Proposal for implementing universal superadiabatic geometric quantum gates in nitrogen-vacancy centers

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We propose a feasible scheme to implement a universal set of quantum gates based on geometric phases and superadiabatic quantum control. Consolidating the advantages of both strategies, the proposed quantum gates are robust and fast. The diamond nitrogen-vacancy center system is adopted as a typical example to illustrate the scheme. We show that these gates can be realized in a simple two-level configuration by appropriately controlling the amplitude, phase, and frequency of just one microwave field. The gate’s robust and fast features are confirmed by comparing the fidelity of the proposed superadiabatic geometric phase (controlled-PHASE) gate with those of two other kinds of phase (controlled-PHASE) gates.

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Because the diamond nitrogen-vacancy (NV) center system has the potential to operate at room temperature, it has attracted a lot of interest in quantum computation [1–5] and quantum sensing [6–9] research in recent years. In order to realize scalable quantum computation based on NV center systems, the fidelity of each quantum gate needs to exceed a certain threshold [10,11]. Geometric phases are believed to be robust against local stochastic noises, which depend solely on certain global geometric features of the executed evolution paths [12–14]. Therefore, quantum gates and quantum control based on geometric phases, which are intrinsically fault tolerant [15–16], have been under consideration for the NV center systems. Very recently, geometric quantum gates based on purely nonadiabatic geometric phases were realized in room temperature NV center systems [17,18] as well as other systems [19,20]. Compared with the initial schemes for geometric quantum computation [21] based on adiabatic non-Abelian holonomies [22], the nonadiabatic geometric phases [23,24] and nonadiabatic non-Abelian holonomies [25,30] allow for high-speed quantum gate operations and thus intrinsically protect against environment-induced decoherence such as decay and dephasing. However, the nonadiabatic geometric quantum gates are susceptible to the systematic errors in the control Hamiltonian [31–33].

On the other hand, the superadiabatic and counteradiabatic [44–46] quantum control proposals are believed to be not only remarkably fast (with speed close to the quantum speed limit) but also highly robust against control parameter variations. In the superadiabatic scheme, the system evolves exactly along the instantaneous eigenstate of an original Hamiltonian at any desired rate by introducing an additional Hamiltonian [41–43]. Interestingly, high-fidelity, robust and fast quantum control based on the superadiabatic protocol has been experimentally realized on the cold atomic ensemble [44], the NV electron qubit [45], and the atomic optical lattice system [46]. It is noteworthy that as adiabatic population transfers [47–49], superadiabatic population transfers are insensitive to the dynamical evolution times, so it is not even necessary to design the exact durations of the controlling fields beforehand.

For scalable quantum computation, the ideal quantum gates should be both robust and fast. Since geometric quantum manipulation has an intrinsic fault tolerant property [12–16] and superadiabatic control is remarkably fast [44–46], the realization of a universal set of quantum gates which consolidates the aforementioned advantages of geometric phases and superadiabatic evolution will be essential in quantum computation and quantum manipulation.

In this paper, we propose an experimentally feasible scheme to implement universal superadiabatic geometric quantum gates (SGQGs) that are both robust and fast. The scheme can be used in many candidates of quantum computation. For the purpose of demonstration, we adopt the NV center system as a typical example to illustrate this approach. This system is controlled by microwave fields. We show that a universal set of SGQGs can be realized in a simple two-level configuration by appropriately controlling the amplitude, phase, and frequency of just one microwave field. On one hand, the evolutions are geometric and thus robust against certain high-frequency fluctuations. On the other hand, the evolutions are superadiabatic and can thus be fast and robust against systematic errors. We compare the fidelities of the proposed SGQGs with those of two other kinds of phase gates, and find that the SGQGs can perform ten times faster but with the fidelities comparable with that of the normal adiabatic geometric phase gate. The fidelities and operation time are comparable with those of the nonadiabatic holonomic gates which are implemented in a three-level structure.

We first address a general approach to achieve SGQGs using a two-level energy structure. We assume that the two-level system couples with a microwave field with frequency \( \omega_m \) and phase \( \varphi \). The energy difference between the states |0⟩ and |1⟩...
is $\hbar \omega$. The system is described by a time-dependent Hamiltonian
\begin{equation}
H_0(t) = \frac{\hbar}{2} \begin{pmatrix}
\Delta(t) & \Omega_R(t) e^{-i\varphi(t)} \\
\Omega_R(t) e^{i\varphi(t)} & -\Delta(t)
\end{pmatrix},
\end{equation}
where $\Delta(t) = \omega - \omega_m(t)$ is the detuning and $\Omega_R(t)$ (real here and hereafter) is the Rabi frequency proportional to the amplitude of the microwave field. The instantaneous eigenstates are
\begin{align*}
|\lambda_+(t)\rangle &= \begin{pmatrix} \cos \frac{\theta}{2} e^{-i\varphi/2} \\ \sin \frac{\theta}{2} e^{i\varphi/2} \end{pmatrix}, \\
|\lambda_-(t)\rangle &= \begin{pmatrix} \sin \frac{\theta}{2} e^{-i\varphi/2} \\ \cos \frac{\theta}{2} e^{i\varphi/2} \end{pmatrix},
\end{align*}
where the mixing angle $\theta = \arctan[\Omega_R(t)/\Delta(t)]$. The corresponding eigenvalues are $E_{\pm} = \pm \hbar \Omega/2$, where $\Omega = \sqrt{\Delta^2(t) + \Omega_R^2(t)}$. With adiabatic approximation, the time evolution takes the following form: $U(t) = \sum_n \exp \left\{ i \int_0^t \Omega_{\pm} (t') dt' \right\} |\lambda_n(t')\rangle \langle \lambda_n(0)| (n = \pm) - \), where $\Omega_{\pm}(t') = i \lambda(t') / \partial t \lambda(t')$ is the effective vector potential. Through the reverse engineering approach, a single superadiabatic Hamiltonian $H_s(t) = H_0(t) + H_1(t)$, where
\begin{equation}
H_1(t) = i\hbar \sum_{n=\pm} \left[ \partial_t |\lambda_n\rangle \langle \lambda_n| - |\lambda_n| \partial_t \langle \lambda_n| \langle \lambda_n| \right]
\end{equation}
is the superadiabatic correction Hamiltonian, will drive all the eigenstates $|\lambda_n(t)\rangle$ of $H_0(t)$ to precisely evolve without transitions between them at any desired rate.

We can further deduce the superadiabatic Hamiltonian. For the given system driven by Hamiltonian (1), when $\varphi$ is kept constant, the superadiabatic correction Hamiltonian reads
\begin{equation}
H_1(t) = \frac{\hbar}{2} \begin{pmatrix}
0 & -i \Omega_{\gamma}(t) e^{-i\varphi} \\
i \Omega_{\gamma}(t) e^{i\varphi} & 0
\end{pmatrix},
\end{equation}
where $\Omega_{\gamma}(t) = \Omega(t) \Delta(t) - \Omega_R(t) \Delta(t)/\Omega^2$. In order to ensure that the system evolves perfectly adiabatically, it seems that another microwave field with phase $\varphi + \pi/2$ is required, which may increase the difficulty of experiments. However, the effect of this extra microwave field can be achieved by appropriately modifying the Rabi frequency (amplitude) and the phase of the original microwave field. Therefore, we recast the wanted Hamiltonian $H_s(t) = H_0(t) + H_1(t)$ in the form
\begin{equation}
H_s(t) = \frac{\hbar}{2} \begin{pmatrix}
\Omega_{\gamma}(t) e^{-i\varphi + \phi(t)} & \Omega_{\gamma}(t) e^{-i\varphi + \phi(t)} \\
\Omega_{\gamma}(t) e^{i\varphi + \phi(t)} & -\Delta(t)
\end{pmatrix},
\end{equation}
where $\Omega_{\gamma}(t) = \sqrt{\Omega_R^2(t) + \Omega_\gamma^2(t)}$ and $\phi(t) = \arctan[\Omega_R(t)/\Omega(t)]$, which eliminates the need for an extra microwave field to realize the $H_1(t)$ term.

The states $|\lambda_{\pm}(t)\rangle$ are a pair of orthogonal states and can be used to realize SGQGs under the cyclic condition $|\lambda_{\pm}(T)\rangle = e^{i\phi} |\lambda_{\pm}(0)\rangle$, where $\phi_{\pm}$ are real phase factors. We first denote an arbitrary initial state as $|\psi_i\rangle = a_+ |\lambda_+(0)\rangle + a_- |\lambda_-(0)\rangle$ with $a_\pm = |\lambda_\pm(0)\rangle / \langle \psi_i|$. Then, we cyclically change the superadiabatic Hamiltonian $H_s(t)$ with period $T$ by suitably manipulating the parameters $\Delta(t)$, $\Omega_R(t)$, and $\varphi(t)$. States $|\lambda_+\rangle$ and $|\lambda_-\rangle$ thus evolve cyclically and gain different phases including both geometric and dynamical components. If a special cyclic evolution path is chosen to erase the accumulated dynamical phases, pure geometric phases can be obtained. Under those conditions, we find the relation $U(T)|\lambda_\pm(0)\rangle = \exp(\pm i\gamma)|\lambda_{\pm}(0)\rangle$, where $\gamma$ is a pure geometric phase given by the vector potential integral in $U(t)$. The final state at time $T$ is found to be $|\psi_f\rangle = U(\chi, \gamma)|\psi_i\rangle$, where
\begin{equation}
U = \begin{pmatrix}
\cos \gamma + i \cos \chi \sin \gamma & i \sin \chi \sin \gamma \\
i \sin \chi \sin \gamma & \cos \gamma - i \cos \chi \sin \gamma
\end{pmatrix},
\end{equation}
is a single-qubit gate depending only on the geometric phase $\gamma$ and the initial value $\chi = 0$.

The system can be valid in many systems. It is important to implement two kinds of noncommutable single-qubit gates and one nontrivial two-qubit gate with realistic physical systems. For demonstration, we illustrate such an implementation based on the control of electron and nuclear spins in a diamond NV center with a proximal $^{13}$C atom. The NV center has a spin-triplet ground state and the nearby nuclear spins ($^{13}$C and the host $^{15}$N) are polarized by a magnetic field of about 500 G along the nitrogen-vacancy axis. Owing to the large energy difference of $|m_s = \pm 1\rangle$ levels shifted by the magnetic field, we take the Zeeman components $|m_s = 0\rangle \equiv |0\rangle$ and $|m_s = -1\rangle \equiv |1\rangle$ as the qubit basis states, as shown in Fig. 1(a). The qubit can be manipulated by a microwave field whose frequency, amplitude, and phase can be adjusted by mixing with an arbitrary waveform generator. Therefore, the superadiabatic Hamiltonian can be straightforwardly realized by driving the microwave field.

We now show schematically how to construct the phase gate $U_1$ in two steps via an “orange slice” scheme as shown in Fig. 1(b), where we plot a designed cyclic evolution path $(ABCD)A$ on the Bloch sphere surface. At this stage, we choose point $A$ (corresponding to $\chi = 0$) in Fig. 1(b) to be the initial state $|\lambda_+\rangle$. In order to drive the state $|\lambda_+\rangle$ ($|\lambda_-\rangle$) to evolve cyclically, with the accumulated dynamical phase being zero, we control the microwave field as follows. In the first step, from $t = 0$ to $t = 2\tau$, the Rabi frequency and detuning of the original Hamiltonian $H_0(0, 2\tau)$ with a constant phase $\varphi_{1}$ are given by
\begin{equation}
\Omega_R(t) = \begin{cases}
\Omega_0[1 - \cos(\frac{\pi t}{\tau})], & 0 \leq t < \tau \\
\Omega_0[1 + \cos(\frac{\pi t - \tau}{\tau})], & \tau \leq t < 2\tau
\end{cases}
\end{equation}
and
\begin{equation}
\Delta(t) = \begin{cases}
\Delta_0[\cos(\frac{\pi t}{\tau}) + 1], & 0 \leq t < \tau \\
\Delta_0[\cos(\frac{\pi t - \tau}{\tau}) - 1], & \tau \leq t < 2\tau.
\end{cases}
\end{equation}
We then show how to achieve the gate $U_2$ geometrically in three steps via an “orange slice” scheme analogous to the gate $U_1$. In Fig. 1(b), we plot the cyclic evolution path $(BCDAB)$ on the Bloch sphere in which point $B$ (corresponding to $\chi = \pi/2$) is the initial state $|\lambda_+\rangle$. From $t = 0$ to $t = \tau$, the Rabi frequency and detuning of the original Hamiltonian $H_0(0, \tau)$ with a constant phase $\varphi'_1$ are given by

$$\Omega_R(t) = \Omega_0[1 + \cos(\frac{\pi t}{\tau})], \quad \Delta(t) = \Delta_0[\cos(\frac{\pi t}{\tau}) - 1]. \quad (9)$$

The system is driven to point $C$ by superadiabatic Hamiltonian $H_s(0, \tau)$ with a constant phase $\varphi'_1$. Thereafter, from $t = \tau$ to $t = 3\tau$, the parameters of the Hamiltonian $H_0(\tau, 3\tau)$ with a constant phase $\varphi'_2$ are given by

$$\Omega_R(t) = \Omega_0[1 - \cos(\frac{\pi (t-\tau)}{\tau})], \quad 2\tau \leq t < 2\tau$$

and

$$\Delta(t) = \Delta_0[\cos(\frac{\pi (t-\tau)}{\tau}) + 1], \quad 2\tau \leq t \leq 3\tau. \quad (10)$$

The system is driven back to point $B$ by superadiabatic Hamiltonian $H_s(3\tau, 4\tau)$ with phase $\varphi'_1$. In these three steps, the $|\lambda_+\rangle$ state evolves along the paths $BC, CA$ and $AB$ on the Bloch sphere and finally returns to the starting point $B$ to form a cyclic loop. Similar to the proof in $U_1$, we can show that the dynamical phases accumulated in these three paths are completely canceled out. Meanwhile, the required geometric phase $\gamma_2 = \pi - (\varphi'_2 - \varphi'_1)$. As a result, the desired SGQG $U_2 = \exp(\gamma_2\sigma_z)$ is achieved.

We now turn to implementing a nontrivial two-qubit gate. We adopt a system with the level structure similar to those used in the recent dynamic\cite{52} and holonomic\cite{53} experiments, which exploit the NV center electron spin as the target qubit and one nearby $^{13}$C nuclear spin as the control qubit (with the computational basis states $|\uparrow\rangle$ and $|\downarrow\rangle$). The single electron spin is coupled to a single $^{13}$C nuclear spin through hyperfine interaction, and the resultant level configuration is shown in Fig. 1(c). The different levels can be coupled by state-selective microwave and radio-frequency fields. In particular, by applying the microwave field $\text{MW}_{\text{qz}}$ with adjustable frequency, Rabi frequency, and phase, we can realize the superadiabatic coupling Hamiltonian $H_{\text{qz}}$ on the two-dimensional subspace spanned by $\{|0, \uparrow\rangle, |1, \uparrow\rangle\}$ of the computational space spanned by $\{|0, \downarrow\rangle, |1, \downarrow\rangle, |0, \uparrow\rangle, |1, \uparrow\rangle\}$. As with the single-qubit gate $U_1$ above, we can achieve the following superadiabatic geometric two-qubit gate:

$$U_{tq} = |\uparrow\rangle\langle\uparrow| \otimes U(\chi_{tq}, \gamma_{tq}) + |\downarrow\rangle\langle\downarrow| \otimes I, \quad (13)$$
with two other kinds of geometric gates. The imperfection of microwave fields as well as the nearby nuclear spins (fluctuations of the amplitude, phase, and frequency of the control fields can be approximately taken as quasistatic noises, a low-frequency noise based on the changes in the operational Material [53]. As a typical case, we can precisely implement of the nuclear spin pointing downward can be neglected when the hyperfine coupling \( A \) is larger than \( 2\pi \times 100 \) MHz under the chosen parameters below, as shown in the Supplemental Material [53]. As a typical case, we can precisely realize the superadiabatic geometric controlled-NOT gate by controlling the microwave field \( \text{MW}_{\text{tq}} \) just as with the implementation of \( U_2 \) (i.e., \( \chi_{\text{tq}} = \pi/2 \)) and by choosing the geometric phase \( \gamma_{\text{tq}} = \pi/2 \). Furthermore, the superadiabatic geometric controlled-PHASE gate \( U_{\text{cp}} \) can be achieved when \( U(\chi_{\text{tq}}, \gamma_{\text{tq}}) = U_1 \), i.e., \( \chi_{\text{tq}} = 0 \). Therefore, \( U_{\text{tq}} \) is sufficient for universal quantum computation when assisted by a combination of the gates \( U_1 \) and \( U_2 \).

We now discuss the performance of SGQGs as compared with two other kinds of geometric gates. The imperfection of a quantum gate is usually due to the fluctuations of the control fields and the NV center environments, specifically, the fluctuations of the amplitude, phase, and frequency of the control microwave fields as well as the nearby nuclear spins (\(^{13}\)C and the host \(^{15}\)N) and far-away random spin bath in the NV center environments. All of these fluctuations may be classified as high- or low-frequency noises based on the changes in the operation time of the quantum gates. The random spin bath can be considered as a high-frequency noise, and the nearby nuclear spins and the fluctuations of the control fields can be approximately taken as quasistatic noises, a low-frequency noise [54]. Previous theories [12,13] and experiments [14] have shown that geometric quantum gates are robust against high-frequency perturbations, and in Supplemental Material [53], we confirm that SGQGs keep this merit. Therefore, here we focus on a typical low-frequency noise, the systematic errors in the control parameters, which effectively include all quasistatic noises.

We choose SGQGs \( U_1 \) and \( U_{\text{cp}} \) as the test cases, comparing them with the adiabatic geometric phase gate without the superadiabatic correction Hamiltonian \( H_1 \), and with the nonadiabatic holonomic phase gate experimentally realized in Ref. [18]. As for \( U_1 \), the isolating two-level system as shown in Fig. 1(a) is studied, with the parameters \( \Omega_0 = 2\pi \times 2 \) MHz and \( \Delta_0 = 6 \) MHz, which have been used to realize the adiabatic geometric phase gate in Refs. [33,55]. The maximum superadiabatic Rabi frequency \( \Omega_{\text{sm}} \) is a function of \( \tau \). Moreover, in order to guarantee that \( \Omega_{\text{sm}} \) is not larger than the peak Rabi frequency \( \Omega_{\text{Rm}} \) of the original Hamiltonian \( H_0 \), we set \( \tau = 0.16 \) \( \mu \) s. The operation time \( T_{\text{sa}} \) of the superadiabatic geometric phase gate is \( 4\tau = 0.64 \) \( \mu \) s. The nonadiabatic holonomic phase gate is realized by setting the parameters \( \theta = 0 \) and \( \varphi = 0 \) of the three-level \( \Lambda \) system Hamiltonian \( H = \hbar\Omega(t)\sin(\theta/2)\eta e^{i\epsilon/2}|0\rangle - \cos(\theta/2)|e\rangle|1\rangle + \text{H.c.} \), as studied in Refs. [17,18,20,25]. The envelope \( \Omega(t) \) is designed as a truncated Gaussian pulse described by \( \Omega_{\text{nh}} \exp(-t^2/\sigma^2) \). We choose \( \Omega_{\text{nh}} = \Omega_{\text{sm}}/1.134 \) as the peak Rabi frequency and \( 2\sigma = 4\sqrt{\pi}/\Omega_{\text{nh}} \), so the operation time \( T_{\text{nh}} \) of the nonadiabatic holonomic phase gate is the same as \( T_{\text{sa}} \).

To implement the \( U_{\text{cp}} \), we control the microwave field \( \text{MW}_{\text{tq}} \) coupled with the subspace \( \{0,\uparrow\}, \{1,\downarrow\}\) to change just as the three different phase gates discussed above; however, the hyperfine coupling between electron spin and \(^{13}\)C nuclear spin is chosen as \( 2\pi \times 127 \) MHz. In the numerical calculation of the fidelities \( F \) below, the effects of \( \{0,\downarrow\}, \{1,\downarrow\}\) are taken into account. All the above parameters are experimentally achievable on the NV center of the recent experiments [52].

The quality of single-qubit (two-qubit) gates is characterized by the “intrinsic fidelity” (fidelity neglecting decoherence) \( F = |\text{Tr}(U_{\text{tq}})|^2/|\text{Tr}(U_{\text{tq}})|^2/4| \) [56], where \( U \) and \( U_0 \) are the operators for an imperfect and ideal single-qubit (two-qubit) gate, respectively. Figure 2 shows the simulated fidelities of the three different kinds of phase (controlled-PHASE) gates as a function of the relative Rabi frequency deviation \( \eta = \Delta\Omega_{\text{sm}}/\Omega_{\text{sm}} \), where \( \Delta\Omega_{\text{sm}} \) is the deviation from its center value \( \Omega_{\text{sm}} \), and relative frequency detuning \( \epsilon = \delta/\Omega_{\text{sm}} \), where \( \delta \) is the static frequency detuning. Clearly, the SGQG \( U_1 \) \( (U_{\text{cp}}) \) is more robust against systematic errors than the nonadiabatic holonomic \( U_1 \) \( (U_{\text{cp}}) \) as shown in Figs. 2(a) and 2(c) [Figs. 2(d) and 2(f)]. Remarkably, the adiabatic geometric \( U_1 \) \( (U_{\text{cp}}) \) without superadiabatic correction Hamiltonian \( H_1 \) is less robust than the SGQG even when the operation time \( T_{\text{sa}}^{	ext{(t)}} = 10T_{\text{sa}}^{	ext{(ph)}} \), as shown in Figs. 2(a) and 2(b) [Figs. 2(d) and 2(e)] [55]. Rather than at \( \eta = 0 \), the highest fidelity in Fig. 2(e) is at the negative \( \eta \), since the effect from \( \{0,\downarrow\}, \{1,\downarrow\}\) is larger when \( \Omega_{\text{sm}} \) is larger. Therefore, our SGQG has both fast and robust features that are significant in quantum manipulation.

FIG. 2: (color online). The fidelities \( F \) versus the deviations of Rabi frequency \( \eta\Omega_{\text{sm}} \) and frequency detuning \( \epsilon\Omega_{\text{sm}} \) from the ideal gates. (a) Superadiabatic geometric \( U_1 \) with operation time \( T_{\text{sa}} = 0.64 \) \( \mu \) s. (b) Adiabatic geometric \( U_1 \) with \( T_a = 10T_{\text{sa}} \). (c) Nonadiabatic holonomic \( U_1 \) with \( T_{\text{nh}} = T_{\text{sa}} \). (d) Superadiabatic geometric \( U_{\text{cp}} \) with operation time \( T'_{\text{sa}} = 0.64 \) \( \mu \) s. (e) Adiabatic geometric \( U_{\text{cp}} \) with \( T_a = 10T_{\text{sa}} \). (f) Nonadiabatic holonomic \( U_{\text{cp}} \) with \( T'_{\text{nh}} = T_{\text{sa}} \).
In conclusion, we have proposed a general scheme to realize universal SGQGs, with application to the NV center system as an example. The designed universal gates are based on geometric phases, which can be robust against certain stochastic errors, such as fluctuations of the driving fields in realistic situations [12–14]. The evolutions are superadiabatic and can be fast and robust against the systematic errors. The physical implementation of the scheme can be realized in the NV center systems with current technology. Therefore, it is promising to experimentally implement these robust and fast universal SGQGs on NV center qubits at room temperature.

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