M02Q.2

(a) When $\alpha = 0$, we have

$$\hat{H} = 2J(\hat{S_1}\hat{S_2} + \hat{S_2}\hat{S_3} + \hat{S_3}\hat{S_1}) + \frac{1}{2}k(x_{12}^2 + x_{23}^2 + x_{31}^2) = \hat{H}_s + \hat{H}_x \tag{1}$$

Since $\hat{x}$ and $\hat{s}$ are independent variables in the Hamiltonian, we should have

$$(\hat{H}_s + \hat{H}_x)|\psi_s > \oplus |\psi_x >= (E_s + E_x)|\psi_s > \oplus |\psi_x > \tag{2}$$

$x_{12} + x_{23} + x_{31} = L$, we can easily have $min(E_x) = E_{x0} = \frac{1}{2}k3(\frac{L}{3})^2 = \frac{kL^2}{6}$
as the ground state energy for spatial part of the Hamiltonian. Corresponding ground state for x is

$$|\psi_{x0} >= |x_{12} = \frac{L}{3}, x_{23} = \frac{L}{3}, x_{31} = \frac{L}{3} > \tag{3}$$

$$< x|\psi_{x0} >= \psi_x(x) = \delta(x_{12} - \frac{L}{3})\delta(x_{23} - \frac{L}{3})\delta(x_{31} - \frac{L}{3}) \tag{4}$$

$$\hat{H}_s|\psi_s >= J(\hat{S_{tot}}^2 - \hat{s_1}^2 - \hat{s_2}^2 - \hat{s_3}^2)|\psi_s >= (J[s_{tot}(s_{tot} + 1)] - \frac{9}{4})|\psi_s > \tag{5}$$

where $\hat{S_{tot}} = \hat{S_1} + \hat{S_2} + \hat{S_3}$ is the total spin operator, and $\hat{s_{tot}}$ is the total spin. $min(s_{tot}) = 1/2$ when 2 of the 3 particles have oppsite spin direction, therefore

$$min(E_s) = E_{s0} = -\frac{3}{2}J \tag{6}$$

From the relationship $\hat{S}_i\hat{S}_j = 1/2\hat{P}_{ij} - 1/4$, we can get the corresponding 4 eigenstates are

$$|\psi_{s0}>=\begin{cases}\frac{1}{\sqrt{2}}(|\uparrow\uparrow\downarrow>-|\uparrow\downarrow\uparrow>)\\ \frac{1}{\sqrt{2}}(|\downarrow\uparrow\uparrow>-|\uparrow\downarrow\uparrow>)\\ \frac{1}{\sqrt{2}}(|\uparrow\downarrow\downarrow>-|\downarrow\uparrow\downarrow>)\\ \frac{1}{\sqrt{2}}(|\downarrow\downarrow\uparrow>-|\downarrow\uparrow\downarrow>)\end{cases} \tag{7}$$

Therefore we have the ground states and ground energy as:

$$|\psi_0>=|\psi_{s0}>\oplus|\psi_{x0}> \tag{8}$$

$$E_0=E_{s0}+E_{x0}=\frac{kL^2}{6}-\frac{3}{2}J \tag{9}$$

where ψ_{s0} and ψ_{x0} are as in (3) and (7), $degeneracy = 4$
\\
(b)When $0<\alpha<<1$, we have perturbation to the ground state.\\
Assume $x_{12}=x_{23}=\frac{L}{3}+\delta x$, $x_{31}=\frac{L}{3}-2\delta x$. Then we have the Hamiltonian:

$$\hat{H}=\hat{H_0}+\delta\hat{H} \tag{10}$$

$$\hat{H_0}=2J(\hat{S_1}\hat{S_2}+\hat{S_2}\hat{S_3}+\hat{S_3}\hat{S_1})+\frac{1}{2}k(x_{12}^2+x_{23}^2+x_{31}^2) \tag{11}$$

$$+2J\alpha\frac{L}{3}(\hat{S_1}\hat{S_2}+\hat{S_2}\hat{S_3}+\hat{S_3}\hat{S_1})$$

$$\delta\hat{H}=2J\alpha\delta x(\hat{S_1}\hat{S_2}+\hat{S_2}\hat{S_3}-2\hat{S_3}\hat{S_1}) \tag{12}$$

Assume we have:

$$\hat{H_0}|\psi_0^i>=E_0|\psi_0^i> \tag{13}$$

$$E_0=-\frac{3}{2}J\hbar^2+\frac{kL^2}{6}-\frac{1}{2}J\alpha L\hbar^2+3k\delta x^2 \tag{14}$$

Where $i\in[1,6]$ denotes a specific isolated state. The states containing 2 up spins have zero cross term with the states containing 2 down spins. We can assume

$$|\psi>=\sum_{i=1}^{6} c_i|\psi_0^i> \tag{15}$$

$$(\hat{H}_0+\delta\hat{H})|\psi>=E_0|\psi>+\delta E|\psi>\Rightarrow \tag{16}$$

$$(\delta\hat{H})|\psi>=\delta E|\psi>\Rightarrow \tag{17}$$

$$\sum_i c_i<\psi_0^j|\delta\hat{H}|\psi_0^i>=\sum_i c_i\delta H_{ji}=c_j\delta E \tag{18}$$

where $\delta H_{ji}=<\psi_0^j|\delta\hat{H})|\psi_0^i>$. For the above equation to have solution for c_i, we require

$$Det|\delta\hat{\hat{H}}_{ij}-\delta E\hat{\hat{I}}|=0 \tag{19}$$

$$\begin{aligned}&\delta\hat{\hat{H}}_{ij}-\delta E\hat{\hat{I}}\\&=J\alpha\delta x\end{aligned} \tag{20}$$

$$\begin{pmatrix} 1-\frac{\delta E}{J\alpha\delta x} & 1 & -2 & 0 & 0 & 0\\ 1 & -2-\frac{\delta E}{J\alpha\delta x} & 1 & 0 & 0 & 0\\ -2 & 1 & 1-\frac{\delta E}{J\alpha\delta x} & 0 & 0 & 0\\ 0 & 0 & 0 & 1-\frac{\delta E}{J\alpha\delta x} & 1 & -2\\ 0 & 0 & 0 & 1 & -2-\frac{\delta E}{J\alpha\delta x} & 1\\ 0 & 0 & 0 & -2 & 1 & 1-\frac{\delta E}{J\alpha\delta x} \end{pmatrix}$$

Therefore we have

$Det|\delta\hat{\hat{H}}_{ij}-\delta E\hat{\hat{I}}|=((\frac{\delta E}{J\alpha\delta x})^3-\frac{9\delta E}{J\alpha\delta x})^2=0\Rightarrow$

$\delta E=\pm 3J\alpha\delta x$

$c_1 = \mp c_3$

Together with E_0, we have:

$$E = -\frac{3}{2}J + \frac{kL^2}{6} - \frac{1}{2}J\alpha L + 3k\delta x^2 \pm 3J\alpha\delta x \tag{21}$$

$$\Xi_0' = min(E) = E(\delta x = \mp\frac{J\alpha}{2k}) = -\frac{3}{2}J + \frac{kL^2}{6} - \frac{1}{2}J\alpha L - \frac{3J^2\alpha^2}{4k} \tag{22}$$

$c_1 = \mp c_3 \Rightarrow$ the ground state is

$$\delta x = \frac{J\alpha}{2k} \tag{23}$$

$$|\psi_s >= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\downarrow> - |\downarrow\uparrow\uparrow>) \tag{24}$$

One thought on “M02Q.2”

December 15, 2013 at 9:07 pm

You move in the right direction, but solution doesn't look finished, and I have some remarks.
In (2) and (8) you should have tensor product $\otimes$ not the direct sum $\oplus$.
In part (a) you say that the degeneracy is 4, but in (b) you act as if there were 6 ground states. Why? Which are those states?
Also, your eigenvalues equation has more solutions, but you consider only two of them. Thus your solution of the part (b) doesn't actually look completed. I suggest you to spend more time on it and make a good comprehensible write-up.

P.S. I don't mean that what you've done in part (b) is completely wrong. But there's definitely lack of explanations, so it doesn't look convincing at all, which is pretty much equivalent to being wrong unless you prove me the opposite.
