QM II
Phys 652

Lecture # 13

Addition of angular momenta

Why study? → how to add orbital angular momentum $\vec{L}$ and spin $\vec{S}$

→ how to add spins of two particles $\vec{S}_1$ and $\vec{S}_2$

⇓

introduce the generalized angular momentum $\vec{J} = \vec{L} + \vec{S} =$

$= \vec{L} \otimes I_s + I_{\vec{r}} \otimes \vec{S}$, $\vec{J} \in \mathcal{E} = \mathcal{E}_{\vec{r}} \otimes \mathcal{E}_s$

identity operator in $\mathcal{E}_s$; in $\mathcal{E}_{\vec{r}}$

(similar could be said about $\vec{J} = \vec{S}_1 + \vec{S}_2$, $\vec{J} \in \mathcal{E} = \mathcal{E}_{S_1} \otimes \mathcal{E}_{S_2}$)

To describe a state of the system with the spin, e.g. a hydrogen atom, we need a set of observables

$\{H, \vec{L}^2, L_z, \vec{S}^2, S_z\} \Rightarrow |n, \ell, m_\ell; s, m_s\rangle$

Can we use a set $\{H, \vec{J}^2, J_z, \vec{L}^2, \vec{S}^2\} \Rightarrow |n, j, m_j; \ell, s\rangle$ instead and would it be useful? ⇒

Example
Consider the Hamiltonian $H_{so} = A\, \vec{L} \cdot \vec{S}$ ← spin-orbit coupling

(total $H = H_{coulomb} + H_{so}$) ↑ const

Recall how in the hydrogen atom problem the fact that $[\vec{L}^2, H] = [L_z, H] = 0$ allowed us to solve the angular part of the Schrödinger's equation separated from the radial part and obtain states $|l, m_l\rangle$ described by orbital angular momentum quantum number l and magnetic quantum number m_l,

$$\vec{L}^2 |l, m_l\rangle = \hbar^2 l(l+1) |l, m_l\rangle \; ; \quad L_z |l, m_l\rangle = \hbar m_l |l, m_l\rangle .$$

Can we still use the same procedure, but take into account the spin? $\Rightarrow$

e.g. $|l, m_l\rangle \Rightarrow |l, m_l; s, m_s\rangle \Rightarrow$

Consider

$$[L_z, H] = \underbrace{[L_z, H_{coulomb}]}_{=0} + [L_z, \overbrace{H_{SO}}^{=A\vec{L}\cdot\vec{S}}] =$$

$$= A[L_z, L_x S_x + L_y S_y + L_z S_z] = A(i\hbar L_y S_x - i\hbar L_x S_y) \neq 0$$

$[L_i, S_j] = 0$ for any i, j

Similarly,

$$[S_z, H] = A[S_z, L_x S_x + L_y S_y + L_z S_z] = A(i\hbar L_x S_y - i\hbar L_y S_x) \neq 0$$

However, $\underline{[J_z, H] = [L_z + S_z, H] = 0} \Rightarrow$

instead of $|l, m_l; s, m_s\rangle$ basis use $|j, m_j; l, s\rangle$ basis

Example: Addition of two spin-1/2 particles

Consider two particles in the ground state ($l_1 = l_2 = 0$)

$S_1 = S_2 = \frac{1}{2}$

The state space of this system

$$\underbrace{\mathcal{E}}_{(2S_1+1)\cdot(2S_2+1) = 4D\text{-space}} = \underbrace{\mathcal{E}_{S_1}}_{2S_1+1} \otimes \underbrace{\mathcal{E}_{S_2}}_{2S_2+1}$$

$|S_1, S_2; m_{S_1}, m_{S_2}\rangle \equiv |m_{S_1}, m_{S_2}\rangle$

4D-space $\Rightarrow$ 4 basis vectors $\Rightarrow$

m_{S_1}, m_{S_2}

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

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

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

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

$$\vec{S}^2_{1,2} |m_{S_1}, m_{S_2}\rangle = \hbar^2 (S_{1,2}+1) S_{1,2} \cdot |m_{S_1}, m_{S_2}\rangle = \underline{= \hbar^2 \cdot \frac{3}{4} |m_{S_1}, m_{S_2}\rangle} ;$$

$$S_{1z,2z} |m_{S_1}, m_{S_2}\rangle = \underline{= \hbar m_{S_1, S_2} |m_{S_1}, m_{S_2}\rangle}$$

Introduce total spin

$\vec{S} = \vec{S}_1 + \vec{S}_2 \Rightarrow$

Check commutation relations:

$$[S_x, S_y] = [S_{1x} + S_{2x}, S_{1y} + S_{2y}] = [S_{1x}, S_{1y}] + [S_{2x}, S_{2y}] = i\hbar (S_{1z} + S_{2z}) = \underline{= i\hbar S_z}$$

$[S_{1x}, S_{2y}] = 0$

$[S_{2x}, S_{1y}] = 0$

(since S_1, S_2 act on different spaces)

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

Can we instead of the basis of operators $\{\vec{S}_1^{\,2}, \vec{S}_2^{\,2}, S_{1z}, S_{2z}\}$

$\Downarrow$

$|s_1, s_2, m_{s_1}, m_{s_2}\rangle$

introduce a basis of $\{\vec{S}_1^{\,2}, \vec{S}_2^{\,2}, \vec{S}^2, S_z\}$?

$\Downarrow$

check: do they all commute?; $|s_1, s_2, s, m_s\rangle \equiv |s, m_s\rangle$ for fixed s_1, s_2

$$[\vec{S}_{1,2}^{\,2}, \vec{S}^2] = [\vec{S}_{1,2}^{\,2}, \vec{S}_1^{\,2} + \vec{S}_2^{\,2} + 2\vec{S}_1 \cdot \vec{S}_2] =$$

$$= 2[\vec{S}_{1,2}^{\,2}, \vec{S}_1 \cdot \vec{S}_2] = 2[\vec{S}_{1,2}^{\,2}, S_{1x}S_{2x} + S_{1y}S_{2y} + S_{1z}S_{2z}]$$

$$= 0$$

$\uparrow$

$$[\vec{S}_{1,2}^{\,2}, S_{i_{1,2}}] = 0$$

$$[\vec{S}_{1,2}^{\,2}, S_z] = [\vec{S}_{1,2}^{\,2}, S_{1z} + S_{2z}] = 0 \quad \checkmark$$

$\Downarrow$

$\vec{S}_1^{\,2}, \vec{S}_2^{\,2}, \vec{S}^2, S_z$ share the same basis

$$\vec{S}_{1,2}^{\,2} \underbrace{|s, m_s\rangle}_{\equiv\, |s_1, s_2, s, m_s\rangle} = \frac{3}{4}\hbar^2 |s, m_s\rangle; \quad \vec{S}^2 |s, m_s\rangle = \hbar^2 s(s+1) \cdot |s, m_s\rangle;$$

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

What are the possible values of s, m_s and how do we relate $|s, m_s\rangle$ with $|m_{s_1}, m_{s_2}\rangle$?

$\Rightarrow$

Since $[\underbrace{S_z}_{S_{1z}+S_{2z}}, S_{\substack{1z\\2z}}] = 0 \Rightarrow |m_{s_1}, m_{s_2}\rangle$ are eigenvectors of S_z (5)

⇓

$$S_z |m_{s_1}, m_{s_2}\rangle = (S_{1z} + S_{2z}) |m_{s_1}, m_{s_2}\rangle = \hbar (m_{s_1} + m_{s_2}) \cdot |m_{s_1}, m_{s_2}\rangle$$

⇓

$$\underline{m_s = m_{s_1} + m_{s_2}}$$

⇓

in the case of $s_1 = s_2 = \frac{1}{2} \Rightarrow m_s = \begin{cases} +1 & (m_{s_1} = m_{s_2} = \frac{1}{2}) \\ 0 & (m_{s_1} = \frac{1}{2}, m_{s_2} = -\frac{1}{2} \text{ or vice verse}) \\ -1 & (m_{s_1} = -\frac{1}{2}, m_{s_2} = -\frac{1}{2}) \end{cases}$

What is a representation of S_z in the $\{|m_{s_1}, m_{s_2}\rangle\}$ basis?

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4×4 matrix $\Rightarrow$ $S_z |\pm\pm\rangle = \pm\hbar |\pm\pm\rangle$

$S_z |\pm\mp\rangle = 0 \, |\pm\mp\rangle$

⇓

$$S_z \doteq \hbar \begin{array}{c} \begin{array}{cccc} |{+}{+}\rangle & |{+}{-}\rangle & |{-}{+}\rangle & |{-}{-}\rangle \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{array} \begin{array}{c} \langle{+}{+}| \\ \langle{+}{-}| \\ \langle{-}{+}| \\ \langle{-}{-}| \end{array}$$

What about $\vec{S}^2$ representation in $\{|m_{s_1}, m_{s_2}\rangle\}$?

⇓

Since $[\vec{S}^2, S_{\substack{1z\\2z}}] \neq 0 \Rightarrow$ <u>don't expect it to be diagonal</u>

show!!

(but, $[\vec{S}^2, \underbrace{S_z}_{S_{1z}+S_{2z}}] = 0$!)

show!!

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

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

$$\vec{S}^2|++\rangle = \vec{S}_1^{\,2}|++\rangle + \vec{S}_2^{\,2}|++\rangle + 2S_{1z}S_{2z}|++\rangle$$

$$+ S_{1+}S_{2-}|++\rangle + S_{1-}S_{2+}|++\rangle = \cancel{2}\cdot\frac{3}{\cancel{4}_{2}}\hbar^2|++\rangle +$$

$$+ \cancel{2}\cdot\hbar^2\cdot\frac{1}{\cancel{2}}\cdot\frac{1}{2}|++\rangle + 0 = 2\hbar^2|++\rangle$$

Similarly, $\vec{S}^2|--\rangle = 2\hbar^2|--\rangle$

$$\vec{S}^2|+-\rangle = \frac{3}{\cancel{4}_{2}}\hbar^2\cdot\cancel{2}|+-\rangle + \cancel{2}\cdot\hbar^2\cdot\frac{1}{\cancel{2}}\cdot\left(-\frac{1}{2}\right)|+-\rangle +$$

$$+ 0 + \hbar\cdot\hbar|-+\rangle = \hbar^2\left(|+-\rangle + |-+\rangle\right)$$

$$S_{1-}S_{2+}|+-\rangle = \hbar^2\sqrt{\frac{1}{2}\cdot\frac{3}{2}-\frac{1}{2}\cdot\left(-\frac{1}{2}\right)}\cdot\sqrt{\frac{1}{2}\cdot\frac{3}{2}+\frac{1}{2}\cdot\frac{1}{2}}\;|-+\rangle$$

$$= \hbar^2|-+\rangle$$

$$\vec{S}^2|-+\rangle = \hbar^2\left(|-+\rangle + |+-\rangle\right) \Rightarrow$$

$$\vec{S}^2 \doteq \hbar^2 \begin{array}{c} \begin{array}{cccc} ++ & +- & -+ & -- \end{array} \\ \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \end{array} \begin{array}{c} ++ \\ +- \\ -+ \\ -- \end{array}$$

So, $|++\rangle$ and $|--\rangle$ are eigenvectors of $\vec{S}^2 \Rightarrow$

$$\vec{S}^2|\underset{+}{m_{s_1}},\underset{+}{m_{s_2}}\rangle = 2\hbar^2|++\rangle\;;\quad \vec{S}^2|--\rangle = 2\hbar^2|--\rangle$$

Other eigenvectors? $\Rightarrow$ diagonalize the submatrix

$$\hbar^2 \begin{array}{c|cc} & +- & -+ \\ \hline +- & 1 & 1 \\ -+ & 1 & 1 \end{array} \Rightarrow \text{eigenvalues are}$$

$$\det\begin{pmatrix} \hbar^2-\lambda & \hbar^2 \\ \hbar^2 & \hbar^2-\lambda \end{pmatrix} = 0$$

$$\Rightarrow (\hbar^2-\lambda)^2 = \hbar^4 \Rightarrow \underline{\lambda = 0 \text{ or } 2\hbar^2}$$

Eigenvectors:

$\underline{\lambda = 0} \Rightarrow \begin{pmatrix} \hbar^2 & \hbar^2 \\ \hbar^2 & \hbar^2 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow C_1 = -C_2 \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \Rightarrow$

$$\underline{\frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)}$$

$\underline{\lambda = 2\hbar^2} \Rightarrow \begin{pmatrix} -\hbar^2 & \hbar^2 \\ \hbar^2 & -\hbar^2 \end{pmatrix}\begin{pmatrix} C_1 \\ C_2 \end{pmatrix} = 0 \Rightarrow C_1 = C_2 \Rightarrow \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\Rightarrow \underline{\frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right)}$$

So, there are two eigenvalues of the operator $\vec{S}^2 \Rightarrow$

$\hbar^2 s(s+1) = 0 \Rightarrow \underline{s = 0}$ and $\hbar^2 s(s+1) = 2\hbar^2 \Rightarrow \underline{s = 1}$

$s = 0$: $\Rightarrow$ non-degenerate $\Rightarrow$ 1 eigenvector $\frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$

$$\overset{s}{|0},\overset{m_s}{0}\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right) \Rightarrow \text{singlet}$$

$s = 1$: $\Rightarrow$ 3-degenerate $\Rightarrow$

$\overset{s}{|1},\overset{m_s}{1}\rangle = |++\rangle$, $|--\rangle = |1,-1\rangle$,

$\frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right) = |\underset{s}{1},\underset{m_s}{0}\rangle$

$\Uparrow$ triplet

Now, $\vec{S}^2$ and S_z in $|S, m_s\rangle$ basis:

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

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

$$\begin{array}{cc} & \begin{array}{cccc} |0,0\rangle & |1,1\rangle & |1,0\rangle & |1,-1\rangle \end{array} \\ S_z \doteq \hbar & \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \end{array}$$

$$\vec{S}^2 \doteq \hbar^2 \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$