

E4852: Dynamics of coupled spins

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The problem:

Two coupled spins are described by the Hamiltonian $H = \mu \vec{S}^A \cdot \vec{S}^B + \text{const}$, when $\vec{S} = \frac{1}{2}\vec{\sigma}$. We prepare the first spin in Z polarization state and the second spin in X polarization state. Without loss of generality we focus here on the movement of the second spin ($\vec{S}^B$). The spin state is described by the polarization vector $\vec{M} = (\langle\sigma_x^B\rangle, \langle\sigma_y^B\rangle, \langle\sigma_z^B\rangle)$. Tip: In the calculations required in sections 4-5, it is convenient to determine the Constant in the Hamiltonian, so that the energy in the Triplet states would be zero.

- (1) If it was possible to freeze the first spin's state, what was the precession frequency of the second spin? And what was the result for the polarization vector $\vec{M}(t)$?
- (2) Write the initial state of the system as a superposition of Singlet and Triplet states.
- (3) Write down the Hamiltonian at the Singlet-Triplet base. What is the motion frequency Ω of the system?
- (4) What is the result for $M_z(t)$?
- (5) What is the result for $M_x(t), M_y(t)$?
- (6) What is the result for the length of the polarization vector? Is it constant?
- (7) In what times the spin can be described by a "wave function"?

The solution:

(1) It is given that the first spin's state remains unchanged, therefore, $\vec{S}^A$ must rotate the first spin along the Z axis so one can write $\vec{S}^A = (0, 0, S_z)$. After inserting $\vec{S}^A$ into the Hamiltonian and assuming $\text{const} = 0$ one gets:

$$H = \mu S^A \cdot S^B + \text{const} = \mu S_z^A S_z^B = \frac{1}{2} \mu \sigma_z^A \sigma_z^B$$

And using the fact that $H = \vec{\Omega} \cdot \vec{S}$ one gets:

$$\vec{\Omega} = (0, 0, \frac{\mu}{2}); \quad |\vec{\Omega}| = \frac{\mu}{2}$$

The polarization vector is defined by $\vec{M} = (\langle\sigma_x^B\rangle, \langle\sigma_y^B\rangle, \langle\sigma_z^B\rangle)$. In order to calculate it one should first write the quantum state for $t = 0$:

$$|\psi^0\rangle = |\uparrow\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

And now one can proceed:

$$\sigma_x^B = \hat{I} \otimes \sigma_x = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \Rightarrow \langle \sigma_x^B \rangle = \langle \Psi^0 | \sigma_x^B | \Psi^0 \rangle = 1$$

$$\sigma_y^B = \hat{I} \otimes \sigma_y = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix} \Rightarrow \langle \sigma_y^B \rangle = \langle \Psi^0 | \sigma_y^B | \Psi^0 \rangle = 0$$

$$\sigma_z^B = \hat{I} \otimes \sigma_z = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \Rightarrow \langle \sigma_z^B \rangle = \langle \Psi^0 | \sigma_z^B | \Psi^0 \rangle = 0$$

So one obtains:

$$\vec{M}(0) = (1, 0, 0)$$

In order to calculate $\vec{M}(t)$ one should use $\vec{M}(t) = R^E(\Phi) \cdot \vec{M}(0)$ while $\Phi = \vec{\Omega}t$ and $\vec{\Omega} = \Omega \hat{z}$ so:

$$R^E(\vec{\Omega}t) = R_z^E(\Omega t) = \begin{pmatrix} \cos(\Omega t) & -\sin(\Omega t) & 0 \\ \sin(\Omega t) & \cos(\Omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

And finally:

$$\vec{M}(t) = R_z^E(\Omega t) \cdot \vec{M}(0) = (\cos(\Omega t), \sin(\Omega t), 0)$$

(2) The Singlet - Triplet states are:

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

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

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

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

So one can write the initial state of the system as:

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

(3) Transferring the Hamiltonian to the Singlet-Triplet base:

$$H|0, 0\rangle = \frac{\mu}{4} \vec{\sigma}^A \cdot \vec{\sigma}^B \left[\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) \right] = -\frac{3}{4}\mu|0, 0\rangle$$

$$H|1, 1\rangle = \frac{\mu}{4}\vec{\sigma}^A \cdot \vec{\sigma}^B |\uparrow\uparrow\rangle = \frac{\mu}{4}|1, 1\rangle$$

$$H|1, 0\rangle = \frac{\mu}{4}\vec{\sigma}^A \cdot \vec{\sigma}^B [\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)] = \frac{\mu}{4}|1, 0\rangle$$

$$H|1, -1\rangle = \frac{\mu}{4}\vec{\sigma}^A \cdot \vec{\sigma}^B |\downarrow\downarrow\rangle = \frac{\mu}{4}|1, -1\rangle$$

So eventually one can write the new Hamiltonian:

$$H_{new} = \begin{pmatrix} -\frac{3}{4}\mu & 0 & 0 & 0 \\ 0 & \frac{\mu}{4} & 0 & 0 \\ 0 & 0 & \frac{\mu}{4} & 0 \\ 0 & 0 & 0 & \frac{\mu}{4} \end{pmatrix}$$

By exploiting the freedom of the constant in the Hamiltonian one can easily obtain that $\Omega = \mu$.

(4) One can define the constant in the Hamiltonian as $const = -\frac{\mu}{4}$ and get:

$$H_{new} = \begin{pmatrix} -\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The time dependant quantum state will be:

$$|\psi^t\rangle = \frac{1}{\sqrt{2}}|1, 1\rangle + \frac{1}{2}|1, 0\rangle + \frac{1}{2}e^{i\mu t}|1, 0\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1/2 + 1/2e^{i\mu t} \\ 1/2 - 1/2e^{i\mu t} \\ 0 \end{pmatrix}$$

And, therefore, one can calculate $M_z(t)$ and get (after some algebra):

$$M_z(t) = \langle\psi^t|\sigma_z^B|\psi^t\rangle = \frac{1}{2}(1 - \cos(\Omega t))$$

(5) In the same way one can calculate $M_x(t)$ and $M_y(t)$ and get:

$$M_x(t) = \langle\psi^t|\sigma_x^B|\psi^t\rangle = \frac{1}{2}(1 + \cos(\Omega t))$$

and

$$M_y(t) = \langle\psi^t|\sigma_y^B|\psi^t\rangle = \frac{1}{2}\sin(\Omega t)$$

(6) The polarization vector is $\vec{M}(t) = (M_x(t), M_y(t), M_z(t))$ so one can use sections 4-5 and write:

$$|\vec{M}(t)|^2 = M_x(t)^2 + M_y(t)^2 + M_z(t)^2 = 1 - \frac{1}{4}\sin^2(\Omega t)$$

It is easy to see that the polarization vector's length is time-dependant so it is NOT a constant.

(7) By examining the polarization vector one can see that its length is not a multiple of $1/2$ and, therefore, we have an entangled quantum state. For the ability to describe the spin as a wave function one must demand that $|\vec{M}(t)| = \frac{1}{2} \cdot integer$ and get the condition:

$$t = \frac{\pi}{\Omega} \cdot integer$$