Problem M02Q.2

(a) When $\alpha = 0$, the spin and motional terms in the Hamiltonian decouple. Thus we must find the ground state of

$$\begin{aligned} H_S &:= 2J \sum_{i=1}^{3} \mathbf{S}_i \cdot \mathbf{S}_{i+1} \\ &= J\left(\mathbf{S}^2 - \sum_i \mathbf{S}_i^2\right) \\ &= J\left(\mathbf{S}^2 - \frac{9}{4}\right), \end{aligned}$$

which occurs when $\mathbf{S} = 1/2$. Letting $\mathbf{n}$ denote the n-dimensional irreducible representation of $SU(2)$, we have the decomposition

$$\begin{aligned} \mathbf{2} \otimes \mathbf{2} \otimes \mathbf{2} &= (\mathbf{1} \oplus \mathbf{3}) \otimes \mathbf{2} \\ &= (\mathbf{1} \otimes \mathbf{2}) \oplus (\mathbf{3} \otimes \mathbf{2}) \\ &= \mathbf{2} \oplus (\mathbf{2} \oplus \mathbf{4}), \end{aligned}$$

so there are two spin-1/2 sectors in the fully coupled basis, yielding a four-fold degenerate ground state.

The first two ground states come from the $\mathbf{1} \otimes \mathbf{2}$ term, and are

$$\begin{aligned} |\psi_1\rangle &:= \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \otimes |\uparrow\rangle, \\ |\psi_2\rangle &:= \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}} \otimes |\downarrow\rangle. \end{aligned}$$

Two other ground states come from the $\mathbf{3} \otimes \mathbf{2}$ term. Using the appropriate Clebsch-Gordan coefficients, we obtain

$$\begin{aligned} |\psi_3\rangle &:= \sqrt{\frac{2}{3}} |\uparrow\uparrow\rangle \otimes |\downarrow\rangle - \sqrt{\frac{1}{3}} \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \otimes |\uparrow\rangle \\ &= \frac{2|\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle}{\sqrt{6}}, \\ |\psi_4\rangle &:= \sqrt{\frac{2}{3}} |\downarrow\downarrow\rangle \otimes |\uparrow\rangle - \sqrt{\frac{1}{3}} \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \otimes |\downarrow\rangle \\ &= \frac{2|\downarrow\downarrow\uparrow\rangle - |\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle}{\sqrt{6}}. \end{aligned}$$

(b) For ease of computation, we will solve the equivalent problem where $x_{2,3} = x_{1,3}$.

Let $x := x_{2,3} = x_{1,3}$, and $y := x_{1,2}$. Then the Hamiltonian from (a) is modified by a term

$$\begin{aligned} H_{\text{int}} &:= \frac{1}{2}k(2x^2 + y^2) - 2J\alpha(x\mathbf{S}_1 \cdot \mathbf{S}_2 + x\mathbf{S}_2 \cdot \mathbf{S}_3 + y\mathbf{S}_3 \cdot \mathbf{S}_1) \\ &= \frac{1}{2}k(2x^2 + y^2) + \frac{1}{2}J\alpha\,(2x + y) - J\alpha\,\underbrace{(xP_{23} + xP_{13} + yP_{12})}_{:=H_{\text{SE}}}. \end{aligned}$$

In the orthonormal basis $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle$, we have

$$P_{12} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = -\sigma_z \otimes I_2,$$

$$P_{23} = \begin{bmatrix} 1/2 & 0 & \sqrt{3}/2 & 0 \\ 0 & 1/2 & 0 & \sqrt{3}/2 \\ \sqrt{3}/2 & 0 & -1/2 & 0 \\ 0 & \sqrt{3}/2 & 0 & -1/2 \end{bmatrix} = \begin{bmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{bmatrix} \otimes I_2,$$

and

$$P_{13} = P_{12}P_{23}P_{12} = \begin{bmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{bmatrix} \otimes I_2.$$

Combining the above, we may write

$$H_{\text{int}} = \frac{1}{2}k\left(2x^2 + y^2\right) I_4 + \frac{J\alpha}{2}\begin{bmatrix} 3y & 0 \\ 0 & 4x - y \end{bmatrix} \otimes I_2.$$

Thus there are two degenerate ground states of the coupled system in general. For $x < y$, these ground states are $|\psi_2\rangle, |\psi_4\rangle$. For $x > y$, these ground states are $|\psi_1\rangle, |\psi_3\rangle$.

We do not need to consider admixtures of excited states as long as $0 < \alpha \ll 1$ is small compared to the energy gap.