Fast magnetic field manipulations and nonadiabatic geometric phases of nitrogen-vacancy center spin in diamond

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Abstract
Fast quantum spin manipulation is needed to design spin-based quantum logic gates and other quantum applications. Here, we construct the exact evolution operator of the nitrogen-vacancy-center (NV) spin in diamond under external magnetic fields, and investigate the nonadiabatic geometric phases—both cyclic and non-cyclic—in these fast-manipulated NV spin systems. It is believed that the nonadiabatic geometric phases can be measured in future experiments, and that these fast quantum manipulations can be useful in designing spin-based quantum applications.

Keywords: quantum spin, geometric phase, fast driving

(Some figures may appear in colour only in the online journal)
2. Exact evolution of quantum states

The NV-center spin has spin value \( s = 1 \), and shows the easy-plane anisotropy; its \( z \)-component \( s_z \) can take three values: \(-1, 0, \) and \(+1 \). As usual, these are taken as the spin basis set for the NV-center spin: \( | -1 \rangle, |0 \rangle, \) and \( | +1 \rangle \). The Hamiltonian of the NV center spin \( \vec{S} \), in the presence of time dependent magnetic field \( \vec{B}(t) = (B_x(t), B_y(t), B_z(t)) \), can be written as

\[
H = DS^2 + \gamma \vec{S} \cdot \vec{B}(t),
\]

where \( h = 1 \) is used, \( D = 2.87 \) GHz is the zero-field splitting, and \( \gamma = 2.8 \) MHz G\(^{-1}\) is the electron gyromagnetic ratio. Accordingly, the Schrödinger equation for time-evolution operator \( U \) is given by

\[
i\hbar \frac{d}{dt} \phi = \left[ H, \phi \right].
\]

By choosing \(|\pm\rangle\), defined as \((|+1\rangle \pm |−1\rangle)/\sqrt{2}\), as the qubit basis of the NV-center spin, we can obtain exact evolution operator of the NV-center spin under time-dependent magnetic field by mapping the three-level system of the NV-center spin under time-dependent magnetic field [18], and using the existing exact analytical solution operator of the NV-center spin under time-dependent magnetic field [18]. The Hamiltonian equation (1) in the new basis of \((|\pm\rangle, |0\rangle, |−\rangle\rangle\) can be expressed as

\[
H_s = \begin{pmatrix}
D & \alpha \gamma B_0 & 0 \\
\alpha \gamma B_0 & 0 & 0 \\
0 & 0 & -i \beta \gamma B_0 \end{pmatrix}.
\]

Then, we can easily derive its exact evolution operator [18]:

\[
U_s(\theta, t) = e^{iH_s t} = \begin{pmatrix}
\alpha \gamma B_0 & 0 & 0 \\
\alpha \gamma B_0 & 0 & 0 \\
0 & 0 & -i \beta \gamma B_0 \end{pmatrix}.
\]

Using the time evolution operator \( U \), we can manipulate the single NV-center spin, exactly and efficiently. Experimentally, the NV-center spin can be easily prepared in state \(|0\rangle\). We try to realize state transfer between \(|0\rangle\) and \(|\pm\rangle\).

With the time evolution operator \( U \), applied the state \(|0\rangle\) will become

\[
U(\theta, t)|0\rangle = \frac{\cos \theta |u^*_{21}(t)\rangle - i \sin \theta |u_{21}(t)\rangle}{\sqrt{2}}.
\]

It is interesting to construct two reasonable functions for \( \Theta(t) \):

\[
\Theta_1(t) = \kappa_1 \sin^2 \left( \frac{\pi}{T_1} t \right),
\]

and

\[
\Theta_2(t) = \kappa_2 \sin^2 \left( \frac{\pi}{T_2} t \right) (1 - \cos \lambda (t - T_2)),
\]

where \( \lambda \) is defined as \( D/2, \) \( \kappa_1 \) and \( \kappa_2 \) are two parameters to be determined, and \( T_1 \) and \( T_2 \) describe the time duration for the two cases. Then, the corresponding magnetic fields \( (B_1(t) \) and \( B_2(t)) \) can be expressed as

\[
B_n(t) = \frac{\Theta_n}{2} + \frac{D}{2} \sin \Theta_n \cot(DW_c(\Theta_n, t))
\]

where \( n = 1 \) or \( 2 \), and the corresponding \( \Theta_n \) is given by equations (8) and (9) respectively.

Because the target state does not contain state \(|0\rangle\), we need to set \( u_{21}(T_1) = 0 \), i.e. \( \cos \left( \frac{\pi}{T_1} \right) = 0 \).

Then the quantity \( \Delta(\Omega) = \lambda \sqrt{W_c(\Omega, T_1)/2} \) contributes an overall phase in the state \( U(\theta, T_1)|0\rangle \) in equation (7). In order to achieve a minimal time value \( T_1 \) and a finite field pulse in the time interval \( t \in (0, T_1) \), we need two conditions: \( \theta < \chi(T_1) \leq \frac{\pi}{2} \) and \( W_c(\Omega, 2 \lambda, T_1) = \pi \). Once we set \( t = T_1 \) and choose a value for \( \chi(T_1) \), the parameter \( \kappa_1 \) and \( T_2 \) can be solved numerically. We can construct arbitrary superposed state [18]

\[
|g\rangle(\phi) = \cos \phi|+\rangle + i \sin \phi|−\rangle \quad (0 \leq \phi \leq \pi)
\]

in the following way. Choosing \( \alpha \) and \( \beta \) in equation (2) to satisfy the equality \( \arctan(\beta/\alpha) = \theta \geq 0 \), we can let \( \theta = \pi - \phi \) in equation (7) and thus obtain the final state

\[
U(\pi - \phi, T_{12})|0\rangle = \begin{pmatrix}
\cos \phi & 0 \\
0 & i \sin \phi \end{pmatrix} e^{-i \theta (T_{12})} e^{-i \pi/2 T_{12}}.
\]

Neglecting the overall factor, we achieve the target state. If we set \( \chi(T_1) = \pi/2 \), we can get a self-consistent result:
\(\kappa_1 = 1.4627998\) and \(T_1 = 2.42412/\lambda\), \(\kappa_2 = 2.01024\) and \(T_2 = 2.442705/\lambda\). The time-dependent function \(\Theta_1(t)\) and the corresponding magnetic field \(B_{12}(t)\) as functions of time \(t\) in units of \(T_{12}\) are shown in the figure 1. For the second function \(\Theta_2(t)\), we use \(1 - \cos \lambda(t - T_2)\) to make the derivation of magnetic field at \(T_2\) equal zero. The magnetic field is anti-symmetrical under the transformation \(t \rightarrow 2T_2 - t\) due to the symmetry of \(\Theta_{12}(t)\). As we have pointed out [18], the arbitrary relative phase \(\phi\) can be realized by constant magnetic field, and it has no contribution to the geometric phase; hence, we do not consider the relative phase.

### 3. Nonadiabatic geometric phases

As usual, the geometric phase is defined as the difference between the total phase and the dynamical phase. We will consider three specific cases. In the first case, the initial state is \(|0\rangle\). This is different from that for non-Abelian holonomic quantum computation [36–38], because the dynamical phase is present during evolution and its geometric phase is independent of magnetic field direction. In the second case, when the initial state is superposed state \(|q\rangle\), the phase evolution depends on magnetic field direction. We can still get a relatively simple result similar to the first one. In the third case, we allow the constant \(\lambda\) to change and then get a very different result.

#### 3.1. Case 1

The state begins from \(|0\rangle\). The total phase can be calculated through \(|0\psi(t)\rangle = e^{-i\lambda t}|0\rangle\). The dynamical phase by integrating \(\Re \langle \psi_0(t)|\psi_0(t)\rangle\) is \(0\). We can express the geometric phase as

\[
\varphi_1^t(\theta_1, t) = \arg(\langle U_0(\theta_1, t)|0\rangle) - \int_0^t \langle U_0^\dagger(\theta_1, \tau')|U_0(\theta_1, \tau')|0\rangle d\tau'.
\]

It can be proved that the integrand is equivalent to \(-\lambda + \frac{\Theta}{2} \sin(2\lambda W_\lambda(\Theta))\) sin \(W_\lambda(\Theta, 2\lambda, t) + \lambda \cos \Theta \cos W_\lambda(\Theta, 2\lambda, t)\). Here, we describe the magnetic field direction with \(\theta_1\). Surprisingly, the geometric phase is independent of parameter \(\theta_1\), and depends only on the parameter \(\Theta\). The state \(|0\rangle\) will evolve into its orthogonal state \(|q\rangle(\pi - \theta_1)\) at time \(T_{12}\). Considering that the total phase is not well-defined when the state is orthogonal, we can consider the phase at time \(T_{12}\) as the left or right limit of \(\varphi_1^t(\theta_1, t)\), i.e. \(\varphi_1^{T_{12}}(\Theta) = \lim_{t \rightarrow T_{12}^-} \varphi_1^t(\theta_1, t)\).

#### 3.2. Case 2

The initial state is supposed to be a qubit state \(|q\rangle\) normal to \(|0\rangle\). It can be derived that \(|q\rangle U_0(\phi_1, t)|q\rangle = e^{-i\lambda t} (\sin^2(\phi_1 + \phi) + \bar{u}_{11}(t) e^{i\lambda t} \cos^2(\phi_1 + \phi))\) and \(\Re \langle \psi_q(\phi_1)|\psi_q(t)\rangle = \Re \langle qU_0^\dagger(\phi_1, t)|U_0(\phi_1, t)|q\rangle\). Here, we mark the magnetic field direction as \(\phi_1\). If \(\phi_1 + \phi = \pi\), the \(|q\rangle\) state will become \(|0\rangle\) at \(T_{12}\), and will return to the initial state \(|q\rangle\) at the time \(2T_{12}\). The geometric phase can be expressed as

\[
\varphi_2^t(\theta_1) = \arg(\langle U_0(\phi_1, t)|q\rangle) - \int_0^t \langle qU_0^\dagger(\phi_1, \tau')|U_0(\phi_1, \tau')|q\rangle d\tau'.
\]
The integrand above can be proved to be equivalent to
\[-\lambda - \cos^2(\phi_1 + \phi) (\lambda \cos \Theta \cos W_s(\Theta, 2\lambda, t) + \frac{\Theta}{\pi} \sin(2\lambda W_c(\Theta, t))) \cos W_s(\Theta, 2\lambda, t) - \lambda \sin^2(\phi_1 + \phi).\]
With the same magnetic field in figure 1, the probability evolution of state \(|0\rangle\) and the geometric phase are presented in figure 3. Comparing figures 2 and 3, it can be seen that the geometric phases seem to be symmetric to each other in these two cases. It can be proved that they are actually the same except for a negative sign. The geometric phases gained at the ending times \(2T_1\) and \(2T_2\) are equivalent to \(\pi\) and \(-4.2705\) respectively.

3.3. Case 3

The parameter \(\lambda\) in the function \(\Theta_2(t)\) can be allowed to change. For convenience, we define \(\eta = \lambda x\), where \(x\) is a variable. Then we can construct the third function: \(\Theta_3(t) = \kappa_3 \sin^2(\frac{x}{T_2})(1 - \cos(\eta(t - T_2)))\). Here, we set the time duration to be the same as \(\Theta_3(t)\), and \(\kappa_3\) and \(\eta(\text{or} \ x)\) are adjustable parameters. The quantity \(\chi(T_2) = \lambda W_c(\Theta, T_2)\). In order to construct a reasonable magnetic field easily, we must set the quantity \(\chi(T_2) \leq \frac{\pi}{4}\) because of the cot function in the magnetic field formula. We set it as \(\frac{\pi}{4}\), and we need to solve the self-consistent equation: \(\chi(T_2) = \frac{\pi}{4}\) and \(W_s(\Theta, 2\lambda, T_2) = \pi\). Consequently, we obtain a reasonable result: \(\kappa_3 = 1.551 569\) and \(x = 2.8671 219\). At this time, there is no simple relation between time \(t\) and \(2T_2 - t\), because of different phase conditions. In figure 4, we present the magnetic field and the probability evolution of state \(|0\rangle\), and the phases (with the two initial states: \(|0\rangle\) and \(|q\rangle\)) as functions of time \(t\). The curves of the phase evolution with \(x = 1\) and \(x = 2.8671 219\) are similar. The small oscillation in the curves is due to the additional...
function factor. The geometric phases gained between $t = 0$ and the ending times $(2T_2)$ are equivalent to 4.54 and −4.54 with $|0⟩$ and $|q⟩$ as the starting states, respectively.

3.4. Geometric interpretation

We use the case of $Θ_t(t)$ to explain the idea of geometric property. We rewrite the equation (7) as the following expression by introducing three real time-dependent functions: $η_i(t)$, $θ_i(t)$, and $ϕ_i(t)$

$$|Ψ(t)⟩ = e^{iη_i(t)}[\cos \frac{θ_i(t)}{2} |0⟩ + e^{iϕ_i(t)} \sin \frac{θ_i(t)}{2} |q⟩].$$

(15)

In the time domain $(0, 2T_1)$, the function $θ_i(t)$ takes values in $(0, \pi)$, and the function $ϕ_i(t)$ in the domain $(-\frac{π}{2}, \frac{π}{2})$. At $t = 0$ the state is $|0⟩$; at $t = T_1$ the state becomes $|q⟩$; and at $t = 2T_1$ the state returns to $|0⟩$. Therefore, we obtain a cyclic process and thus the path of the state in the unit sphere spanned by the $(θ_i, ϕ_i)$ parameters makes a closed curve. Then we can obtain the solid angle for the time duration $(0, 2T_1)$:

$$\int \int \sin θ_1 dθ_2 dϕ_2 = 2π.$$ Our geometric phase $π$ in this case is equivalent to half the solid angle, as it should be. It is interesting that the geometric interpretation of the quantum phase is still true, although the quantum process is nonadiabatic.

4. Conclusion

It is believed that the study of geometric phases is an attempt to understand quantum mechanics better. Geometric phase is an observable quantity in experiments with a solid-state spin qubit, via spin echo interferometry [41–43]. It has been proposed to use Berry phase in mechanically rotating diamond crystal [44]. Geometric phase has many potential applications [45, 46]. With the development of quantum techniques, geometric quantum computation makes a hot research field in quantum physics, because of its fault tolerance property [40, 47, 48], and will be relevant to qubit control. Our main results include: (1) we have constructed the exact evolution operator of the NV spin system with the more transparent method, and then found three physically reasonable pulses for designing fast quantum logic gates based on the NV spin in diamond; and (2) we have investigated nonadiabatic geometric phases of the fast-driven NV spin systems, and shown that for the first pulse $(Θ_1(t))$, the nonadiabatic geometric phase for the cyclic path $(t = 0 → T_1 → 2T_1)$ is equivalent to half the solid angle spanned by the corresponding two angle variable in the definition of the qubit state. In addition, the controlling pulse and the geometric phase can be manipulated through choosing different $Θ(t)$ functions. We believe that these manipulations can be useful in designing practical quantum applications, and that nonadiabatic geometric phases, measurable in future experiments, could be used in quantum applications.

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