Quantum control of NV center using counter-diabatic driving

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1 Introduction

The ground state of the NV center is a spin triplet with $|0\rangle, |-1\rangle, |1\rangle$ spin sub-levels. They are defined in S_z basis , where $\hat{z}$ direction is along the NV center axis. The Hamiltonian for the ground state of the NV center can be written as [1]:

$$H_{NV} = \hbar\Delta S_z^2 + g\mu_B \vec{S}.\vec{B}_{ext} \tag{1}$$

where $\Delta = 2\pi \times 2.87$ GHz is zero-field splitting, $g \approx 2$ is the g-factor of electron in the NV center and μ_B is Bohr magneton. If there is no external magnetic field, then $|-1\rangle$ and $|1\rangle$ levels are degenerate, and $\hbar^3\Delta$ is the energy difference between $|0\rangle$ and $|\pm 1\rangle$ energy levels.

2 Eigenvalues

Let's choose magnetic field to be in x-direction. Then we have:

$$\begin{aligned} H_{NV} &= \hbar\Delta S_z^2 + g\mu_B S_x B \\ &= \Lambda S_z^2 + \lambda S_x \end{aligned}$$

where $\Lambda = \hbar\Delta$ and $\lambda = g\mu_B B$. Magnetic field is going to be our control parameter in this problem. Using spin algebra (appendix B), we obtain Hamiltonian in the S_z basis ($|-1\rangle$, $|0\rangle$, $|1\rangle$):

$$H = \begin{bmatrix} \beta & \alpha & 0 \\ \alpha & 0 & \alpha \\ 0 & \alpha & \beta \end{bmatrix} \tag{2}$$

where $\alpha = \hbar\lambda/\sqrt{2}$ and $\beta = \hbar^2\Lambda$.

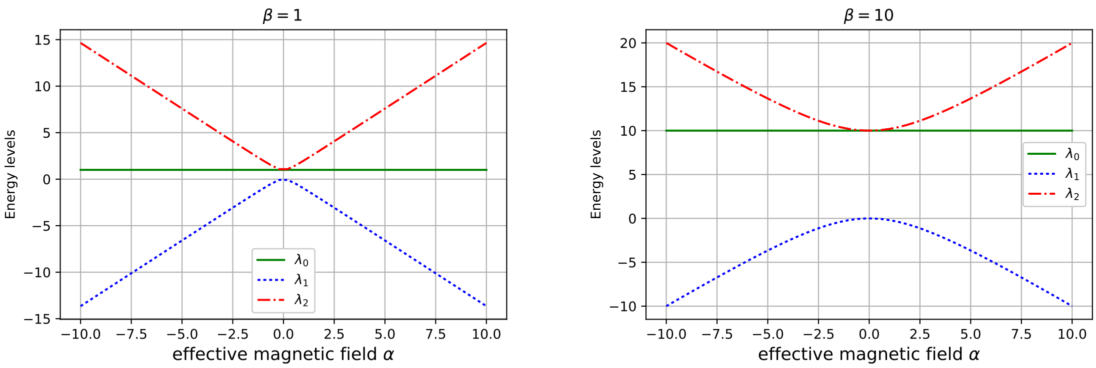

Figure 1: Avoided level crossing as a function of effective magnetic field

Energy eigenvalues are given by:

$$\lambda_0 = \beta, \quad \lambda_1 = (\beta - \sqrt{\beta^2 + 8\alpha^2})/2, \quad \lambda_2 = (\beta + \sqrt{\beta^2 + 8\alpha^2})/2$$

We should remember that $\alpha \propto B$. Hence, it makes sense that when $\alpha = 0$, there is a two -fold degeneracy and zero field energy gap is given by $\beta = \hbar^3\Delta$. Now let's have a look at eigenvectors:

$$\nu_0 = (-1, 0, 1), \quad \nu_1 = (1, -(\beta + \sqrt{\beta^2 + 8\alpha^2})/2\alpha, 1), \quad \nu_2 = (1, -(\beta - \sqrt{\beta^2 + 8\alpha^2})/2\alpha, 1)$$

3 Adiabatic gauge potential

Now let's compute adiabatic gauge potential $A_\lambda = i\hbar\partial_\lambda$. Its' equation of motion is given by:

$$[H, \partial_\lambda H + \frac{i}{\hbar}[A_\lambda, H]] = 0 \tag{3}$$

We would choose a gauge such that diagonal elements of diabatic gauge potential A_λ is zero. We can derive off- diagonal elements by using the identity $\langle m|H(\lambda)|n\rangle = 0 \quad , n \neq m$ and then differentiate it with respect to λ to obtain:

$$\boxed{\langle m|A_\lambda|n\rangle = -i\hbar\frac{\langle m|\partial_\lambda H|n\rangle}{E_m - E_n}} \tag{4}$$

where both energies (E_m, E_n) and eigenvectors $(|m\rangle, |n\rangle)$ depend on λ.

Here $\partial_\lambda H = S_x$ whose matrix representation is given in appendix B. After doing calculation in S_z basis $(|-1\rangle, |0\rangle\ , |1\rangle)$, we find that

$$A_\lambda = \hbar N \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix} \tag{5}$$

where N is given by

$$N = \frac{4\sqrt{2}\alpha\beta\hbar}{\sqrt{8\alpha^2 + \beta^2}\sqrt{8\alpha^2 + \left(\beta - \sqrt{8\alpha^2 + \beta^2}\right)^2}\sqrt{8\alpha^2 + \left(\beta + \sqrt{8\alpha^2 + \beta^2}\right)^2}} \tag{6}$$

What I don't know is that the above gauge potential is composed of which spin operators. I am still working on it.

Expression involving commutators

Another way to express this formula is:

$$A_\lambda(\mu) = -i\hbar \lim_{\mu \to 0} \sum_{n=0}^{\infty} (-1)^n \frac{C^{(2n+1)}}{\mu^{2n+2}} \tag{7}$$

where $C^{(n)}$ is n- commutator of H and $\partial_\lambda H$, i.e. $C^{(n)} = [H, [H, \text{ n times} \ldots, [H, \partial_\lambda H]]]]$. We define the first term as $C^{(1)} = [H, \partial_\lambda H]$, second term as $C^{(2)} = [H, [H, \partial_\lambda H]] = [H, C^{(1)}]$ and so on and forth.

Let's find out A_λ for this Hamiltonian for which we need to compute different odd-powered commutator $[H, \partial_\lambda H]$, where $\partial_\lambda H = S_x$. It turns out that I am not able to compute the summation as the expressions of commutators is pretty involved (details are given in appendix A). I would need to think of some smarter way to compute adiabatic gauge potential.

A Computation of gauge potential

Here we begin:

$$\begin{aligned} C^{(1)} = [H, S_x] &= \Lambda[S_z^2, S_x] \\ &= S_z[S_z, S_x] + [S_z, S_x]S_z \\ &= i\hbar(S_zS_y + S_yS_z) \\ &= i\hbar([S_z, S_y] + 2S_yS_z) \\ &= i\hbar(-i\hbar S_x + 2S_yS_z) \end{aligned}$$

$$\begin{aligned} C^{(2)} = [H, C^{(1)}] &= \hbar^2[H, S_x] + i\hbar[H, S_yS_z] \\ &= \hbar^2 C^{(1)} + i\hbar S_y[H, S_z] + i\hbar[H, S_y]S_z \\ &= \hbar^2 C^{(1)} + i\hbar\lambda S_y[S_x, S_z] + i\hbar T \\ &= \hbar^2 C^{(1)} - \hbar^2\lambda S_y^2 + i\hbar T \end{aligned}$$

$$\begin{aligned} T = [H, S_y]S_z &= \Lambda[S_z^2, S_y]S_z + \lambda[S_x, S_y]S_z \\ &= \Lambda S_z[S_z, S_y]S_z + \Lambda[S_z, S_y]S_z^2 + i\hbar\lambda S_z^2 \\ &= -i\hbar\Lambda(S_zS_xS_z + S_xS_z^2) + i\hbar\lambda S_z^2 \\ &= -i\hbar\Lambda([S_z, S_x]S_z + 2S_xS_z^2) + i\hbar\lambda S_z^2 \\ &= -i\hbar\Lambda(i\hbar S_yS_z + 2S_xS_z^2) + i\hbar\lambda S_z^2 \end{aligned}$$

Hence, we get:

$$\begin{aligned} C^{(2)} = [H, C^{(1)}] &= \hbar^2 C^{(1)} - \hbar^2\lambda(S_y^2 + S_z^2) + \hbar^2\Lambda(i\hbar S_yS_z + S_xS_z^2) \\ &= \hbar^2 C^{(1)} - \hbar^2\lambda(S^2 - S_x^2) + \hbar^2\Lambda(i\hbar S_yS_z + S_xS_z^2) \end{aligned}$$

Further,

$$\begin{aligned} C^{(3)} = [H, C^{(2)}] &= [H, \hbar^2 C^{(1)} - \hbar^2\lambda(S^2 - S_x^2) + \hbar^2\Lambda(i\hbar S_yS_z + S_xS_z^2)] \\ &= \hbar^2 C^{(2)} - \hbar^2\lambda[H, (S^2 - S_x^2)] + \hbar^2\Lambda[H, (i\hbar S_yS_z + S_xS_z^2)] \\ &= \hbar^2 C^{(2)} + \hbar^2\lambda[H, S_x^2] + i\hbar^3\Lambda[H, S_yS_z] + \hbar^2\Lambda[H, S_xS_z^2] \\ &= \hbar^2 C^{(2)} + \hbar^2\lambda^2[S_z^2, S_x^2] + i\hbar^3\Lambda T_1 + \hbar^2\Lambda T_2 \\ &= \hbar^2 C^{(2)} + \hbar^2\lambda T_0 + i\hbar^3\Lambda T_1 + \hbar^2\Lambda T_2 \end{aligned}$$

$$\begin{aligned} T_0 = [S_z^2, S_x^2] &= S_z[S_z, S_x^2] + [S_z, S_x^2]S_z \\ &= S_zS_x[S_z, S_x] + S_z[S_z, S_x]S_x + S_x[S_z, S_x]S_z + [S_z, S_x]S_xS_z \\ &= i\hbar(S_zS_xS_y + S_zS_yS_x + S_xS_yS_z + S_yS_xS_z) \\ &= i\hbar(S_z[S_x, S_y] + 2S_zS_yS_x + [S_x, S_y]S_z + 2S_yS_xS_z) \\ &= 2i\hbar(i\hbar S_z^2 + S_zS_yS_x + S_yS_xS_z) \\ &= -2\hbar^2 S_z^2 + 2i\hbar(S_zS_yS_x + S_yS_xS_z) \end{aligned}$$

$$T_1 = [H, S_yS_z] = -\hbar^2\lambda S_y^2 + i\hbar T = -\hbar^2\lambda S_y^2 + \hbar^2\Lambda(i\hbar S_yS_z + 2S_xS_z^2) - \hbar^2\lambda S_z^2$$

$$= -\hbar^2\lambda(S_y^2 + S_z^2) + \hbar^2\Lambda(i\hbar S_y S_z + 2S_x S_z^2)$$

$$\begin{aligned}
T_2 = [H, S_x S_z^2] &= [H, S_x]S_z^2 + S_x[H, S_z^2] \\
&= C^{(1)} S_z^2 + \lambda S_x[S_x, S_z^2] \\
&= C^{(1)} S_z^2 + \lambda S_x[S_x, S_z]S_z + \lambda S_x S_z[S_x, S_z] \\
&= C^{(1)} S_z^2 - i\hbar\lambda(S_x S_y S_z + S_x S_z S_y) \\
&= C^{(1)} S_z^2 - i\hbar\lambda(S_x[S_y, S_z] + 2S_x S_z S_y) \\
&= C^{(1)} S_z^2 - i\hbar\lambda(i\hbar S_x^2 + 2S_x S_z S_y) \\
&= C^{(1)} S_z^2 + \hbar^2\lambda S_x^2 - 2i\hbar\lambda S_x S_z S_y
\end{aligned}$$

Finally, we get

$$\begin{aligned}
C^{(3)} &= \hbar^2 C^{(2)} + \hbar^2\lambda T_0 + i\hbar^3\Lambda T_1 + \hbar^2\Lambda T_2 \\
&= \hbar^2 C^{(2)} + 2i\hbar^3\lambda(i\hbar S_z^2 + S_z S_y S_x + S_y S_x S_z) + \hbar^2\Lambda(i\hbar T_1 + T_2)
\end{aligned}$$

Let's simplify the last term $i\hbar T_1 + T_2$:

$$\begin{aligned}
i\hbar T_1 + T_2 &= -i\hbar^3\lambda(S_y^2 + S_z^2) + i\hbar^3\Lambda(i\hbar S_y S_z + 2S_x S_z^2) + C^{(1)} S_z^2 + \hbar^2\lambda S_x^2 - 2i\hbar\lambda S_x S_z S_y \\
&= -i\hbar^3\lambda(S_y^2 + S_z^2) + \hbar^2\lambda S_x^2 + i\hbar^3\Lambda(i\hbar S_y S_z + 2S_x S_z^2) - 2i\hbar\lambda S_x S_z S_y + C^{(1)} S_z^2 \\
&= -i\hbar^3\lambda(S_y^2 + S_z^2) + \hbar^2\lambda S_x^2 + i\hbar^3\Lambda(i\hbar S_y S_z + 2S_x S_z^2) - 2i\hbar\lambda S_x S_z S_y + i\hbar(-i\hbar S_x + 2S_y S_z)S_z^2 \\
&= -i\hbar^3\lambda(S_y^2 + S_z^2) + \hbar^2\lambda S_x^2 + i\hbar^3\Lambda(i\hbar S_y S_z + 2S_x S_z^2) - 2i\hbar\lambda S_x S_z S_y + \hbar^2 S_x S_z^2 + 2i\hbar S_y S_z^3 \\
&= -i\hbar^3\lambda(S_y^2 + S_z^2) + \hbar^2\lambda S_x^2 + \hbar^2 S_x S_z^2(1 + 2i\hbar\Lambda) - \hbar^4\Lambda S_y S_z - 2i\hbar\lambda S_x S_z S_y + 2i\hbar S_y S_z^3
\end{aligned}$$

Now, let's write:

$$C^{(2)} = \hbar^2 C^{(1)} - \hbar^2\lambda(S^2 - S_x^2) + \hbar^2\Lambda(i\hbar S_y S_z + S_x S_z^2)$$

B Spin Algebra

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x \quad [S_z, S_x] = i\hbar S_y \tag{8}$$

$$S^2|s, m\rangle = \hbar^2 s(s+1)|s, m \pm 1\rangle \quad S_z|s, m\rangle = \hbar m|s, m\rangle \tag{9}$$

$$S_\pm|s, m\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)}|s, m \pm 1\rangle \tag{10}$$

where $S_+ = S_x + iS_y$ and $S_- = S_x - iS_y$. Hence, we get $S_x = (S_+ + S_-)/2$ and $S_y = (S_+ - S_-)/2i$

$$S_+ = \sqrt{2}\hbar \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix} \quad S_- = \sqrt{2}\hbar \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \tag{11}$$

Hence,

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad S_y = i\frac{\hbar}{\sqrt{2}} \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix} \tag{12}$$

References

[1] Shonali Dhingra and Brian D'Urso. Nitrogen vacancy centers in diamond as angle-squared sensors. *Journal of Physics: Condensed Matter*, 29(18):185501, 2017.