Homework #7: Brief solutions

***** (about lecture #5) *****

1. (9points) For $j_1 = 2$, $j_2 = 1$, $j = 1$, *compute all the nonzero Clebsch-Gordon coefficients,* $\langle j, m|j_1, m_1; j_2, m_2\rangle$. [Hint: think of this as an "addition of angular momentum" problem, define angular momentum operators $\hat{\boldsymbol{J}}_1$ and $\hat{\boldsymbol{J}}_2$ for $|j_1, m_1\rangle$ and $|j_2, m_2\rangle$ Hilbert spaces respectively, $m_i = -j_i, -j_i+1, \ldots, j_i$, define total angular momentum operators $\hat{\boldsymbol{J}} = \hat{\boldsymbol{J}}_1 + \hat{\boldsymbol{J}}_2$, then solve the total angular momentum eigenbasis $|j, m\rangle$ in terms of tensor product basis $|j_1, m_1\rangle|j_2, m_2\rangle$]

Solution:

Consider highest $m = j = 1$ state $|j = 1, m = 1\rangle$ first, it should be a linear superposition of $|j_1, m_1\rangle|j_2, m_2\rangle$ states with $m_1 + m_2 = m$.

Assume $|j = 1, m = 1\rangle = c_1|2, 2\rangle|1, -1\rangle + c_2|2, 1\rangle|1, 0\rangle + c_3|2, 0\rangle|1, 1\rangle$.

From $\hat{J}_+|j = 1, m = 1\rangle = 0$, and $\hat{J}_+ = \hat{J}_{1,+} + \hat{J}_{2,+}$.

$c_1 \cdot (0 + \sqrt{2}|2, 2\rangle|1, 0\rangle) + c_2 \cdot (2|2, 2\rangle|1, 0\rangle + \sqrt{2}|2, 1\rangle|1, 1\rangle) + c_3 \cdot (\sqrt{6}|2, 1\rangle|1, 1\rangle + 0) = 0.$

Therefore $\sqrt{2}c_1 + 2c_2 = 0$, and $\sqrt{2}c_2 + \sqrt{6}c_3 = 0$.

We can choose $c_1 = \sqrt{\frac{6}{10}}$, $c_2 = -\sqrt{\frac{3}{10}}$, $c_3 = \sqrt{\frac{1}{10}}$, up to overall phase factor.

Namely $\langle 2, 2; 1, -1|1, 1\rangle = \sqrt{\frac{6}{10}}$, $\langle 2, 1; 1, 0|1, 1\rangle = -\sqrt{\frac{3}{10}}$, $\langle 2, 0; 1, 1|1, 1\rangle = \sqrt{\frac{1}{10}}$.

$|j = 1, m = 0\rangle = \frac{1}{\sqrt{2}}\hat{J}_-|j = 1, m = 1\rangle$
$= \frac{1}{\sqrt{2}}\left[(2c_1 + \sqrt{2}c_2)|2, 1\rangle|1, -1\rangle + (\sqrt{6}c_2 + \sqrt{2}c_3)|2, 0\rangle|1, 0\rangle + (\sqrt{6}c_3)|2, -1\rangle|1, 1\rangle\right]$
$= \sqrt{\frac{3}{10}}|2, 1\rangle|1, -1\rangle - \sqrt{\frac{4}{10}}|2, 0\rangle|1, 0\rangle + \sqrt{\frac{3}{10}}|2, -1\rangle|1, 1\rangle.$
Namely, $\langle 2, 1; 1, -1|1, 0\rangle = \sqrt{\frac{3}{10}}$, $\langle 2, 0; 1, 0|1, 0\rangle = -\sqrt{\frac{4}{10}}$, $\langle 2, -1; 1, 1|1, 0\rangle = \sqrt{\frac{3}{10}}$.

$|j = 1, m = -1\rangle = \frac{1}{\sqrt{2}}\hat{J}_-|j = 1, m = 0\rangle$
$= (\sqrt{6}c_1 + 2\sqrt{3}c_2 + c_3)|2, 0\rangle|1, -1\rangle + (3c_2 + 2\sqrt{3}c_3)|2, -1\rangle|1, 0\rangle + (\sqrt{6}c_3)|2, -2\rangle|1, 1\rangle$
$= \sqrt{\frac{1}{10}}|2, 0\rangle|1, -1\rangle - \sqrt{\frac{3}{10}}|2, -1\rangle|1, 0\rangle + \sqrt{\frac{6}{10}}|2, -2\rangle|1, 1\rangle.$
Namely $\langle 2, 0; 1, -1|1, -1\rangle = \sqrt{\frac{1}{10}}$, $\langle 2, -1; 1, 0|1, -1\rangle = -\sqrt{\frac{3}{10}}$, $\langle 2, -2; 1, 1|1, -1\rangle = \sqrt{\frac{6}{10}}$.

Note that $\langle j, m|j_1, m_1; j_2, m_2\rangle = (\langle j_1, m_1; j_2, m_2|j, m\rangle)^*$.

2. (21points) Consider a spin-1 moment, denote the spin angular momentum operators by $\hat{\boldsymbol{S}}$. Then $[\hat{S}_a, \hat{S}_b] = \sum_c \mathbb{i}\epsilon_{abc}\hat{S}_c$. A complete orthonormal basis for the 3-dimensional Hilbert space is the S_z-eigenbasis $|S_z = +1, 0, -1\rangle$. Define "magnetic quadrupole" operators, $\hat{Q}_1 = \hat{S}_y\hat{S}_z + \hat{S}_z\hat{S}_y$, $\hat{Q}_2 = \hat{S}_z\hat{S}_x + \hat{S}_x\hat{S}_z$, $\hat{Q}_3 = \hat{S}_x\hat{S}_y + \hat{S}_y\hat{S}_x$, $\hat{Q}_4 = \hat{S}_x\hat{S}_x - \hat{S}_y\hat{S}_y$, $\hat{Q}_5 = \frac{1}{\sqrt{3}}(\hat{S}_x\hat{S}_x + \hat{S}_y\hat{S}_y - 2\hat{S}_z\hat{S}_z)$. They are obviously hermitian.

(a) (5pts) *Check that* $\sum_{a=x,y,z}[\hat{S}_a, [\hat{S}_a, \hat{Q}_i]] = 6 \cdot \hat{Q}_i$, $i = 1, \ldots, 5$. [Therefore the $\hat{Q}_i$ operators "angular momentum" quantum number is $k = 2$, because $6 = 2 \cdot (2+1)$] [The commutators $[\hat{S}_a, \hat{Q}_i]$ will be useful later]

(b) (7pts) By making linear combinations of $\hat{Q}_i$, we can form "irreducible tensor operators" $\hat{T}_q^{(k=2)}$, $q = -2, -1, 0, 1, 2$. And $[\hat{S}_z, \hat{T}_q^{(k=2)}] = q \cdot \hat{T}_q^{(k=2)}$, $[\hat{S}_\pm, \hat{T}_q^{(k=2)}] = \sqrt{(k \mp q)(k \pm q + 1)} \cdot \hat{T}_{q\pm1}^{(k=2)}$. *Solve* $\hat{T}_q^{(k=2)}$ *as linear combinations of* $\hat{Q}_i$. [Hint: find $\hat{T}_{q=0}^{(k=2)}$ first, then generate others]

(c) (9pts) *Compute the matrix elements* $\langle S_z = m|\hat{T}_{q=m_1}^{(k=2)}|S_z = m_2\rangle$, *for* $m = -1, 0, 1$, $m_1 = -2, -1, 0, 1, 2$, $m_2 = -1, 0, 1$. *Show that this is proportional to the C-G coefficients* $\langle j = 1, m|j_1 = 2, m_1; j_2 = 1, m_2\rangle$ *solved in Problem 1.*

Solution:

Under the $|S_z = +1, 0, -1\rangle$ basis, $\hat{Q}_1 = \begin{pmatrix} 0 & -\frac{\mathbb{i}}{\sqrt{2}} & 0 \\ \frac{\mathbb{i}}{\sqrt{2}} & 0 & \frac{\mathbb{i}}{\sqrt{2}} \\ 0 & -\frac{\mathbb{i}}{\sqrt{2}} & 0 \end{pmatrix}$, $\hat{Q}_2 = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ 0 & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$,

$\hat{Q}_3 = \begin{pmatrix} 0 & 0 & -\mathbb{i} \\ 0 & 0 & 0 \\ \mathbb{i} & 0 & 0 \end{pmatrix}$, $\hat{Q}_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$, $\hat{Q}_5 = \begin{pmatrix} -\frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 & -\frac{1}{\sqrt{3}} \end{pmatrix}$.

[Side remarks: define $\hat{Q}_6 = \hat{S}_x$, $\hat{Q}_7 = \hat{S}_y$, $\hat{Q}_8 = \hat{S}_z$, then $\mathrm{Tr}(\hat{Q}_i) = 0$, $\mathrm{Tr}(\hat{Q}_i\hat{Q}_j) = 2\delta_{i,j}$, for $i, j = 1, \ldots, 8$. They are related to the Gell-Mann matrices. Any 3×3 traceless matrix $\hat{M}$ can be represented as a unique linear combination $\sum_{i=1}^{8}(\hat{Q}_i \cdot \frac{1}{2}\mathrm{Tr}(\hat{Q}_i\hat{M}))$.]

Use the commutation relations of spin operators, we have

$[\hat{S}_x, \hat{Q}_1] = 2\mathbb{i}(\hat{S}_z^2 - \hat{S}_y^2) = \mathbb{i}\hat{Q}_4 - \sqrt{3}\mathbb{i}\hat{Q}_5$; $[\hat{S}_y, \hat{Q}_1] = \mathbb{i}(\hat{S}_y\hat{S}_x + \hat{S}_x\hat{S}_y) = \mathbb{i}\hat{Q}_3$; $[\hat{S}_z, \hat{Q}_1] = -\mathbb{i}(\hat{S}_x\hat{S}_z + \hat{S}_z\hat{S}_x) = -\mathbb{i}\hat{Q}_2$;

$[\hat{S}_x, \hat{Q}_2] = -\mathbb{i}(\hat{S}_y\hat{S}_x + \hat{S}_x\hat{S}_y) = -\mathbb{i}\hat{Q}_3$; $[\hat{S}_y, \hat{Q}_2] = 2\mathbb{i}(\hat{S}_x^2 - \hat{S}_z^2) = \mathbb{i}Q_4 + \sqrt{3}\mathbb{i}\hat{Q}_5$; $[\hat{S}_z, \hat{Q}_2] = \mathbb{i}(\hat{S}_z\hat{S}_y + \hat{S}_y\hat{S}_z) = \mathbb{i}\hat{Q}_1$;

$[\hat{S}_x, \hat{Q}_3] = \mathbb{i}(\hat{S}_x\hat{S}_z + \hat{S}_z\hat{S}_x) = \mathbb{i}\hat{Q}_2$; $[\hat{S}_y, \hat{Q}_3] = -\mathbb{i}(\hat{S}_z\hat{S}_y + \hat{S}_y\hat{S}_z) = -\mathbb{i}\hat{Q}_1$; $[\hat{S}_z, \hat{Q}_3] = 2\mathbb{i}(\hat{S}_y^2 - \hat{S}_x^2) = -2\mathbb{i}\hat{Q}_4$;

$[\hat{S}_x, \hat{Q}_4] = -\mathbb{i}(\hat{S}_y\hat{S}_z + \hat{S}_z\hat{S}_y) = -\mathbb{i}\hat{Q}_1$; $[\hat{S}_y, \hat{Q}_4] = -\mathbb{i}(\hat{S}_z\hat{S}_x + \hat{S}_x\hat{S}_z) = -\mathbb{i}\hat{Q}_2$; $[\hat{S}_z, \hat{Q}_4] = 2\mathbb{i}(\hat{S}_y\hat{S}_x + \hat{S}_x\hat{S}_y) = 2\mathbb{i}\hat{Q}_3$;

$[\hat{S}_x, \hat{Q}_5] = \sqrt{3}\mathbb{i}(\hat{S}_z\hat{S}_y + \hat{S}_y\hat{S}_z) = \sqrt{3}\mathbb{i}\hat{Q}_1$; $[\hat{S}_y, \hat{Q}_5] = -\sqrt{3}\mathbb{i}(\hat{S}_z\hat{S}_x + \hat{S}_x\hat{S}_z) = -\sqrt{3}\mathbb{i}\hat{Q}_2$; $[\hat{S}_z, \hat{Q}_5] = 0$.

These relations can be written as $[\hat{S}_a, \hat{Q}_i] = \sum_j \hat{Q}_j (M_a)_{j,i}$, where the 5×5 matrices M_a are
$$M_x = \begin{pmatrix} 0 & 0 & 0 & -\mathbb{i} & \sqrt{3}\mathbb{i} \\ 0 & 0 & \mathbb{i} & 0 & 0 \\ 0 & -\mathbb{i} & 0 & 0 & 0 \\ \mathbb{i} & 0 & 0 & 0 & 0 \\ -\sqrt{3}\mathbb{i} & 0 & 0 & 0 & 0 \end{pmatrix},\ M_y = \begin{pmatrix} 0 & 0 & -\mathbb{i} & 0 & 0 \\ 0 & 0 & 0 & -\mathbb{i} & -\sqrt{3}\mathbb{i} \\ \mathbb{i} & 0 & 0 & 0 & 0 \\ 0 & \mathbb{i} & 0 & 0 & 0 \\ 0 & \sqrt{3}\mathbb{i} & 0 & 0 & 0 \end{pmatrix},\ M_z = \begin{pmatrix} 0 & \mathbb{i} & 0 & 0 & 0 \\ -\mathbb{i} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2\mathbb{i} & 0 \\ 0 & 0 & -2\mathbb{i} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

(a) use $[\hat{S}_a, \hat{Q}_i]$ results above, you can check that $\sum_{a=x,y,z}(M_a)^2 = 6\cdot \mathbb{1}_{5\times 5}$ (steps omitted)

(b) We can obviously choose $\hat{T}^{(k=2)}_{q=0} = \hat{Q}_5$, because $[\hat{S}_z, \hat{Q}_5] = 0$. Then

$\hat{T}^{(k=2)}_{q=1} = \frac{1}{\sqrt{6}}[\hat{S}_+, \hat{T}^{(k=2)}_{q=0}] = \frac{1}{\sqrt{2}}(\mathbb{i}\hat{Q}_1 + \hat{Q}_2)$.

$\hat{T}^{(k=2)}_{q=2} = \frac{1}{2}[\hat{S}_+, \hat{T}^{(k=2)}_{q=1}] = \frac{1}{\sqrt{2}}(-\hat{Q}_4 - \mathbb{i}\hat{Q}_3)$.

$\hat{T}^{(k=2)}_{q=-1} = \frac{1}{\sqrt{6}}[\hat{S}_-, \hat{T}^{(k=2)}_{q=0}] = \frac{1}{\sqrt{2}}(\mathbb{i}\hat{Q}_1 - \hat{Q}_2)$.

$\hat{T}^{(k=2)}_{q=-2} = \frac{1}{2}[\hat{S}_-, \hat{T}^{(k=2)}_{q=-1}] = \frac{1}{\sqrt{2}}(-\hat{Q}_4 + \mathbb{i}\hat{Q}_3)$.

Note: if we replace $\hat{S}_{x,y,z}$ by x, y, z in the definition of $\hat{Q}_i$, then $\hat{T}^{(k=2)}_q$ becomes functions proportional to spherical harmonics, $(-4\sqrt{\frac{\pi}{15}})\cdot r^2 \cdot Y^{m=q}_{l=2}(\theta,\phi)$.

(c) Under the $|S_z = +1, 0, -1\rangle$ basis,

$$\hat{T}^{(k=2)}_{q=2} = \begin{pmatrix} 0 & 0 & -\sqrt{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \hat{T}^{(k=2)}_{q=1} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix},\ \hat{T}^{(k=2)}_{q=0} = \begin{pmatrix} -\frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 & -\frac{1}{\sqrt{3}} \end{pmatrix},$$
$$\hat{T}^{(k=2)}_{q=-1} = \begin{pmatrix} 0 & 0 & 0 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},\ \hat{T}^{(k=2)}_{q=-2} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\sqrt{2} & 0 & 0 \end{pmatrix}.$$

We can check that

$\langle S_z = m|\hat{T}^{(k=2)}_{q=m_1}|S_z = m_2\rangle = \langle j = 1, m|j_1 = 2, m_1; j_2 = 1, m_2\rangle \cdot (-\sqrt{\frac{10}{3}})$. .

***** (about lecture #5 & #6) *****

3. (20points) Consider two spin-1 moments, $\hat{\boldsymbol{S}}_1$ and $\hat{\boldsymbol{S}}_2$. They satisfy $[\hat{S}_{i,a}, \hat{S}_{j,b}] = \delta_{i,j} \sum_c \mathbb{i}\epsilon_{abc}\hat{S}_{i,c}$ (here a, b, c label x, y, z components), and $\hat{\boldsymbol{S}}_1^2 = \hat{\boldsymbol{S}}_2^2 = 1 \cdot (1+1) = 2$. A complete orthonormal basis for the 9-dimensional Hilbert space is the S_z-basis, $|s_1, s_2\rangle$, with $s_{1,2} = -1, 0, 1$ and $\hat{S}_{1,z}|s_1, s_2\rangle = s_1|s_1, s_2\rangle$ and $\hat{S}_{2,z}|s_1, s_2\rangle = s_2|s_1, s_2\rangle$. The matrix elements of $\hat{S}_{i,x}$ and $\hat{S}_{i,y}$ under this basis follow the Condon-Shortley convention.

(1) (9pts) Consider $\hat{H}_0 = -J \cdot \hat{\boldsymbol{S}}_1 \cdot \hat{\boldsymbol{S}}_2 \equiv -J \sum_a \hat{S}_{1,a}\hat{S}_{2,a}$. Here $J > 0$ is a positive real constant. *Solve all the eigenvalues and eigenstates (in terms of S_z-basis) of $\hat{H}_0$.* [Hint: $\hat{H}_0 = -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + \frac{J}{2}\hat{\boldsymbol{S}}_1^2 + \frac{J}{2}\hat{\boldsymbol{S}}_2^2$.]

(2) (6pts) Define vector spin chirality $\hat{\boldsymbol{\chi}} = \hat{\boldsymbol{S}}_1 \times \hat{\boldsymbol{S}}_2$ (namely $\hat{\chi}_x = \hat{S}_{1,y}\hat{S}_{2,z} - \hat{S}_{1,z}\hat{S}_{2,y}$, ...). Define total spin operator (spin rotation generator) $\hat{\boldsymbol{S}} = \hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2$. *Check that $\hat{\boldsymbol{\chi}}$ transforms like a vector under spin rotation, namely $[\hat{S}_a, \hat{\chi}_b] = \mathbb{i}\epsilon_{abc}\hat{\chi}_c$. Evaluate the matrix elements of $\hat{\chi}_a$ ($a = x, y, z$) between the degenerate ground states of $\hat{H}_0$ solved in (1).* [Hint: certain symmetry may help, and you can use the "projection theorem"]

(3) (5pts) Add a small staggered magnetic field term to the Hamiltonian as perturbation, $\hat{H} = \hat{H}_0 - B \cdot (\hat{S}_{1,z} - \hat{S}_{2,z})$. Treat the real constant B as a small parameter. *Solve the second order perturbation results for the energies of the original ground states of $\hat{H}_0$.* [NOTE: the unperturbed ground states of $\hat{H}_0$ are degenerate, but degenerate perturbation theory can be avoided by dividing the Hilbert spaces by symmetry (conserved quantity)]

Solution:

(1) $\hat{H}_0 = -\frac{J}{2}(\hat{\boldsymbol{S}}_1 + \hat{\boldsymbol{S}}_2)^2 + 2J$. The total spin can be 2 or 1 or 0, "$\mathbf{1} \otimes \mathbf{1} = \mathbf{2} \oplus \mathbf{1} \oplus \mathbf{0}$".

The basis states $|S_{1+2}, S_{1+2,z}\rangle$ are eigenstates, and can be built in similar way as that of Homework #5 Problem 3(a,b). First solve the highest S_z state in each total S_{1+2} subspace, then the other states can be obtained by applications of lowering ladder operators.

$|S_{1+2} = 2, S_{1+2,z} = 2\rangle = |1, 1\rangle$.

Suppose $|S_{1+2} = 1, S_{1+2,z} = 1\rangle = c_1|1, 0\rangle + c_2|0, 1\rangle$, then by $0 = \hat{S}_{1+2,+}|S_{1+2} = 1, S_{1+2,z} = 1\rangle = (\hat{S}_{1,+} + \hat{S}_{2,+})(c_1|1, 0\rangle + c_2|0, 1\rangle) = \sqrt{2}(c_1 + c_2)|1, 1\rangle$, we have $c_2 = -c_1$. The normalized state $|S_{1+2} = 1, S_{1+2,z} = 1\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle - |0, 1\rangle)$.

Suppose $|S_{1+2}=0, S_{1+2,z}=0\rangle = c_1|1,-1\rangle + c_2|0,0\rangle + c_3|-1,0\rangle$, then by $0 = \hat{S}_{1+2,+}|S_{1+2}=0, S_{1+2,z}=0\rangle = (\hat{S}_{1,+}+\hat{S}_{2,+})(c_1|1,-1\rangle + c_2|0,0\rangle + c_3|-1,0\rangle) = \sqrt{2}(c_1+c_2)|1,0\rangle + \sqrt{2}(c_2+c_3)|0,1\rangle$, we have $c_2 = -c_1$ and $c_3 = -c_2$. The normalized state $|S_{1+2}=0, S_{1+2,z}=0\rangle = \frac{1}{\sqrt{3}}(|1,-1\rangle - |0,0\rangle + |-1,1\rangle)$.

$\hat{H}_0$ eigenvalue	S_{1+2}	$S_{1+2,z}$	state
$-J$	2	2	$\|1,1\rangle$
$-J$	2	1	$\frac{1}{\sqrt{2}}(\|1,0\rangle + \|0,1\rangle)$
$-J$	2	0	$\frac{1}{\sqrt{6}}(\|1,-1\rangle + 2\|0,0\rangle + \|-1,1\rangle)$
$-J$	2	-1	$\frac{1}{\sqrt{2}}(\|0,-1\rangle + \|-1,0\rangle)$
$-J$	2	-2	$\|-1,-1\rangle$
J	1	1	$\frac{1}{\sqrt{2}}(\|1,0\rangle - \|0,1\rangle)$
J	1	0	$\frac{1}{\sqrt{2}}(\|1,-1\rangle - \|-1,1\rangle)$
J	1	-1	$\frac{1}{\sqrt{2}}(\|0,-1\rangle - \|-1,0\rangle)$
$2J$	0	0	$\frac{1}{\sqrt{3}}(\|1,-1\rangle - \|0,0\rangle + \|-1,1\rangle)$

(2)

Use Einstein convention, $\hat{\chi}_a = \epsilon_{abc}\hat{S}_{1,b}\hat{S}_{2,c}$.

Use $[\hat{S}_a, \hat{S}_{i,b}] = \mathbb{i}\epsilon_{abc}\hat{S}_{i,c}$, and $\epsilon_{abc}\epsilon_{cdf} = \delta_{ad}\delta_{bf} - \delta_{af}\delta_{bd}$. Then

$[\hat{S}_a, \hat{\chi}_b] = [\hat{S}_a, \epsilon_{bcd}\hat{S}_{1,c}\hat{S}_{2,d}] \ = \epsilon_{bcd}\mathbb{i}\epsilon_{acf}\hat{S}_{1,f}\hat{S}_{2,d} + \epsilon_{bcd}\hat{S}_{1,c}\mathbb{i}\epsilon_{adf}\hat{S}_{2,f}$

$= \mathbb{i}(\delta_{ba}\delta_{df} - \delta_{bf}\delta_{da})\hat{S}_{1,f}\hat{S}_{2,d} + \mathbb{i}(\delta_{bf}\delta_{ca} - \delta_{ba}\delta_{cf})\hat{S}_{1,c}\hat{S}_{2,f} = \mathbb{i}(\hat{S}_{1,a}\hat{S}_{2,b} - \hat{S}_{1,b}\hat{S}_{2,a}) = \mathbb{i}\epsilon_{abc}\hat{\chi}_c$.

Ground states of $\hat{H}_0$ are $|S_{1+2}=2, S_{1+2,z}\rangle$ states. All the matrix elements of $\hat{\chi}_a$ between these states vanish, $\langle S_{1+2}=2, S_{1+2,z}=m|\hat{\chi}_a|S_{1+2}=2, S_{1+2,z}=m'\rangle = 0$.

Method #1: brute-force evaluation (omitted).

Method #2: use "projection theorem",

$\hat{\boldsymbol{\chi}}$ transform like a vector, so $\langle S_{1+2}=2, S_{1+2,z}=m|\hat{\chi}_a|S_{1+2}=2, S_{1+2,z}=m'\rangle$

$= \langle S_{1+2}=2, S_{1+2,z}=m|\hat{S}_{1+2,a}|S_{1+2}=2, S_{1+2,z}=m'\rangle \cdot \frac{\langle S_{1+2}=2, S_{1+2,z}=m|\hat{\boldsymbol{S}}_{1+2}\cdot\hat{\boldsymbol{\chi}}|S_{1+2}=2, S_{1+2,z}=m\rangle}{2\cdot(2+1)}$.

But $\hat{\boldsymbol{S}}_{1+2}\cdot\hat{\boldsymbol{\chi}} = \epsilon_{abc}(\hat{S}_{1,a}+\hat{S}_{2,a})\hat{S}_{1,b}\hat{S}_{2,c} = \mathbb{i}\hat{S}_{1,c}\hat{S}_{2,c} + \hat{S}_{1,b}\cdot(-\mathbb{i}\hat{S}_{2,b}) = 0$. Here we have used the Einstein convention, and $\epsilon_{abc}\hat{S}_{i,a}\hat{S}_{i,b} = \mathbb{i}\hat{S}_{i,c}$.

Method #3: use "parity selection rule",

consider unitary transformation $\hat{I}$: $|s_1, s_2\rangle \mapsto |s_2, s_1\rangle$, $\hat{S}_{1,a} \leftrightarrow \hat{S}_{2,a}$,

then $\hat{I}^2 = \mathbb{1}$, it generates a Z_2 group $\{\mathbb{1}, \hat{I}\}$, with two irreps: $R_{\Gamma_1}(\hat{I}) = (+1)$, $R_{\Gamma_2}(\hat{I}) = (-1)$.

Note that all $|S_{1+2} = 2, S_{1+2,z}\rangle$ states belong to the trivial(even) irrep of this group, $\hat{I}|S_{1+2} = 2, S_{1+2,z}\rangle = |S_{1+2} = 2, S_{1+2,z}\rangle \cdot (+1)$, but the operators $\hat{\boldsymbol{\chi}}$ belong to the non-trivial(odd) irrep, $\hat{I}\hat{\chi}_a\hat{I}^\dagger = \hat{\chi}_a \cdot (-1)$. Therefore the matrix element $\langle S_{1+2} = 2, S_{1+2,z} = m|\hat{\chi}_a|S_{1+2} = 2, S_{1+2,z} = m'\rangle$ belongs to the "(even)* $\otimes$ (odd) $\otimes$ (even) = (odd)" irrep, so must vanish by the selection rule.

(3) Note that the perturbed Hamiltonian still conserves total $\hat{S}_{1+2,z} \equiv \hat{S}_{1,z} + \hat{S}_{2,z}$, $[\hat{H}, \hat{S}_{1+2,z}] = 0$. Therefore $\hat{H}$ is block-diagonalized by dividing the 9-dimensional Hilbert space into different total-S_z subspaces.

The $S_{1+2,z} = \pm 2$ subspaces are 1-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = \pm 2\rangle)$ respectively.

The $S_{1+2,z} = \pm 1$ subspaces are 2-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = \pm 1\rangle, |S_{1+2} = 1, S_{1+2,z} = \pm 1\rangle)$ respectively.

The $S_{1+2,z} = 0$ subspace is 3-dimensional with the complete orthonormal basis $(|S_{1+2} = 2, S_{1+2,z} = 0\rangle, |S_{1+2} = 1, S_{1+2,z} = 0\rangle, |S_{1+2} = 0, S_{1+2,z} = 0\rangle)$.

In each subspace, the ground state is non-degenerate, $|S_{1+2} = 2, S_{1+2,z}\rangle$, so one can use non-degenerate perturbation theory.

$S_{1+2,z}$	$\hat{H}$ in subspace	2nd order ground state energy
2	$(-J) + (0)$	$-J$
1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & -B \\ -B & 0 \end{pmatrix}$	$\approx -J + \frac{(-B)\cdot(-B)}{-J-J} = -J - \frac{B^2}{2J}$
0	$\begin{pmatrix} -J & 0 & 0 \\ 0 & J & 0 \\ 0 & 0 & 2J \end{pmatrix} + \begin{pmatrix} 0 & -\frac{2}{\sqrt{3}}B & 0 \\ -\frac{2}{\sqrt{3}}B & 0 & -\frac{4}{\sqrt{6}}B \\ 0 & -\frac{4}{\sqrt{6}}B & 0 \end{pmatrix}$	$\approx -J + \frac{(-2B/\sqrt{3})\cdot(-2B/\sqrt{3})}{-J-J} = -J - \frac{2B^2}{3J}$
-1	$\begin{pmatrix} -J & 0 \\ 0 & J \end{pmatrix} + \begin{pmatrix} 0 & B \\ B & 0 \end{pmatrix}$	$\approx -J + \frac{(B)\cdot(B)}{-J-J} = -J - \frac{B^2}{2J}$
-2	$(-J) + (0)$	$-J$