Lecture # 14

Examples of addition of angular momenta and dealing with spinors

Last time: $|s_1, s_2, m_{s_1}, m_{s_2}\rangle \Rightarrow \underbrace{|s_1, s_2, s, m_s\rangle}_{\equiv\, |s, m_s\rangle}$

For $s_1 = s_2 = \frac{1}{2} \Rightarrow m_{s_1, s_2} = \pm\frac{1}{2} \Rightarrow$

$s = \left.\begin{array}{l} s_1 + s_2 = 1 \\ |s_1 - s_2| = 0 \end{array}\right\}$ two possible values $\quad m_s = m_{s_1} + m_{s_2} = -1, 0, 1$

$\vec{S}^2 |s_1, s_2, s, m_s\rangle = \hbar^2 s(s+1) |s_1, s_2, s, m_s\rangle$

$S_z |s, m_s\rangle = \hbar m_s |s, m_s\rangle$, where $\vec{S} = \vec{S}_1 + \vec{S}_2$

$S_z = S_{1z} + S_{2z}$

When is such a change of basis useful? $\Rightarrow$

Example 1 (Comprehensive exam, U Wisconsin)

A system of two particles each with spin 1/2 is described by an effective Hamiltonian

$H = A(S_{1z} + S_{2z}) + B\,\vec{S}_1 \cdot \vec{S}_2$, where $\vec{S}_1$ & $\vec{S}_2$ are the spin operators for the particles 1 and 2 and A & B are constants. Find the energy levels of this Hamiltonian

Solution:

Choose a C.S.C.O. $\{H, \vec{S}_1^2, \vec{S}_2^2, \vec{S}^2, S_z\} \Rightarrow |s, m_s\rangle$ basis

$\vec{S} = \vec{S}_1 + \vec{S}_2$, $\quad S_{1z} + S_{2z} = S_z$;

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

$H|s, m_s\rangle = \underset{\substack{\uparrow \\ \text{find it!}}}{E}|s, m_s\rangle$; $\quad \vec{S}^2|s, m_s\rangle = \hbar^2 s(s+1)|s, m_s\rangle$

$S_z|s, m_s\rangle = \hbar m_s|s, m_s\rangle$

$$H = A S_z + B\,\frac{\vec{S}^2 - \vec{S}_1^2 - \vec{S}_2^2}{2}$$

$$H|s, m_s\rangle = A\hbar m_s|s, m_s\rangle + \frac{B}{2}\left[\hbar^2 s(s+1) - \frac{3}{4}\hbar^2 \cdot 2\right]\cdot$$

$$\cdot|s, m_s\rangle = \underbrace{\left(A\hbar m_s + \frac{B}{2}\hbar^2\left(s(s+1) - \frac{3}{2}\right)\right)}_{= E}|s, m_s\rangle$$

$$E_{singlet} \underset{\substack{\uparrow \\ s=0 \\ m_s=0}}{=} -\frac{B}{2}\hbar^2 \cdot \frac{3}{2} = \underbrace{-\frac{3}{4}\hbar^2 B}$$

$$E_{triplet} \underset{\substack{\uparrow \\ s=1 \\ m_s=-1,0,1}}{=} \begin{cases} -A\hbar + \frac{B}{2}\hbar^2\left(2 - \frac{3}{2}\right) = -A\hbar + \frac{B}{4}\hbar^2 \leftarrow m_s = -1 \\ \frac{B\hbar^2}{4} \leftarrow m_s = 0 \\ A\hbar + \frac{B\hbar^2}{4} \leftarrow m_s = 1 \end{cases}$$

Example 2 (comprehensive exam, U Chicago)

Two electrons are tightly bound to different neighbouring sites in a certain solid. They are, therefore, distinguishable particles which can be described in terms of their respective Pauli spin matrices $\hat{\vec{\sigma}}^{(1)}$ and $\hat{\vec{\sigma}}^{(2)}$

The Hamiltonian is $H = -\underset{\substack{\uparrow \\ \text{const}}}{A}\left(\hat{\sigma}_x^{(1)}\hat{\sigma}_x^{(2)} + \hat{\sigma}_y^{(1)}\hat{\sigma}_y^{(2)}\right)$

(a) What are the energy levels and their degeneracy

$\Downarrow$

$$\hat{\sigma}_x^{(1)}\hat{\sigma}_x^{(2)} + \hat{\sigma}_y^{(1)}\hat{\sigma}_y^{(2)} = \hat{\vec{\sigma}}^{(1)}\cdot\hat{\vec{\sigma}}^{(2)} - \hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)} = ? \; =$$

Recall: $\vec{S}^{(i)} \doteq \frac{\hbar}{2}\hat{\vec{\sigma}}^{(i)}$

$$\hat{\vec{\sigma}}^{(1)}\cdot\hat{\vec{\sigma}}^{(2)} = \frac{\left(\hat{\vec{\sigma}}^{(1)}+\hat{\vec{\sigma}}^{(2)}\right)^2 - \left(\hat{\vec{\sigma}}^{(1)}\right)^2 - \left(\hat{\vec{\sigma}}^{(2)}\right)^2}{2} = \frac{\left(\hat{\vec{\sigma}}^{(1)}+\hat{\vec{\sigma}}^{(2)}\right)^2 - 6I}{2}$$

$$\left(\hat{\vec{\sigma}}^{(1)}\right)^2 = \underbrace{\left(\hat{\sigma}_x^{(1)}\right)^2}_{= I} + \underbrace{\left(\hat{\sigma}_y^{(1)}\right)^2}_{= I} + \underbrace{\left(\hat{\sigma}_z^{(1)}\right)^2}_{= I} = 3I$$

$$\hat{\sigma}_z^{(1)}\hat{\sigma}_z^{(2)} = \frac{\left(\hat{\sigma}_z^{(1)}+\hat{\sigma}_z^{(2)}\right)^2 - \left(\hat{\sigma}_z^{(1)}\right)^2 - \left(\hat{\sigma}_z^{(2)}\right)^2}{2} = \frac{\left(\hat{\sigma}_z^{(1)}+\hat{\sigma}_z^{(2)}\right)^2 - 2I}{2}$$

$$= \frac{\left(\hat{\vec{\sigma}}^{(1)}+\hat{\vec{\sigma}}^{(2)}\right)^2 - \left(\hat{\sigma}_z^{(1)}+\hat{\sigma}_z^{(2)}\right)^2}{2} - 2I \doteq \frac{2}{\hbar^2}\left(\vec{S}^2 - S_z^2\right) - 2I$$

$\uparrow$ $\vec{S} = \vec{S}^{(1)} + \vec{S}^{(2)} = \frac{\hbar}{2}\left(\hat{\vec{\sigma}}^{(1)} + \hat{\vec{\sigma}}^{(2)}\right)$

So, $H = -\frac{2A}{\hbar^2}\left(\vec{S}^2 - S_z^2\right) + 2\cancel{A}I$

$$H\,|s, m_s\rangle = \left(-\frac{2A}{\cancel{\hbar^2}}\left(\cancel{\hbar^2}s(s+1) - \cancel{\hbar^2}m_s^2\right) + 2A\right)|s, m_s\rangle$$

$$E = -2A\left[s(s+1) - m_s^2 - 1\right]$$

$s=0$ (singlet) : $E = 2A$
($m_s = 0$)

$s=1$ (triplet):

$$E = -2A\left[2 - m_s^2 - 1\right] = -2A\left[1 - m_s^2\right] = \begin{cases} 0 & m_s = 1 \\ -2A & 0 \\ 0 & -1 \end{cases}$$

$E = 0$ → double-degenerate
($m_s = 1$ or -1)
$\uparrow\uparrow$ $\downarrow\downarrow$

$E = -2A$ ~~double degenerate~~

(b) HW
Add magnetic field ⇒ $H_{\text{magnetic}} = -\frac{e}{mc}\vec{S}\cdot\vec{B}$

Example 3 Dealing with spinors

Consider a spin 1/2 particle, whose state is described by a spinor $[\Psi(\vec{r})] = \begin{pmatrix} \Psi_+(\vec{r}) \\ \Psi_-(\vec{r}) \end{pmatrix}$

Ψ_+: $m_s = +\frac{1}{2}$

Ψ_-: $m_s = -\frac{1}{2}$

(S_z-basis)

where
$$\Psi_+(\vec{r}) = R(r)\left[Y_0^0 + \frac{1}{\sqrt{3}} Y_1^0\right]$$
$$\Psi_-(\vec{r}) = \frac{R(r)}{\sqrt{3}}\left[Y_1^1 - Y_1^0\right]$$

(a) What condition does $R(r)$ have to satisfy for $[\Psi(\vec{r})]$ to be normalized?

$\Downarrow$

$$\int\left(|\Psi_+|^2 + |\Psi_-|^2\right) dV = 1 = \int_0^\infty |R(r)|^2 \left(|Y_0^0|^2 + \frac{1}{3}|Y_1^0|^2 + \frac{1}{3}|Y_1^1|^2 + \frac{1}{3}|Y_1^0|^2\right) r^2 dr\, d\Omega = 2\underline{\int_0^\infty |R(r)|^2 r^2 dr = 1}$$

$$\int |Y_\ell^m|^2 d\Omega = 1$$

$\Downarrow$

$$\underline{\int_0^\infty |R(r)|^2 r^2 dr = \frac{1}{2}}$$

(b) S_z is measured. What results can be found and with what probabilities?

$$\mathcal{P}\left(S_z = +\frac{\hbar}{2}\right) = \int |\Psi_+|^2 dV = \int_0^\infty |R(r)|^2 \left(|Y_0^0|^2 + \frac{1}{3}|Y_1^0|^2\right) \cdot r^2 dr\, d\Omega = \frac{4}{3} \cdot \frac{1}{2} = \frac{2}{3}$$

$$\mathcal{P}\left(S_z = -\frac{\hbar}{2}\right) = \int |\Psi_-|^2 dV = \frac{1}{3}\cdot\frac{1}{2}\cdot 2 = \underset{\sim}{\frac{1}{3}}$$

Check: $\frac{2}{3} + \frac{1}{3} = 1$ ✓

What would be a result of the measurement on average? $\Rightarrow$

$$\langle S_z \rangle = \frac{\hbar}{2}\cdot\mathcal{P}\left(S_z = +\frac{\hbar}{2}\right) - \frac{\hbar}{2}\cdot\mathcal{P}\left(S_z = -\frac{\hbar}{2}\right) =$$

$$= \frac{\hbar}{\cancel{2}}\cdot\frac{\cancel{2}}{3} - \frac{\hbar}{2}\cdot\frac{1}{3} = \underset{\sim}{\frac{\hbar}{6}}$$

Note: Since $[\Psi(\vec{r})] = \begin{bmatrix}\Psi_+(\vec{r})\\ \Psi_-(\vec{r})\end{bmatrix} = \Psi_+(\vec{r})\underbrace{\begin{bmatrix}1\\0\end{bmatrix}}_{\substack{\shortparallel\\ |+\rangle = \\ = |S_z = +\frac{\hbar}{2}\rangle}} + \Psi_-(\vec{r})\underbrace{\begin{bmatrix}0\\1\end{bmatrix}}_{\substack{\shortparallel\\ |-\rangle = |S_z = -\frac{\hbar}{2}\rangle}}$,

we can clearly "read out" the probabilities to find a particle in the $|S_z = \pm\frac{\hbar}{2}\rangle$ states as $\int |\Psi_\pm(\vec{r})|^2 dV$.

What <u>if</u> we need to find the probability of finding a particle in the state $|S_x = \pm\frac{\hbar}{2}\rangle$?

$\Rightarrow$

First, find the eigenvectors $|S_x = \pm \frac{\hbar}{2}\rangle$:

$$S_x \doteq \frac{\hbar}{2}\hat{\sigma}_x \doteq \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \text{eigenvalues: } \lambda = \pm\frac{\hbar}{2} \Rightarrow$$

$$|S_x = \frac{\hbar}{2}\rangle: \begin{pmatrix} -\frac{\hbar}{2} & \frac{\hbar}{2} \\ \frac{\hbar}{2} & -\frac{\hbar}{2} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0 \Rightarrow \underline{c_1 = c_2}$$

$$\Leftarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$|S_x = -\frac{\hbar}{2}\rangle \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Let's present our spinor $[\Psi(\vec{r})] = \begin{bmatrix} \Psi_+(\vec{r}) \\ \Psi_-(\vec{r}) \end{bmatrix}$ in terms of $|S_x = \pm\frac{\hbar}{2}\rangle$ basis;

$$\begin{bmatrix} \Psi_+(\vec{r}) \\ \Psi_-(\vec{r}) \end{bmatrix} = \alpha \cdot \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}}_{= |S_x = +\frac{\hbar}{2}\rangle} + \beta \cdot \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}}_{= |S_x = -\frac{\hbar}{2}\rangle} \Rightarrow$$

$$\begin{aligned} \frac{\alpha}{\sqrt{2}} + \frac{\beta}{\sqrt{2}} &= \Psi_+ \\ \frac{\alpha}{\sqrt{2}} - \frac{\beta}{\sqrt{2}} &= \Psi_- \end{aligned} \Rightarrow \begin{aligned} \alpha &= \frac{\sqrt{2}}{2}(\Psi_+ + \Psi_-) \\ \beta &= \frac{\sqrt{2}}{2}(\Psi_+ - \Psi_-) \end{aligned}$$

So, $$\begin{bmatrix} \Psi_+(\vec{r}) \\ \Psi_-(\vec{r}) \end{bmatrix} = \frac{\sqrt{2}}{2}(\Psi_+ + \Psi_-) \cdot \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}}_{|S_x = +\frac{\hbar}{2}\rangle} +$$

$$+\ \frac{\sqrt{2}}{2}\left(\Psi_+ - \Psi_-\right)\cdot \underbrace{\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix}}_{|S_x = -\frac{\hbar}{2}\rangle}$$

HW: finish the problem and determine the probability to measure $S_x = \pm\frac{\hbar}{2}$ as well as find $\langle S_x \rangle$.