NV Centers

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1 NV centers

Following the Charles' note and the reference [1]. We consider the evolution of an NV center system made of the electronic spin coupled to the nitrogen nuclear spin. The dynamics of such a system is governed by the following Hamiltonian:

$$H = \omega_S S_z + \omega_I I_z + A S_z I_z + u(t) S_x + v(t) I_z \tag{1}$$

where ω_S and ω_I denote the respective Larmor frequencies[1] of the electron and the nuclear spin. A represents the strength of the secular hyperfine coupling, $u(t)$ and $v(t)$ are the amplitudes of the control fields. Here, $S_j = (\sigma_j \otimes \mathbb{I})/2$ acts on the electron spin and $I_k = (\mathbb{I} \otimes \sigma_k)/2$ acts on the nuclear spin with $j, k \in \{x, y, z\}$.

1.1 Contrability

We can write the hamiltonian 1 in other way

$$2\pi(H_0 + uH_1 + vH_2) \tag{2}$$

were

$$\begin{aligned}
H_0 &= i(\omega_S S_z + \omega_I I_z + A_{\|} S_z I_z + A_{\perp} S_z I_x),\\
H_1 &= i(S_x),\\
H_2 &= i(I_x).
\end{aligned}$$

Remark 1. From the Schrödinger equation with $\hbar = 1$,

$$\begin{aligned}
i\hbar \frac{d}{dt}|\Psi(t)\rangle &= H(t)|\Psi(t)\rangle\\
\frac{d}{dt}|\Psi(t)\rangle &= -2\pi i(H_0 + H_1 + H_2)|\Psi(t)\rangle
\end{aligned}$$

Notation 1. For future purposes, I will use H_j for iH_j. And for commutators

$$H_{jk} := [H_j, H_k] \qquad H_{jkl} := [H_j, [H_k, H_l]]$$

and so on.

Proposition 1. *A system with Hamiltonian* (2) *is controllable. The propagator can be an arbitrary element of* $SU(4)$*.*

Proof. Since H_0 is always recurrent, it is enough to prove that the Lie span

$$Lie\{H_0, H_1, H_2\}$$

[1]The Larmor Frequency refers to the precession frequency of electron spins in a material, which is influenced by the effective magnetic fields generated by polarized nuclei through hyperfine interactions.

is equal to $su(4)$, which has a natural basis

$$su(4) = \text{span}\{S_u I_v : (u,v) \neq (0,0)\}.$$

We have

$$H_{10} = i(\omega_S S_y + A_\parallel S_y I_z + A_\perp S_y I_x)$$
$$H_{110} = -i(\omega_s S_z + A_\parallel S_z I_z + A_\perp S_z I_x)$$

Hence

$$H_0 + H_{110} = i\omega_I I_z = H_3 \sim I_z$$

Similarly we find

$$H_{22110} = iA_\parallel S_z I_z$$

and

$$[H_3, [H_3, H_{110}]] = i\omega_I A_\perp S_z I_x \sim iA_\perp S_z I_x.$$

Therefore

$$H_{110} + H_{22110} + [H_3, [H_3, H_{110}]]/\omega_I = -xi\omega_S S_z \sim S_z$$

Taking the commutator of S_x and S_z gives S_y. Therefore, the Lie span contains all S_u with $u \neq 0$. Similarly, it contains all I_u. Taking the commutators of S_u, I_v with H_{22110} gives all possible pairs $S_u I_v$ with non-zero u, v.

□

Next, let us assume that we can only control the electron, which means that $v = 0$. First, we treat a subcase.

Proposition 2. *Let $A_\perp = 0$. In this case a system with Hamiltonian (2) and $v = 0$ is not controllable. Its Lie span is isomorphic to $su(2) \oplus su(2) \oplus u(1)$ as* ***complex Lie algebras****.*

Proof. Now, we have the following hamiltonians

$$H_0 = i(\omega_S S_z + \omega_I I_z + A_\parallel S_z I_z),$$
$$H_1 = iS_x.$$

Lets start to see what we can generate with H_0 and H_1, i.e., span$\{H_0, H_1\}$. We have

$$H_{10} = i(\omega_S S_y + A_\parallel S_y I_z)$$
$$H_{110} = -i(\omega_S S_z + A_\parallel S_z I_z)$$

Hence

$$H_0 + H_{110} = i\omega_I I_z = H_3 \sim I_z$$

we see that $I_z \in Lie\{H_0, H_1\}$. Next, we compute

$$[H_{110}, H_{10}] = i(\omega_S^2 + A_\parallel^2/4)S_x + i2\omega_S A_\parallel S_x I_z$$

and one more commutator

$$\begin{aligned}
[[H_{110}, H_{10}], H_{10}] &= -i\omega_S(\omega_S^2 + A_\parallel^2/4)S_z - iA_\parallel(\omega_S^2 - A_\parallel^2/4)S_z I_z - i2\omega_S^2 A_\parallel S_z I_z - i(\omega_S A_\parallel^2/2)S_z \\
&= -i\omega_S(\omega_S^2 - 3A_\parallel^2/4)S_z - iA_\parallel(3\omega_S^2 + A_\parallel^2/4)S_z I_z
\end{aligned}$$

Now, lets see if the vectors H_{110} and $[[H_{110}, H_{10}], H_{10}]$ are independent.

$$\begin{vmatrix} \omega_s & -i\omega_S(\omega_S^2 - 3A_\parallel^2/4) \\ A_\parallel & -A_\parallel(3\omega_S^2 + A_\parallel^2/4) \end{vmatrix} S_z \wedge S_z I_z = \omega_s A_\parallel (A_\parallel^2/2 - 2\omega_s^2) S_z \wedge S_z I_z$$

So, the two vectors are independent if the determinant is different of zero. This means, that

$$A_{\|}^2/2 - 2\omega_S^2 \neq 0 \Leftrightarrow A_{\|} \neq 2\omega_S, \quad \text{note that } A_{\|}, \omega_S \geq 0$$

Then, we can write

$$\begin{pmatrix} S_z \\ S_z I_z \end{pmatrix} = \begin{pmatrix} \omega_s & -i\omega_S(\omega_S^2 - 3A_{\|}^2/4) \\ A_{\|} & -A_{\|}(3\omega_S^2 + A_{\|}^2/4) \end{pmatrix}^{-1} \begin{pmatrix} H_{110} \\ [[H_{110}, H_{10}], H_{10}] \end{pmatrix}$$

Hence we can generate S_z and $S_z I_z$. This implies that for $A_{\|} \neq 2\omega_S$, H_0 and H_1 generated the subalgebra

$$L_1 = \text{span}\{iS_u I_z, iS_v : u \in \{0, x, y, z\}, v \in \{x, y, z\}\}.$$

For the case $A_{\|} = 2\omega_S$, the vectors H_{110} and $[[H_{110}, H_{10}], H_{10}]$ are dependent and generate the subalgebra

$$L_2 = \text{span}\{iS_x, iI_z, i(S_u + S_u I_z) : u \in \{x, y, z\}\}.$$

Therefore,

$$Lie\{H_0, H_1\} = \begin{cases} L_1 & \text{if } A_{\|} \neq 2\omega_S \\ L_2 & \text{if } A_{\|} = 2\omega_S \end{cases}$$

which is a subalgebra of $su(4)$. ☐

Proposition 3. *Let $A_\perp \neq 0$. In this case a system with Hamiltonian (2) and $v = 0$ is controllable.*

Proof. We will show that a part of the argument can be reduced to the proof of the previous Proposition 1. We compute

$$H_{10} = i(\omega_S S_y + A_{\|} S_y I_z + A_\perp S_y I_x)$$
$$H_{110} = -i(\omega_S S_z + A_{\|} S_z I_z + A_\perp S_z I_x)$$

Hence

$$H_0 + H_{110} = i\omega_I I_z = H_3 \sim I_z$$

Similarly we find

$$[H_3, [H_3, H_{110}]] = i\omega_I A_\perp S_z I_x \sim iA_\perp S_z I_x.$$

and

$$[H_3, [H_3, H_{10}]] = i\omega_I A_\perp S_y I_x \sim iA_\perp S_y I_x.$$

Hence $H_{10} - [H_3, [H_3, H_{10}]] = i(\omega_S S_y + A_{\|} S_y I_z)$ and $H_{110} - [H_3, [H_3, H_{110}]] = i(\omega_S S_z + A_{\|} S_z I_z)$ are equal to H_{10} and H_{110} from the previous case (when $A_\perp = 0$). Then, it is easy to see that $Lie\{H_0, H_1\}$ contains L_1 and L_2. For the case $A_{\|} \neq 2\omega$, we use the same arguments as in the previous proof. For the case $A_{\|} = 2\omega$, less find $S_u + S_u I_Z$, with $u \in \{y, z\}$:

$$H_{10} - H_{3310} \sim i(\omega_S S_y + A_{\|} S_y I_z)$$
$$H_{110} - H_{33110} \sim i(\omega_S S_z + A_{\|} S_z I_z)$$

With this, we can compute

$$[iI_x, i(S_z + S_z I_z)] = -([I_x, S_z] + [I_x, S_z I_z]) = -(0 - iS_z I_y) = iS_z I_y$$

and one more commutator

$$[iI_x, [iI_x, i(S_z + S_z I_z)]] \sim iS_z I_z.$$

With this, we can compute

$$[iI_z, [iS_z I_z, iS_z I_x]] = [iI_z, -iI_y] = -iI_x \sim iI_x$$

and iI_x is equal to H_2 in Proposition 1. So, $Lie\{H_0, H_1\} = Lie\{H_0, H_1, H_2\}$ and the system is controllable by Proposition 1. ☐

References

[1] Haidong Yuan et al. "Time-optimal polarization transfer from an electron spin to a nuclear spin". In: *Physical Review A* 92.5 (Nov. 2015). ISSN: 1094-1622. DOI: 10.1103/physreva.92.053414. URL: http://dx.doi.org/10.1103/PhysRevA.92.053414.