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Identifying different mechanisms in the control of a nitrogen–vacancy center system

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ABSTRACT

The nitrogen–vacancy (NV) center system has shown great potential in quantum computing due to its long decoherence time at room temperature by encoding the qubit in dressed states [28]. The corresponding control mechanisms, which is expressed by the pathways linking the initial and target states, can be naturally investigated with the Hamiltonian-encoding and observable-decoding (HE–OD) method in the interaction adiabatic representation. This is proved by the fact that the mechanisms change slightly with different detunings, magnetic and driving field intensities, and the dominant pathway is always $|g\rangle \rightarrow |d\rangle \rightarrow |g\rangle$, with $|g\rangle$ and $|d\rangle$ as the first two lowest dressed states. Cases are different in the diabatic representation. The orders of dominant pathways increase the driving field intensities. Tendencies of quantum pathway amplitudes with driving fields, magnetic fields and detunings change at different conditions, which can be analyzed from the Dyson series. HE–OD analysis show that the two states $|g\rangle$ and $|d\rangle$ in the interaction adiabatic representation are preferable to be employed as a qubit than the state pair $|0\rangle$ and $|-1\rangle$ in the diabatic representation under the current Hamiltonian and parameters.

1. Introduction

How to achieve an optimal and effective control of quantum systems has always been a hot topic due to its wide and potential application [1–12]. The corresponding control mechanism analysis is important to understand the underlying physics and can give hints to improve the control effect. The Hamiltonian-encoding and observable-decoding (HE–OD) technique has provided such a feasible means, and expressed the mechanism in terms of different pathways linking the initial and target states [12–21]. In the experiment, a signal function is firstly encoded in the Hamiltonian in a specific manner, and then the information of pathways is extracted by decoding the resultant nonlinear distortion of the output signal.

Quantum computation requires good control of quantum qubits. The nitrogen–vacancy (NV) center is an important candidate of solid-state quantum computing because of its special nature [22], such as long decoherence time at room temperature [23], good scalability and microwave manipulation [24]. In this context, we will perform a mechanism analysis on the NV center system with HE–OD.

This paper is organized as follows. Section 2 introduces the HE–OD method for mechanism analysis and the two representations for the NV center system. Section 3 gives the results. The final conclusions are presented in Section 4.

2. Methodology

2.1. The HE–OD method

It is known that the state of a quantum system can be described by the Schrödinger equation

$$i\frac{d|\Psi(t)\rangle}{dt} = H|\Psi(t)\rangle. \tag{1}$$

The state $\Psi(t)$ at time t can be obtained from the propagator $U(t)$ and the initial state $|\Psi(0)\rangle$ as $|\Psi(t)\rangle = U(t)|\Psi(0)\rangle$. The time evolution of $U(t)$ satisfies

$$i\frac{dU(t)}{dt} = HU(t). \tag{2}$$

Its Dyson expansion is

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$$U(t) = I + (-i)\int_0^t H(t_1)\,dt_1 + (-i)^2\int_0^t H(t_2)\int_0^{t_2} H(t_1)\,dt_1 dt_2 + \cdots. \quad (3)$$

The transition amplitude from the initial state $|a\rangle$ to the target state $|b\rangle$ is given by $\langle b|U(t)|a\rangle$. So the n-th order pathway $|a\rangle \to |l_1\rangle \to \cdots \to |l_{n-1}\rangle \to |b\rangle$ has the amplitude

$$U_{ba}^{n(l_1,\ldots,l_{n-1})}(t) = (-i)^n \int_0^t \langle b|H(t_n)|l_{n-1}\rangle \times \int_0^{t_n} \langle l_{n-1}|H(t_{n-1})|l_{n-2}\rangle \times \cdots \times \int_0^{t_2} \langle l_1|H(t_1)|a\rangle\, dt_1 dt_2 \cdots dt_n. \quad (4)$$

The HE–OD method introduces a dimensionless time-like variable s, and the Hamiltonian is encoded as $H(t) \to H(t,s)$, which leads to a distorted output signal $\langle b|U(t,s)|a\rangle$. Then the method tries to extract the desired pathway amplitudes from these signals. In practice, each element of the original Hamiltonian H is modulated as

$$H_{ij}(t) \to H_{ij}(t)\, m_{ij}(s).$$

Here the modulation function $m_{ij}(s)$ is taken to be the Fourier form

$$m_{ij}(s) = \exp\left(2\pi i \gamma_{ij} s/N\right), s = 1, 2, \cdots, N.$$

The propagator under the new Hamiltonian $H(t) \to H(t,s)$ evolves as

$$i\frac{dU(t,s)}{dt} = \begin{pmatrix} H_{11}(t)\,m_{11}(s) & \cdots & H_{1d}(t)\,m_{1d}(s) \\ \vdots & \vdots & \vdots \\ H_{d1}(t)\,m_{d1}(s) & \cdots & H_{dd}(t)\,m_{dd}(s) \end{pmatrix} U(t,s). \quad (5)$$

The transition amplitude from the initial state to the target state becomes

$$\langle b|U(t,s)|a\rangle = \sum_{n=1}^{\infty}\sum_{l_1,\cdots,l_{n-1}=1}^{d} U_{ba}^{n(l_1,\ldots,l_{n-1})}(t) \times M_{ba}^{n(l_1,\ldots,l_{n-1})}(s) \quad (6)$$

with

$$M_{ba}^{n(l_1,\ldots,l_{n-1})}(s) = m_{bl_{n-1}}(s)\, m_{l_{n-1}l_{n-2}}(s)\cdots m_{l_1 a}(s) = \exp\left(2\pi i \gamma_{n(l_{n-1},l_{n-2},\cdots,l_1)} s/N\right), \quad (7)$$

and

$$\gamma_{n(l_{n-1},l_{n-2},\cdots,l_1)} = \gamma_{bl_{n-1}} + \gamma_{l_{n-1}l_{n-2}} + \cdots + \gamma_{l_1 a}. \quad (8)$$

Due to the orthogonality of encoding functions $M_{ba}^{n(l_1,\ldots,l_{n-1})}(s)$, the pathway amplitudes $U_{ba}^{n(l_1,\ldots,l_{n-1})}(t)$ featured by the frequency of $\gamma_{n(l_{n-1},l_{n-2},\cdots,l_1)}$ can be obtained by performing an inverse fast Fourier transform (IFFT) of $U_{ba}(t,s)$.

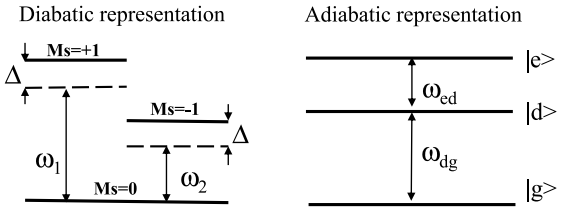

Fig. 1. Energy-level diagram of the NV center in diabatic and IA representations. The electronic spin-triplet states are labeled with $|M_s\rangle$, and the dressed states are denoted with $|g\rangle$, $|d\rangle$ and $|e\rangle$.

2.2. Diabatic and interaction adiabatic representations

A nitrogen–vacancy (NV) center is actually a spin defect consisting of a substitutional nitrogen impurity adjacent to a carbon vacancy in diamond. According to the electronic structure theory, its property is determined by six electrons, with two from the nitrogen atom, three from the carbon atoms surrounding the vacancy and one from the lattice [25–27]. The net spin is one due to the unpaired electron of the vacancy, leading to three energy levels with the magnetic quantum number M_s equal to 0, 1 or −1. As shown in Fig. 1, the two levels with $M_s = \pm 1$ are degenerate due to the axial symmetry, while the state $M_s = 0$ is energetically lower.

In the diabatic representation, the electronic spin ground states of an NV center in an external field B_z along the symmetry axis can be described by the following Hamiltonian [28]:

$$H = DS_z^2 + \gamma_e B_z S_z, \quad (9)$$

where $D = 2.87$ GHz is the so-called zero-field splitting [22], and the second Zeeman term $\gamma_e = 2.802$ MHz/G determines the eigenstates $|M_s\rangle$.

In experiment, two off-resonant continuous microwave driving fields are usually applied to transitions $|0\rangle \to |\pm 1\rangle$ at the same time. In the interaction picture, the Hamiltonian of the NV center driven by two microwaves with the same off-resonance Δ can be obtained by using rotating-wave approximation:

$$H_{NV} = H_a + H_b \quad (10)$$

with

$$H_a = \begin{bmatrix} \Delta + \gamma_e b & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \Delta - \gamma_e b \end{bmatrix},$$

$$H_b = \begin{bmatrix} 0 & \frac{1}{2}\Omega_1(t) & 0 \\ \frac{1}{2}\Omega_1(t) & 0 & \frac{1}{2}\Omega_2(t) \\ 0 & \frac{1}{2}\Omega_2(t) & 0 \end{bmatrix}.$$

Here Ω_1 and Ω_2 are the Rabi frequencies of the two transitions. Then the Hamiltonian is transformed to eliminate its nonzero diagonal elements

$$H_I = e^{iH_a t}\cdot H_b \cdot e^{-iH_a t} = \frac{1}{2}\begin{bmatrix} 0 & \Omega_1(t)e^{i(\Delta+\gamma_e b)t} & 0 \\ \Omega_1(t)e^{-i(\Delta+\gamma_e b)t} & 0 & \Omega_2(t)e^{-i(\Delta-\gamma_e b)t} \\ 0 & \Omega_2(t)e^{i(\Delta-\gamma_e b)t} & 0 \end{bmatrix}. \quad (11)$$

The encoding in the diabatic representation is performed to this Hamiltonian.

In the following, we will introduce how to encode in the interaction adiabatic (IA) representation [14]. The time varying transformation that diagonalizes $H_{NV}(t)$ is $R_A(t)$, which links the dressed states and eigenstates $|M_s\rangle$. Then in the adiabatic representation, the evolution of the propagator becomes

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