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 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 $\beta = \hbar^2\Lambda$.

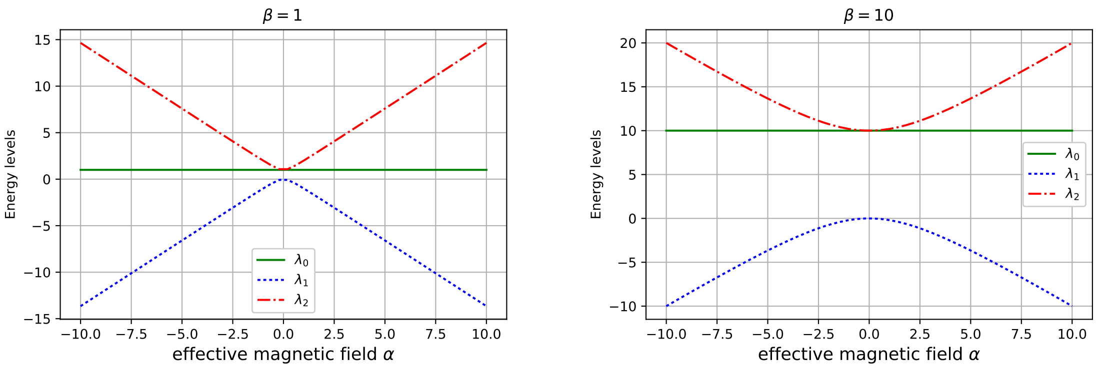

Figure 1: Avoided level crossing as a function of effective magnetic field

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_λ whose equation of motion is given by:

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

Another way to express this formula is:

$$A_\lambda(\mu) = -i\hbar \lim_{\mu \to 0} \sum_{n=0}^{\infty} (-1)^n \frac{C^{(2n+1)}}{\mu^{2n+2}} \tag{4}$$

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:

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

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

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

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

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,

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

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

$$
\begin{aligned}
T_1 = [H, S_yS_z] = -\hbar^2\lambda S_y^2 + i\hbar T &= -\hbar^2\lambda S_y^2 + \hbar^2\Lambda(i\hbar S_yS_z + 2S_xS_z^2) - \hbar^2\lambda S_z^2 \\
&= -\hbar^2\lambda(S_y^2 + S_z^2) + \hbar^2\Lambda(i\hbar S_yS_z + 2S_xS_z^2)
\end{aligned}
$$

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

Finally, we get

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

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

$$
i\hbar T_1 + T_2 = -i\hbar^3\lambda(S_y^2 + S_z^2) + i\hbar^3\Lambda(i\hbar S_yS_z + 2S_xS_z^2) + C^{(1)}S_z^2 + \hbar^2\lambda S_x^2 - 2i\hbar\lambda S_xS_zS_y
$$

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

Now, let's write:

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

B Spin Algebra

$$[S_x,S_y]=i\hbar S_z,\quad [S_y,S_z]=i\hbar S_x\quad [S_z,S_x]=i\hbar S_y \tag{5}$$

$$S^2|s,m\rangle=\hbar^2s(s+1)|s,m\pm 1\rangle\quad S_z|s,m\rangle=\hbar m|s,m\rangle \tag{6}$$

$$S_\pm|s,m\rangle=\hbar\sqrt{s(s+1)-m(m\pm 1)}|s,m\pm 1\rangle \tag{7}$$

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

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.