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PH3102 - Assgn-08 -

Q.3) $|\chi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right)$ ← singlet state.

(i)

(i)

Let us denote the orthonormal sets of 1st and 2nd spin as

$\{|\psi_{1A}\rangle, |\psi_{2A}\rangle\} = \{|\uparrow_1\rangle, |\downarrow_1\rangle\}$ ∵ ½ spin 2 particle

& $\{|\phi_{1B}\rangle, |\phi_{2B}\rangle\} =$

$= \{|\downarrow_2\rangle, |\uparrow_2\rangle\}$

So, we can write

$$|\chi\rangle = \sum_{i=1}^{2} k_i \, |\psi_{iA}\rangle \, |\phi_{iB}\rangle \quad \text{s.t} \quad \sum_{i=1}^{2} k_i^2 = 1$$

$$= \frac{1}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle \right)$$

∴ The density matrix,

$$\rho^{AB} = |\chi\rangle\langle\chi| = \frac{1}{2}\left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right)\left(\langle\uparrow,\downarrow| - \langle\uparrow,\downarrow|\right)$$

$$= \frac{1}{2}\left(|\uparrow,\downarrow\rangle\langle\uparrow,\downarrow| - |\uparrow,\downarrow\rangle\langle\uparrow,\downarrow| - |\downarrow,\uparrow\rangle\langle\uparrow,\downarrow| + |\downarrow,\uparrow\rangle\langle\uparrow,\downarrow| \right).$$

The density matrix describes the probabilities of finding a system in various configurations.

(ii) Now, we obtain the reduced density matrix ρ_1 (or ρ^A) for the first spin. We obtain it by taking partial trace of ρ^{AB} over the subsystem B.

i.e, $\rho^A = Tr_B(\rho^{AB})$

$$= \sum_{l=1}^{2} \langle \phi_{lB} | \rho^{AB} | \phi_{lB} \rangle.$$

we have

$$\rho^{AB} = \left(\sum_i k_i \, |\psi_{iA}\rangle |\phi_{iB}\rangle \right)\left(\sum_j k_j^* \langle \psi_{jA}| \langle \phi_{jB}| \right)$$

$$\therefore \rho^A = \sum_l \left\{ \langle \phi_{lB}| \left[\sum_{i,j} k_i k_j^* \, |\phi_{iB}\rangle |\psi_{iA}\rangle \langle \psi_{jA}| \langle \phi_{jB}| \right] |\phi_{lB}\rangle \right\}$$

(δ_{li} connects $|\phi_{iB}\rangle$ and $\langle\phi_{jB}|$; δ_{jl} connects $\langle\phi_{jB}|$ and $|\phi_{lB}\rangle$)

$$= \sum_l |k_l|^2 \, |\psi_{lA}\rangle\langle\psi_{lA}| \qquad \therefore \underline{i = l = j}$$

$$= \frac{1}{2}\left(|\uparrow_1\rangle\langle\uparrow_1| + |\downarrow_1\rangle\langle\downarrow_1| \right)$$

Q3(iii)

$$\rho^A = \frac{1}{2}\left(\begin{pmatrix} 1 \\ 0 \end{pmatrix}(1,\ 0) + \begin{pmatrix} 0 \\ 1 \end{pmatrix}(0,\ 1) \right)$$

$$= \frac{1}{2}\left(\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \right) = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \frac{1}{2}\, \mathbb{I} \quad \phi$$

This is the reduced density matrix for 1st spin.

(iii) Entanglement entropy of 1st spin.

$$S_{EE} = -\mathrm{Tr}\left[\rho_1 \ln \rho_1\right] = -\sum_i \lambda_i \ln \lambda_i$$

we calculate eigen values for ρ_1 (or ρ^A).

↳ roots of eq^n: $|\chi I - \rho^A| = 0$.

$$= \begin{vmatrix} \chi - 1/2 & 0 \\ 0 & \chi - 1/2 \end{vmatrix} = (\chi - 1/2)^2 = 0.$$

$$\chi = 1/2 = \lambda_i \ \forall\, i$$

$$\therefore S_{EE} = -2 \times \frac{1}{2} \ln\left(\frac{1}{2}\right) = \cancel{2} \times \frac{1}{\cancel{2}} \times \ln 2 = \boxed{\ln 2} \quad \phi$$

which is maximum for two-component system. This means singlet state is a maximally mixed state. we can infer that more mixed a density matrix is, the more will be it's VNE.

If S_{AB} → denotes von-Neumann ~~error~~ entropy of complete system, it can be shown.

$$S_{AB} \leq S_A + S_B.$$

↳ ↓

Entanglement entropies of subsystems A and B

since $S_A = S_B = \ln 2$ (symmetry).

$\therefore S_{AB} \leq 2\ln 2$ ← upper bound on the entropy of the singlet state.

(iv) $|\chi(\theta)\rangle = \cos\theta\,|\uparrow,\downarrow\rangle + \sin\theta\,|\downarrow,\uparrow\rangle$

$\therefore \rho(\theta) = |\chi(\theta)\rangle\langle\chi(\theta)|$

$= (\cos\theta\,|\uparrow,\downarrow\rangle + \sin\theta\,|\downarrow,\uparrow\rangle)(\cos\theta\langle\uparrow,\downarrow| + \sin\theta\langle\downarrow,\uparrow|)$

$= \cos^2\theta\,|\uparrow,\downarrow\rangle\langle\uparrow,\downarrow| + \frac{1}{2}\sin 2\theta\,|\uparrow,\downarrow\rangle\langle\downarrow,\uparrow|$

$+ \frac{1}{2}\sin 2\theta\,(|\downarrow,\uparrow\rangle\langle\uparrow,\downarrow|) + \sin^2\theta\,|\downarrow,\uparrow\rangle\langle\downarrow,\uparrow|$

Similarly we can calculate,

$\rho_{A1}(\theta) = \sum_i k_i^2\,|\psi_{iA}\rangle\langle\psi_{iA}|$

$= \cos^2\theta\,|\uparrow\rangle\langle\uparrow| + \sin^2\theta\,|\downarrow\rangle\langle\downarrow|$

$= \cos^2\theta \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \sin^2\theta \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$

$= \begin{bmatrix} \cos^2\theta & 0 \\ 0 & \sin^2\theta \end{bmatrix}$

Computing it's eigen value.

$\Rightarrow |\chi I - \rho_1(\theta)| = \begin{vmatrix} \chi - \cos^2\theta & 0 \\ 0 & \chi - \sin^2\theta \end{vmatrix} = (\chi - \cos^2\theta)(\chi - \sin^2\theta) = 0.$

$\lambda_1 = \cos^2\theta$

$\lambda_2 = \sin^2\theta.$

$\therefore S_{EE}(\theta) = -\sum \lambda_i \ln(\lambda_i)$

$= -2\sin^2\theta \ln|\sin\theta| - 2\cos^2\theta \ln|\cos\theta|$

Parameterising $\sin^2\theta = t^2$. (or $\cos^2\theta = t^2$)

$S_{EE}(t) = -t^2 \ln t^2 - (1-t^2)\ln(1-t^2).$

$\frac{dS_{EE}}{dt} = 2t\left[\ln(1-t^2) - \ln(t^2)\right]$

$\frac{dS_{EE}}{dt} = 0$ when $t = 0$ i.e when $\sin\theta = 0 \Rightarrow \theta = 0$ | $\cos\theta = 0$ | $\theta = \pi/2$

Now,

Also $t^2 = 1 - t^2$

$\therefore 2t^2 = 1$

$\therefore \sin^2\theta \ (\text{or } \cos^2\theta) = 1/2 \Rightarrow \theta = \pi/4 \text{ or } 3\pi/4$.

For $\theta = 0, (\text{or } \pi/2)$

$SEE(\theta) = 0$.

For $\theta = \pi/4 \ (\text{or } 3\pi/4)$

$= -2 \times \frac{1}{2} \ln\left(\frac{1}{2}\right) = \ln 2$

Clearly, For $\theta = 0, \pi/2$ SEE is minimum. → pure states

$\theta = \pi/4, 3\pi/4$ SEE is maximum → mixed states

(b) $H = J \bar{S}_1 \cdot \bar{S}_2$

$J > 0 \rightarrow$ strength of interaction is given by the ~~so called~~ interaction coupling

or

(a) since the Hilbert space of each of the 2 spins ~~will be~~ is 2-dimensional. (S, S_z).

$\therefore$ The total system will have $2 \times 2 = 4$ eigenstates.

S_tot = 0, S_z = 0
S_tot = 0; S_z = 0,1,-1
Total 4 states

$\bar{S}_{tot} = \bar{S}_1 + \bar{S}_2$

(b) ~~Sto~~ Now $\vec{S}_{tot}^{\,2} = S_1^2 + S_2^2 + 2\bar{S}_1 \cdot \bar{S}_2 \quad [\because [S_1, S_2] = 0]$

$\therefore H = \frac{J}{2}\left[S_{tot}^2 - S_1^2 - S_2^2\right]$. ✓

$$\boxed{\hat{H} = \frac{J}{2}\left[S_{tot}^2 - \bar{S}_1^2 - \bar{S}_2^2\right]}$$ ✓

iii) We know $[S_{tot}^2, S_z] = 0$

S_z - z^{th} component of total spin angular momentum.

$\therefore [H, S_z] = 0$ So, S_z's eigenvalues are good quantum number.

Also $[H, S_{tot}^2] = 0$ $\therefore$ same for S_{tot}.

Now note that since, $H \propto \vec{S}_i$ $[H, S_{iz}] \neq 0$ $(i = 1, 2)$

hence, states of definite S_{iz} cannot be eigenstates of the above Hamiltonian H.

However, also, $[H, S_1^2] = [H, S_2^2] = 0$

$\Rightarrow$ The eigenvalues of ~~S_1, S_2, S_1~~ S_{tot}^2, S_z, S_1^2, S_2^2 are 'good' quantum numbers to label eigen states.

like $-|s, m_s; s_1, s_2\rangle$

Since, $s_1, s_2 = 1/2$ in this problem and are fixed we can drop them.

The possible values of $s := |s_1 - s_2|, \ldots s_1 + s_2$.

$\equiv 0, 1$.

$\therefore$ $s = 0 \Rightarrow m_s = 0$ (Singlet state)

& $s = 1 \Rightarrow m_s = -1, 0, 1$ (Triplet state)

$\therefore$ We have a total of 4

$\therefore$ In general we have.

$$H|s, m_s\rangle = \frac{J}{2}\left[S_{tot}^2 - S_1^2 - S_2^2\right]|s, m_s\rangle.$$

$$= \frac{J\hbar^2}{2}\left[s(s+1) - 2\times\left(\frac{1}{2}\right)\left(\frac{1}{2}+1\right)\right]|s, m_s\rangle$$

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

clearly the energy eigenvalue is independent of m_s.

All the states with same s, but different m_s are thus degenerate.

$$E_s = \frac{J\hbar^2}{2}\left[s(s+1) - \frac{3}{2}\right]$$

∴ Eigenstates are →

$$\left\{\begin{array}{l} |s=1, m_s=-1\rangle \\ |s=1, m_s=1\rangle \\ |s=1, m_s=0\rangle \end{array}\right\} \Rightarrow E|_{s=1} = \frac{J}{4}\hbar^2$$

And.

$$|s=0, m_s=0\rangle \qquad E|_{s=0} = -\frac{3}{4}J\hbar^2$$

↓ ground state.

∴ we have, triply degenerate 1st Excited states.

we already calculated the eigenstates. (from prev. assignments)

$$|s=1, m_s=1\rangle = |\uparrow\uparrow\rangle$$

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

$$|s=1, m_s=-1\rangle = |\downarrow\downarrow\rangle$$

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

(iv) ~~The grou~~ In the ground state, $S = 0$

⇒ All the electrons are paired, and thus their spins cancel out.

Since, there is only one orientation ~~for~~ this can happen (i.e ~~S_z~~ $m_s = 0$) ~~or S_z~~, this is referred to as <u>singlet state</u>.

To see SU(2) symmetry, we have to calculate total magnetisation in any arbitrary direction ($\hat{n}$)

Total Magnetisation = $\langle \hat{S}_{tot}(\hat{n}) \rangle_{\psi_0}$ | $\hat{S}_{tot}(\hat{n}) = \hat{n} \cdot \vec{S}_{tot}$.

$\psi_0 \equiv |s = 0, m_s = 0\rangle$.

$\therefore$ $S_{tot}(\hat{n}) = n_x S^x_{tot} + n_y S^y_{tot} + n_z S^z_{tot}$.

$S_+ = S^x_{tot} + i S^y_{tot}$

$S_- = S^x_{tot} - i S^y_{tot}$

$S^x_{tot} = \frac{S_+ + S_-}{2}$, $S^y_{tot} = \frac{S_+ - S_-}{2i}$

Note, $S_\pm |s, m_s\rangle = \hbar \sqrt{s(s+1) - m_s(m_s \pm 1)}\, |s, m_s \pm 1\rangle$

$\therefore \langle 0,0 | \left(n_x \left(\frac{S_+ + S_-}{2} \right) + \frac{n_y}{2i} \left(S_+ - S_- \right) + n_z S^z_{tot} \right) | 0,0 \rangle$.

$= n_z \langle 0,0 | \left(S^z_{tot} \right) | 0,0 \rangle$

$= n_z \hbar \times 0 = 0$

Thus the total magnetisation in any arbitrary direction ($\hat{n}$) is 0. (constant), Thus singlet state remains unchanged when we rotate our frame of reference, $\rightarrow$ SU(2) symmetry.

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(v) Now we find the expectation values of $S_{tot}(\hat{n})$ in the 3 triplet states in the spectrum

a)

$$\langle 1,0| \left(n_x \left(\frac{S_+ + S_-}{2} \right) + \frac{n_y}{2i} \left(S_+ - S_- \right) + n_z S^2_{tot} \right) |1,0\rangle$$

Note carefully that

$S_+ |1,0\rangle \sim |1,1\rangle$

& $S_- |1,0\rangle \sim |1,-1\rangle$

Both of which are orthogonal to $|1,0\rangle$.

Also, $S^2_{tot} |1,0\rangle = 0 \times \hbar |1,0\rangle \to 0$.

$\therefore$

$$= \langle 1,0| \left(c_1 |1,1\rangle + c_2 |1,-1\rangle \right)$$

for some $c_1, c_2 \in \mathbb{C}$

which is $= 0$!

(b) For other 2 states, same way action of S_+, S_- will result in annihilation of $|1,1\rangle$ and $|1,-1\rangle$ respectively, and in the rest will produce orthogonal state, which results $\to 0$.

Remaining

$$= n_z \langle 1,\pm 1 | S^2_{tot} | 1,\pm 1 \rangle$$

$$= \pm \boxed{n_z \hbar}$$

This means the total magnetisation in these excited states depend on n_z, which means it has symmetry only in x-y plane.

$I = I(m_s, m_s)$ magnitude

we may conclude, the fact that the total magnetisation (I) is maximum along z-direction is a consequence of the fact that we have used S_z-axis to label the states.

If we instead have chosen x-axis, then also $I(s, 0) = 0$ but, $I(\cdot, \pm 1)$ i.e polarised states will now have maximum along x-axis.

⇒ The polarised states have a preferred axis along which (I) is maximum.

Nature of Magnetism

https://solidstate.quantumtinkerer.tudelft.nl/lecture_8/#paramagnetism-free-spin-12

By definition,

- Ferromagnet - A state where $\langle S_{tot}(\vec{n}) \rangle_{|s,m_s\rangle} \neq 0$ in the absence of field.
- Antiferromagnet - states where the staggered magnetisation $\langle S_1^z - S_2^z \rangle \neq 0$ in absence of any field
- Paramagnet - states where both $\langle S_{tot}(\vec{n}) \rangle = \langle S_1^z - S_2^z \rangle = 0$.

Note that,

state $|s=1, m_s=1\rangle = |\uparrow, \downarrow\rangle$

& $|s=1, m_s=-1\rangle = |\downarrow, \downarrow\rangle$

are ferromagnetic

Claim: $|s=1, m_s=0\rangle$ & $|s=0, m_s=0\rangle$ are paramagnetic.

Proof: We already showed that total magnetisation of these states are zero.

It remains to show they have vanishing staggered magnetisation as well.

$$|1,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

$$|0,0\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

singlet

$$\therefore \langle 1,0|\left(S_{1z} - S_{2z}\right)|1,0\rangle$$

$$= \frac{1}{2}\left[\langle\uparrow\downarrow| + \langle\downarrow\uparrow|\right]\left(S_{1z} - S_{2z}\right)\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right]$$

$$= \frac{\hbar}{2}\left[\langle\uparrow\downarrow| + \langle\downarrow\uparrow|\right]\left(\frac{1}{2}|\uparrow\downarrow\rangle + \frac{1}{2}|\uparrow\downarrow\rangle - \frac{1}{2}|\downarrow\uparrow\rangle - \frac{1}{2}|\downarrow\uparrow\rangle\right)$$

$$= \frac{\hbar}{2}\left[\frac{1}{2} + \frac{1}{2} - \frac{1}{2} - \frac{1}{2}\right] = 0 !$$

$$\& \langle 0,0|\left(S_{1z} - S_{2z}\right)|0,0\rangle .$$

$$= \frac{1}{2}\left[\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right]\left(S_{1z} - S_{2z}\right)\left[|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right]$$

$$= \frac{\hbar}{2}\left[\langle\uparrow\downarrow| - \langle\downarrow\uparrow|\right]\left(\frac{1}{2}|\uparrow,\downarrow\rangle + \frac{1}{2}|\downarrow\uparrow\rangle + \frac{1}{2}|\uparrow,\downarrow\rangle + \frac{1}{2}|\downarrow,\uparrow\rangle\right)$$

$$= \frac{\hbar}{2}\left[\frac{1}{2} + \frac{1}{2} - \frac{1}{2} - \frac{1}{2}\right] = 0 .$$

□

Hence our claim is proved!

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Problem 2

$$H = J\bar{S}_1 \cdot \bar{S}_2 + B(S_1^z + S_2^z), \quad J \geq 0$$

(i) Let us denote this Hamiltonian by H_B.

From prev problem we have

$$H_B = \frac{J}{2}\left(\bar{S}_{tot}^2 - S_1^2 - \bar{S}_2^2\right) + B\left(S_1^z + S_2^z\right)$$

$$= H + B(S_1^z + S_2^z) = H + B(S_{tot}^z)$$

Similarly, as prev problem we find that

Notice $[H_B, S_{tot}^2] = 0$, $[H_B, S_{tot}^z] = 0$.

$\therefore$ s, m_s → good quantum numbers.

So, we have the same eigen states as before. (Also, $[H_B, H] = 0$).

Eigenstates

$S_{tot}^z |s, m_s\rangle = m_s |s, m_s\rangle$

$S_{tot}^2 |s, m_s\rangle = s(s+1)|s, m_s\rangle$

(a) $|s=0; m_s=0\rangle$.

$$H_B|0,0\rangle = (H + BS_{tot}^z)|0,0\rangle$$
$$= \left(-\frac{3}{4}JB + 0\right)|0,0\rangle$$

$\therefore E_{0,0} = -\frac{3}{4}J$.

(b) $|s=1; m_s=0\rangle$

$$H_B|1,0\rangle = (H + BS_{tot}^z)|1,0\rangle$$
$$E_{1,0} = \frac{J}{4}.$$

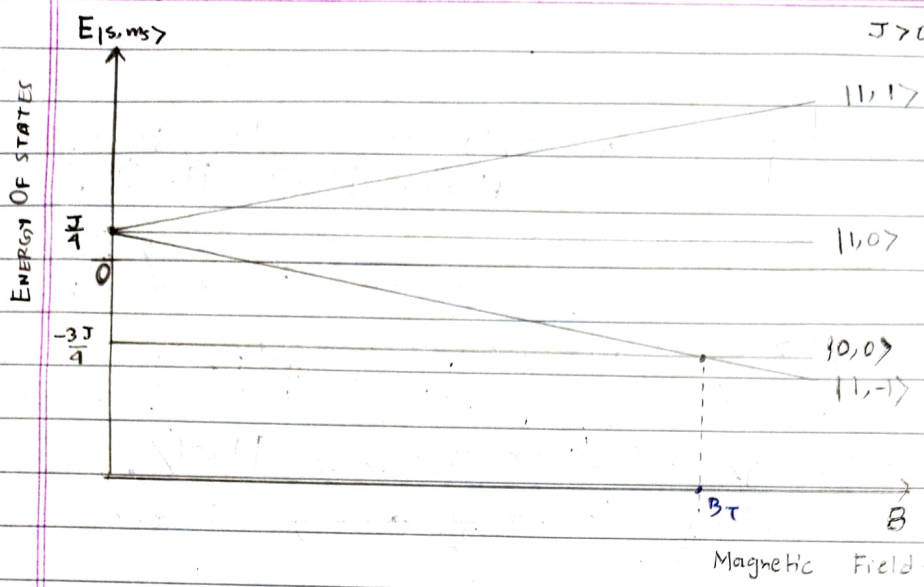
(c) $|s=1, m_s=1\rangle$

$$H_B|1,1\rangle = \left(\frac{J}{4} + B\right)|1,1\rangle. \Rightarrow E_{1,1} = \frac{J}{4} + B$$

(d) $|s=1, m_s=-1\rangle$

$$H_B|1,-1\rangle = \left(\frac{J}{4} - B\right)|1,-1\rangle \Rightarrow E_{1,-1} = \frac{J}{4} - B$$

Taking $t = 1$ in all calculations.



Note that, the presence of magnetic field lifts the degeneracy of triplet states.

(ii) Let us denote magnetic field ~~at~~ where this quantum transition occurs as B_T.

$$\therefore \frac{J}{4} - B_T = -\frac{3}{4}J \Rightarrow \boxed{B_T = J}$$

For

$B < B_T$: $|\psi_{ground}\rangle = $ ~~$|0,0\rangle$~~ $|s=0, m_s=0\rangle$

$B > B_T$: $|\psi_{ground}\rangle = |s=1, m_s=-1\rangle$.

So ∴ Earlier ground state was a singlet, ~~which had~~ which had SU(2) symmetry. After ~~that~~ 'level crossing', the ground state became $|\downarrow\downarrow\rangle$, thus breaking SU(2) or spin-rotation symmetry.

(iii) When $J<0$, let $J' \equiv -J$.
The eigen values become.

$$E'_{0,0} = +\frac{3}{4}J \; ; \; E'_{1,0} = -\frac{J}{4} \; ; \; E'_{1,1} = \frac{-J}{4} + B$$

$$E'_{1,-1} = \frac{-J}{4} - B$$

At $B = 0$,

We have

$E_g = -\frac{J}{4}$ → triply degenerate ground state,
$|1,0\rangle$, $|1,1\rangle$, $|1,-1\rangle$.

Now
as, $B > 0$. we turn the field,

The new ground state is, only $|1,-1\rangle$,
thus lifting the ~~degeneracy~~ degeneracy

There is no transition ground state,
However, the energy levels of
state. $|0,0\rangle$ and $|1,1\rangle$ switches
at $B = B'_T$

$$-\frac{J}{4} + B'_T = \frac{3}{4}J$$

$$\boxed{B'_T = J} \quad (J > 0)$$

↖ +ve.