Lecture 17: Addition of two spins - Singlets + Triplets

Let us explicitly calculate the coupled basis for two spins $\frac{1}{2}$, by diagonalizing the matrices for the operators $\hat{\vec{S}}^2$ and $\hat{S}_z$

Matrix representations in product basis:

$$\hat{S}_z \,|s_A\, m_{s_A};\, s_B\, m_{s_B}\rangle = \left(\hat{S}_{z_A} + \hat{S}_{z_B}\right) |s_A\, m_{s_A}\rangle \otimes |s_B\, m_{s_B}\rangle$$

$$= \left(m_{s_A} + m_{s_B}\right) |s_A\, m_{s_A}\rangle \otimes |s_B\, m_{s_B}\rangle$$

$\Rightarrow$ $\hat{S}_z$ is diagonal in this bas

$$\hat{S}_z = \begin{array}{c} \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & 0 & \\ & & & -1 \end{bmatrix} \end{array}$$

However, $\hat{\vec{S}}^2 |s_A, m_{s_A};\, s_B\, m_{s_B}\rangle = \left(\hat{\vec{S}}_A^2 + \hat{\vec{S}}_B^2 + 2\vec{S}_A \cdot \vec{S}_B\right) |\quad\rangle$

$$= \left(\tfrac{3}{4} + \tfrac{3}{4}\right) |s_A, m_{s_A};\, s_B, m_{s_B}\rangle$$

$$+ 2\, \hat{\vec{S}}_A \cdot \hat{\vec{S}}_B \,|s_A, m_{s_A};\, s_B, m_{s_B}\rangle$$

Aside: $\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B = \frac{1}{4}\left(\hat{\sigma}_x^A \otimes \hat{\sigma}_x^B + \hat{\sigma}_y^A \otimes \hat{\sigma}_y^B + \hat{\sigma}_z^A \otimes \hat{\sigma}_z^B\right)$

$$\hat{\sigma}_x = \hat{\sigma}_+ + \hat{\sigma}_- \qquad \hat{\sigma}_y = -i(\hat{\sigma}_+ - \hat{\sigma}_-)$$

$$\Rightarrow \hat{\vec{S}}_A \cdot \hat{\vec{S}}_B = \frac{1}{4}\Big[(\hat{\sigma}_+^A + \hat{\sigma}_-^A) \otimes (\hat{\sigma}_+^B + \hat{\sigma}_-^B) - (\hat{\sigma}_+^A - \hat{\sigma}_-^A) \otimes (\hat{\sigma}_+^B - \hat{\sigma}_-^B) + \hat{\sigma}_z^A \otimes \hat{\sigma}_z^B\Big]$$

$$\Rightarrow 2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B = \hat{\sigma}_+^A \otimes \hat{\sigma}_-^B + \hat{\sigma}_-^A \otimes \hat{\sigma}_+^B + \frac{1}{2}\hat{\sigma}_z^A \otimes \hat{\sigma}_z^B$$

$$\Rightarrow 2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B |\uparrow\uparrow\rangle = \frac{1}{2}\hat{\sigma}_z|\uparrow\rangle_A \otimes \hat{\sigma}_z|\uparrow\rangle_B = \frac{1}{2}|\uparrow\uparrow\rangle$$

$$2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B |\uparrow\downarrow\rangle = \hat{\sigma}_-^A|\uparrow\rangle_A \otimes \hat{\sigma}_+^B|\downarrow\rangle + \frac{1}{2}\hat{\sigma}_z|\uparrow\rangle_A \otimes \hat{\sigma}_z|\downarrow\rangle_B$$

$$= |\downarrow\uparrow\rangle - \frac{1}{2}|\uparrow\downarrow\rangle$$

$$2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B |\downarrow\uparrow\rangle = \hat{\sigma}_+|\downarrow\rangle_A \otimes \hat{\sigma}_-|\uparrow\rangle_B + \frac{1}{2}\hat{\sigma}_z|\downarrow\rangle \otimes \hat{\sigma}_z|\uparrow\rangle$$

$$= |\uparrow\downarrow\rangle - \frac{1}{2}|\downarrow\uparrow\rangle$$

$$2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B |\downarrow\downarrow\rangle = \frac{1}{2}\hat{\sigma}_z|\downarrow\rangle_A \otimes \hat{\sigma}_z|\downarrow\rangle_B = \frac{1}{2}|\downarrow\downarrow\rangle$$

Now on the two spin-½ systems

$$\hat{\vec{S}}^2 = \frac{3}{2}\hat{\mathbb{1}}_{AB} + 2\hat{\vec{S}}_A \cdot \hat{\vec{S}}_B$$

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Thus,

$$\hat{S}^2|\uparrow\uparrow\rangle = \tfrac{3}{2}|\uparrow\uparrow\rangle + \tfrac{1}{2}|\uparrow\uparrow\rangle = 2|\uparrow\uparrow\rangle$$

$$\hat{S}^2|\downarrow\downarrow\rangle = \tfrac{3}{2}|\downarrow\downarrow\rangle + \tfrac{1}{2}|\downarrow\downarrow\rangle = 2|\downarrow\downarrow\rangle$$

$$\hat{S}^2|\uparrow\downarrow\rangle = \tfrac{3}{2}|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle - \tfrac{1}{2}|\uparrow\downarrow\rangle$$
$$= |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle$$

$$\hat{S}^2|\downarrow\uparrow\rangle = \tfrac{3}{2}|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle - \tfrac{1}{2}|\downarrow\uparrow\rangle$$
$$= |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle$$

$$\Rightarrow \hat{S}^2 = \begin{array}{c} \begin{array}{cccc} |\uparrow\uparrow\rangle & |\uparrow\downarrow\rangle & |\downarrow\uparrow\rangle & |\downarrow\downarrow\rangle \end{array} \\ \left[\begin{array}{c|cc|c} 2 & & & \\ \hline & 1 & 1 & \\ & 1 & 1 & \\ \hline & & & 2 \end{array}\right] \end{array}$$

$\Rightarrow$ $\hat{S}^2$ is "block-diagonal"

The states $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are eigenvectors of $\hat{S}^2$

We must diagonalize the block in the subspace spanned by $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$

<u>Note:</u> the two states $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ have degenerate eigenvalues for $\hat{S}_z$, $M = 0$

Any linear combination of these states still have $M = 0$ for $\hat{S}_z$ total

In this subspace

$$\hat{\vec{S}}^2 \doteq \begin{array}{cc} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \\ |\uparrow\downarrow\rangle \quad |\downarrow\uparrow\rangle \end{array}$$

seek solution to $\hat{\vec{S}}^2 |\lambda\rangle = \lambda |\lambda\rangle$

Characteristic equation

$$\det(\hat{\vec{S}}^2 - \lambda \hat{\mathbb{1}}) = \det \begin{bmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{bmatrix} = (1-\lambda)^2 - 1 = 0$$

$$\Rightarrow \lambda^2 - 2\lambda = 0$$

Eigenvalues: $\lambda = 0$, $\vec{S}^2 |\lambda\rangle = S(S+1)|\lambda\rangle = 0 \Rightarrow S = 0$

$\lambda = 2$, $\hat{\vec{S}}^2 |\lambda\rangle = S(S+1)|\lambda\rangle \Rightarrow S = 1$

Eigenvectors: $S = 0$: $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} = \frac{1}{2}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

$S = 1$: $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \frac{1}{2}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$

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Thus we arrive at the eigenvectors ~~for~~ the Coupled representation expanded in the product basis:

$$\boxed{\begin{array}{l} \underline{\text{Singlet:}} \\ |S=0, M=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right) \\ \\ \underline{\text{Triplet:}} \\ |S=1, M=1\rangle = |\uparrow\uparrow\rangle \\ |S=1, M=0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right) \\ |S=1, M=-1\rangle = |\downarrow\downarrow\rangle \end{array}}$$

Note: the New eigenstates for $M=0$ are symmetric and antisymmetric combinations of the product states.

These are ~~eigen~~ entangled states.

Note: In triplet subspace, the state is invariant under exchange of spins ("symmetric under exchange")

In singlet subspace, the state picks up a negative sign under exchange ("anti-symmetric" under exchange)

Note: Given two spin-$\frac{1}{2}$ particles, each characterized by $s = \frac{1}{2}$, the total angular momentum has magnitude with possible eigenvalue

$$S = s_A + s_B = 1 \quad \text{or} \quad S = s_A - s_B = 0$$

This is an example of the "triangle rule"

Classically, given two vectors $\vec{L}_A$ and $\vec{L}_B$

$$\vec{L} = \vec{L}_A + \vec{L}_B$$

$$\Rightarrow |\vec{L}|^2 = |\vec{L}_A|^2 + |\vec{L}_B|^2 + \underbrace{2\vec{L}_A \cdot \vec{L}_B}_{2|\vec{L}_A||\vec{L}_B|\cos\theta}$$

$$\Rightarrow \cos\theta_{max} = +1 \qquad \cos\theta_{min} = -1$$

$$(|\vec{L}_A| - |\vec{L}_B|)^2 \leq |\vec{L}|^2 \leq (|\vec{L}_A| + |\vec{L}_B|)^2$$

triangle inequality $\Rightarrow$ $$\boxed{\big|\, |\vec{L}_A| - |\vec{L}_B| \,\big| \leq |\vec{L}| \leq |\vec{L}_A| + |\vec{L}_B|}$$

General addition of angular momentum

Given two angular momenta $\hat{\vec{j}}_1$ and $\hat{\vec{j}}_2$, the total angular momentum operator is

$$\hat{\vec{J}} = \hat{\vec{j}}_1 + \hat{\vec{j}}_2 = \hat{\vec{j}}_1 \otimes \hat{\mathbb{1}}_2 + \hat{\mathbb{1}}_1 \otimes \hat{\vec{j}}_2$$

Two representations

- Uncoupled $|j_1, m_1 ; j_2 m_2\rangle = |j_1 m_1\rangle \otimes |j_2 m_2\rangle$

  Simultaneous eigenvectors of

  $$\{\hat{\vec{j}}_1^{\,2}, \hat{j}_{1z} ; \hat{\vec{j}}_2^{\,2}, \hat{j}_{2z}\}$$

- Coupled $|J, M_J ; j_1 j_2\rangle$

  Simultaneous eigenvectors of

  $$\{\hat{\vec{J}}^{\,2}, \hat{J}_z ; \hat{\vec{j}}_1^{\,2}, \hat{\vec{j}}_2^{\,2}\}$$

Change of basis $\Longrightarrow$ Clebsch-Gordan coef.

$$|J M_J ; j_1 j_2\rangle = \sum_{m_1, m_2} |j_1 m_1 j_2 m_2\rangle \underbrace{\langle j_1 m_1 ; j_2 m_2 | J M_J\rangle}_{\text{CG coeff}}$$

Dimension of Hilbert space

$$\mathcal{H}_{12} = h_1 \otimes h_2$$

$$D_{12} = d_1 d_2 = (2j_1+1)(2j_2+1)$$

There must be D_{12} different basis vectors in the coupled representation

$$D_{12} = \sum_{J=J_{min}}^{J_{max}} (2J+1)$$

What are the possible values of J?

$$\boxed{\text{Triangle inequality} \quad |j_1 - j_2| \leq J \leq j_1 + j_2 \quad \text{in integer steps}}$$

^ Proof requires group theory

Check $\displaystyle\sum_{J=J_{min}}^{J_{max}} (2J+1) = 2\sum_{J_{min}}^{J_{max}} J + (J_{max} - J_{min} + 1)$

$$= 2\left[\tfrac{1}{2}(J_{max}+J_{min})(J_{max}-J_{min}+1)\right] + (J_{max}-J_{min}+1)$$

$$= (J_{max}+J_{min}+1)(J_{max}-J_{min}+1)$$

Assume $j_1 > j_2$ $\quad = (2j_1+1)(2j_2+1)$ ✓

Examples

- Spin + Orbital angular momentum of electron

$j_1 = 1/2$ $\longrightarrow$ $l = 0$ $J = 1/2$ only

$j_2 = l$ $\quad$ $l > 0$ $J = l + \frac{1}{2}, \ l - 1/2$

- Two spin-1 particles

$j_1 = 1$ $\longrightarrow$ $J = 0, 1, 2$

$j_2 = 1$

- Spin 3/2 nucleus + $l = 2$ orbital

$j_1 = 3/2$ $\longrightarrow$ $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \frac{7}{2}$

$j_2 = 2$