The basis of individual particles

System of two spin-$\frac{1}{2}$ particle

The basis of total spin $\vec{J} = \vec{J}_1 + \vec{J}_2$

$|m_1\rangle \otimes |m_2\rangle$

Possible states

$|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$,
$|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$

$|j, m\rangle$

Possible states

$|j=1, m=0,\pm 1\rangle$ (triplet)

$|j=0, m=0\rangle$ (singlet)

We have used operators $\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$

and $\hat{J}^2 = \hat{J}_1^2 + \hat{J}_2^2 + 2\hat{\vec{J}}_1 \cdot \vec{J}_2$ $\quad \hat{\vec{J}}_{1,2} = \{\hat{J}_{1,2x}, \hat{J}_{1,2y}, \hat{J}_{1,2z}\}$

to verify that the state $|\uparrow\uparrow\rangle \equiv |1, 1\rangle$

and $|\downarrow\downarrow\rangle \equiv |1, -1\rangle$

$$\hat{J}_z |\uparrow\uparrow\rangle = \hbar |\uparrow\uparrow\rangle \qquad m = 1$$

$$\hat{J}^2 |\uparrow\uparrow\rangle = 2\hbar^2 |\uparrow\uparrow\rangle \qquad j(j+1) = 2 \qquad j = 1$$

However, we discovered that

$$\hat{J}^2 |\uparrow\downarrow\rangle = \hbar^2 |\uparrow\downarrow\rangle + \hbar^2 |\downarrow\uparrow\rangle$$

$$\hat{J}^2 |\downarrow\uparrow\rangle = \hbar^2 |\downarrow\uparrow\rangle + \hbar^2 |\uparrow\downarrow\rangle$$

So $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ are not eigenstates of $\hat{J}^2$

However $|\pm\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle \pm |\downarrow\uparrow\rangle)$ are!

$$\hat{J}^2 |\pm\rangle = \frac{1}{\sqrt{2}} (\hat{J}^2 |\uparrow\downarrow\rangle \pm \hat{J}^2 |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}} \hbar^2 \left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle \pm (|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle) \right)$$

$$\hat{J}^2 |+\rangle = 2\hbar^2 \cdot \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) = 2\hbar^2 |+\rangle$$

and

$$\hat{J}_z |+\rangle = 0 \cdot |+\rangle \quad \Rightarrow \quad |+\rangle \equiv |j=1, m=0\rangle$$

$$\hat{J}^2 |-\rangle = 0$$
$$J_z |-\rangle = 0 \quad \Rightarrow \quad |-\rangle \equiv |j=0, m=0\rangle$$

How to deside which basis to use?
For non-interacting particle it doesn't matter. Two particles in magnetic field

$$\hat{H} = \omega_0 \hat{S}_{1z} + \omega_0 \hat{S}_{2z} = \omega_0 (\hat{S}_{1z} + \hat{S}_{2z}) = \omega_0 \hat{S}_z$$

If two particles are in state $|m_1\rangle \otimes |m_2\rangle$

$$\langle E \rangle = \langle \psi | \hat{H} | \psi \rangle = \omega_0 \langle m_1 | \hat{S}_{1z} | m_1 \rangle + \omega_0 \langle m_2 | \hat{S}_{2z} | m_2 \rangle =$$

$$= m_1 \omega_0 + m_2 \omega_0 = (m_1 + m_2)\omega_0 = m\omega_0 \qquad m = m_1 + m_2$$

However, if two spin interact, the two-particle basis is no longer eigenbasis of the hamiltonian

$$\hat{H} = \frac{2A}{\hbar^2} \vec{\hat{S}}_1 \cdot \vec{\hat{S}}_2$$

Spin-spin interaction (magn. field of one spin acts on the other)

Textbook provides direct treatment of how to find the eigenstates of $\hat{H}$ (sec. 5.2)

~~However~~ 4×4 Hamiltonian matrix: 4 basis states
$|1\rangle = |\uparrow\uparrow\rangle$, $|2\rangle = |\uparrow\downarrow\rangle$, $|3\rangle = |\downarrow\uparrow\rangle$, $|4\rangle = |\downarrow\downarrow\rangle$

$$H_{ij} = \langle i | \hat{H} | j \rangle$$

$\hat{H}|1\rangle = \frac{A}{2}|1\rangle \Rightarrow H_{11} = \frac{A}{2}$, $H_{12,3,4} = 0$

$\hat{H}|4\rangle = \frac{A}{2}|4\rangle \Rightarrow H_{44} = \frac{A}{2}$, $H_{41,23} = 0$

$H_{22} = H_{33} = -\frac{A}{2}$ $\qquad H_{23} = H_{32} = A$ $\qquad$ all other matrix elements are zero

$$\hat{H} = \begin{pmatrix} A/2 & 0 & 0 & 0 \\ 0 & -A/2 & A & 0 \\ 0 & A & -A/2 & 0 \\ 0 & 0 & 0 & A/2 \end{pmatrix}$$

States $|2\rangle$ & $|3\rangle$ get mixed up

The central part looks similar to the hamiltonian we used when discussing ammonia molecule

$$\hat{H}_{NH_3} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix}$$

Just like then, we will find that symmetric and anti-symmetric ~~sy~~ superpositions of states are the eigenstates of the hamiltonian

Alternative solution

$$\hat{\vec{S}} = (\hat{\vec{S}}_1 + \hat{\vec{S}}_2) \qquad \hat{S}^2 = (\hat{\vec{S}}_1 + \hat{\vec{S}}_2)^2 = \hat{S}_1^2 + \hat{S}_2^2 + 2\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2$$

$$\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2 = (\hat{S}^2 - \hat{S}_1^2 - \hat{S}_2^2)/2$$

Thus, any eigenstate of $\hat{S}^2$, $\hat{S}_1^2$ & $\hat{S}_2^2$ are also eigenstates of $\hat{\vec{S}}_1 \cdot \hat{\vec{S}}_2$

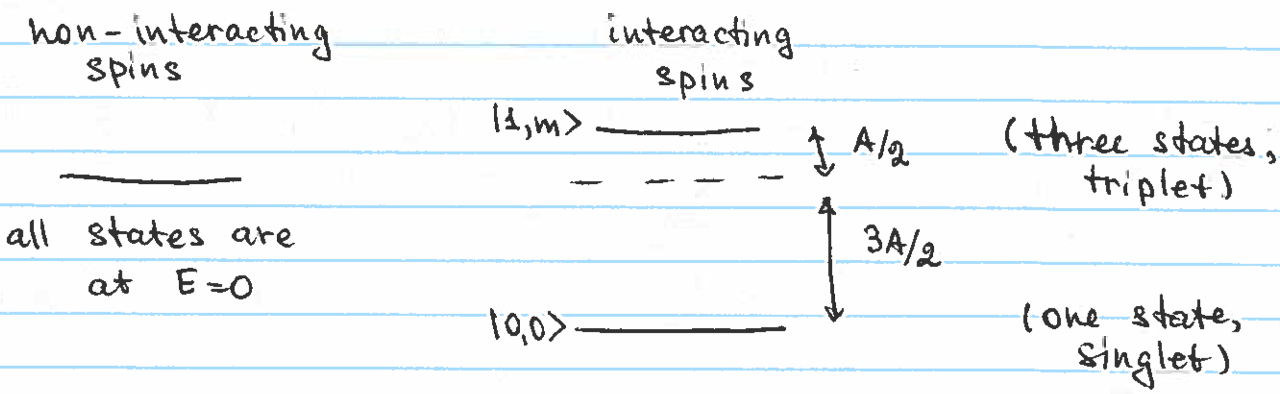
Luckily, we just discover that $|s,m\rangle$ states of the total spin fit the bill!

$$\hat{S}^2 |s,m\rangle = \hbar^2 s(s+1) |s,m\rangle$$
$$\hat{S}_1^2 |s,m\rangle = \hbar^2 s_1(s_1+1) |s,m\rangle = \frac{3}{4}\hbar^2 |s,m\rangle$$
$$\hat{S}_2^2 |s,m\rangle = \hbar^2 s_2(s_2+1) |s,m\rangle = \frac{3}{4}\hbar^2 |s,m\rangle$$

Thus $$\hat{S}_1 \cdot \hat{S}_2 = \frac{1}{2}\hbar^2 \left[s(s+1) - \frac{3}{2} \right]$$

$$\hat{H}|1,m\rangle = \frac{2A}{\hbar^2}\cdot\frac{1}{2}\cdot\hbar^2\left[1\cdot 2-\frac{3}{2}\right] = \frac{A}{2}$$

$$\hat{H}|0,0\rangle = \frac{2A}{\hbar^2}\cdot\frac{1}{2}\hbar^2\left[0-\frac{3}{2}\right] = -\frac{3A}{2}$$



What if there is also magnetic field?

$$\hat{H} = \omega_0\hat{S}_{1z} + \omega_0\hat{S}_{2z} + \frac{2A^2}{\hbar^2}\hat{\vec{S}}_1\cdot\hat{\vec{S}}_2 =$$

$$= \omega_0\hat{S}_z + \frac{2A^2}{\hbar^2}\cdot\frac{1}{2}\left(\hat{S}^2-\hat{S}_1^2-\hat{S}_2^2\right)$$

Luckily the eigenstates $|s,m\rangle$ of the total spin $\hat{S}^2$ and the z-component of the total spin $\hat{S}_z$ are still the eigenstates of the Hamiltonian