State-independent Nonadiabatic Geometric Quantum Gates

Yan Liang,† Pu Shen,‡ Li-Na Ji,† and Zheng-Yuan Xue†,‡,∗

†Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, and School of Physics and Telecommunication Engineering, South China Normal University, Guangzhou 510006, China
‡Guangdong-Hong Kong Joint Laboratory of Quantum Matter, and Frontier Research Institute for Physics, South China Normal University, Guangzhou 510006, China

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Quantum computation has demonstrated advantages over classical computation for special hard problems, where a set of universal quantum gates is essential. Geometric phases, which have built-in resilience to local noise, have been used to construct quantum gates with excellent performance. However, this advantage has been smeared in previous schemes. Here, we propose a state-independent nonadiabatic geometric quantum-gate scheme that is able to realize a more fully geometric gate than previous approaches, allowing for the cancelation of dynamical phases accumulated by an arbitrary state. Numerical simulations demonstrate that our scheme has significantly stronger gate robustness than the previous geometric and dynamical ones. Meanwhile, we give a detailed physical implementation of our scheme with the Rydberg atom system based on the Rydberg blockade effect, specifically for multiqubit control-phase gates, which exceeds the fault-tolerance threshold of multiqubit quantum gates within the considered error range. Therefore, our scheme provides a promising way for fault-tolerant quantum computation in atomic systems.

I. INTRODUCTION

As a recently emerged computation pattern based on quantum mechanics [1], quantum computation has powerful parallel computing capabilities that enable it to exceed classical computation in principle and provide potential solutions to hard computation problems, such as quantum chemistry [2], quantum many-body physics [3], and quantum machine learning [4]. Moreover, the computational power of a quantum computer increases exponentially with the increase of the qubit number. It is well known that operating qubits to obtain a universal set of quantum gates is the building block for large-scale quantum computation in a fault-tolerant way. However, due to the inevitable noise and the decoherence effect, the physical implementation of quantum computation remains a great challenge. Therefore, realizing quantum gates with high fidelity and strong robustness is essential, especially for two-qubit gates.

Benefiting from global properties, geometric phases can naturally combat certain local noise, and geometric quantum computation (GQC) utilizing either Abelian or non-Abelian holonomy is considered to be an effective way to improve the robustness of quantum gates [5–10]. A GQC based on the Abelian phase is relatively straightforward experimentally, as it only needs the operation of nondegenerate two-level quantum systems to realize quantum gates. However, early GQC schemes were based on adiabatic evolution [11–14], which required longer operating times and imposed additional constraints that introduced more noise and decoherence. To relax the constraints of adiabatic evolution, nonadiabatic GQC (NGQC) was proposed naturally [15–16]. Owing to the combination of fast manipulation and strong robustness, NGQC has been developed rapidly [17–26], and has been experimentally demonstrated in various quantum systems [27–30].

Achieving NGQC requires the elimination of the accompanying dynamical phases. This can be done by setting the dynamical phase to zero at all times, by driving two auxiliary basis vectors to cyclically evolve along the geodesic paths on the Bloch sphere, such as the orange-slice-shaped geometric path [8]. Another approach is to allow the existence of the dynamical phase during the evolution process, but then to set the accumulated dynamical phase at the final time to zero [18, 22, 24]. However, in all these schemes, an arbitrary superposition state of two auxiliary basis vectors still holds a nonzero dynamical phase [16,18]. Additionally, the gate robustness of these schemes is only second order, which is the same as that of the dynamical scheme, in the presence of systematic errors. In particular, when the rotation angle is π, the geometric rotating gate has the same robustness against systematic errors as the dynamical scheme [8,21,30]. Therefore, it is worth exploring whether there exists a more rigorous geometric quantum gate scheme that eliminates the dynamical phase accumulated by an arbitrary initial state, which could lead to significantly stronger gate robustness compared with previous NGQC and dynamical schemes.

Here, we propose a state-independent NGQC (SINGQC) scheme that not only eliminates dynamical phases accumulated by two auxiliary basis vectors, but also eliminates dynamical phases accumulated by any state. Numerical results show that the gate robustness of our scheme is significantly stronger than both conventional dynamical gate (DG) and previous NGQC schemes. In addition, we present a physical implementation of our scheme in the Rydberg atom system, based on the Rydberg blockade effect. From numerical results, our control phase (CZ) gates are exceptionally robust to systematic errors and possess strong immunity to the Rydberg state lifetime, making them more robust than the DG scheme. Without optimization, the fidelities of our SINGQC multi-qubit gates still exceed 99% within the considered error range, representing a major advancement for atomic multi-qubit gates. Overall, our scheme provides an alternative for realizing fault-tolerant quantum computing in atomic systems.

† These two authors contributed equally to this work.
‡ zyxue83@163.com
II. STATE-INDEPENDENT GEOMETRIC GATES

In this section, we first derive the SINGQC condition realizing the state-independent geometric quantum gates. Then, we design special evolution paths satisfying the SINGQC condition to construct single-qubit gates. Finally, the robustness of our scheme is discussed and compared with the previous single-loop NGQC (SLNGQC) scheme [8, 19, 20] and the DG scheme driven by simple resonant pulses (see Appendix A and B for details).

A. The SINGQC condition

We first proceed to the condition for realizing the state-dependent geometric quantum gates (SINGQG), using the reverse engineering of the target Hamiltonian [31, 32]. For a two-level system, a set of orthogonal auxiliary vectors can be generated by rotating the state-independent geometric quantum gates. Then, the state-independent geometric quantum gates are constructed.

|ψ(t)⟩ = H(t)|ψ(t)⟩,
|ψ(0)⟩ = |ψ(0)⟩, the accumulated phase. We assume that the quantum system is controlled by the following Hamiltonian [23]

H(t) = Δ(t)σ_z + [Ω(t)|0⟩⟨1| + H.c.],

where Δ(t) = \frac{1}{2} sin^2(\theta(t)) \hat{ϕ}(t) + Δ(t) and \hat{Ω}(t) = -\frac{1}{2} e^{-iϕ(t)}[\theta(t) - i sin \theta(t) cos \phi(t) \hat{ϕ}(t)]. It is easy to verify that the evolution states |ψ(t)⟩ only accumulate geometric phase, i.e., γ_k(t) = i \int_0^t (μ_k(t))^{−1} dτ. When the auxiliary vectors move cyclic evolution at the final time τ, i.e., |μ_k(τ)⟩ = |μ_k(0)⟩ = |ψ_k(0)⟩, the corresponding evolution operator is

U(τ) = \sum_{k=1}^2 |ψ_k(τ)⟩⟨ψ_k(0)| = \sum_{k=1}^2 e^{iγ_k(τ)}|μ_k(0)⟩⟨μ_k(0)|.

where γ_k(τ) = −γ_0(τ) = −\frac{1}{2} \int_0^τ [1 - cos(θ(t))] dτ. By setting θ_0 = 0, \phi_0 = 0 and γ = γ_k(τ), we further obtain the evolution operator in the computation space spanned by {0, 1} as

U(τ) = e^{iγnσ},

where n = (sin θ_0 cos φ_0, sin θ_0 sin φ_0, cos θ_0) is a unit vector and σ = (σ_x, σ_y, σ_z) is a vector of standard Pauli operators. Obviously, the evolution operation U(τ) is an arbitrary rotation gate around the rotation axis n by the rotation angle −2γ. However, considering an arbitrary initial state |

|Ψ(0)⟩ = C_1|ψ_1(0)⟩ + C_2|ψ_2(0)⟩, where C_1 and C_2 are the nonzero complex numbers that satisfy |C_1|^2 + |C_2|^2 = 1, we find that, during the evolution time [0, τ], the accumulated dynamical phase γ_0(τ) is no longer zero, but

γ_0(τ) = \int_0^τ \langle Ψ(t)|H(t)|Ψ(t)⟩ dt

= \int_0^τ \{iC_1^∗C_2 e^{i[γ_2(τ)−γ_1(τ)]}|μ_1(t)⟩|μ_2(t)⟩ + iC_2^∗C_1 e^{i[γ_1(τ)−γ_2(τ)]}|μ_2(t)⟩|μ_1(t)⟩\} dt.

To obtain γ_0(τ) = 0, which is equivalent to \int_0^τ iexp[i(\gamma_2(t)−\gamma_1(t))]|μ_1(t)⟩|μ_2(t)⟩ dt = 0, the following SINGQC condition should be met:

\int_0^τ e^{i\int_0^t [1−cos(θ'(t))] \hat{ϕ}(t') dt'} e^{-i\hat{ϕ}(t)} [i\hat{θ}(t) + sin(θ(t)) \hat{ϕ}(t) dt] = 0.

FIG. 1. The evolution path of |ψ_1(t)⟩ on the Bloch sphere for different gates, where (a) and (b) belong to Path 1 corresponding to the condition in Eq. (5). (c) and (d) belong to Path 2 corresponding to the condition in Eq. (12). (a) Path 1 for the S gate. (b) Path 1 for the H gate. (c) Path 2 for the S gate. (d) Path 2 for the H gate. The evolution process can be described using spherical coordinates [Θ(θ), Φ(φ)]. Start from point A (θ_0, 0) of Path 1 (Path 2). First, rotate (θ_0 − θ_0) [i(2π − θ_0 − θ_0)] counterclockwise around the y-axis to point B (θ_0, 0) [B’ (θ_0, π)]. Then, rotate (θ_0 - θ_0) [i(2π - θ_0)] clockwise around the axis of m = [cos(π/2 + 2π/θ_0), sin(π/2 + 2π/θ_0), 0] to point D (0, 0) [D’ (0, 0)]. Finally, return to the initial point A(θ_0, 0) [A'(θ_0, 0)] by rotating (θ_0 - θ_0) counterclockwise around the y-axis. Note that the fourth segment is unnecessary for the S gate since θ_0 = 0.
B. Arbitrary single-qubit gate

In fact, to realize the SINGQC scheme, there are many ways to satisfy Eq. (6). Here, we design special evolution paths satisfying the SINGQC condition to construct arbitrary single-qubit gates. Without loss of generality, we divide the evolution process into four segments, and the Hamiltonian from Eq. (2) in each segment is

\[
\begin{aligned}
H_1(t) &= \Omega_1 e^{-i(\frac{\pi}{2} + \varphi_0)}|0\rangle\langle 1| + \text{H.c.}, \quad t \in [0, \tau_1], \\
H_2(t) &= \left[\Omega_2 e^{-i(\varphi(t))} + \Delta \sigma_z\right]|0\rangle\langle 1| + \text{H.c.}, \quad t \in (\tau_1, \tau_2], \\
H_3(t) &= \Omega_3 e^{-i(\frac{\pi}{2} + \varphi(t))}|0\rangle\langle 1| + \text{H.c.}, \quad t \in (\tau_2, \tau_3), \\
H_4(t) &= \Omega_4 e^{-i(\frac{\pi}{2} + \varphi(t))}|0\rangle\langle 1| + \text{H.c.}, \quad t \in [\tau_3, \tau],
\end{aligned}
\]

and the requirements of the parameters are

\[
\begin{aligned}
\int_{0}^{\tau_1} \Omega_1 dt &= \int_{0}^{\tau_2} \Omega_2 dt = \int_{0}^{\tau_3} \Omega_3 dt = \int_{0}^{\tau_4} \Omega_4 dt = \frac{\theta_0}{2}, \\
\Omega_2 &= -\frac{1}{2} \sin \theta_1 \cos \theta_1 \dot{\varphi}(t); \quad \Delta = \frac{1}{2} \sin^2 \theta_1 \dot{\varphi}(t), \\
\int_{\tau_2}^{\tau_3} \Omega_3 dt &= \int_{\tau_3}^{\tau_4} \Omega_4 dt = \frac{\theta_0 - \theta_2}{2}.
\end{aligned}
\] (7)

with \(\theta_1 = \theta(\tau_1)\). In the implementation of the Hamiltonian, the variable \(\varphi(t)\) is set to be time dependent in the second segment and time independent in the other three segments, while \(\theta(t)\) is set to be time independent in the second segment and time dependent in the other three segments. Under these settings, Eq. (6) reduces to

\[
\int_{\tau_1}^{\tau_2} e^{-i \int_{0}^{\tau_1} \cos \theta_1 \dot{\varphi}(t) dt'} \sin \theta_1 \varphi(t) dt = 0.
\] (9)

Thus, to satisfy Eq. (6), we choose \(\varphi(t) = \frac{2\pi(t - \tau_1)}{\cos \theta_1(\tau_2 - \tau_1)} + \varphi_0\) \((t \in (\tau_1, \tau_2))\) in the second segment, and the modulation of this time-dependent phase can be realized with a phase modulator \([33,35]\). Meanwhile, we can obtain the specific expression of the half rotation angle \(\gamma\) in the evolution operator, i.e.,

\[
\gamma = \frac{1}{2} \int_0^\tau \left[1 - \cos \theta(t)\right] \dot{\varphi}(t) dt
= \frac{1}{2} \int_{\tau_1}^{\tau_2} \left[1 - \cos \theta_1\right] \dot{\varphi}(t) dt
= \left(\frac{1}{\cos \theta_1} - 1\right) \pi,
\] (10)

where \(\theta_1 = \arccos \frac{\pi}{\gamma + \pi}\) depends on the specific \(\gamma\). Therefore, after setting gate parameters \((\theta_0, \varphi_0, \gamma)\), we can construct the arbitrary single-qubit gates for the SINGQC scheme by applying the Hamiltonian in Eq. (7). It is worth noting that, under the control of the Hamiltonian in Eq. (7), \(|\psi_1(t)\rangle\) and \(|\psi_2(t)\rangle\) from an arbitrary evolution state \(|\Psi(t)\rangle\) will cyclically evolve on Bloch sphere, where \(|\Psi(t)\rangle = C_1|\psi_1(t)\rangle + C_2|\psi_2(t)\rangle\).

To illustrate the evolution process more clearly, we use the \(S\) and Hadamard \((H)\) gates as examples, with \((\theta_0, \varphi_0, \gamma)\) set to \((0, 0, \pi/4)\) and \((\pi/4, 0, \pi/2)\), respectively. We plot the evolution trajectories (Path 1) of \(|\psi_1(t)\rangle\) on the Bloch sphere, as shown in Figs. (a) and (b) for the \(S\) and \(H\) gates, respectively. From the perspective of \(|\psi_1(t)\rangle\), the evolution process can be described as follows. First, \(|\psi_1(t)\rangle\) evolves from point \(A\) to \(B\) under the control of Hamiltonian \(H_1(t)\) in Eq. (7) for a time duration of \([0, \tau_1]\) with \(\tau_1 = \frac{|\theta_0 - \theta_3|}{2\Omega_1}\). Then, from point \(B\), the system Hamiltonian is switched to \(H_2(t)\), and \(|\psi_1(t)\rangle\) reaches point \(C\) after a time duration of \(\tau_2 - \tau_1 = \frac{\pi}{2} \sin \theta_1 / \Omega_2\). Next, from point \(C\), the quantum system is governed by the Hamiltonian \(H_3(t)\) and \(|\psi_1(t)\rangle\) reaches point \(D\) after a time duration of \(\tau_3 - \tau_2 = \frac{|\theta_0|}{2\Omega_4}\). Finally, \(|\psi_1(t)\rangle\) will be back to the starting point \(A\) by applying a control field \(\Omega_1\) for a duration of \([\tau_3, \tau]\) with \(\tau - \tau_3 = \frac{|\theta_0|}{2\Omega_4}\), where the corresponding Hamiltonian is \(H_4(t)\) in Eq. (7). It is worth noting that the fourth segment is not necessary for the \(S\) gate since \(\theta_0 = 0\), resulting in a duration of \(\tau - \tau_3 = \frac{|\theta_0|}{2\Omega_4}\).

C. Gate performance

We turn to test the performance of the implemented SINGQC gates and compare it with the previous schemes. The performance of quantum gates in an open quantum system can be evaluated by the Lindblad master equation

\[
\dot{\rho} = -i[H'(t), \rho] + \frac{1}{2} \sum_{j=-,+} \Gamma_j L_j(\sigma_j),
\] (11)

where the quantum system is controlled by

\[
H'(t) = (1 + \epsilon)H(t) + \frac{\eta}{2} \Omega_i \sigma_z
\]

with \(\epsilon\) and \(\eta\) being the error fractions of the control and detuning errors, respectively; \(\rho\) is the density matrix of the quantum system; \(L(A) = 2A\rho A^\dagger - A^\dagger A\rho - \rho A^\dagger A\) is the Lindbladian operator with \(\sigma_- = |0\rangle\langle 1|, \sigma_z = |1\rangle\langle 1| - |0\rangle\langle 0|\); \(\Gamma_-\) and \(\Gamma_+\) are the decay and dephasing rates, respectively. We also
consider the influence of phase error ($\Omega e^{i\phi} \rightarrow \Omega e^{i(1+\chi)\phi}$) in Appendix C.

To show the noise-resilient advantage of our SINGQC scheme, we first consider only the influence of the control error, which destroys the cyclic evolution and introduces a nonzero dynamical phase. The gate fidelity is defined as $F = \frac{1}{\Delta} \sum_{i=1}^{\Delta} \langle \Psi_i(0) | U(\tau) \rho U(\tau) | \Psi_i(0) \rangle$, where the six initial states $| \Psi_i(0) \rangle$ are $|0\rangle$, $|1\rangle$, $(|0\rangle + |1\rangle)/\sqrt{2}$, $(|0\rangle - |1\rangle)/\sqrt{2}$, $(|0\rangle + i|1\rangle)/\sqrt{2}$ and $(|0\rangle - i|1\rangle)/\sqrt{2}$, respectively. For simplicity, we set $|\Omega, t\rangle = \Omega$ to be the time-independent driving amplitude. Figures 2(a) and 2(b) show plots of the fidelities of the $S$ and $H$ gates as a function of $\epsilon$, respectively. Our scheme exhibits excellent robustness to control error, and the gate fidelity of the $S$ gate remains above 99.9% in the range of the error ratio $\epsilon \in [-0.2, 0.2]$, which far exceeds that of the DG and SLNGQC schemes. The $H$ gate also far outperforms the SLNGQC and DG schemes in terms of robustness to control error and, when the error ratio is $\epsilon = 0.2$, the gate fidelity of the SINGQC scheme is 6% higher than that of the corresponding SLNGQC and DG schemes. On the other hand, we also plot gate fidelities as a function of the detuning error of the $S$ and $H$ gates, as shown in Figs. 2(c) and 2(d), respectively. However, the results are not satisfactory.

**D. An alternative scheme and its performance**

In order to make our scheme robust to both control and detuning errors, we modify the requirements for the parameters in Eq. (8) as follows:

\[
\begin{align*}
\int_{0}^{\tau_1} \Omega_1 dt & = \int_{0}^{\tau_1} \frac{\dot{\theta}(t)}{2} dt = \frac{2\pi - \theta_1 - \theta_0}{2}, \\
\Omega_2 & = \frac{1}{2} \sin \theta_1 \cos \theta_1 \dot{\varphi}(t); \quad \Delta = \frac{1}{2} \sin^2 \theta_1 \dot{\varphi}(t), \\
\int_{\tau_2}^{\tau_3} \Omega_3 dt & = \int_{\tau_2}^{\tau_3} \frac{\dot{\theta}(t)}{2} dt = 0 - \frac{(2\pi - \theta_1)}{2}, \\
\int_{\tau_3}^{\tau} \Omega_4 dt & = \int_{\tau_3}^{\tau} \frac{\dot{\theta}(t)}{2} dt = \frac{\theta_0 - \theta_1}{2}.
\end{align*}
\] (12)

Under these settings, the evolution trajectories (Path 2) of $|\psi_3(t)\rangle$ on the Bloch sphere are shown in Figs. 1(c) and 1(d), for the $S$ and $H$ gates, respectively. The evolution process can be described as follows: In the first step, $|\psi_1(t)\rangle$ evolves from point $A'$ to $B'$ by the control of Hamiltonian $H_1(t)$ in Eq. (7) for a duration of $[0, \tau_1]$, with $\tau_1 = |(2\pi - \theta_1 - \theta_0)/(2\Omega_1)|$. Subsequently, the system Hamiltonian is changed to $H_2(t)$, and $|\psi_3(t)\rangle$ reaches point $C'$ after a duration of $\tau_2 - \tau_1 = \pi \sin \theta_1 / \Omega_2$. Next, $|\psi_3(t)\rangle$ reaches point $D'$ by the control of Hamiltonian $H_3(t)$ for a duration of $\tau_3 - \tau_2 = |(\theta_1 - 2\pi)/(2\Omega_3)|$. Finally, the system Hamiltonian is changed to be $H_4(t)$ during $[\tau_3, \tau]$ with $\tau - \tau_3 = |\theta_0/(2\Omega_4)|$, and thus $|\psi_4(t)\rangle$ will be back to the starting point $A'$.

The gate robustness against the control error for the $S$ and
$H$ gates are shown in Figs. 3(a) and (b), respectively. The results indicate that Path 1 and Path 2 have similar robustness to control error and are far superior to SLNQC and DG schemes. Furthermore, Path 2 also achieves satisfactory results in terms of robustness to detuning errors, with a fidelity higher than 99.3% for all gates across the error rate range of $\eta \in [-0.2, 0.2]$, as shown in Figs. 3(c) and (d). Therefore, our scheme can possess stronger robustness to both control and detuning errors than previous schemes.

E. Gate performance under decoherence

However, since the evolution along Path 2 experiences a longer trajectory, it inevitably requires a longer operation time. Therefore, considering the decoherence, the evolution method of Path 1 is more suitable for an actual physical system affected greatly by control error, while the evolution method of Path 2 is more inclined to be selected for a physical system affected greatly by detuning error. Next, taking the $S$ gate as an example, we comprehensively analyze the effects of systematic error and decoherence (with uniform rates $\Gamma$). As shown in Fig. 4, our SINGQC scheme performs best in both control and detuning error. Remarkably, even with a decoherence rate of $\Gamma = 4 \times 10^{-4}\Omega$, the gate fidelities of our scheme can exceed 99.5% within the control error range of $\epsilon \in [-0.2, 0.2]$ and the detuning error range of $\eta \in [-0.15, 0.15]$, as shown in Figs. 4(a) and (b), respectively.

III. PHYSICAL REALIZATION

By exciting neutral atoms into the high principal quantum number state, Rydberg atoms have received extensive theoretical and experimental attention because of their excellent atomic properties. In this section, we propose to implement the SINGQC scheme in the Rydberg atomic system by encoding qubit bases with a pair of long-lived hyperfine ground clock states of typical alkali atoms.

A. Single-qubits quantum gate

As shown in Fig. 5(a), quantum information is encoded in two magnetic-field-insensitive hyperfine ground states $|0\rangle \equiv |5S_{1/2}, F = 1, m_F = 0\rangle$ and $|1\rangle \equiv |5S_{1/2}, F = 2, m_F = 0\rangle$, which can be controlled by a two-photon Raman transition. This process can be realized by using a single ground-state Rabi laser with two frequency components generated by current modulation of a diode laser. The laser is detuned from the $5F_{3/2}$ excited state by $\delta$. Usually, the Raman lasers are far detuned from the short-lived electronically excited states $5P_{3/2}$, so the decoherence of excited states can be neglected. In this case, the Hamiltonian of the single-qubit gate is in the same form as Eq. (2), with $\omega = \Omega_A \Omega_B / \delta$, and $\Delta \approx \omega_A + \omega_B - \omega_0 + (\Omega_A^2 - \Omega_B^2) / \delta$, where $\Omega_A, \Omega_B$ characterize the coupling strengths for the two Raman fields, $\omega_A, \omega_B$ are the corresponding coupling field frequencies, $\phi(t)$ is the local phase, and $\omega_0$ is the atomic resonance frequency. When $\Omega = 2\pi \times 1.36$ MHz, and $\Gamma = 1.15$ kHz $\approx \Omega / 7400$, the gate fidelity can exceed 99.9% within the control error range of $\epsilon \in [-0.2, 0.2]$, and over 99.3% within the detuning error range of $\eta \in [-0.2, 0.2]$, as shown in Figs. 4(a) and (b), respectively.

B. Multiqubit quantum gate

In addition to single-qubit quantum gates, the implementation of nontrivial two-qubit gates is crucial for universal quantum computation. While an arbitrary multiqubit quantum gate can be decomposed into several single- and two-qubit quantum gates, it is still worthwhile to directly implement the $N$-qubit ($N > 3$) quantum gate because it can reduce the complexity of a large quantum circuit. Rydberg atoms are promising platforms for the implementation of multiqubit quantum gates owing to their excellent interaction properties. In the following, we pay attention to directly realizing SINGQC multiqubit quantum gates with the CZ gate being one of the typical examples.

As shown in Fig. 5(b), we consider $N + 1$ Rubidium atoms, where $N$ is the number of control atoms and $T$ denotes the target atom. The related energy levels of each atom are $|0\rangle \equiv |5S_{1/2}, F = 1, m_F = 0\rangle$, $|1\rangle \equiv |5S_{1/2}, F = 2, m_F = 0\rangle$, and $|r\rangle \equiv |83S, J = 1/2, m_J = 1/2\rangle$. The quantum information is encoded in two stable ground states $|0\rangle$ and $|1\rangle$, and the Rydberg state $|r\rangle$ is acting as the auxiliary state. The states $|0\rangle$ and $|r\rangle$ of the control atoms are coupled resonantly by the Rabi frequency $\Omega_r(t)$, and states $|1\rangle$ and $|r\rangle$ of the target atom are coupled nonresonantly via the Rabi frequency $\Omega_t(t)$ with a detuning $\Delta'$, as shown in Fig. 5(c). The Rydberg-Rydberg interaction strength $V$ can be adjusted by precise control of atom positions with optical tweezer arrays. The total Hamiltonian of the multiqubit system reads

$$H_2(t) = (1 + \epsilon_c)H_c(t) + (1 + \epsilon_i)H_I(t) + H_V + \eta'\Omega'(|r\rangle_c\langle r| + |r\rangle_t\langle r|),$$

where $H_c(t) = \sum_{k=1}^{N} \Omega_c(t)|r_k\rangle\langle r_k| + \text{H.c.}$ is the Hamiltonian of the control atoms with a time-dependent Rabi frequency of $\Omega_c(t) = \Omega_c \cos \omega t$ and $H_I(t) = \Omega_I(t)e^{-i\Delta'}|r\rangle_c\langle 1| + \text{H.c.}$ is...
the Hamiltonian of the target qubit. The interaction Hamiltonian between the Rydberg states is represented by

\[ \mathcal{H}_V = \sum_{k>j=1}^N (V_{jk}|rr\rangle_{jk}\langle rr| + V_{kt}|rr\rangle_{kt}\langle rr|), \]

where \( V_{jk} \) is the Rydberg-Rydberg interaction between control atoms, and \( V_{kt} \) is the Rydberg-Rydberg interaction between the \( k \)th control atom and the target atom. For the sake of simplicity, we suppose that \( V_{jk} = V_c \) and \( V_{kt} = V_t = \omega \). \( \Omega' \) represents the amplitude of the Rabi frequency \( \Omega(t) \). \( \epsilon_c \) (\( \epsilon_t \)) represents the control error of the control (target) atoms, and \( \eta^2 \) is the detuning error. Under the conditions of a strong Rydberg-Rydberg interactions mechanism \( V_t >> \Omega_c, \Omega' \), and when \( \Omega_c >> \Omega' \), we can derive the effective Hamiltonian of the multiqubit system as [42]

\[ \mathcal{H}_{eff}(t) = \left( \otimes_j^N |1\rangle_j \right) \otimes \mathcal{H}_t(t). \]  

In the rotation frame of unitary transformation \( \exp(-iht) \) with \( h = \sum_{j=1}^N (|1\rangle_{ct}\langle 1| - |11\rangle_{ct}\langle 11|) \), the effective Hamiltonian becomes

\[ \mathcal{H}'_{eff}(t) = \left[ \Omega_c(t)|11\rangle_{ct}\langle 1r| + \text{H.c.} \right] + \frac{\Delta}{2} (|11\rangle_{ct}\langle 11| - |1r\rangle_{ct}\langle 1r|), \]  

where \( |i\rangle_{ct} = |1\rangle_c \otimes |i\rangle_t \) (\( i = 1, r \)) and \( |1\rangle_c \) means all control atoms are in the \( |1\rangle \) state. It is obvious that Eq. (15) with basis vectors \( |11\rangle_{ct}, |1r\rangle_{ct} \) possesses the same form as Eq. (2), thereby we can implement a geometric phase only on the computation basis \( |11\rangle_{ct} \). As a result, a multiqubit controlled-phase gate \( (C^N_Z) \) can be obtained, and what is more, the operation time here is independent of the involved number of atoms.

For the realization of the proposed multiqubit model with Rydberg atoms, we need the atomic arrangement structure as depicted in Fig. 5(b). This structure can be realized by a defect-free three-dimensional array with the control atoms distributed on the spherical surface [51][52]. Based on this array, one can greatly increase the available number of control atoms.

C. Gate performance

Finally, we numerically test the performance of the SINGQC multiqubit gates that evolve along Path 1 by defining the gate fidelity as \( F' = \frac{1}{N!} \sum_{j=1}^{N+1} |\Psi_j(0)\rangle \langle U^* \rho U | \Psi_j(0)\rangle \), where \( |\Psi_j(0)\rangle = \otimes_i^{N+1} |\psi'_i(0)\rangle \) represents one of the initial states of the \( N+1 \) atom system and \( |\psi'_i(0)\rangle \) denotes the \( i \)th atom initially in one of the states \( \{ |0\rangle, |1\rangle, (|0\rangle + |1\rangle)/\sqrt{2}, (|0\rangle - |1\rangle)/\sqrt{2} \} \) [29]. Here \( U^* \) is the evolution operator, and \( \rho \) is the density matrix of the multiqubit quantum system under consideration. Here we choose \( \Omega_c = 2\pi \times 36 \text{ MHz} \), which can be obtained experimentally by using a higher power in the blue beam and increasing the detuning from the intermediate level

FIG. 6. The performance of the CZ gate implemented with the SINGQC scheme (solid red line) and the DG scheme (dashed black line). (a) Fidelities of the CZ gate under different Rydberg state lifetimes. Fidelities of the CZ gate with respect to the (b) control error of the target atom, (c) the control error of the control atoms, and (d) the detuning error.

FIG. 7. The performance of the \( C_NZ \) gate implemented with the SINGQC scheme, where the solid blue line and the dashed purple line represent the results of the \( C_2Z \) and \( C_3Z \) gates, respectively. (a) Fidelities of the \( C_NZ \) gate under different Rydberg state lifetimes. Fidelities of the \( C_NZ \) gate with respect to the (b) control error of the target atom, (c) the control error of control atoms, and (d) the detuning error.
Other parameters are $\Omega' = 2\pi \times 0.75$ MHz, $V_l = \omega = 2\pi \times 400$ MHz, and $V_c = V_l/7$. The decoherence operators of the $k$ atom are $\sigma_0^k = |0\rangle_k\langle 0|$, $\sigma_+^k = |1\rangle_k\langle 0|$ and $\sigma_-^k = |0\rangle_k\langle 1|$, where $|2\rangle$ is an additional ground state representing the remainder of the Zeeman magnetic sublevels out of the computational states $|0\rangle$ and $|1\rangle$. For simplicity, we suppose that the decay rates of the Rydberg state to eight Zeeman ground states are the same. Thus, the decoherence rates are $\Gamma_0 = \Gamma/8$, and $\Gamma_\pm = 3\Gamma/4$, where $\Gamma = 1/\tau_r$ with $\tau_r$ being the Rydberg state lifetime. Figure 6(a) plots the fidelities of the $\text{CZ}$ gate as a function of Rydberg state lifetime, where we find that the $\text{CZ}$ gate constructed in the SINGQC manner is more resistant to the control error of control atoms than the DG gate within the considered error range, as shown in Figs. 6(b)-(d).

In conclusion, based on the inverse engineering of the Hamiltonian, we propose the SINGQC scheme, where arbitrary input states accumulate only geometric phases, which is different from the previous NGQC schemes. Numerical results indicate that our scheme can significantly improve the gate robustness against control error, and it can also enhance robustness against detuning errors through an alternative evolution path. In particular, the gate robustness of our scheme can outperform the DG scheme even when the rotation angle of the geometric gate is $\pi$, which breaks the limitation that the gate robustness of geometric schemes cannot exceed the DG scheme for the rotation angle of $\pi$ as was the case in previous schemes.

In addition, we construct the SINGQC multiqubit gates in the Rydberg atom system, where the gate operation time does not increase with the increase of the involved atom number. Numerical simulations show that the $\text{CZ}$ gate of our protocol is more robust than the DG scheme. Even for $C_2Z$ and $C_3Z$ gates, the gate fidelities of our scheme almost entirely exceed the fault tolerance threshold of the multiqubit gate within the considered error range. Moreover, our SINGQC scheme can also be applied to other solid-state platforms.

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Appendix A: The dynamical scheme

In a generic two-level model, the dynamical gate is constructed by a simple resonant pulse, so the Hamiltonian of the system is

$$H_d = \Omega e^{-i\varphi_d}|0\rangle\langle 1| + \text{H.c.} \tag{A1}$$

The corresponding evolution operator can be expressed as

$$U_d(\Theta_d, \varphi_d) = \cos \Theta_d I - i \sin \Theta_d (\cos \varphi_d \sigma_x + \sin \varphi_d \sigma_y), \tag{A2}$$

where $\Theta_d = \Omega t$. The $S$ gate and $H$ gate can be implemented as

$$U_d^S(\Theta_d, \varphi_d) = U_d(\frac{\pi}{4}, \varphi_d)U_d(\frac{\pi}{4}, \frac{3\pi}{2})U_d(\frac{\pi}{4}, 0), \tag{A3a}$$

$$U_d^H(\Theta_d, \varphi_d) = U_d(\frac{\pi}{4}, \frac{3\pi}{2})U_d(\frac{\pi}{4}, 0). \tag{A3b}$$

In the presence of errors, the Hamiltonian in Eq. (A1) becomes $H_d' = (1 + \epsilon)H_d + \eta \Omega \sigma_z/2$.

Appendix B: The conventional single-loop NGQC scheme

In single-loop NGQC scheme, the Hamiltonian in each segment is set to be

$$H_s = \Omega e^{-i\varphi_s}|0\rangle\langle 1| + \text{H.c.} \tag{B1}$$

The corresponding evolution operator is similar to that of Eq. (A2), i.e., $U_s(\Theta_s, \varphi_s) = \cos \Theta_s I - i \sin \Theta_s (\cos \varphi_s \sigma_x + \sin \varphi_s \sigma_y)$ with $\Theta_s = \Omega t$. For the $S$ gate, the implementation is divided into two segments, that is,

$$U_s^S(\Theta_s, \varphi_s) = U_s(\frac{\pi}{2}, \frac{3\pi}{4})U_s(\frac{\pi}{2}, -\frac{\pi}{2}). \tag{B2}$$
FIG. 8. Gate fidelity as function of the phase error $\chi$ in the absence of decoherence. The results of the $S$ and $H$ gates are shown in (a) and (b), respectively, which indicate that our scheme is more robust against phase error than both the dynamical and single-loop NGQC schemes.

For the $H$ gate, three segments are needed and the evolution operator is

$$U_H^s(\Theta_s, \varphi_s) = U_s\left(\frac{3\pi}{8}, -\frac{\pi}{2}\right)U_s\left(\frac{\pi}{2}, \pi\right)U_s\left(\frac{\pi}{8}, -\frac{\pi}{2}\right). \quad (B3)$$

Considering both types of error, the Hamiltonian becomes

$$H_s' = (1 + \epsilon)H_s + \eta\Omega\sigma_z/2.$$
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