Plug-and-Play Approach to Non-adiabatic Geometric Quantum Computation

Bao-Jie Liu,† Xue-Ke Song,† Zheng-Yuan Xue,‡ Xin Wang,‡,† and Man-Hong Yung†,‡,†

†Institute for Quantum Science and Engineering, and Department of Physics,
Southern University of Science and Technology, Shenzhen 518055, China
‡Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, and School of Physics
and Telecommunication Engineering, South China Normal University, Guangzhou 510006, China

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Geometrical phases acquired in cyclic quantum evolutions can be utilized as natural resources for constructing robust logic gates for quantum information processing, which was originally proposed through adiabatic changes of the driving Hamiltonian. Practically, much efforts have been made to shorten the construction times of geometrical gates, known as non-adiabatic holonomic quantum computation (NHQC). However, previous NHQC gates require the driving Hamiltonian to satisfy a set of rather restrictive conditions, reducing the robustness of the resulting geometric gates against control errors. Here we show that non-adiabatic geometric gates can be constructed in an alternative way where the driving Hamiltonian can exhibit a high degree of flexibility for retaining the robustness of the geometric phases. Consequently, this approach makes it possible to incorporate most of the existing optimal control methods, such as dynamical decoupling, composite pulses, and shortcut to adiabaticity, into the construction of geometrical gates, to further address different types of errors. Furthermore, this extensible approach of geometric quantum computation can be applied to various physical platform such as superconducting qubits and nitrogen-vacancy (NV) centers. Specifically, we performed numerical simulation to show how the noise robustness in the recent experimental implementations [Phys. Rev. Lett. 119, 140503 (2017)] and [Nat. Photonics 11, 309 (2017)] of NHQC with NV centers can be significantly improved by our optimized NHQC approach. These results cover a large class of new techniques combing the noise robustness of both geometric phase and optimal control theory.

I. INTRODUCTION

Methods of constructing precise and noise-resistant quantum gates are of fundamental importance to quantum information processing. Geometric quantum computation (GQC) utilizes a peculiar property of quantum theory: the Abelian or non-Abelian geometric phases [1–3] of quantum states, acquired after a cyclic evolution. The geometrical phase depends only on the global properties of the evolution trajectories. Consequently, quantum gates based on the geometric phases are immune to local disturbances during the evolution [4–8]. More precisely, a geometric phase can either be a real number (i.e., Abelian), known as the "Berry phase" [9], or a matrix (non-Abelian holonomy) [10] that is the key ingredient in constructing quantum operations for holonomic quantum computation (HQC).

Early applications of GQC involves adiabatic evolutions to avoid transitions between different sets of eigenstates [11–13]. However, the adiabatic condition necessarily implies lengthy gate operation time; the effectiveness of adiabatic GQC therefore becomes severely limited by the environment-induced decoherence. Later, it was found that geometric quantum gates can be realized non-adiabatically, if we construct a driving Hamiltonian with time-independent eigenstates [14–19], and build geometric gates confined to the Hilbert subspace [11, 12, 17, 18], a method known as NHQC (non-adiabatic holonomic quantum computation). However, this condition imposes stringent requirements on the driving Hamiltonian; the systematic errors would introduce additional fluctuating phase shifts, smearing the geometric phases [20–23]. Furthermore, the restriction imposed in the previous NHQC schemes excludes the flexibility for incorporating most of the optimization techniques, limiting its applicability. These problems motivate us to search for a new approach to GQC that is (i) non-adiabatic, (ii) robust against the control errors (iii) compatible with other optimization techniques for maximizing the gate fidelity against other noises and/or environmental induced decoherence.

Here, we shall demonstrate that non-adiabatic GQC is also possible under much general conditions, relative to traditional NHQC. Specifically, instead of a time-independent basis, we focus on a set of eigenstates of the dynamical invariant [24], where the driving Hamiltonian can be always diagonalized during the gate operations. In this way, we can achieve a new form of GQC with the capability of performing pulse-shape optimization that is compatible with most of the existing optimal control methods, including Derivative Removal by Adiabatic Gate (DRAG) [25], shortcut to adiabaticity (STA) [26, 27], dynamical decoupling [28–30], dynamically corrected gates [31–33] and optimal control using machine learning [34, 35], etc, shown in Fig 1a. Given the extensibility of this approach and the fact that the traditional NHQC method can be regarded as a special case, we refer to this method as NHQC+. For example, when combined with STA, we label it as NHQC+STA.

Specifically, we shall discuss how this new approach of
GQC can be applied to general three-level quantum systems. Previously, STA-based non-Abelian gates require at least four energy levels for an implementation [36–38]. Recently, a restricted form of NHQC+STA has already been demonstrated experimentally, using only three energy levels of a superconducting qubit [39], where the theoretical proposal was contributed by the first and last authors of this work. Here we shall present how our methods can be applied to nitrogen-vacancy (NV) centers. In particular, we are interested in comparing our method with the NHQC gates implemented in recent experiments with NV centers [40, 41]. We numerically found that our optimized NHQC+ method can achieve a significant improvement over the NHQC gates in Refs. [40, 41], subject to the experimental parameters.

II. RESULTS

The NHQC+ approach developed here shares the same advantages of NHQC over adiabatic GQC in speeding up the operation times of quantum gates. In terms of systematic errors, NHQC+ can become potentially more robust; this is due to the fact that NHQC+ removes the limitation of the pulse shape. In addition, NHQC+ is compatible with many optimization techniques, which may further make it robust to other types of noises. For the previous approaches [17, 18] of NHQC, there is a set of rather strict constraints imposed to the driving Hamiltonian, in order to ensure the dynamical phase to vanish all the time during the gate operations. Practically, one can only choose fixed pulses for NHQC. For NHQC+, however, the parameter paths leading to a dynamical invariant are typically not unique, as we can choose from a family of solutions. Consequently, we can design pulse sequences using optimal control theory to increase the robustness against different types of errors. Therefore, by removing the pulse-shape limitation of NHQC and being compatible with many existing optimization techniques, NHQC+ can become potentially more robust against different types of errors.

To illustrate how we deviate from the traditional treatments of GQC, we shall succinctly derive various forms of GQCs in the same framework; the goal is to provide a unified view on GQC, subject to a different set of time-dependent basis, \{\ket{\phi_m (t)}\}, which satisfies the boundary conditions at time \(t = 0\) and \(t = \tau\):

\[
\ket{\phi_m (\tau)} = \ket{\phi_m (0)} = \ket{\psi_m (0)} ,
\]

but in general their time dependence do not follow Schrödinger’s equation. In this way, we can always write,

\[
\ket{\psi_m (t)} = \sum_k v_{km} (t) \ket{\phi_k (t)} ,
\]

which means that the time-evolution operator becomes,

\[
U (t) = \sum_{m,k} v_{km} (t) \ket{\phi_k (t)} \bra{\psi_m (0)} ,
\]

where the matrix elements \(v_{mk} (\tau)\) can be determined by taking the time derivative in Eq. (3), and yields,

\[
\frac{d}{dt} v_{km} (t) = i \sum_i (A_{kl} (t) - H_{kl}) v_{im} (t) ,
\]

where \(H_{kl} (t) \equiv \bra{\phi_k (t)} H (t) \ket{\phi_l (t)}\) and \(A_{kl} (t) \equiv i \bra{\phi_k (t)} \frac{d}{dt} \ket{\phi_l (t)}\), which can be combined to form an effective Hamiltonian:

\[
H_{\text{eff}} (t) \equiv V (t)^\dagger H (t) V (t) - i V (t)^\dagger \frac{d}{dt} V (t) ,
\]

where \(V (t) \equiv \sum_k \ket{\phi_k (t)} \bra{\phi_k (0)}\). In other words, written in the initial basis \{\ket{\phi_k (0)}\}, the matrix elements are given by \(H_{kl} (t) + A_{kl} (t)\). With these tools, various forms of GQC can emerge as different settings (or approximations) of these equations.

In the following, let us focus on NHQC (comparable with e.g. Ref. [17, 18]) using this language; for the adiabatic cases, including Abelian and non-Abelian cases, the details are discussed see in the Appendix A. First, we choose the auxiliary state to be proportional to the dynamical states, i.e.,

\[
\ket{\phi_m (t)} \equiv e^{-i f_m (t)} \ket{\psi_m (t)} ,
\]

where \(f_m (t)\) is a phase angle satisfying \(f_m (0) = 0\). The basis vectors are chosen as

\[
\ket{\psi_m (t)} = \sum_t e^{i f_m (t)} E_t (t) e^{-i f_m (t)} \ket{e_t} ,
\]

where \(E_t (t)\) and \(\ket{e_t}\) are the instantaneous eigenvalue and eigenstate of the Hamiltonian \(H (t)\). Consequently, the effective Hamiltonian in Eq. (5) becomes diagonal, i.e., \(A_{ml} (t) - H_{ml} (t) = \delta_{ml} f_m (t)\), which implies that

\[
U (\tau) = \sum_m e^{i f_m (\tau)} \ket{\psi_m (0)} \bra{\psi_m (0)} .
\]

The point is that \(f_m (\tau)\) represents an overall phase, including both dynamical phase and geometrical phase. In order to obtain a pure geometric gate, an additional constraint is often
imposed for NHQC \cite{17, 18}: for all \( j \) and \( k \), and at all times \( t \),
\begin{equation}
\langle \psi_m (t) | H (t) | \psi_k (t) \rangle = 0 , \tag{10}
\end{equation}
which means that, at least for a certain subspace, the Hamiltonian acts as a null matrix, and represents a rather strong restriction for the choice of the time-evolution Hamiltonian and weaken the noise robustness. Our work aims to relax such a condition.

B. Construction of NHQC+

Let us now focus on the effective Hamiltonian in Eq. (6). Our strategy is to find an auxiliary basis \( \{ | \phi_k (t) \rangle \} \) such that for all \( k \neq m \), the effective Hamiltonian \( H_{\text{eff}} \) is always diagonal in the initial basis, i.e.,
\begin{equation}
\langle \phi_m (0) | H_{\text{eff}} (t) | \phi_k (0) \rangle = 0 , \tag{11}
\end{equation}
Consequently, Eq. (5) implies that \( v_{mk} (t) = \delta_{mk} \) \( v_{kk} (t) \) is diagonal and hence the unitary operator
\begin{equation}
U (t) = \sum_k v_{kk} (t) | \phi_k (t) \rangle \langle \psi_k (0) | \tag{12}
\end{equation}
are all diagonal. Explicitly, we have \( v_{kk} (t) = e^{-i \int_0^t \langle \phi_k (t) | H (t) | \phi_k (t) \rangle dt - \int_0^t \langle \phi_k (t) | \dot{\phi}_k (t) \rangle dt} \). Note particularly that if the following condition,
\begin{equation}
\int_0^t \langle \phi_k (t) | H (t) | \phi_k (t) \rangle dt = 0 . \tag{13}
\end{equation}
is further satisfied for each \( k \), then the resulting unitary evolution becomes purely geometrical, i.e.,
\begin{equation}
U (\tau) = \sum_k e^{-i \int_0^\tau \langle \phi_k (t) | \dot{\phi}_k (t) \rangle dt} | \psi_k (0) \rangle \langle \psi_k (0) | , \tag{14}
\end{equation}
which is the main goal to be achieved below.

In order to satisfy the condition in Eq. (11), let us employ the eigenbasis of the the dynamical invariant \( I (t) \) associated with \( H (t) \) as the auxiliary basis for constructing the geometrical gates, i.e.,
\begin{equation}
I (t) = \sum_k \lambda_k | \phi_k (0) \rangle \langle \phi_k (0) | . \tag{15}
\end{equation}
Note that the the dynamical invariant \( I (t) \) has time-independent eigenvalues \( \{ \lambda_k \} \), (see Appendix B), and obeys the following equation of motion,
\begin{equation}
\frac{dI}{dt} = \frac{\partial I}{\partial t} + \frac{1}{i \hbar} [I, H] = 0 , \tag{16}
\end{equation}
which implies that \( \frac{\partial}{\partial \tau} (V^I V^\dagger) = i [V^I V^\dagger, V^I H V - i V^\dagger \dot{V}] \) (see details in Appendix B). However, the resulting operator, \( V^I V = \sum_k \lambda_k | \phi_k (0) \rangle \langle \phi_k (0) | \), is time-independent. Consequently, we conclude that
\begin{equation}
\left[ \sum_k \lambda_k | \phi_k (0) \rangle \langle \phi_k (0) | , H_{\text{eff}} (t) \right] = 0 \tag{17}
\end{equation}
and hence the condition in Eq. (11). In summary, we have just demonstrated that non-adiabatic geometric quantum gates can be constructed by a class of Hamiltonians \( H (t) \) satisfying
eq. (13), where the eigenvectors of the corresponding dynamical invariant satisfy the boundary conditions in Eq. (2).

Note that the key difference between the previous NHQC schemes and the NHQC+ approach introduced here is that the Hamiltonians are subject to different constraints. In the NHQC case, the Hamiltonian is required to satisfy a set of constraints at each moment of time (see Eq. (10)). For NHQC+, the Hamiltonian needs to vanish only in the integral sense (see Eq. (13)). More importantly, the NHQC+ removes the limitation of \( k \neq m \) in Eq. (10) by using the eigenbasis of the dynamical invariant as the evolution states, which is the reason why our method can be compatible with most of the optimization schemes.

C. Demonstration with three-level systems

To continue, we shall make our discussion explicit by demonstrating its application to three-level systems with a one-photon detuning \( \Delta(t) \). The goal of this section is to show how to determined the dynamical invariant for a class of Hamiltonians that can be realized experimentally.

The energy structure of the Hamiltonian is not important; it can be in any form, including, the \( \Xi, V, \) and \( \Lambda \) structures. We keep the following construction relevant to a variety of physical platforms, including superconducting qubit [42], NV center in diamond [40, 41], and atomic systems [27], respectively. A sketch of the energy-level structure is shown in Fig 1 b. For all cases, a driven three-level system can generally be described by the following Hamiltonian [43], in the interaction picture,

\[
H_0(t) = \Delta(t)|e\rangle\langle e| + \frac{1}{2} \left[ (\Omega_P(t)|0\rangle + \Omega_S(t)|1\rangle \right] \langle e| + H.c.,
\]

where \( \Omega_P(t) \) and \( \Omega_S(t) \) denote, respectively, the pumping and Stokes pulses driving the \(|0\rangle \leftrightarrow |e\rangle \) and \(|1\rangle \leftrightarrow |e\rangle \) transitions.

For our purpose, it is sufficient to assume that the pumping \( \Omega_P(t) \) and Stokes \( \Omega_S(t) \) pulses have the same time dependence, which means that we choose the pulses to have the following form, \( \Omega_P(t) = \Omega(t) \sin(\theta/2)e^{i\phi(t)} \) and \( \Omega_S(t) = \Omega(t) \cos(\theta/2)e^{i[\phi(t)+\alpha]} \), but we maintain the ratio \( \Omega_P(t)/\Omega_S(t) \) of the two pulses to be time-independent, i.e.,

\[
\Omega_P(t)/\Omega_S(t) \equiv \frac{\sin(\theta/2)}{\cos(\theta/2)} e^{-i\phi},
\]

where \( \theta \) and \( \phi \) are parameters to be determined later. Consequently, the Hamiltonian in Eq. (18) can be simplified as follows,

\[
H_0(t) = \Delta(t)|e\rangle\langle e| + \frac{\Omega(t)}{2} \left[ e^{i\phi(t)} |\Phi\rangle \langle e| + H.c. \right],
\]

where the time-independent bright state,

\[
|\Phi\rangle \equiv \sin(\theta/2)|0\rangle + \cos(\theta/2)e^{i\phi}|1\rangle,
\]

is orthogonal to the excited state \(|e\rangle\). Note that dark state \(|\varphi_0\rangle = \cos(\theta/2)|0\rangle - \sin(\theta/2)e^{i\phi}|1\rangle \) is now decoupled from states \(|\Phi\rangle \) and \(|e\rangle\).

For this Hamiltonian, the explicit form of the dynamical invariant \( \mathcal{I}(t) \) is found to be \( \mathcal{I}(t) = \Omega_0/2 \mathcal{I}(t) \) (see Appendix A), where \( \Omega_0/2 \) is a constant with units of frequency and is also related to the driving amplitude. In order to seek the dynamical invariant \( \mathcal{I}(t) \) of the Hamiltonian \( H_0(t) \) in Eq. (18), we need to first apply the following unitary transformation,

\[
U_T = \begin{pmatrix}
\sin \frac{\theta}{2} & 0 & e^{-i\phi} \\
0 & 1 & 0 \\
e^{i\phi} & 0 & -\sin \frac{\theta}{2}
\end{pmatrix}.
\]

After the transformation, we obtain an equivalent Hamiltonian in basis \{\( |\Phi\rangle, |e\rangle, |\varphi_0\rangle \},

\[
\mathcal{H}_0 = U_T H_0 U_T^\dagger + i \dot{U}_T U_T^\dagger,
\]

which results in the following expression,

\[
\mathcal{H}_0 = \Omega(t) \cos \phi_1 T_1 + \Omega(t) \sin \phi_1 T_2 - \Delta(t) T_3.
\]

Substituting Eq. (23) and (25) into Eq. (16), we can obtain the related functions between \( \chi(t) \), \( \alpha(t) \) and \( \Omega(t) \), \( \Delta(t) \) to be shown later. Moreover, we can inverse \( \mathcal{I}(t) \) from the basis \{\( |\Phi\rangle, |e\rangle, |\varphi_0\rangle \} \) to basis \{\( |0\rangle, |e\rangle, |1\rangle \} \) by the unitary transformation \( U_T \), i.e., 

\[
\mathcal{I} = \begin{pmatrix}
-s_c s_{\phi/2} & s_{\chi} s_{\phi/2} e^{i\alpha} & 0 \\
s_{\phi/2} s_{\chi} e^{i\alpha} & c_{\chi} s_{\phi/2} e^{-i(\alpha-\phi)} & 0 \\
c_{\phi} s_{\chi} e^{i\phi} & c_{\chi} s_{\phi} e^{i(\alpha-\phi)} & -c_{\chi} s_{\phi/2}^2
\end{pmatrix},
\]

where with a short-hand notation, \( c_{\chi} \equiv \cos \chi(t), s_{\phi} \equiv \sin(\theta/2) \), and so on, the matrix form of \( \mathcal{I} = \mathcal{I}(t) \). Here the functions, \( \chi(t) \) and \( \alpha(t) \), obey the following differential equations, \( \dot{\chi}(t) = \Omega(t) \sin(\phi_1(t) - \alpha(t)) \) and \( \dot{\alpha}(t) = \Omega(t) \cos(\chi(t) \cos(\phi_1(t) - \alpha(t)) \). One possible set of solution is found to be,

\[
\chi(t) = \pi \left| \frac{\text{erf}(T/2) + 1}{\text{erf}(T/2) + 1} \right|
\]

\[
\alpha(t) = \phi_1(t) - \arctan[\chi(t)/(\Omega_0 \sin \chi(t))],
\]

where the parameter \( T \) controls the effective duration of the protocol. As we are considering the driving pulses have a finite duration, we have chosen \( T = 4T \) as a cutoff. In this way, the time dependence of \( \Omega(t) \) and \( \Delta(t) \) can be determined numerically. On the other hand, the eigenvectors of Eq. (26) can be solved by the following solutions,

\[
|\varphi_+ (t) \rangle = \sin[\chi(t)/2]|\Phi \rangle + \cos[\chi(t)/2] e^{i\alpha(t)} |e \rangle,
\]

\[
|\varphi_- (t) \rangle = \cos[\chi(t)/2]|\Phi \rangle - \sin[\chi(t)/2] e^{i\alpha(t)} |e \rangle,
\]

\[
|\varphi_0 \rangle = \cos(\theta/2)|0\rangle - \sin(\theta/2)e^{i\phi}|1\rangle.
\]
Note that the eigenstate $|\varphi_0\rangle$ is time-independent. This set of orthogonal basis vectors play the role of the auxiliary states discussed in Eq. (3) for NHQC+.

### D. NHQC+ gates in three-level systems

We are now ready to demonstrate how to build up universal non-Abelian geometric single-qubit gates, i.e., holonomic quantum gates. Let us start with the following set of basis states, $\{|\varphi_0\rangle, |\varphi_+\rangle(0)\}$, which is two of the eigenstates of the dynamical invariant $I(t)$ at time $t = 0$ (see Eq. (28)).

The corresponding evolution operator takes the form, $U_2 = |\varphi_0\rangle\langle\varphi_0| + e^{i\gamma/2}|\varphi_+(\tau/2)\rangle\langle\varphi_+(\tau/2)|$, where we defined another phase factor $f_2 \equiv -f(\tau)$.

Finally, applying the boundary condition Eq. (2), we obtain the following unitary transformation matrix in the basis states $\{|\varphi_0\rangle, |\varphi_+(0)\rangle\}$ at the final time $t = \tau$,

$$U(\tau) = U_2U_1 = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\gamma} \end{pmatrix}.$$ 

where the phase factor, $\gamma = f_1 + f_2$, is purely a geometric phase, as the condition in Eq. (11) has been satisfied for eliminating the dynamical phase, i.e., $\int_0^\tau (|\varphi_+(t)|H_1(t)|\varphi_+(t)\rangle dt + \int_0^\tau (|\varphi_+(t)|H_2(t)|\varphi_+(t)\rangle dt = 0$. Explicitly, the geometric phase $\gamma$ can be determined by the Eq. (5), i.e.,

$$\gamma = i\int_0^\tau \langle \varphi_+(t)|\frac{\partial}{\partial t}|\varphi_+(t)\rangle dt = -\int_0^\alpha(\tau) \cos^2 \frac{\chi(t)}{2} d\alpha(t).$$ 

In fact, one can show that the geometric phase $\gamma$ is exactly equal to half of the solid angle $\Omega_{\text{angle}}$ shown in Fig 1 b, i.e., $\gamma = \Omega_{\text{angle}}/2$. Considering two stages, a closed path in the parameter space is formed. The solid angle enclosed by the closed path is evidently $2(\gamma_2 - \gamma_1)$ and thus, the geometric phase acquired is simply $\gamma = \gamma_2 - \gamma_1$, as sketched in Fig 1 b. Consequently, the holonomy matrix can be obtained in the computational space spanned by $\{|0\rangle, |1\rangle\}$, $U(\tau)$ is the non-Abelian geometric single-qubit gate as

$$U(\gamma, \theta, \phi) = e^{i\frac{\gamma}{2}} e^{-i\gamma_2 \pi \sigma},$$ 

where $\sigma = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$, $\sigma$ are the Pauli matrices. We can see that Eq. (35) describes a rotation operation around the $n$ axis by a $\gamma/2$ angle, up to a global phase factor $e^{-i\frac{\gamma}{2}}$. As $n$ and $\gamma/2$ are arbitrary values, Eq. (35) denotes a set of universal single-qubit gates in the qubit subspace.

### E. Reduction to NHQC

For completeness, we also demonstrate how our framework can be reduced to previous approaches to NHQC [17, 18]. For this purpose, we simply set $\alpha = \phi_1 - \frac{\pi}{2}$ and $\Delta = 0$, we obtain $\chi(t) = \int_0^\tau \Omega(t') dt'$ in Eq. (27). Similar to the above cyclic evolution, we choose $|\varphi_-(t)\rangle$ and $|\varphi_0\rangle$ as the two computational states, and set the pulse area to fulfill the cyclic
condition on the Bloch sphere that
\[ \chi(\tau) = \int_0^\tau \Omega(t)dt = 2\pi. \] (36)

In this setting, the state \( |\varphi_-(\tau)\rangle \) will acquire a pure \( \pi \) geometric phase. Therefore, in the computational space spanned by \( \{|0\rangle, |1\rangle\} \), the non-Abelian geometric single-qubit gate \( U(\pi, \theta, \phi) \) will be obtained. However, the above realization needs at least two NHQC gates to realize an arbitrary single-qubit gate. Such a limitation can be overcome with the method introduced in Ref. [45].

F. Example 1: NHQC+SSSP

Here, we demonstrate how our method can be compatible with other pulse optimization techniques. First, we consider a way to generate robust pulses against the systematic error. Suppose the system is initialized in the state starts \( |\psi(0)\rangle \), and the time evolution is driven by the perturbed Hamiltonian \( H_0(t) + H_\beta(t) \), where
\[ H_\beta(t) = \beta \Omega(t) |\Phi\rangle \langle e| + H.c., \] (37)
is the perturbing Hamiltonian, with a small unknown parameter \( \beta \).

Taking perturbation theory up to the second order \( O(\beta^2) \), we have \( \Phi_+ (\tau) = \Phi_0 (\tau) + \Phi_1 (\tau) + \Phi_2 (\tau) + \ldots \) where \( \Phi_0 (t) \) is the unperturbed term, \( \Phi_1 (\tau) = -i \int_0^\tau dt U_0 (t, \tau) H_\beta(t) \Phi_0 (t), \) and \( \Phi_2 (\tau) = -\int_0^\tau dt \int_0^\tau dt' U_0 (t, \tau) H_\beta(t) U_0 (t, t') H_\beta(t') \Phi_0 (t') \).

Note that \( U(v, t) = \langle \Phi_0 (v) | \Phi_0 (t) + \Phi_0 (v) | \Phi_1 (t) \rangle \) is the unperturbed time evolution operator, and \( \Phi_0 (t) \) is also a solution of the Schrödinger equation. Assuming that the error-free (\( \beta = 0 \)) scheme works perfectly, i.e., \( \Phi_0 (\tau) = e^{i\Omega(\tau)} |\varphi_+ (\tau)\rangle \), we have the probability \( P = |\langle \Phi_+ (\tau) | \Phi_+ (\tau) \rangle|^2 \), i.e.,
\[ P = 1 - \beta^2 \int_0^\tau |\Phi_0 (t) | H_\beta(t) |\Phi_0 (t)| dt \] (38).

Let us define the sensitivity of the systematic error to be [46, 47]
\[ q_s = -\frac{1}{2} \frac{\partial^2 P(\beta)}{\partial \beta^2} \big|_{\beta=0} = -\frac{\partial P(\beta)}{\partial \beta} \bigg|_{\beta=0}, \] (39)
which means that \( q_s = \int_0^\tau \chi(t) | H_1(t) | \Phi_0 (t) | dt \). Explicitly, we have
\[ q_s = \left| \int_0^\tau \chi(t) | H_1(t) | \Phi_0 (t) | dt \right|^2. \] (40)

To minimize \( q_s \), we can choose the \( f(t) \) as a function of \( \chi(t) \) with a simple Fourier series type of Ansatz [48], i.e.,
\[ f(t) = 2 \chi(t) + \sum_{n=1}^3 A_n \sin[2n \chi(t)], \] (41)
with \( \chi = \pi [\text{erf}(t/T) + 1] = A_n \) being an arbitrary real number. Furthermore, we can use high-order perturbation theory up to \( O(\beta^3) \), \( O(\beta^5) \), and \( O(\beta^7) \), etc., by adjusting the coefficients of \( A_n \) to make \( q_s \) = 0, and thus be able to realize ultrahigh fidelity with respect to the systematic parameter \( \beta \).

The next step, we need to find invariant to inverse engineer the Hamiltonian (see details in Appendix C) for numerical simulation. From Fig. 2a, we can clearly find the Single-Shot Shaped Pulse (SSSP) to take a broad region of deviations with ultrahigh fidelity. At the same time, we compare both the variation of maximum Rabi frequency \( \Omega_{\text{max}} \) and the static detuning \( \delta \) with the recent experiment with the single shot [40, 41]. The corresponding resonant NHQC pulses, SSSP 3rd order pulse of moderate area, demonstrate a remarkably high robustness of the fidelity except NHQC pulse, shown in Fig. 2b and c for large deviations of the original Rabi frequency \( \beta \) (up to 10\%) and a range of the static detuning \( \delta \) of the same order as the peak value of the Rabi frequencies.

G. Example 2: NHQC+KDD

On the other hand, we can further combine our method with dynamical decoupling (DD) [28], e.g., XY4 (PDD), Knill DD (KDD) [29], and universally robust (UR) DD [30], to simultaneously compensate pulse imperfections and dephasing to an arbitrary order. As an example, we shall combine KDD pulse and non-Abelian geometric phase. DD sequences consist of repetitive trains of \( \pi \) pulses. The delay between the pulse and their phases are important parameters for the performance of the DD sequences. In particular, the relative phases, which correspond to the directions of the rotation axes, are important for making the sequences robust against pulse imperfection and unwanted environmental interactions. The KDD pulses use this design principle and is given as [29]
\[ \Omega(t) = \left\{ \begin{array}{ll}
\frac{\pi^2}{2W} \cos \left[ \frac{\pi(t-T/2)}{W} \right] e^{i\beta_k} & \text{for } t_1 \leq t \leq t_2 \\
0 & \text{otherwise}
\end{array} \right., \] (43)
where \( t_1 = (1-W)T/2, t_2 = (1+W)T/2, W \ll 1 \) for DD pulse. For the robust pulses against control errors, we take a 20 self-correcting pulse by combining 5-pulse blocks to form \( [\text{KDD}_n - KDD_{n+\pi/2} - KDD_n - KDD_{n+\pi/2}] \) [29]. According to Eq. (27), we can choose parameters \( \alpha = \phi_1 - \pi/2, \phi_1 = \delta_k \) to realize non-Abelian geometric quantum gates with KDD pulse. For numerical simulation, we plot the NOT gate to against control errors for holonomic gate with \( W = 0.05 \) in Fig. 2a, and we can clearly see this gate is robust to the error.
A. Application of NHQC+ in NV centers

Let us now analyze the noise robustness of the quantum gate performance of NHQC+ in a realistic physical system, namely, NV center, which is a defect in diamond consisting of a substitutional nitrogen atom and an adjacent vacancy, trapping an electron with spin \( S = 1 \) ground state. The energy level configuration of a solid-state NV center electron spin is schematically shown in Fig. 1(c). The spin states can be labelled as \(|E_{\nu}⟩ \otimes |m_s⟩\), with \(|E_{\nu}⟩\) and \(|m_s⟩\) being the orbital state, spin state and \( \nu \) being the angular momentum projection quantum number along the NV center axis and the spin state with eigenvalue \( m_s \hbar \). For our purpose, we choose \(|0⟩ \equiv |E_0⟩ \otimes |1⟩\), \(|1⟩ \equiv |E_0⟩ \otimes |−1⟩\) and \(|2⟩ \equiv |E_0⟩ \otimes |0⟩\).

In this way, the NV center can be modeled as a three-level \( \Lambda \) system [51] with the center level structure consisting of long-lived states \(|i⟩\) (\( i = 0, 1 \)) coupled to another long lived state \(|2⟩\) by microwave driving fields \( \Omega_j(t) \), with a phase difference \( \pi \).

Here, we choose the parameters of the light-NV-center interaction in a two-photon resonant way as \( \Delta_i = \omega_{2i} - \omega_i = \Delta \), with \( \Delta \) being the one-photon detuning, \( \omega_{2i} \) is the transitions of \(|2⟩ \rightarrow |i⟩\) and \( \omega_i \) is the frequency of driving lasers. In this case, the Hamiltonian of a driving NV center in the basis of \( \{0, 1, 2\} \) can be written as

\[
H_1(t) = \sum_{m=0}^{m=1} \Omega_{m}(t)|m⟩⟨2| + H.c.] + \Delta(t)|2⟩⟨2|, \tag{44}
\]

which becomes essentially the same as Eq. (18). Consequently, we can realize arbitrary geometric single-qubit gate in the framework of NHQC+.

Additionally, we can further construct a nontrivial two-qubit controlled-phase (CP) gate, when the coupling between two NV centers is available. For example, let us consider the scenario of two NV centers coupled to a fused-silica microsphere optical cavity [52, 53] with a large detuning. The coupling configuration of a NV center for nontrivial two-qubit gates is shown in Fig. 1(d), where the NV centers can be attached around the equator of the cavity, and the light-matter interaction \( G_j \) is induced via the evanescent field of the cavity mode [52]. The coupling between the two NV centers is mediated by a cavity in the Raman resonant regime, with driving laser field, with Rabi frequency \( \Omega_j \) \( (j = 1, 2) \). By choosing the proper parameter, the cavity and driving field with frequency \( \omega_c \) and \( \omega_{d,j} \) couple to the transition \(|0⟩ \rightarrow |A_2⟩\) and \(|j⟩ \rightarrow |A_2⟩\) with \( \omega_{A_2j,j} \) of \( j \)th NV center with coupling strength \( G_j \) and \( \Omega_j \), respectively. The detuning \( \delta_j = \omega_{A_2j,j} - \omega_c \) are the same with each other for every NV center. Therefore, when the coupling between the two NV centers is mediated by a cavity in the Raman resonant regime, the effective Hamiltonian of the two-qubit gate becomes,

\[
H_2(t) = \sum_{j=1}^{2} g_j \left( a \sigma_j^+ + H.c. \right), \tag{45}
\]

where \( \sigma_j^\dagger(a) \) is the creation (annihilation) operator of the cavity, \( \sigma_j^\dagger(j) |0⟩= |j⟩ |0⟩ \) is an electronic flip operator, and the effective cavity assisted coupling strength \( g_j = G_j(1, 2) / \delta_j \) can be conveniently tuned via the amplitude of the corresponding external driven laser field \( \Omega_j \).

In this way, the Hamiltonian in Eq. (45) is equivalent to a resonant three-level system, working in the single excitation subspace \( \{000, 010, 002\} \) of the coupled Hamiltonian,

\[
H_3(t) = g_1(t)|000⟩⟨001| + g_2(t)|002⟩⟨010| + H.c., \tag{46}
\]

where \(|nnq⟩ \equiv |m_n⟩ |n⟩ |q⟩ \) with the subscript 1, 2, and 3 indicate the states belong to NV centers 1 and 2, and the cavity, respectively. Note that there exists a dark eigenstate of dynamical invariant with zero eigenvalue [50], it can be written as: \( |\varphi_0(t)⟩ = \cos \mu(t)|0⟩ + i \sin \mu(t)|0⟩ \), with the effective coupling strengths given by \( \Omega_1(t) = \eta(t) \cot \mu(t)|0⟩\rangle(t) - \mu(t)|0⟩\rangle(t) \), and \( \Omega_2(t) = \eta(t) \cot \mu(t)|0⟩\rangle(t) + \mu(t)|0⟩\rangle(t) \).

Subject to the boundary conditions: \( \eta(0) = \eta(\tau) = 0 \) and \( \mu(0) = \mu(\tau) = 0(2\pi) \) for the cyclic evolution, there are many possible solutions to \( \mu(t) \) and \( \eta(t) \) for optimizing the time evolution. In particular, when the initial state is set as \(|100⟩\), after a cyclic evolution, the state \(|100⟩\) acquires a geometric phase \( \gamma \), while the other states remain unchanged. In the computing space spanned by \( \{000, 010, 100, 110\} \), a holonomic CP gate can be expressed as

\[
U_{CP}(\gamma) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & e^{i\gamma} & 0 \\
0 & 0 & 0 & 1 \\
\end{pmatrix}. \tag{47}
\]

In general, the nontrivial two-qubit holonomic logical gate can be realized by controlling the \( \gamma \), that is, adjusting the phase of one of the two steps similar to the realization of single qubit. In other words, we can achieve a universal set of holonomic gates for the NV-center system in the framework of NHQC+.

B. Robustness of NHQC+

When considering the realistic case, i.e., taking the decoherence effect into consideration, the performance of a single-qubit gate in Eq. (35), induced from the Hamiltonian in Eq. (18), can be evaluated by using a master equation in the Lindblad form [54], which in many cases represents a good approximation and the use of it has been justified by the experiments [55, 56], i.e.,

\[
\dot{\rho}_1 = i[\rho_1, H_1] + \sum_{j=0}^{1} \left[ \frac{\Gamma_j^j}{2} L(\sigma_j^-, e) + \frac{\Gamma_j^j}{2} L(\sigma_j^-, e) \right], \tag{48}
\]

where \( \rho_1 \) is the density matrix of the considered system and \( L(A) = 2A\rho_1 A^\dagger - A^\dagger A\rho_1 - \rho_1 A^\dagger A \) is the Lindbladian of the operator \( A \), \( \sigma_{0,e}^\dagger = |0⟩⟨e|, \sigma_{1,e}^\dagger = |e⟩⟨1| \) and \( \sigma_j^\dagger = (-1)^j (|e⟩⟨1| - |j⟩⟨j|) \). In addition, \( \kappa, \Gamma_j^1 \) and \( \Gamma_j^2 \) are the decay rate of the cavity, the decay and dephasing rates of the \( \{j, e\} \)
two-level systems, respectively. In our simulation, we have used the following set of experimental parameters. The Rabi frequency and gate time is set as \( \Omega = 2\pi \times 20 \text{ MHz}, \tau = 40 \text{ ns}, \) and \( \Gamma'_1 = \Gamma'_2 \approx 2\pi \times 10 \text{ KHz} \) [57].

Suppose that the qubit is initially prepared in the \( |0\rangle \) state, the time-dependence of the state populations and the state fidelities of realizing the Hadamard and NOT gates with NHQC+ are depicted in Fig. 3a and 3b, where the state fidelities are obtained to be 99.74% and 99.35%, respectively. Furthermore, we have also investigated the gate fidelity of the Hadamard and NOT gates for initial states of the form \( |\psi\rangle = \cos \Theta |0\rangle + \sin \Theta |1\rangle \), where a total of 1001 different values of \( \Theta \) were uniformly chosen in the range of \([0, \pi/2]\) as shown in Fig. 3c. The gate fidelities of the Hadamard and NOT gates can reach, respectively, 99.58% and 99.57%, subject to the experimental parameters.

Meanwhile, in practice, any gate implementation will inevitably encounter different source of errors, such as random error, systemic error, and dephasing error, etc. As it is well-known, geometric quantum gates have been proved to be insensitive to fast varying random fluctuations [4–6]. Here we focus on the systematic errors in the control parameters, which effectively include all quasi-static noises.

Compared with the traditional NHQC methods, where the cyclic condition requires the integration of Rabi frequency over time should be exactly \( 2\pi \), which makes the operation not robust against certain systematic error, e.g., the fluctuation of the Rabi frequencies. In the presence of pulse errors, the systemic variation of maximum Rabi frequency \( \Omega_{\text{max}} \) is set to be \( \Omega'_{\text{max}} = (1 + \beta)\Omega_{\text{max}} \) with the variation parameter being set to be \( \beta \in [-0.1, 0.1] \). We simulate the performance of our non-abelian quantum gate and the NHQC scheme with the same error pulse and time. For the NOT gate as a test case, as shown in Fig. 3d, the gate of our proposal is also more robust than the NHQC scheme.

\section*{IV. CONCLUSION}

In summary, we have proposed a new framework of non-adiabatic geometric quantum computation that is compatible with optimal control. This is made possible by relaxing the constraint imposed for the driving Hamiltonian in the previous approach of NHQC. We present an explicit way to construct non-adiabatic non-abelian geometric gates using three level systems. We have also focused on the performance of pulse optimization in systems of nitrogen-vacancy center.

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Appendix A: Abelian and non-Abelian adiabatic GQC

Let us first consider the diagonal form of the time-dependent Hamiltonian $H(t)$, by the time-dependent basis \{\ket{e_k(t)}\}, i.e.,

$$H(t) = \sum_k E_k(t) \ket{e_k(t)} \bra{e_k(t)} , \quad (A1)$$

where \{\ket{E_k(t)}\} are the instantaneous eigenvalues of $H(t)$ at time $t$. In this case, we consider the auxiliary basis states \{\ket{\phi_m(t)}\} to be identical to the eigenstates \{\ket{e_m(t)}\} of $H(t)$. For simplicity, suppose the eigenvalues are non-degenerate, then we have,

$$\bra{\phi_k(t)} H(t) \ket{\phi_l(t)} = \delta_{kl} E_k(t) . \quad (A2)$$

Furthermore, the adiabatic theorem [58] suggests that there is no transition occurs when the variation of $H(t)$ is sufficiently slow, which implies that, $A_k(t) = 0$ whenever $k \neq l$. Consequently, after a cycle where $H(t) = H(0)$, the unitary transformation in Eq. (4) becomes an Abelian transformation [11], i.e.,

$$U(\tau) = \sum_k e^{i\varphi_k} \ket{\phi_k(0)} \bra{\phi_k(0)} , \quad (A3)$$

where $\varphi_k \equiv i \int_0^\tau \langle \kkt{e_k(t)}{\dot{\kkt{e_k(t)}}} \rangle dt = \int_0^\tau E_k(t) dt$ is the sum of the geometric and dynamical phases.

Derivation of the results for non-Abelian GQC [12] is straightforward in this approach under the adiabatic approximation, where transition away from a degenerate subspace is not allowed. In this subspace, the Hamiltonian is diagonal in a certain basis, i.e.,

$$H_{sub}(t) \equiv E(t) \sum_k \ket{e_k(t)} \bra{e_k(t)} . \quad (A4)$$

In this case, $H_{kl}(t) = \delta_{kl} E(t)$, and the vector potential no longer acting trivially in this subspace,

$$U(\tau) = e^{-i \int_0^\tau E(t) dt} T e^{i \int_0^\tau A(t) dt} , \quad (A5)$$

where $A(t) \equiv \sum_{kl} A_{kl}(t) \ket{e_k(0)} \bra{e_l(0)}$. This forms the basis for constructing adiabatic geometric gates.

Appendix B: Dynamical invariant

For a general time-dependent Hamiltonian $H(t)$, a common property is described by the existence of time-dependent Hermitian Lewis-Riesenfeld invariants [24], $I(t) = I(t)$, that satisfies the following dynamical equation:

$$\frac{dI}{dt} = \frac{\partial I}{\partial t} + \frac{1}{i\hbar} [I, H] = 0 . \quad (B1)$$

A normal quantum state satisfies Schrödinger’s equation, $i\hbar \frac{\partial}{\partial t} \ket{\psi(t)} = H(t) \ket{\psi(t)}$, which implies that the product $I(t) \ket{\psi(t)}$ also follows a similar equation of motion:

$$i\hbar \frac{\partial}{\partial t} (I(t) \ket{\psi(t)}) = H(t) (I(t) \ket{\psi(t)}) . \quad (B2)$$

Furthermore, the eigenvectors \{\ket{\varphi_n(t)}\} of $I(t)$,

$$I(t) \ket{\varphi_n(t)} = \lambda_n \ket{\varphi_n(t)} , \quad (B3)$$

are assumed to form a complete set, $\bra{\varphi_m(t)} \varphi_k(t) \rangle = \delta_{mk}$, and the eigenvalues $\lambda_n$ are time-independent real numbers, which can be justified as follows.

First, we note that the equation of motion of the dynamical invariant $I(t)$ implies that,

$$i\hbar \bra{\varphi_m(t)} \frac{\partial I}{\partial t} \ket{\varphi_n(t)} + (\lambda_m - \lambda_n) \bra{\varphi_m(t)} H \ket{\varphi_n(t)} = 0 , \quad (B4)$$

which means that the diagonal entries of $\frac{\partial I}{\partial t}$ are all zero, i.e.,

$$\bra{\varphi_n(t)} \frac{\partial I}{\partial t} \ket{\varphi_n(t)} = 0 . \quad (B5)$$

Next, suppose the eigenvalues $\lambda$ are time dependent. Then, the eigenvalue equation of the dynamical invariant $I(t)$ implies that

$$\frac{\partial I}{\partial t} \ket{\varphi_n(t)} + \lambda_n \ket{\varphi_n(t)} = \lambda_n \ket{\varphi_n(t)} , \quad (B6)$$

which further implies that the diagonal elements is just the same the derivative of $\lambda_n$, i.e., $\bra{\varphi_n(t)} \frac{\partial I}{\partial t} \ket{\varphi_n(t)} = \frac{\partial \lambda_n}{\partial t}$, and leads to the conclusion that

$$\frac{\partial \lambda_n}{\partial t} = 0 . \quad (B7)$$

Here, we will show that the eigenvectors \{\ket{\varphi_n(t)}\} are what we’re looking for to realize GQC. This comes from the following result.

Result: Here, we move the Hamiltonian $H(t)$ from the bare basis to the basis of dynamical invariant eigenvectors. The related unitary is $U_R(t) = \sum_n \ket{\varphi_n(t)} \bra{\varphi_n(t)}$, where $U_R(t)$ maps the dynamical invariant eigenvectors $\ket{\varphi_n(t)}$ onto the time-independent state $\ket{\varphi_n}$ all the time. In this new frame, the Hamiltonian, $H_R(t) = U_R H(t) U_R^\dagger + iU_R \dot{U}_R^\dagger$, has no off-diagonal matrix elements connecting the various eigenvectors.

Proof. According to the dynamical invariant equation Eq. (B1), we take an identical transformation as

$$U_R \frac{\partial I}{\partial t} U_R^\dagger = i[U_R I U_R^\dagger, U_R H U_R^\dagger] , \quad (B8)$$

It is easily found that

$$U_R \frac{\partial I}{\partial t} U_R^\dagger = \frac{\partial(U_R I U_R^\dagger)}{\partial t} - \frac{\partial U_R}{\partial t} I U_R^\dagger - U_R I \frac{\partial U_R^\dagger}{\partial t} , \quad (B9)$$

and

$$\frac{\partial(U_R U_R^\dagger)}{\partial t} = \frac{\partial U_R}{\partial t} U_R^\dagger + U_R \frac{\partial U_R^\dagger}{\partial t} = 0 . \quad (B10)$$
Combining Eq. (B10) and (B9) with Eq. (B8), we get,

\[
\frac{\partial (U_R \rho U_R^\dagger)}{\partial t} = i[U_R \rho U_R^\dagger, U_R H U_R^\dagger + iU_R U_R^\dagger]. \tag{B11}
\]

Taking \( I(t) = \lambda_n|\varphi_n(t)\rangle \langle \varphi_n(t) | \) into above equation, the Eq. (B11) reduces to

\[
\sum_n \lambda_n |\varphi_n\rangle \langle \varphi_n | H_R] = 0. \tag{B12}
\]

From the Eq. (B12), we can conclude that \( H_R \) is diagonal in the basis of eigenvectors of dynamical invariant \( I(t) \). Based on the result, in order to seek the eigenvectors \( \{|\varphi_n(t)\rangle\} \) to realize GQC, we only need to find dynamical invariant.

**Appendix C: Robust pulses with quantum optimal control**

Here, in order to construct the solution of time-dependent Schrödinger equation, we can combine the eigenstates of dynamical invariant \([46]\) with dynamical phase and geometric phase, i.e., \( |\Phi^0_+(t)\rangle = e^{i\int_0^t f(t')|\varphi_+(t')\rangle dt'} \), with \( f(t) = \int_0^t \langle \varphi_+(t')|i\partial_\tau - H_0(t)|\varphi_+(t')\rangle dt \). Combining \( |\Phi^0_+(t)\rangle \) and the time-dependent Schrödinger equation, we find

\[
f(t) = \int_0^t \frac{\Omega(t') \cos[\phi_1(t') - \alpha(t')]}{\sin \chi(t')} dt'. \tag{C1}
\]

Now, we need to inverse engineer the Hamiltonian with the invariant-based evolution states. For achieving a cyclic evolution for GQC, we have the cyclic evolution condition \( \chi(0) = \pi \) and \( \chi(\tau) = 3\pi \). Then we get the Hamiltonian with help of the Eq. (B1) and Eq. (C1), i.e.,

\[
\Omega(t) = \sqrt{\chi^2(t) + f^2(t) \sin^2 \chi(t)},
\Delta(t) = -f(t) \cos \chi(t) - \dot{\alpha}(t),
\phi_1(t) = \alpha(t) + \arctan \left( \frac{\chi(t)}{f(t) \sin \chi(t)} \right). \tag{C2}
\]

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