

Addition of spin-1/2 particles

Let us first review quantum mechanics of a single spin-1/2 particle

Assuming that the S^2 and S_z are good quantum numbers

~~then~~ Since, $[S^2, S_z] = 0$ but $[S_x, S_y] = i\hbar S_z$ and so on

we cannot find simultaneous eigenstates of S^2, S_x, S_y, S_z

we pick S^2 and S_z .

For spin 1/2 particles $s = 1/2$ and $S_z = \pm 1/2$

So, we will denote $S = 1/2$ and $S_z = +1/2$ state by $|\uparrow\uparrow\rangle$

$$|S, S_z\rangle \equiv \left|\frac{1}{2}, \pm\frac{1}{2}\right\rangle = |\uparrow\rangle; \left|\frac{1}{2}, -\frac{1}{2}\right\rangle = |\downarrow\rangle$$

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

$$S^2 |\downarrow\rangle = \frac{3}{4}\hbar^2 |\downarrow\rangle; S_z |\uparrow\rangle = +\frac{\hbar}{2} |\uparrow\rangle$$

$$S_z |\downarrow\rangle = -\frac{\hbar}{2} |\downarrow\rangle$$

In matrix notation

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ and } |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; S_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

What about S_x and S_y ?

We introduce them in terms of the ladder operators

$S_{\pm} = S_x \pm iS_y$ where S_+ increases S_z by \hbar and

S_- lowers S_z by \hbar . But since $S_z = \pm 1/2$ only...

ie $S_+ |\uparrow\rangle = 0$ and $S_- |\downarrow\rangle = 0$

But $S_+ |\downarrow\rangle = c_+ |\uparrow\rangle$ and $S_- |\uparrow\rangle = c_- |\downarrow\rangle$

S_{\pm} does not change S , only S_z .

In general $S_{\pm} |s, S_z\rangle = \hbar \sqrt{s(s \pm 1) - m(m \pm 1)} |s, S_z \pm 1\rangle$

In matrix notation: - $S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

$$\Rightarrow S_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; S_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

So, specifically $S_+ |\downarrow\rangle = \hbar \sqrt{\frac{1}{2}(\frac{1}{2}+1) - (-\frac{1}{2})(-\frac{1}{2}+1)} |\uparrow\rangle$
 $= \hbar \sqrt{\frac{3}{4} + \frac{1}{4}} = \hbar |\uparrow\rangle$

and $S_- |\uparrow\rangle = \hbar \sqrt{\frac{3}{4} - \frac{1}{2}(\frac{1}{2}-1)} |\downarrow\rangle = \hbar \sqrt{\frac{3}{4} + \frac{1}{4}} |\downarrow\rangle = \hbar |\downarrow\rangle$

Let's proceed to addition of two spin $1/2$ particles

we can use the classical picture to add spins

consider spins \vec{S}_1 and \vec{S}_2 of two particles

Total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$ If $|\vec{S}_1| = |\vec{S}_2|$ we have

two max. values are $\vec{S} = \vec{S}_1 + \vec{S}_2$ or $\vec{S} = \vec{S}_1 - \vec{S}_2$

For spin $1/2$ particles $|\vec{S}| = \frac{1}{2} - \frac{1}{2}$ or $\frac{1}{2} + \frac{1}{2} \Rightarrow 0$ or 1

The two particles have their own Hilbert spaces. So

the ^{spin} wave function of their combination can be a product

$$|S\rangle = |s_1, s_{z1}\rangle \otimes |s_2, s_{z2}\rangle \quad (\text{we will drop the outer product notation})$$

There can be four possible combinations based on $S_z = \pm \frac{1}{2}$

$$|\frac{1}{2}, \frac{1}{2}\rangle |\frac{1}{2}, \frac{1}{2}\rangle = |\uparrow\uparrow\rangle$$

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

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

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

These are the four basis states of the 2 spin $1/2$ system

Symmetric and Antisymmetric wavefunction by adding 2 spin $-\frac{1}{2}$ particles

	S	S _z	
$ \uparrow\uparrow\rangle$	1	1	Triplet state $ \uparrow\uparrow\rangle, \uparrow\downarrow\rangle, \downarrow\uparrow\rangle$ (S=1) $ \uparrow, 0\rangle$
$ \downarrow\downarrow\rangle$	1	-1	
$\frac{ \uparrow\downarrow\rangle + \downarrow\uparrow\rangle}{\sqrt{2}}$	1	0	
$\frac{ \uparrow\downarrow\rangle - \downarrow\uparrow\rangle}{\sqrt{2}}$	0	0	Singlet state $ 0, 0\rangle$ (S=0)

Lets show these explicitly...

Note $S=1 \Rightarrow S^2 = 1(1+1)\hbar^2 \Rightarrow 2\hbar^2$

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

$$2\vec{S}_1 \cdot \vec{S}_2 = 2S_{1x}S_{2x} + 2S_{1y}S_{2y} + 2S_{1z}S_{2z}$$

$$S_{1x}S_{2x} + S_{1y}S_{2y} = \frac{S_1^+ S_2^- + S_1^- S_2^+}{2}$$

$$\Rightarrow 2\vec{S}_1 \cdot \vec{S}_2 = S_1^+ S_2^- + S_1^- S_2^+ + 2S_{1z}S_{2z}$$

$$|\uparrow\uparrow\rangle \left[S_1^2 |\uparrow\uparrow\rangle = \frac{3}{4}\hbar^2 |\uparrow\uparrow\rangle \quad S_2^2 |\uparrow\uparrow\rangle = \frac{3}{4}\hbar^2 |\uparrow\uparrow\rangle \right]$$

$$2\vec{S}_1 \cdot \vec{S}_2 = S_1^+ S_2^- |\uparrow\uparrow\rangle + S_1^- S_2^+ |\uparrow\uparrow\rangle + 2S_{1z}S_{2z} |\uparrow\uparrow\rangle$$

since $S_1^+ |\uparrow\rangle = 0$ & $S_2^+ |\uparrow\rangle = 0$

$$2 \times \frac{1}{2} \times \frac{1}{2} \hbar^2 |\uparrow\uparrow\rangle$$

$$\Rightarrow \langle 2|\uparrow\uparrow\rangle = (3/4 + 3/4 + 1/2)\hbar^2 |\uparrow\uparrow\rangle = 2\hbar^2 |\uparrow\uparrow\rangle$$

$$\boxed{|\downarrow\downarrow\rangle} \quad S_1^2 |\downarrow\downarrow\rangle = S_2^2 |\downarrow\downarrow\rangle = \frac{3}{4} \hbar^2 |\downarrow\downarrow\rangle$$

$$2 S_{1x} S_{2x} = \underbrace{S_1^+ S_2^- |\downarrow\downarrow\rangle + S_1^- S_2^+ |\downarrow\downarrow\rangle}_0 + 2 S_{1z} S_{2z} |\downarrow\downarrow\rangle$$

$2 \left(\frac{1}{2}\right) \left(-\frac{1}{2}\right) \hbar^2 = -\frac{1}{2} \hbar^2$

$$\Rightarrow S^2 |\downarrow\downarrow\rangle = \left(\frac{3}{2} + \frac{1}{2}\right) \hbar^2 |\downarrow\downarrow\rangle$$

$$\boxed{\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{2}} = |\uparrow\downarrow\rangle \quad \text{we will use both notation.}$$

$$S_1^2 |\uparrow\downarrow\rangle = S_2^2 |\uparrow\downarrow\rangle = \frac{3}{4} \hbar^2 |\uparrow\downarrow\rangle$$

$$\text{Similarly } S_1^2 |\downarrow\uparrow\rangle = S_2^2 |\downarrow\uparrow\rangle = \frac{3}{4} \hbar^2 |\downarrow\uparrow\rangle$$

$$\text{So, } \left. \begin{aligned} S_1^2 \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) &= \frac{3}{4} \hbar^2 \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) \\ S_2^2 \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) &= \frac{3}{4} \hbar^2 \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) \end{aligned} \right\} \begin{aligned} (S_1^2 + S_2^2) |\uparrow\downarrow\rangle \\ = \frac{3}{2} \hbar^2 |\uparrow\downarrow\rangle \end{aligned}$$

$$\begin{aligned} \overline{S_1 \cdot S_2} |\uparrow\downarrow\rangle &= S_1^+ S_2^- |\uparrow\downarrow\rangle + S_1^- S_2^+ |\uparrow\downarrow\rangle + 2 S_{1z} S_{2z} |\uparrow\downarrow\rangle \\ &= 0 + \hbar^2 |\downarrow\uparrow\rangle + 2 \left(\frac{1}{2}\right) \left(-\frac{1}{2}\right) \hbar^2 |\uparrow\downarrow\rangle \\ &= \hbar^2 |\downarrow\uparrow\rangle - \frac{\hbar^2}{2} |\uparrow\downarrow\rangle \end{aligned}$$

$$\begin{aligned} \overline{S_1 \cdot S_2} |\downarrow\uparrow\rangle &= S_1^+ S_2^- |\downarrow\uparrow\rangle + S_1^- S_2^+ |\downarrow\uparrow\rangle + 2 S_{1z} S_{2z} |\downarrow\uparrow\rangle \\ &= \hbar^2 |\uparrow\downarrow\rangle + 0 + 2 \left(-\frac{1}{2}\right) \left(\frac{1}{2}\right) \hbar^2 |\downarrow\uparrow\rangle \\ &= \hbar^2 |\uparrow\downarrow\rangle - \frac{\hbar^2}{2} |\downarrow\uparrow\rangle \end{aligned}$$

$$\begin{aligned} 2 \overline{S_1 \cdot S_2} \left(\frac{|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle}{\sqrt{2}} \right) &= \hbar^2 \left(\frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \right) - \frac{\hbar^2}{2} \left(\frac{|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle}{\sqrt{2}} \right) \\ &= \frac{\hbar^2}{2} |\uparrow\downarrow\rangle \end{aligned}$$

$$\rightarrow S^2 |\uparrow\downarrow\rangle = \frac{3}{2} \hbar^2 |\uparrow\downarrow\rangle + \frac{\hbar^2}{2} |\uparrow\downarrow\rangle = 2 \hbar^2 |\uparrow\downarrow\rangle \Rightarrow \boxed{S=1}$$

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} = |00\rangle$$

$$S_1^2 |00\rangle = \frac{3}{4} \hbar^2 \frac{|\uparrow\downarrow\rangle}{\sqrt{2}} - \frac{3}{4} \hbar^2 \frac{|\downarrow\uparrow\rangle}{\sqrt{2}} = \frac{3}{4} \hbar^2 |00\rangle$$

Similarly $S_2^2 |00\rangle = \frac{3}{4} \hbar^2 |00\rangle$

$$2S_1 \cdot S_2 \left(\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \right) = \left[\frac{\hbar^2}{\sqrt{2}} |\downarrow\uparrow\rangle - \frac{\hbar^2}{2} \frac{|\uparrow\downarrow\rangle}{\sqrt{2}} \right] - \left[\frac{\hbar^2}{\sqrt{2}} |\uparrow\downarrow\rangle - \frac{\hbar^2}{2} \frac{|\downarrow\uparrow\rangle}{\sqrt{2}} \right]$$

$$= -\hbar^2 \left[\frac{|\uparrow\downarrow\rangle}{\sqrt{2}} - \frac{|\downarrow\uparrow\rangle}{\sqrt{2}} \right] - \frac{\hbar^2}{2} \left[\frac{|\uparrow\downarrow\rangle}{\sqrt{2}} - \frac{|\downarrow\uparrow\rangle}{\sqrt{2}} \right]$$

$$= -\frac{3\hbar^2}{2} |00\rangle$$

$$\Rightarrow S^2 = \frac{3}{4} \hbar^2 |00\rangle + \frac{3}{4} \hbar^2 |00\rangle - \frac{3}{2} \hbar^2 |00\rangle = 0$$

Also note $S^- = S_1^- + S_2^-$

$$S^- |\uparrow\uparrow\rangle = (S_1^- + S_2^-) |\uparrow\uparrow\rangle = |\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle \rightarrow |10\rangle \text{ state.}$$

Now the $s=1$ (Triplet) state and $s=0$ (singlet) are not degenerate and will have different energies say E_s and E_t .

We want to find the Hamiltonian which generates the triplet and singlet states as eigenvectors with E_t & E_s