Quantum control of NV center using counter-diabatic driving

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1 Introduction

The Hamiltonian for the ground state of the NV center can be written as :

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

where $\Delta = 2\pi \times 2.87$ GHz is zero-field splitting, γ_e is the gyromagnetic ratio of electron in the NV center, γ_n is the gyromagnetic ratio of nuclear spin, $\vec{S}$ ($\vec{J}$) is the spin of electron (nucleus).

Since $\gamma \propto 1/m$ and nucleus is heavier than electron, we have $\gamma_e \gg \gamma_n$. To simplify our model, we will ignore the last term resulting in the following Hamiltonian [1]:

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

The ground state of electron in 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. 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 Static magnetic field

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

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

where $\Lambda = \hbar\Delta$ and $\lambda = \hbar\gamma_e B$. Magnetic field is going to be our control parameter in this problem.

2.1 Energy levels as a function of magnetic field

Using spin algebra (appendix A), we obtain Hamiltonian in the S_z basis ($|-1\rangle$, $|0\rangle$, $|1\rangle$):

$$H = \begin{pmatrix} \beta & \alpha & 0 \\ \alpha & 0 & \alpha \\ 0 & \alpha & \beta \end{pmatrix} \tag{3}$$

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

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:

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

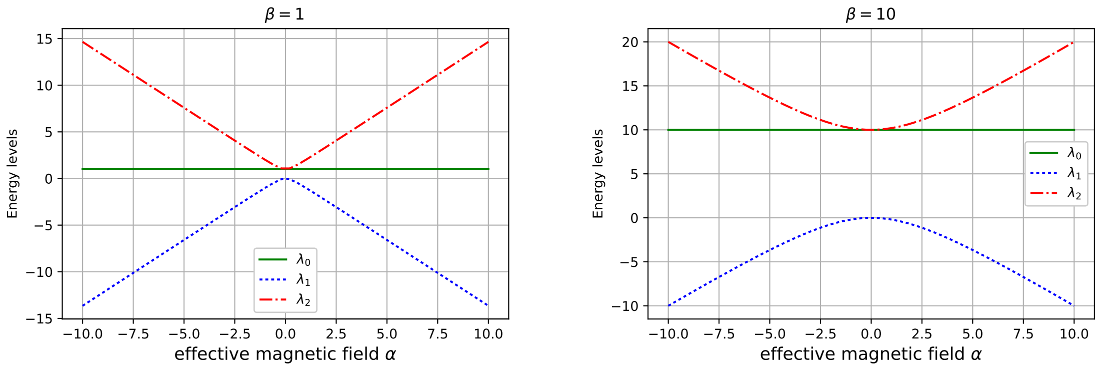

Figure 1: Avoided level crossing as a function of effective magnetic field

2.2 Adiabatic gauge potential

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

$$[H, \partial_\lambda H + \frac{i}{\hbar}[A_\lambda, H]] = 0 \tag{4}$$

Eigen-value equation is given by $H(\lambda)|n(\lambda)\rangle = E_n(\lambda)|n(\lambda)$. Let's derive diagonal and off-diagonal elements:

- **n-th diagonal element:** $A^n_\lambda = \langle n|A_\lambda|n\rangle = i\hbar\langle n|\partial_\lambda|n\rangle$
  Now since $\alpha = \hbar\lambda/\sqrt{2}$, we have $\partial_\lambda = \frac{d\alpha}{d\lambda}\partial_\alpha = \frac{\hbar}{\sqrt{2}}\partial_\alpha$.
  Now let's have a look at eigenvectors:
  $$|n=0\rangle = \begin{bmatrix} -1 \\ 0 \\ 1 \end{bmatrix}, \quad |n=1\rangle = \begin{bmatrix} 1 \\ \nu_1 \\ 1 \end{bmatrix}, \quad |n=2\rangle = \begin{bmatrix} 1 \\ \nu_2 \\ 1 \end{bmatrix}$$
  where $\nu_1 = -(\beta + \sqrt{\beta^2 + 8\alpha^2})/2\alpha$ and $\nu_2 = -(\beta - \sqrt{\beta^2 + 8\alpha^2})/2\alpha$.
  Hence, $A^{n=0}_\lambda = 0$

- **off- diagonal element:** We use the identity $\langle m|H(\lambda)|n\rangle = 0 \quad , n \neq m$ and then differentiate with respect to λ to obtain:
  $$\langle m|A_\lambda|n\rangle = -i\hbar\frac{\langle m|\partial_\lambda H|n\rangle}{E_m - E_n} \tag{5}$$
  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 A. After doing calculation in S_z basis $(|-1\rangle, |0\rangle, |1\rangle)$, we find that off-diagonal elements are:
  $$A^{od}_\lambda = i\hbar N \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{6}$$
  where
  $$N = \frac{4\sqrt{2}\alpha\beta\hbar}{\sqrt{8\alpha^2+\beta^2}\sqrt{8\alpha^2 + \left(\beta - \sqrt{8\alpha^2+\beta^2}\right)^2}\sqrt{8\alpha^2 + \left(\beta + \sqrt{8\alpha^2+\beta^2}\right)^2}}$$
  $$= \frac{4\sqrt{2}\alpha\beta\hbar}{(8\alpha^2+\beta^2)\sqrt{8}\alpha} = \frac{2\beta\hbar}{8\alpha^2+\beta^2}$$

The above matrix of A_λ can be expanded in the basis of $SU(3)$ to expand. This basis is composed of Gell–Mann matrices [2], which are represented as λ_i. For our purpose, most important Gell-Mann matrix is λ_7 whose representation is given below [3, 4]:

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} = \frac{1}{\sqrt{2}\hbar^2}(\hbar S_y - S_y S_z - S_z S_y) \tag{7}$$

Hence, we get

$$\boxed{A_\lambda = \frac{N}{\sqrt{2}\hbar}(\hbar S_y - S_y S_z - S_z S_y)} \tag{8}$$

To be doubly sure, I should verify if the above gauge potential satisfies equation 4.

3 Periodic magnetic field with noise

Let's choose magnetic field to be $\vec{B} = (B_x(t), 0, 0)$ where $B_x(t) = B_0 \sin(\omega t) + \epsilon(t)$ and $\epsilon(t)$ is an infinitesimal white noise which satisfies $\overline{\epsilon(t)\epsilon(t')} = \kappa\delta(t - t')$ [1].

Then we have:

$$\begin{aligned} H_{NV} &= \Lambda S_z^2 + \hbar\gamma_e S_x B_x(t) \\ &= \Lambda S_z^2 + \lambda S_x \end{aligned}$$

where $\Lambda = \hbar\Delta$ and $\lambda = \hbar\gamma_e(B_0 \sin(\omega t) + \epsilon(t))$. For now on, we will work in the unit in which $\hbar\gamma_e = 1$ so that $\lambda = (B_0 \sin(\omega t) + \epsilon(t))$ and $\Lambda = \Delta/\gamma_e$.

Using Fermi Golden rule, we can derive transition rate $\langle \Gamma_n \rangle$ [5] as follows:

$$\Gamma_n(\omega) = \kappa \sum_{m \neq n} |\langle n|G_\lambda|m\rangle|^2 \delta(E_n - E_m - \hbar\omega) \tag{9}$$

where $G_\lambda = \partial_\lambda H + \dfrac{i}{\hbar}[A_\lambda, H]$ and ω is frequency of the periodic external drive. More details are given in appendix.

A Spin Algebra

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x \quad [S_z, S_x] = i\hbar S_y \tag{10}$$

$$S^2|s, m\rangle = \hbar^2 s(s+1)|s, m \pm 1\rangle \quad S_z|s, m\rangle = \hbar m|s, m\rangle \tag{11}$$

$$S_\pm|s, m\rangle = \hbar\sqrt{s(s+1) - m(m \pm 1)}|s, m \pm 1\rangle \tag{12}$$

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

$$S_+ = \sqrt{2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \qquad S_- = \sqrt{2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{13}$$

Hence,

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S_y = i\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{14}$$

[1] If the system is in equilibrium, then fluctuation -dissipation theorem dictates $\kappa = T$

B Gell-Mann matrices

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$
$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$
$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

These matrices are traceless and Hermitian.

C transition rate

Let's consider a Hamiltonian:

$$\mathcal{H}_{\mathcal{X}} = \mathcal{H}(\lambda) + \dot{\lambda}\mathcal{X} \tag{15}$$

where $\lambda = \lambda_0 + \epsilon(t)$ and $\epsilon(t)$ is an infinitesimal white noise which satisfies $\overline{\epsilon(t)\epsilon(t')} = \kappa\delta(t-t')$ [2]. A system under white noise would lead to transitions between all eigenstates. We will see how much there is reduction in transition and dissipation rate with our approximate gauge potential.

We can simplify the above expression:

$$\mathcal{H}_{\mathcal{X}} \approx \mathcal{H}(\lambda_0) + \epsilon\partial_\lambda\mathcal{H} + \dot{\epsilon}\mathcal{X} \tag{16}$$

Our expressions will involve G_λ which is given as $G_\lambda(\mathcal{X}) = \partial_\lambda H + \frac{i}{\hbar}[\mathcal{X}, H]$ where $\mathcal{X} = A_\lambda$.

Now we would drive the system periodically in addition to the white noise we have in the system. So, in this protocol, time dependence of λ is given as $\lambda(t) = \lambda_0 \sin(\omega t) + \epsilon(t)$. We can use Fermi's golden rule (using results from [6]) to derive transition rate $\langle \Gamma_n \rangle$ [5] as follows:

$$\Gamma_n(\omega) = \kappa \sum_{m \neq n} |\langle n|G_\lambda|m\rangle|^2 \delta(E_n - E_m - \hbar\omega) \tag{17}$$

where ω is frequency of the periodic external drive.

D Gauge potential: expression involving commutators

Another way to express the formula of adiabatic gauge potential:

$$A_\lambda(\mu) = -i\hbar \lim_{\mu\to 0} \sum_{n=0}^{\infty} (-1)^n \frac{C^{(2n+1)}}{\mu^{2n+2}} \tag{18}$$

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 D). I would need to think of some smarter way to compute adiabatic gauge potential.

[2] If the system is in equilibrium, then fluctuation -dissipation theorem dictates $\kappa = T$

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:

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

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