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 :

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

where $\Delta = 2\pi \times 2.87$ GHz is zero-field splitting, $\gamma_e = 2.8MHz/G$ is the gyromagnetic ratio of electron in the NV center, $\gamma_n \simeq 1kHz/G$ is the gyromagnetic ratio of nuclear spin, $\vec{S}$ ($\vec{I}$) is the spin of electron (nucleus) and $A \simeq 3MHz$ is magnitude of spin-spin coupling which leads to hyperfine splitting. The second and third terms are due to Zeeman effect.

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 two terms resulting in the following Hamiltonian :

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

It seems that the above Hamiltonian should be experimentally realizable [1]. Moreover, 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 $\hbar\Delta$ 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 [1]. Then we have:

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

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 B), we obtain Hamiltonian in the S_z basis ($|-1\rangle$, $|0\rangle$, $|1\rangle$):

$$H = \begin{pmatrix} \beta & \alpha & 0 \\ \alpha & 0 & \alpha \\ 0 & \alpha & \beta \end{pmatrix} \quad \text{where } \alpha = \lambda/\sqrt{2},\ \beta = \Lambda \tag{3}$$

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 $\beta = \hbar\Delta$. Now let's have a look at eigenvectors:

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

[1] If magnetic field is in z-direction, then gauge potential is zero. This is so because increasing B_z does not induce any excitations.

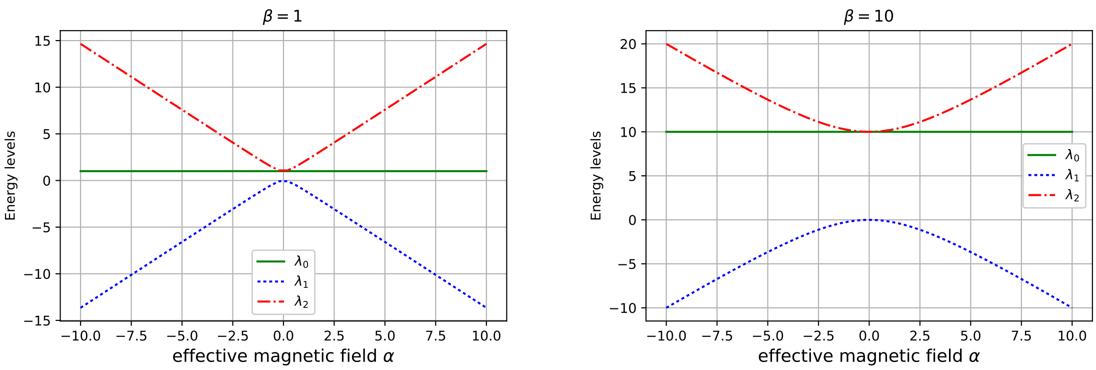

Figure 1: Avoided level crossing as a function of effective magnetic field

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:** $A^n_\lambda = \langle n|A_\lambda|n\rangle = i\hbar\langle n|\partial_\lambda|n\rangle$
- **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 B. We find that $\tilde{A_\lambda}$ in energy basis is given by :

$$\tilde{A_\lambda} = i\hbar\tilde{N}\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \text{where } \tilde{N} = \frac{\beta\hbar}{8\alpha^2 + \beta^2} \tag{6}$$

In S_z basis, we have $A_\lambda = U\tilde{A_\lambda}U^T$ where U is the unitary transformation that diagonalizes Hamiltonian, i.e. $H_d = U^T HU$. A_λ is given below:

$$A_\lambda = i\hbar N\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}, \quad \text{where } N = \frac{\beta\hbar}{\sqrt{16\alpha^2 + 2\beta^2}}$$

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 matrices are λ_2 and λ_7 whose representation is given below [3, 4]:

$$\lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \frac{1}{\sqrt{2}\hbar^2}(\hbar S_y + S_y S_z + S_z S_y)$$

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

Hence, we find that $A_\lambda = \hbar N(\lambda_2 - \lambda_7)$ which can be written as:

$$\boxed{A_\lambda = N_0(S_y S_z + S_z S_y)} \tag{7}$$

where $N_0 = \dfrac{\beta}{\sqrt{8\alpha^2 + \beta^2}} = \dfrac{\Delta}{\sqrt{4\gamma_e^2 B^2 + \Delta^2}}$.

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 $\overline{\epsilon(t)\epsilon(t')} = \kappa\delta(t - t')$ [2].

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:

$$\Gamma_n(\omega) = \kappa \sum_{m \neq n} |\langle n|G_\lambda|m\rangle|^2 \delta(E_n - E_m - \hbar\omega) \tag{8}$$

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 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.

B Spin Algebra

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x \quad [S_z, S_x] = i\hbar S_y \tag{9}$$

$$S^2|s, m\rangle = \hbar^2 s(s+1)|s, m \pm 1\rangle \quad S_z|s, m\rangle = \hbar m|s, m\rangle \tag{10}$$

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

$$S_{\pm}|s,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}|s,m\pm 1\rangle \tag{11}$$

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

$$S_+ = \sqrt{2}\hbar \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad S_- = \sqrt{2}\hbar \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{12}$$

Hence,

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \quad S_y = i\frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \tag{13}$$

C Fidelity of ground state of two and three level problem

Two level system

The Hamiltonian for Landau-Zener problem is :

$$H = \hbar\Delta\sigma_z + \hbar\lambda(t)\sigma_x \tag{14}$$

where $\lambda(t) = 2(t-1)/\tau$. Hence, $\dot{\lambda} = 2/\tau$. We are going to start off ground-state of Hamiltonian with $\lambda = -2$ at time $t_i = 1-\tau$ and end our protocol with $\lambda = 2$ at $t_f = 1+\tau$. Hence, duration of our protocol is 2τ.

Here condition for time-evolution to be adiabatic is $1/\tau \ll E/\hbar$ which comes out to be $1/\tau \ll \Delta^2$

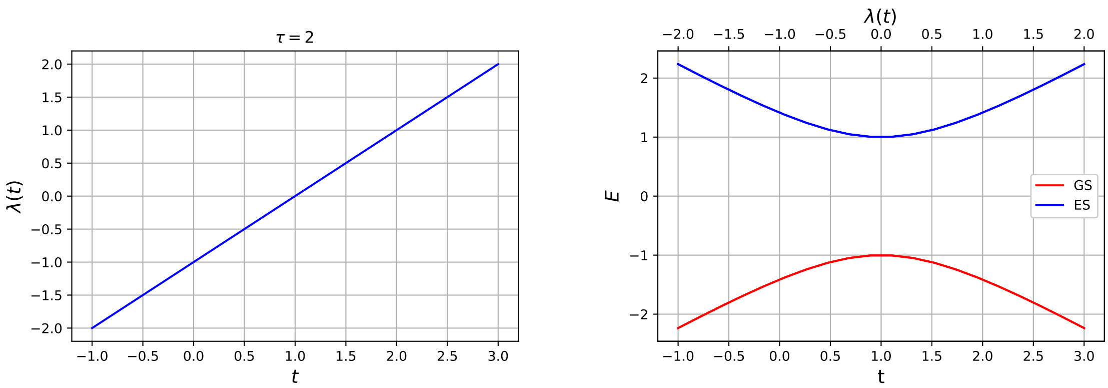

Figure 2: a) Protocol of magnetic field b) Avoided level crossing as we change λ for $\Delta = 1$ and $\tau = 2$

We would numerically compute fidelity F as we run our simulation from $t = t_i$ to $t = t_f$ units, where $F = \langle\psi_{GS}(t_f)|\psi(t_f)\rangle$.

Two level system: rotating magnetic field

The Hamiltonian for Landau-Zener problem is ($\hbar = 1$):

$$H = \Delta\sigma_z + \lambda(t)(\sigma_x\cos(\omega t) + \sigma_y\sin(\omega t)) \tag{15}$$

Going to rotating frame, we find:

$$\begin{aligned} H_{rot} &= V^\dagger H V - iV^\dagger\dot{V} \\ &= (\Delta - \frac{\omega}{2})\sigma_z + \lambda(t)\sigma_x \end{aligned}$$

where $V = \exp(-i\omega t\sigma_z/2)$

We would choose $\omega = 2\Delta$ so that $H_{rot} = \lambda(t)\sigma_x$.

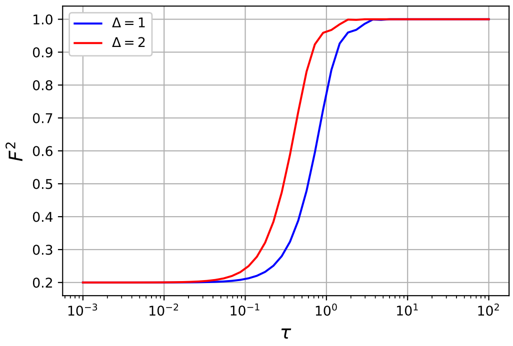

Figure 3: Fidelity (probability to find the wave-function to be in ground state) as increase the duration of protocol

Three level system

Let's choose magnetic field to be in x-direction. Then we have Hamiltonian of NV center given by:

$$\begin{aligned} H_{NV} &= \hbar \Delta S_z^2 + \hbar \gamma_e S_x B \\ &= \hbar \Delta (S_z^2 + \frac{\gamma_e}{\Delta} S_x B) \\ &= \hbar \Delta (S_z^2 + \lambda(t) S_x) \\ &= \Delta H_0(t) \end{aligned}$$

where $\lambda = \gamma_e B/\Delta$. We would choose $\lambda(t) = t/2T$. Hence, $\dot{\lambda} = 1/(2T)$. We are going to start off ground-state of Hamiltonian with $\lambda = -2$ at time $t_i = -T$ and end our protocol with $\lambda = 2$ at $t_f = T$. Hence, duration of our protocol is $2T$.

Let's suppose our Hamiltonian commutes at different time. Then unitary operator $U(t) = \exp(-i\Delta \int H_0(\Delta t) dt$. We can define $\tau = \Delta t$ so that $U(\tau)$. Since $\Delta \sim 10^9 s^{-1}$, this technique helps us numerically because then we don't have to deal with matrices that has huge numbers of the order of Δ.

Hence, for this purpose, we should convert $\lambda(t) = \Delta t/2(\Delta T) = \tau/(2\tilde{T}) = \lambda(\tau)$. This means that actual time of duration of protocol would be $2T = 2\tilde{T}/\Delta$.

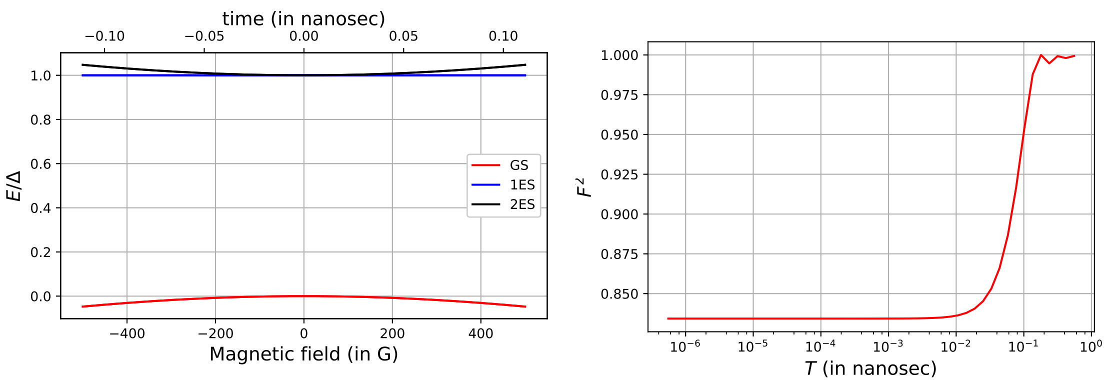

Figure 4: a)Avoided level crossing as we change λ with $T = 2/\Delta$ seconds b) Fidelity (probability to find the wave-function to be in ground state) as we increase the duration of protocol

In this numerical simulation, range of magnetic field has been chosen to be what's accessible in lab. We see that it's there is almost no transition from ground state to excited states.

Three level system: rotating magnetic field

Let's choose magnetic field to be in x-direction. Then we have Hamiltonian of NV center given by:

$$\begin{aligned} H_{NV} &= \hbar\Delta S_z^2 + \hbar\gamma_e S_x B_x \cos(\Delta t) \\ &= \hbar\Delta(S_z^2 + \frac{\gamma_e}{\Delta} S_x B_x \cos(\Delta t)) \\ &= \hbar\Delta(S_z^2 + \lambda(t)\cos(\Delta t) S_x) \\ &= \hbar\Delta H_0(t) \end{aligned}$$

where $\lambda(t) = \gamma_e B_x(t)/\Delta$. We would choose $\lambda(\Delta t) = 2\Delta t/(\Delta T) = 2\tau/\tilde{T}$. Hence, $H_0(\tau) = S_z^2 + \lambda(\tau) S_x \cos(\tau)$. With $\hbar = 1$, we have $H_{NV} = \Delta H_0(\tau)$

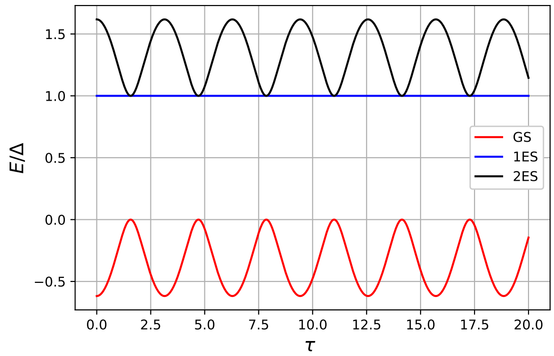

Figure 5: Energy levels

D Transition rate for periodically driven noisy system

Let's consider a Hamiltonian:

$$\mathcal{H}_{\mathcal{X}} = \mathcal{H}(\lambda) + \dot{\lambda}\mathcal{X} \tag{16}$$

where $\lambda = \lambda_0 + \epsilon(t)$ and $\epsilon(t)$ is an infinitesimal white noise which satisfies $\overline{\epsilon(t)\epsilon(t')} = \kappa\delta(t - t')$ [3]. 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:

$$\mathcal{H}_{\mathcal{X}} \approx \mathcal{H}(\lambda_0) + \epsilon\partial_\lambda\mathcal{H} + \dot{\epsilon}\mathcal{X} \tag{17}$$

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:

$$\Gamma_n(\omega) = \kappa \sum_{m\neq n} |\langle n|G_\lambda|m\rangle|^2 \delta(E_n - E_m - \hbar\omega) \tag{18}$$

where ω is frequency of the periodic external drive.

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

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