_x(t) \rangle$?

$$\langle + | S_x | + \rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{+i \frac{\mu_B B_z t}{\hbar}} & e^{-i \frac{\mu_B B_z t}{\hbar}} \end{bmatrix} \frac{\hbar}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-i \frac{\mu_B B_z t}{\hbar}} \\ e^{+i \frac{\mu_B B_z t}{\hbar}} \end{bmatrix}$$

$$= \frac{\hbar}{4} \left(e^{2i \frac{\mu_B B_z t}{\hbar}} + e^{-2i \frac{\mu_B B_z t}{\hbar}} \right) = \frac{\hbar}{2} \cos \frac{2\mu_B B_z t}{\hbar} \left. \vphantom{\frac{\hbar}{2} \cos \frac{2\mu_B B_z t}{\hbar}} \right\} \text{precession!}$$

$$\text{Similarly, } \langle + | S_y | + \rangle = \frac{\hbar}{2} \sin \frac{2\mu_B B_z t}{\hbar}$$

Adding orbital and spin angular momentum

$$H = \frac{\mu_B}{\hbar} \vec{L} \cdot \vec{B} + 2 \frac{\mu_B}{\hbar} \vec{S} \cdot \vec{B} = \frac{\mu_B}{\hbar} (\vec{L} + 2\vec{S}) \cdot \vec{B}$$

Only $\vec{J} = \vec{L} + \vec{S}$ is conserved, not $\vec{L} + 2\vec{S}$. Does $E = "g" \mu_B B_z m_J$??

$$H = \frac{\mu_B}{\hbar} \frac{(\vec{L} + 2\vec{S}) \cdot \vec{J}}{|\vec{J}|} \cdot \frac{\vec{B} \cdot \vec{J}}{|\vec{J}|} = \frac{\mu_B}{\hbar} \frac{(\vec{L} + 2\vec{S}) \cdot (\vec{L} + \vec{S})}{J^2} J_z B_z$$

$$= \frac{\mu_B}{\hbar} \frac{(L^2 + 2S^2 + 3\vec{S} \cdot \vec{L})}{J^2} J_z B_z$$

$$L^2 = \hbar^2 l(l+1), \quad l = 0, 1, 2, \dots$$

$$S^2 = \hbar^2 s(s+1) = \frac{3}{4} \hbar^2$$

$$J^2 = \hbar^2 j(j+1), \quad j = l-s, l+s$$

What is $\vec{S} \cdot \vec{L}$?

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

$$\text{So } \vec{S} \cdot \vec{L} = \frac{J^2 - L^2 - S^2}{2}$$

Landé g-factor

$$E = \frac{\mu_B}{\hbar} \frac{(L^2 + 2S^2 + \frac{3}{2}(J^2 - L^2 - S^2))}{J^2} \hbar m_J B_z$$

$$= \mu_B \frac{\frac{3}{2}J^2 - \frac{1}{2}L^2 + \frac{1}{2}S^2}{J^2} m_J B_z = \left(1 + \frac{J^2 - L^2 + S^2}{2J^2}\right) \mu_B m_J B_z$$

$$= g_L \mu_B m_J B_z$$

where g_L (Landé g-factor) is given by

$$g_L = 1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$$

Lande g-factor examples

$$\underline{l=0}$$

$$j=s=\frac{1}{2}$$

$$g_L = 1 + \frac{\frac{1}{2}(\frac{3}{2}) - 0(0+1) + \frac{1}{2}(\frac{3}{2})}{2 \cdot \frac{1}{2}(\frac{3}{2})} = 2$$

$$\underline{l=1}$$

$$j = \frac{1}{2} \text{ or } \frac{3}{2}$$

$$g_L = \begin{cases} 1 + \frac{\frac{1}{2}(\frac{3}{2}) - 1(2) + \frac{1}{2}(\frac{3}{2})}{2 \cdot \frac{1}{2}(\frac{3}{2})} = 1 + \frac{\frac{3}{4} - \frac{8}{4} + \frac{3}{4}}{\frac{6}{4}} = \frac{2}{3} \quad (j=\frac{1}{2}) \\ \text{or} \\ 1 + \frac{\frac{3}{2}(\frac{5}{2}) - 1(2) + \frac{1}{2}(\frac{3}{2})}{2 \cdot \frac{3}{2}(\frac{5}{2})} = 1 + \frac{\frac{15}{4} - \frac{8}{4} + \frac{3}{4}}{\frac{30}{4}} = \frac{4}{3} \quad (j=\frac{3}{2}) \end{cases}$$

Anomalous Zeeman Effect

$l=1$	$m_j = +\frac{3}{2}$	$\frac{j}{3/2}$	$\frac{g_L}{4/3}$
	$m_j = +\frac{1}{2}$	$\frac{3}{2}$	$\frac{4}{3}$
	$m_j = +\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{3}$
	$m_j = -\frac{1}{2}$	$\frac{1}{2}$	$\frac{2}{3}$
	$m_j = -\frac{1}{2}$	$\frac{3}{2}$	$\frac{4}{3}$
	$m_j = -\frac{3}{2}$	$\frac{3}{2}$	$\frac{4}{3}$

$$l=0 \begin{cases} m_j = \frac{1}{2} \\ m_j = -\frac{1}{2} \end{cases} \quad (g_L = 2)$$
$$j = \frac{1}{2}$$

$j = \frac{3}{2} \rightarrow j = \frac{1}{2}$ transitions:

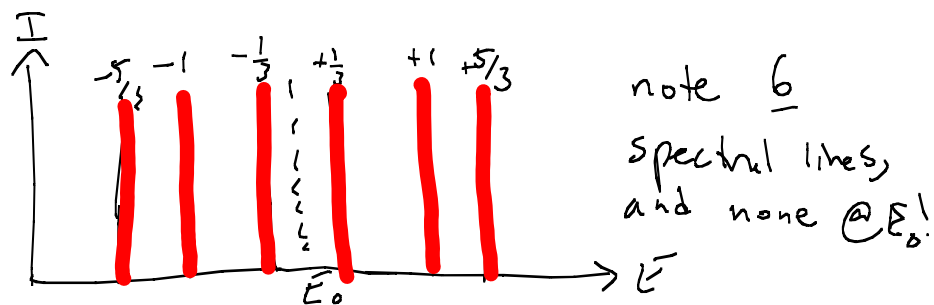
$$\frac{\Delta E \propto (g_L m_j)^i - (g_L m_j)^f}{2 - 1} = +1$$

$$\frac{2}{3} - 1, \frac{2}{3} + 1 = -\frac{1}{3}, \frac{5}{3}$$

$$-\frac{2}{3} + 1, -\frac{2}{3} - 1 = \frac{1}{3}, -\frac{5}{3}$$

$$-2 + 1 = -1$$

Spectroscopy in B-field:



All because g_L is different for different states!

In terms of matrices

Example: $l=1, s=\frac{1}{2}$

Then (without proof)

$$L_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad L_y = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad L_z = \hbar \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

what is $J^2 = L^2 + S^2 + 2\vec{S} \cdot \vec{L}$? a 6×6 matrix!!

$$\begin{aligned} &= (\mathbb{I}_2 \otimes L_x)^2 + (S_x \otimes \mathbb{I}_3)^2 + 2S_x \otimes L_x \\ &+ (\mathbb{I}_2 \otimes L_y)^2 + (S_y \otimes \mathbb{I}_3)^2 + 2S_y \otimes L_y \\ &+ (\mathbb{I}_2 \otimes L_z)^2 + (S_z \otimes \mathbb{I}_3)^2 + 2S_z \otimes L_z \end{aligned}$$

 Kronecker product merges the 2×2 space w/ 3×3 space to create a larger 6×6 space!

Numerical Calculation

```
Sx=1/2*[0 1;1 0];
Sy=1/2*[0 -i ; i 0];
Sz=1/2*[1 0; 0 -1];
Lx=1/sqrt(2)*[0 1 0; 1 0 1; 0 1 0];
Ly=1/sqrt(2)*[0 -i 0; i 0 -i; 0 i 0];
Lz=[1 0 0; 0 0 0 ; 0 0 -1];
```

```
Ssqrd=kron(eye(3), Sx)^2+kron(eye(3), Sy)^2+kron(eye(3), Sz)^2;
Lsqrd=kron(Lx, eye(2))^2+kron(Ly, eye(2))^2+kron(Lz, eye(2))^2;
SdotL=kron(Lx,Sx)+kron(Ly,Sy)+kron(Lz,Sz);
```

```
Jsqrd=Ssqrd+Lsqrd+2*SdotL;
```

```
[v,d]=eig(Jsqrd);
diag(d)
```

```
gL=(Lsqrd+2*Ssqrd+3*SdotL)/Jsqrd;
eig(gL)
```

$$\frac{J^2}{\hbar^2} = \begin{bmatrix} 3.75000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 1.75000 & 1.41421 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 1.41421 & 2.75000 & 0.00000 & 0.00000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 2.75000 & 1.41421 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 1.41421 & 1.75000 & 0.00000 \\ 0.00000 & 0.00000 & 0.00000 & 0.00000 & 0.00000 & 3.75000 \end{bmatrix}$$

eigenvalues of $\frac{J^2}{\hbar^2} = \begin{matrix} 0.75000 \\ 0.75000 \\ 3.75000 \\ 3.75000 \\ 3.75000 \\ 3.75000 \end{matrix} \left\{ \begin{matrix} = \frac{3}{4} = \frac{1}{2}(\frac{1}{2}+1) \\ = \frac{15}{4} = \frac{3}{2}(\frac{3}{2}+1) \end{matrix} \right.$

$\langle g_L \rangle = \begin{matrix} 0.66667 \\ 1.33333 \\ 1.33333 \\ 0.66667 \\ 1.33333 \\ 1.33333 \end{matrix}$

i.e. $\frac{2}{3}$ or $\frac{4}{3}$, same as calculation w/ $j = l \pm s$ and $1 + \frac{j(j+1) - l(l+1) + s(s+1)}{2j(j+1)}$.