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<th>Title</th>
<th>Unconventional Geometric Quantum Computation</th>
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Quantum computation takes its power from superposition and entanglement, which are two main features distinguishing the quantum world from the classical world. But they are also very fragile and may be destroyed easily by a process called decoherence. The suppression of these decoherence effects in a large-scalable quantum computer is essential for construction of workable quantum logical devices. Quantum error-correcting codes [1] enable quantum computers to operate despite some degree of decoherence and may make quantum computers experimentally realizable, provided that the noise in individual quantum gates is below a certain constant threshold. The recently estimated threshold is that the individual gate infidelity should be of the order $10^{-4}$ [2]. In order for this precision to be possible, quantum gates must be operated in a built-in fault-tolerant manner.

Apart from the decoherence-free subspace scheme [3], a promising approach to achieve built-in fault-tolerant quantum gates is based on geometric phase shifts [4–6]. A universal set of quantum gates [7] may be realized using geometric phase shifts when the Hamiltonian of the qubit system changes along suitable loops in a control space [8–15]. A quantum gate is expressed by a unitary evolution operator $U(\gamma)$, where the set $\gamma$ are phases acquired in a particular evolution in realization of the gate, and usually these phases consist of both geometric ($\gamma^g$) and dynamic ($\gamma^d$) components [4–6]. $U(\gamma)$ is specified as a geometric gate if the phase $\gamma$ in the gate operation is a pure geometric one (i.e., with zero dynamic phase in the evolution), and quantum computation implemented in this way is referred to as geometric quantum computation (GQC) in a general sense [8–15]. GQC demands that logical gates in computing are realized by using geometric phase shifts, so that it may have the inherently fault-tolerant advantage due to the fact that the geometric phases depend only on some global geometric features. Although this property was doubted by some numerical calculations with certain decohering mechanisms [16], an analytical result showed that geometric phases may be robust against dephasing [17]. Several basic ideas of adiabatic GQC by using NMR [9], superconducting nanocircuits [10], trapped ions [11], or semiconductor nanostructure [12] were proposed, and the generalization to nonadiabatic case was also suggested [13–15].

According to conventional wisdom, a key point in GQC [8–15] is to remove/avoid the dynamic phase. One simple method is to choose the dark states as qubit space, thus the dynamic phase is always zero [11]. A more general method to cancel the dynamic phase is the so-called multiloop scheme, i.e., let the evolution be dragged by the Hamiltonian along several special closed loops, then the dynamic phases accumulated in different loops may be canceled, with the geometric phases being added [9,10,15]. These methods to cancel the dynamic phase need subtle choice of the control parameters and/or more operations than that needed in dynamic phase gates, and thus may induce additional errors in the operations. On the other hand, since the central idea of the GQC is that the phase accumulated in the gate evolution has global geometric features, it is natural to ask whether we can design and implement a quantum gate with geometric features but a nonzero/nontrivial dynamic phase. Clearly, this kind of gate differs from the conventional geometric quantum gates addressed previously [8–15] and is of significance in physical implementation of the built-in fault-tolerant quantum computation.

In this Letter, we not only answer the above important question for the first time, but also propose a new class of unconventional geometric quantum gates, in which the total phase $\gamma$ consists of both a geometric component and a nonzero dynamic one. Our novel idea is simply that, despite its nonzero dynamic component, the total phase is still dependent only on global geometric features if we ensure that the dynamic phase $\gamma^d$ is proportional to the geometric phase $\gamma^g$ [4–6] as

$$\gamma^d = \eta \gamma^g, \quad (\eta \neq 0, -1),$$

(1)
where $\eta$ is a proportional constant independent on (or at least some) parameters of the qubit system. Equation (1) may be rewritten as $\gamma = (1 + \eta)\gamma^s$ with $\gamma$ the total phase accumulated in the gate operation, and the corresponding quantum gate should possess global geometric features, which we hereafter specify as the unconventional geometric gate. These gates would have advantages that conventional geometric gates have. Comparing with conventional geometric gates, unconventional geometric gates proposed here can simplify experimental operations, since the additional operations required to cancel the dynamic phase are not necessary in certain physical systems. In the following, we illustrate in detail that unconventional nontrivial two-qubit geometric gates with inherent fault-tolerant geometric features can be really implemented in physical systems [18–21], and specify the recently reported two-qubit phase gate [19] as an unconventional geometric gate proposed here.

Let us consider a realistic physical system proposed quite earlier in implementing quantum computers [18]. In this system, two ions are confined in a harmonic trap potential and interact with laser radiation. Two internal states of each ion denoted by $|\uparrow\rangle$ or $|\downarrow\rangle$ represent the qubit states. By choosing the laser beams appropriately, the trap potential may excite a stretch mode with the frequency $\omega$, when the ions are in the different internal state, while nothing happened when they are in the same internal state [19]. If the internal states are in $|\uparrow\rangle$ or $|\downarrow\rangle$, within the rotating wave approximation, the Hamiltonian of this system in the rotating frame reads ($\hbar = 1$)

$$
H(t) = i\Omega_D(a_\uparrow^\dagger e^{-i\delta t+i\phi_L} - a_\downarrow e^{i\delta t-i\phi_L}),
$$

(2)

where $a_\uparrow^\dagger$ and $a_\downarrow$ are the usual harmonic oscillator raising and lowering operators, $\delta$ is the detuning, $\phi_L$ represents the phase of the driving field and $\Omega_D = -(F_0 - F_{0\dagger})z_0/2$ with $z_0$, being the spread of the ground state wave function of the stretch mode. $F_0$ ($F_{0\dagger}$) is the dipole force acting on the $|\downarrow\rangle$ ($|\uparrow\rangle$) state. The quantum state $|\Psi\rangle$ under this force can be coherently displaced in position-momentum phase space. It is clear that the populations of the two ions would not change when the system is governed by the Hamiltonian (2); thus the two-qubit gate achieved in the cyclic evolution should be a phase gate described by

$$
U(\gamma) = \text{diag}[1, \exp(i\gamma_\uparrow), \exp(i\gamma_\downarrow), 1]
$$

(3)

in the computational basis $\{|\uparrow\rangle, |\uparrow\rangle, |\downarrow\rangle, |\downarrow\rangle\}$. $\gamma_\uparrow = \gamma_\downarrow = \gamma$ [20–22]. The phase gate (3) is a nontrivial two-qubit gate when $\gamma \neq n\pi$ with $n$ an integer [7].

To explicitly express the geometric and dynamic phases, we employ here the coherent-state path integral formulation in the phase space to derive them. The phase change associated with cyclic evolution in $[0, T]$ is defined by $|\Psi(T)\rangle = \exp(i\gamma)|\Psi(0)\rangle$ with $\gamma$ a real number. In order to evaluate $\gamma$, we may rewrite the relation as

$$
\exp(i\gamma) = \langle \Psi(0)|U(T, 0)|\Psi(0)\rangle
$$

with the evolution operator being written as the standard time-ordered product:

$$
U(T, 0) = \hat{T} e^{-i\int_0^T H(t)dt} = \prod_{n=1}^N e^{-iH(n)T/N}.
$$

(4)

Here $\hat{T}$ is the time ordering operator, and $H(n)$ denotes the Hamiltonian at time $t = nT$. In the system we consider here, we may use the coherent states $|\alpha_I\rangle$, which are the eigenstates of the destruction operator $a$ with eigenvalues $\alpha_I$. If $H(a^\dagger, a; t)$ is normally ordered (a more general case than that addressed here), by inserting $N$ resolutions of the identity $(1/\pi) \int |\alpha_I\rangle\langle\alpha_I| d^2\alpha_I |\alpha_I\rangle = 1$ into $U(T, 0)$ with $d^2\alpha_I = d\text{Re}(\alpha_I) d\text{Im}(\alpha_I)$ and $N \to \infty$, we find that the propagator, defined as $K(\alpha_I(T); \alpha_I(0)) = \langle \alpha_I(0)|\alpha_I(T)\rangle$, is given by [23]

$$
K(\alpha_I(T); \alpha_I(0)) = \int e^{i(\gamma^s + \gamma^d)} D[\alpha_I(t)],
$$

(5)

where $D[\alpha_I(t)] = \lim_{N \to \infty} (1/\pi)^N \prod_{n=1}^N d^2\alpha_I(t_n)$,

$$
\gamma^s = \frac{i}{2} \int_0^T \alpha_I^* D\alpha_I - \alpha_I^* D\alpha_I dt
$$

(6)

is just the geometric phase in a closed path in the phase space [5], and

$$
\gamma^d = -\int_0^T H(\alpha_I^*; \alpha_I; t) dt
$$

(7)

is the dynamic phase with $H(\alpha_I^*; \alpha_I; t) = \langle \alpha_I|H(t)|\alpha_I\rangle$ [24]. $\gamma^s$ in Eq. (6) can also be expressed as $(i/2) \int [\alpha_I^* D\alpha_I - \alpha_I^* D\alpha_I^*]$, which is the area enclosed by the closed path of $\alpha_I(t)$. In the present system, we have

$$
\alpha_I(t) = i\frac{\Omega_D}{\delta} (e^{-i\delta t} - 1) e^{i\phi_L},
$$

(8)

$$
H(\alpha_I^*; \alpha_I; t) = \frac{2\Omega_D^2}{\delta} [1 - \cos(\delta t)],
$$

(9)

under the natural initial condition $\alpha_I(0) = 0$, with the requirement that the evolution operator satisfies $U(t = 0) = 1$ [see Eq. (11)]. Therefore, the phases accumulated in one cycle are found to satisfy Eq. (1):

$$
\gamma^d = -2\gamma^s = 2\gamma = 2\Phi_{II},
$$

(10)

with $\Phi_{II} = -2\pi(\Omega_D/\delta)^2$. Thus, a universal unconventional geometric gate described by Eq. (3) can be achieved once $\alpha_I(t)$ forms a closed path in the gate operation. For instance, $\Phi_{II} = -\pi/2$ is obtained by choosing $|\Omega_D/\delta| = 1/2$; then $U(\pi/2)$ is a universal controlled $\pi$ phase gate after rotating $-\pi/2$ on the $|\uparrow\rangle$ states.

At this stage, it is worth pointing out that the unconventional geometric phase gate is unreachable in this system since only a nontrivial $\gamma^d = \pm \pi$ can be obtained under the condition of the trivial dynamic phase ($\gamma^d = 2\pi n \times \mathrm{integer}$). But $U(\gamma)$ is a trivial gate when $\gamma = \pm \pi$ [7]. However, most intriguingly, the total phase is exactly equal to the minus geometric phase, namely, $U(\gamma)$ achieved here is an unconventional geometric logical gate with $\eta = -2$ proposed before. Interestingly, the
proportional constant in this example is indeed independent of any parameters in the system, such as the speed of the gate, the detuning, the phase, and the density of the laser beams used etc. Consequently, the phase $\gamma$ in the gate (3) has really all the features dependent only on the geometry. Remarkably, the phase gate addressed here was experimentally demonstrated very recently [19], and the high fidelity of the two-qubit phase gate achieved in the reported experiment benefits from its geometric features: The phase is determined only by the path area, not on the exact starting state distributions, path shape, orientation in phase space, or the passage rate to traverse the closed path [19]. All these features are global properties which motivated one to study the conventional GQC [8–15]. To our knowledge, a conventional geometric quantum gate has not been achieved experimentally, though the conditional geometric phase was observed in Ref. [9].

Also intriguingly, we find that Eq. (10) is valid even in noncyclic cases, which has close relevance to the robustness of the (cyclic phase) gate against the small noncyclic perturbations. When a quantum system evolves from an initial state $|\Psi(0)\rangle$ to a final state $|\Psi(t)\rangle$ with $\langle\Psi(0)|\Psi(t)\rangle = e^{\gamma t} \langle\Psi(0)|\Psi(0)\rangle$, $\gamma$ is specified as the total phase and the noncyclic geometric phase can be defined as $\gamma^g = \gamma - \gamma^d$, where $\gamma^d = -\int_0^t \langle\Psi(t)|H(t')|\Psi(t')\rangle dt'$ is the dynamic phase [5,6]. In the present system, the wave function $|\Psi(t)\rangle$ at time $t$ is $|\Psi(t)\rangle = U(t)|\psi(0)\rangle$, and the evolution operator $U_t$ can be found as

$$U_t = \tilde{U} e^{-it\int_0^t H(t')dt'},$$

$$= e^{-it\int_0^t H(t')dt'}(1/2) \int_0^t dt_1 \int_0^{t_1} [H(0),H(t_1)]dt_1 + \cdots$$

$$= e^{\Phi_{II}(t)}D(\alpha_{II}),$$

(11)

where $\Phi_{II}(t) = (\Omega_{D}/\delta)^2[\sin(\delta t) - \delta t]$, $D(\alpha_{II}) = \exp[\alpha_{II}(t)a^\dagger - \alpha_{II}^\dagger(t)a]$, and $\alpha_{II}(t)$ is given by Eq. (8).

The commutator of the Hamiltonian (2) at different time is a number, not an operator. Then the last equation is exactly derived by expanding the magnus’ formula [Eq. (11)] [25] to the second term, since the higher-order terms in the expansion vanish. Then it is straightforward to derive $\gamma(t) = \Phi_{II}(t)$ at any time $t$. On the other hand, the dynamic phase accumulated during $[0, t]$ can be obtained explicitly $\gamma^d(t) = -\int_0^t \langle n|D^\dagger(\alpha_{II})H(t') \times D(\alpha_{II})|n\rangle dt'' = 2\Phi_{II}(t)$, where $|n\rangle$ is an eigenstate in the Fock space. Therefore, we conclude that Eq. (10) is valid at any time. Because of this very special property, the total phase still depends only on the geometric features even in the presence of a slight deviation of the period $T$ and thus the illustrated geometric gate is also insensitive to the error in controlling the cyclic time in this respect [26], which is an extra advantage of this kind of gate and is believed to be one of the factors leading to high fidelity of the unconventional phase gate reported experimentally [19]. The robustness of GQC to noncyclic perturbations is also addressed in Ref. [27].

We now turn to another interesting example [20]. In the ions trapped quantum computer model, the Hamiltonian for ions interacting with the vibrational mode can be controlled by using different kinds of Raman laser pulses. In the case of two ions with each driven by identical Raman lasers, the system may be described by a special case of the interaction Hamiltonian given by

$$H(t) = -i[f(t)a^\dagger - f^*(t)a]J_z,$$

(12)

where $J_z = \sigma_z^{(1)} + \sigma_z^{(2)}$ is the collective spin operator with $\sigma_z^{(j)}$ being the $z$-component Pauli matrix for the $j$th ion. The conditional phase gate in the system has been proposed by using a specific four pulse sequence [20]. We suggest a more general gate achieved by this Hamiltonian than that addressed there. The gate governed by the Hamiltonian (12) is clearly a phase gate $U(|\gamma\rangle) = \exp[i\gamma D_{II}|\gamma\rangle]$, where $D_{II}$ is a special Hamiltonian than that addressed there. The gate governed by the Hamiltonian would not lead the spins to flip in the computational basis. Denoting $\beta_{II}(j, l = 1, \text{or } 2)$ as the eigenvalues for $J_z$ in this basis, it is straightforward to find that

$$D^\dagger(\beta_{II})a^\dagger\beta_{II}D(\beta_{II}) = \beta_{II}^2[a^\dagger + \alpha^*(t)],$$

$$D^\dagger(\beta_{II})a\beta_{II}D(\beta_{II}) = \beta_{II}^2[a + \alpha(t)],$$

where $D(\beta_{II}) = \exp[[\alpha(t)a^\dagger - \alpha^*(t)a]\beta_{II}]$ with $\alpha(t) = -\int_0^t f(t)dt'$. Then we have

$$H(\alpha^*, \alpha; t) = \langle n|D^\dagger(\beta_{II})H(t)D(\beta_{II})|n\rangle$$

$$= -i\beta_{II}^2[f(t)\alpha^*(t) - f^*(t)\alpha(t)].$$

Substituting this result into Eq. (7), the dynamic phase is given by

$$\gamma_{II}^d(\tau) = 2\beta_{II}^2\gamma^0(\tau),$$

(13)

with $\gamma^0(\tau) = (1/2) \int_0^\tau f(t)\alpha^*(t) - \alpha(t)f^*(t) dt$. The geometric phase is then found to be

$$\gamma_{II}^g(\tau) = -\beta_{II}^2\gamma^0(\tau).$$

(14)

Comparing Eq. (13) with Eq. (14), we have

$$\gamma_{II}^d(\tau) = -2\gamma_{II}^g(\tau) = 2\gamma_{II}(\tau).$$

(15)

Thus, a universal phase gate $U(|\gamma\rangle)$ may also be realized if $\alpha(t)$ forms a closed path, noting that $U(|\gamma\rangle)$ is nontrivial under the condition $\gamma_{II} + \gamma_{II} = \gamma_{II} + \gamma_{II} (\text{mod } 2\pi)$.

Similarly, by appropriately choosing laser beams, the ions in a Paul trap may be described by the Hamiltonian given by

$$H(t) = -i[f(t)a^\dagger - f^*(t)a]J_y,$$

with $J_y = \sigma_y^{(1)} + \sigma_y^{(2)}$. Comparing with the Hamiltonian (12), only a basis changes from $J_z$ to $J_y$. Using a similar method, we find a gate given by $U(\gamma) = \exp(-i\gamma J_y\vec{J})$ with $\gamma(\tau) = \gamma^0(\tau)$ [21], and also have $\gamma^d(\tau) = -2\gamma^g(\tau) = 2\gamma(\tau)$.
Clearly, the quantum gates demonstrated above are just the unconventional geometric gates with a parameter-independent proportional constant. Therefore, they not only possess all geometric advantages that conventional geometric gates have but also are independent of initial states in the system, enabling one to reach the high fidelity. Nevertheless, we should note that the uncertainty of the phase in a general unconventional geometric quantum gate comes from two factors: fluctuations due to the conventional geometric phase term and the $\eta$ term. Generally speaking, an unconventional geometric gate is robust to the fluctuations or perturbations from the parameters which $\eta$ (and $\gamma^s$) is independent of. This is the reason why $\eta$ is required to be independent on at least some parameters of the qubit system; a perfect unconventional geometric gate is just the example illustrated above: $\eta$ is independent on all parameters of the system.

In conclusion, we have proposed a new class of unconventional geometric quantum gates. Comparing with conventional GQC, our proposal may simplify experimental operations, because additional operations to remove/avoid the dynamic phase are no longer required. Apart from the above-addressed systems related to the harmonic oscillators, it is of great significance to design and to implement this class of unconventional geometric gates in other physical systems.

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[26] Note that in the presence of small noncyclic perturbations the gate operator (3) may be modified as $\text{diag}[1, \nu \exp(i\gamma), \nu \exp(i\gamma), 1]$ with $\nu (\in [0, 1])$ the visibility being slightly less than unit, which may lead to a weak decoherence effect; but it is negligible, even inevitable. Quantitatively, for a small deviation $\Delta \tau$ of the period $T$, $\nu$ is estimated to be $1 - (2 \pi \Omega_D / \sqrt{2} \delta^2)(\Delta \tau / T)^2$ and the deviation of $\gamma$ is about $-2 \pi (2 \pi \Omega_D / \sqrt{6} \delta^2)(\Delta \tau / T)^2$.