High-Fidelity Single-Shot Toffoli Gate via Quantum Control

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A single-shot Toffoli, or controlled-controlled-NOT, gate is desirable for classical and quantum information processing. The Toffoli gate alone is universal for reversible computing and, accompanied by the Hadamard gate, forms a universal gate set for quantum computing. The Toffoli gate is also a key ingredient for (nontopological) quantum error correction. Currently Toffoli gates are achieved by decomposing into sequentially implemented single- and two-qubit gates, which require much longer times and yields lower overall fidelities compared to a single-shot implementation. We develop a quantum-control procedure to construct a single-shot Toffoli gate for three nearest-neighbor-coupled superconducting transmon systems such that the fidelity is 99.9% and is as fast as an entangling two-qubit gate under the same realistic conditions. The gate is achieved by a nongreedy quantum control procedure using our enhanced version of the differential evolution algorithm.

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Scalable quantum computing [1,2] requires a set of high-fidelity universal quantum gates with which to construct the circuit [2–4]. Experimental progress towards a high-fidelity universal set of gates comprising single- and two-qubit operations has been impressive, exceeding 99.9% for single-qubit gates and 99% for an entangling two-qubit gate [3], but an outstanding problem is that (nontopological) quantum error correcting codes require a gate acting on at least three qubits [5,6], with the Toffoli gate [7–9] being optimal. The Toffoli gate is also a key component for reversible arithmetic operations, such as the modular exponentiation, which is a necessary step in Shor's factoring algorithm [10].

The quantum Toffoli gate is to effect a three-qubit controlled-controlled-NOT (CCNOT) gate, which means that the third qubit is flipped only if the first two qubits are in the $|1\rangle$ state and not flipped otherwise. Thus far Toffoli gates are achieved by decomposing into single- and two-qubit gates with resultant fidelities limited to 81% in a postselected photonic circuit [11], 71% in an ion-trap system [7], 68.5% in a three-qubit circuit QED system [8], and 78% in a four-qubit circuit QED system [6]. We here introduce a nongreedy quantum-control approach for directly constructing Toffoli gates based on an enhanced version of the differential evolution (DE) algorithm [12,13]. We show that our scheme applied to the three nearest-neighbor-coupled superconducting transmon systems should produce a Toffoli gate operating with 99.9% fidelity and operating as fast as an entangling two-qubit gate under the same conditions. As our quantum-control-based approach [14] to realizing the Toffoli gate does not resort to decomposition, a fast Toffoli gate enables error correction with high fidelity under this scheme. An additional valuable benefit of realizing CCNOT directly is that the Hadamard (H) and CCNOT together make a universal gate set [15] with significant advantages over the oft-studied H, $\pi/8$ gate, and CNOT universal set [2].

Superconducting circuits offer a promising medium for realizing a high-fidelity CCNOT gate based on quantum control of three nearest-neighbor-coupled superconducting artificial atoms [3]. Our approach is to vary the energy levels for each of three individual superconducting atoms using time-dependent control electronics, which conveniently do not require additional microwave control [16]. A similar strategy has recently been employed successfully to design two-qubit controlled-Z gates, for which optimal pulses are found via a greedy algorithm [17]. We, however, have observed that existing optimization algorithms (including greedy algorithms) are insufficient to generate an optimal pulse for high-fidelity Toffoli gates, and, therefore, developed a nongreedy optimization scheme, referred to here as subspace-selective self-adaptive DE or SuSSADE.

We consider a linear chain of three nearest-neighbor-coupled superconducting artificial atoms, realized as transmons [3] with distinct locations labeled $k = 1, 2, 3$. The transmons have nondegenerate discrete energy levels, labeled $\{|j\rangle_k\}$, with $j = 0$ for the ground state. The energies are anharmonically spaced, with this spacing

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allowed to be dependent on the specific transmon. Whereas superconducting atoms contain many energy levels, we truncate all energy levels for $j > 3$ for each transmon as a CCNOT operates on at most three excitations.

Although the Toffoli gate acts on three qubits as per definition, our quantum-control procedure operates on the first four levels of each transmon. The Hamiltonian that generates Toffoli acts on the 4^3-dimensional Hilbert space $\mathcal{H}_4^{\otimes 3}$ with energy basis $\{|j \in \{0,1,2,3\}\rangle^{\otimes 3}\}$. We follow the standard practice of specifying transmon energy levels instead as frequencies with these atomic frequencies shifted by the frequency of a rotating-frame basis transformation: the shifted frequency of the kth transmon is Δ_k, and the anharmonicity of the jth level of the kth transmon is η_{jk}. Therefore, the energy of the kth transmon's jth level at time t is $h[j\Delta_k(t) - \eta_{jk}]$.

Nearest-neighbor transmons couple via an XY interaction with coupling strength between the kth and $(k+1)$th transmons denoted by g_k. The three-transmon Hamiltonian is thus [16]

$$\frac{\hat{H}(t)}{h} = \sum_{k=1}^{3}\sum_{j=0}^{3}(j\Delta_k(t) - \eta_{jk})|j\rangle_k\langle j|_k + \sum_{k=1}^{2}\frac{g_k}{2}(X_k X_{k+1} + Y_k Y_{k+1}), \tag{1}$$

for coupling operators

$$X_k = \sum_{j=1}^{3}\sqrt{j}\,|j-1\rangle_k\langle j|_k + \text{H.c.},$$
$$Y_k = -\sum_{j=1}^{3}\sqrt{-j}\,|j-1\rangle_k\langle j|_k + \text{H.c.}, \tag{2}$$

which are higher-dimensional generalizations of Pauli spin matrices [16,18], and H.c. denotes the Hermitian conjugate.

Here we employ Hamiltonian evolution to realize the CCZ gate, which effects $\alpha|0\rangle + \beta|1\rangle \mapsto \alpha|0\rangle - \beta|1\rangle$ on the third qubit only if the first two qubits are $|1\rangle$. The CCNOT and CCZ operations are equivalent under the local transformation $\text{CCNOT} = [\mathbb{1}\otimes\mathbb{1}\otimes H]\text{CCZ}[\mathbb{1}\otimes\mathbb{1}\otimes H]$ (similar to the equivalence between two-qubit CNOT and CZ gates), with H straightforward to implement as a fast single-qubit operation [19,20]. The CCZ gate is achieved by varying Δ_k of each superconducting atom over duration Θ with the resultant Hamiltonian-generated time-ordered $(\mathcal{T})$ evolution operator

$$U(\Theta) = \mathcal{T}\exp\left(-\mathrm{i}\int_0^\Theta \hat{H}(\tau)d\tau\right). \tag{3}$$

Whereas our approach enables generating any desirable pulse shape for Δ_k, here we consider two types of pulses: piecewise-constant and piecewise-error function. These time-dependent control pulses are constrained within the frequency range of a superconducting transmon system. We employ the less computationally expensive piecewise-constant function to demonstrate the existence of an optimal pulse for a high-fidelity Toffoli gate. However, the control electronics for superconducting systems is only capable of generating smooth pulses, which motivated us to consider a realistic case for which the control parameters are connected together via smooth error functions [16,21]. We show that the gate fidelity does not depend on the pulse shape, and only depends on the number of control parameters. Therefore, without any loss of generality, we choose the less computationally expensive piecewise-constant control function to analyze the fidelity of the designed gate against other parameters.

The Hamiltonian evolution (3) describes the unitary dynamics of the system in the absence of decoherence. Decoherence is incorporated by treating each atom as a damped harmonic oscillator characterized by amplitude and scattering induced phase-damping rates for each oscillator. The corresponding time scales are relaxation time T_1 and dephasing time T_2, analogous to the rates employed for two-level systems [2,22]. We here assume $T \coloneqq T_1 \equiv T_2$, which is valid for frequency-tunable transmons [16]. These decohering processes modify the unitary evolution (3) to a completely positive trace-preserving map $\mathcal{E}(\Theta)$, which is decomposable into an operator sum as discussed in the Supplemental Material [23].

A high-fidelity quantum gate is usually designed by determining an optimal control pulse for each frequency Δ_k neglecting open-system effects such as decoherence. Performance is assessed for the unitary evolution (3) projected to the computational subspace: $U_{\mathcal{P}}(\Theta) \coloneqq \mathcal{P}U(\Theta)\mathcal{P}$. The standard figure of merit for performance of $U_{\mathcal{P}}(\Theta)$ is the "intrinsic fidelity" (fidelity neglecting decoherence) with respect to the ideal gate, in this case CCZ, so the intrinsic fidelity is [13] $\mathcal{F} = \frac{1}{8}|\text{Tr}(\text{CCZ}^\dagger U_{\mathcal{P}}(\Theta))|$ with $\mathcal{F} = 1$ if $U_{\mathcal{P}}(\Theta) = \text{CCZ}$ and $0 \leq \mathcal{F} < 1$ otherwise. After determining control pulses that maximize $\mathcal{F}$, decoherence is then incorporated into the calculation to assess the performance under open-system conditions [16].

In the presence of decoherence, the efficacy of the nonunitary evolution compared to the target gate is quantified by the average state fidelity $\bar{\mathcal{F}}$, which is calculated as follows. For $\{|\psi_k\rangle \in \mathcal{H}_2^{\otimes 3}\}$ the set of three-transmon computational basis states, the nonunitary extension of the unitary evolution (3) transforms a pure computational basis state $|\psi_k\rangle\langle\psi_k|$ into a mixed state ρ_k^{final}. As each basis state $|\psi_k\rangle\langle\psi_k|$ remains invariant under an ideal CCZ gate, average state fidelity $\bar{\mathcal{F}} = \frac{1}{8}\sum_k\sqrt{|\langle\psi_k|\rho_k^{\text{final}}|\psi_k\rangle|}$ quantifies the efficacy of a quantum gate in the presence of intrinsic as well as decoherence-induced noise for a given optimal pulse. Whereas $\bar{\mathcal{F}} \approx 99.9\%$ is considered to be a threshold for topological (surface-code) fault tolerance for single- and two-qubit gates [3], our approach achieves this fidelity even for the three-qubit CCZ gate subject to realistic constraints of the control pulses. In this work, unless otherwise stated, the average state fidelity is referred to as fidelity.

The strategy for controlling the evolution (3) is to vary the frequencies so that energy levels approach each other but then avoid degeneracies, known as avoided level crossings. These avoided crossings mix energy-level populations and dynamical phases together. This avoided-crossing effect enables shaping the evolution toward the final time-evolution operator objective, which is obtained by maximizing $\mathcal{F}$.

Optimal pulse shapes for each Δ_k are obtained by discretizing the time duration Θ into N constant intervals of duration $\Delta\tau \coloneqq \Theta/N$, and the control-problem parameter space is spanned by the set of variables $\{\Delta_k(\ell\Delta\tau);\ \ell = 1, \ldots, N\}$ for each k. These control points are then connected via step functions or error functions to construct the pulse shapes as we described earlier. The CCZ optimization problem is nonconvex with a $3N$-dimensional parameter space corresponding to N parameters for each of the three frequencies $\Delta_{1,2,3}$. For a fixed $\Delta\tau$, therefore, the dimension of the parameter space increases linearly with the total time duration Θ, which influences which optimization methods work and which do not.

We devise a quantum-control procedure that designs an optimal pulse for a Toffoli gate, which operates as fast as a two-qubit gate [16] with a target intrinsic fidelity of 0.9999. We first use the existing optimization algorithms, namely, the quasi-Newton approach, which employs the Broyden-Fletcher-Goldfarb-Shanno (BFGS) approximation of the Hessian [35–39], simplex methods [40], several versions of particle swarm optimization [41,42], and differential evolution (DE) algorithms [13,43]; however, they all failed to reach the target intrinsic fidelity under the time constraint of the fast Toffoli gate. Therefore, we construct a new optimization algorithm here to realize a Toffoli gate that reaches our target.

Of these optimization approaches, DE yielded the best fidelity but failed to reach the target due to the well-known problems of searching high-dimensional parameter spaces [44]. This drawback motivated us to enhance DE for such high-dimensional problems by instead breeding over randomly selected low-dimensional subspaces, hence our name subspace-selective self-adaptive DE (SuSSADE) algorithm (see Supplemental Material [23]). One of our objectives is to demonstrate (numerically) the capability of SuSSADE with respect to finding a solution equally successfully regardless of parameter-space dimension within the regime that is relevant for current superconducting experiments.

To understand our enhancement, we first briefly review standard DE [43]. DE cooperatively evolves a collection of trial solutions, called chromosomes, towards an optimal solution. Chromosomes are labeled by their location in the parameter space, and optimization is thus a search for the best chromosome in this space. Evolution from one generation (i.e., chromosomes for one iteration step) to the next is achieved by breeding each chromosome with three other randomly chosen chromosomes from the same generation. Breeding yields a single daughter chromosome, and only the fittest of the original and daughter chromosome survives. This breeding-and-survival procedure continues until either a chromosome reaches the requisite $\mathcal{F}$ or the number of generations reaches a specified upper bound.

Whereas standard DE breeds chromosomes randomly selected from the entire space, our SuSSADE algorithm is much faster due to breeding being restricted some of the time to a subset of chromosomes drawn from a low-dimensional subspace, i.e., some fixed parameters and some variable parameters. Our algorithm randomly switches breeding between the subspace and the whole space according to the value of an input switch parameter $S \in [0, 1]$ such that a uniformly distributed random number $r_j \in [0, 1]$ at generation j restricts breeding to the subspace if $r_j < S$ and breeds in the whole space otherwise.

In the extreme case of restricting to one-dimensional subspaces, chromosomes can breed only if all but one of the parameters are the same. We refer to this one-dimensional extreme case as 1DSuSSADE. Henceforth, we use only 1DSuSSADE as it works well with $S = 0.14$ for designing the Toffoli gate.

Here we present two types of pulses that achieve the target intrinsic fidelity, and we explore how the performance of piecewise constant pulses vary with respect to the total gate time, coupling strength, and decoherence-induced noise. The success of our quantum control procedure corresponds to a target intrinsic fidelity of 0.9999 and a time scale comparable to a two-qubit gate [16].

Figure 1 shows both the piecewise constant as well as piecewise-error-function pulses that achieve the target intrinsic fidelity obtained by optimizing all the parameters within the experimental constraints. The CCZ gate corresponding to Fig. 1 requires a total gate time of 26 ns given a coupling strength of $g = 30$ MHz [16,17]. Comparing the intrinsic fidelities of Figs. 1(a) and 1(b) shows that the target fidelity does not depend on the shape of the pulse; rather it depends on the number of control parameters. In what follows, therefore, we consider only the piecewise-constant pulse shapes as these are computationally less expensive to handle and also do not compromise the generality of our results. We show in Fig. 2 how the (maximized) intrinsic fidelity changes when the parameters g and Θ are varied within a range commensurate with currently available superconducting circuits [3]. Figure 2(a) gives the intrinsic fidelity as a function of total gate time for various coupling strengths g. Figure 2(b) shows that the total gate time changes linearly with the coupling g, in order to achieve a given fidelity. Finally, we consider the effect of decoherence on the approximate CCZ gate obtained by optimal pulses shown in Fig. 1(a), and compute the fidelity $\bar{\mathcal{F}}$. Amplitude-damping

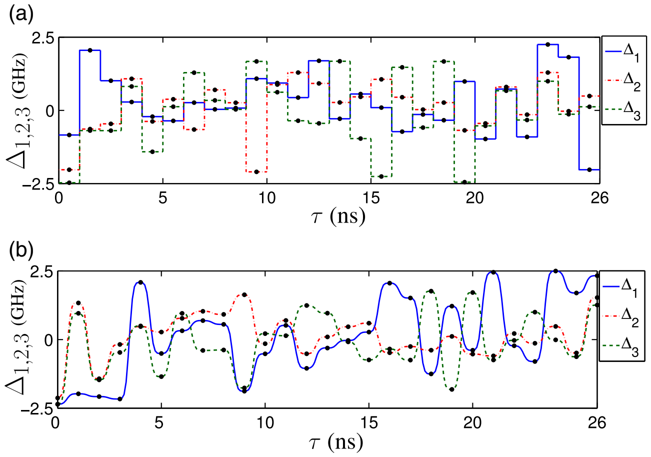

FIG. 1 (color online). Optimal pulse shapes for the Toffoli gate given as frequency detunings Δ_i (for the $i = 1, 2, 3$) of the superconducting atoms, corresponding to the (a) piecewise-constant and (b) error-function-based pulse profiles, as a function of time τ with constant step-size time interval $\Delta\tau = 1$ ns and with $\mathcal{F} = 0.9999$ and $g = 30$ MHz. The black dots on both plots show the control parameters used to optimize the shape of the pulses.

and phase-damping rates (T_1^{-1} and T_2^{-1}) are treated as the dominant forms of decoherence. For fast gates with $\Theta \ll T$, but with decoherence more significant than intrinsic errors, an order-of-magnitude estimate yields $1 - \bar{\mathcal{F}} \sim \Theta/T$ [16], which is consistent with the numerically evaluated plot of $\bar{\mathcal{F}}$ vs T in Fig. 3. We have employed our quantum control procedure to determine the optimal pulse (Fig. 1) for a high-fidelity single-shot three-qubit Toffoli gate. We computed a smooth pulse [Fig. 1(b)], for which the control parameters are separated by 1 ns and connected via error functions, thereby ensuring that the pulse is compatible with the power and bandwidth specifications of standard control electronics. Applying our approach to the three nearest-neighbor-coupled superconducting transmon systems produces a fast and high-fidelity Toffoli gate in 26 ns, which matches the time scale for the two-qubit avoided-crossing-based CZ gate.

The longer total gate time, with a fixed $\Delta\tau$, generates a higher-dimensional parameter space for the optimization algorithm. The monotonically increasing optimized intrinsic fidelity in Fig. 2(a) with increasing total time thus demonstrates the capability of our algorithm for a parameter regime relevant to superconducting experiments, for which alternative algorithms fail. The linear relationship between $1/\Theta$ and g demonstrates that faster gate speed requires higher coupling. This relation is a characteristic signature for avoided-crossing-based gates (as also obtained for avoided-crossing-based two-qubit gates [16]) assuming the corresponding optimization algorithm is capable of finding the optimal solution regardless of the parameter space dimension.

The effect of decoherence on the performance of the optimal Toffoli gate has been explored (Fig. 3), and we interpret the corresponding result as follows: when $T \gg \Theta$, the effect of thermal noise becomes less dominant, and the fidelity of a quantum gate is almost entirely contributed by the intrinsic fidelity. Here we have been able to design a fast and optimal pulse for a Toffoli gate using our quantum control approach for which the intrinsic fidelity is so high (~99.99%), that the fidelity ($\bar{\mathcal{F}} \sim 99.9\%$) is significantly contributed by the decoherence-induced noise, which is also very small (compared to previous realizations) for the state-of-the-art superconducting atoms with $T \sim 20$–$60\ \mu$s [3].

In summary, we have devised a powerful quantum control scheme, named SuSSADE, to design a fast and high-fidelity single-shot Toffoli gate for a scalable chain of the nearest-neighbor-coupled three-transmon system. The time required for the Toffoli operation is comparable with the time scale of the two-qubit avoided-crossing-based CZ gate, which is the key advantage our quantum-control approach offers compared to decomposition-based approaches requiring many such two-qubit gates to implement a single CCZ operation. Our three-transmon system serves as a module for all 1D and 2D quantum computing architectures [45], and, therefore, one can realize our scheme in a large-scale multiqubit architecture, if the undesired couplings are turned off [46]. Our approach demonstrates the efficacy of SuSSADE for

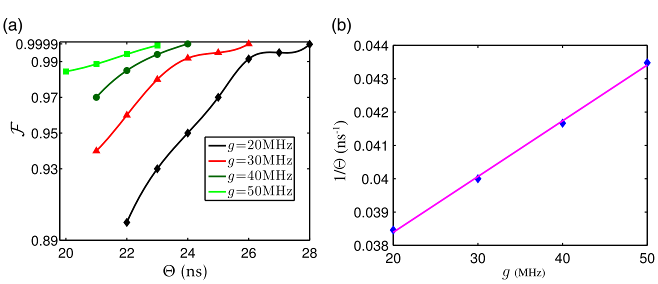

FIG. 2 (color online). (a) Intrinsic fidelity $\mathcal{F}$ vs total gate time Θ for various coupling strengths g and (b) $1/\Theta$ vs g for $\mathcal{F} = 0.999$. The ◇, △, ∘, and □ denote the actual numerical computations using 1DSuSSADE, and solid lines depict cubic-fit curves.

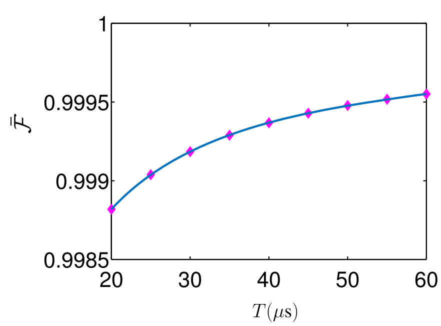

FIG. 3 (color online). The fidelity $\bar{\mathcal{F}}$ is plotted against the coherence times T. We assume $T = T_1 = T_2$, with T_1 and T_2 the relaxation time and dephasing time of each transmon, respectively. This assumption is valid for tunable transmons. Each ◇ denotes an actual numerical result obtained from the decoherence calculation. The solid line depicts the cubic-fit curve.

designing quantum gates as well as yielding the concrete example of a three-qubit gate required for scalable quantum-error correction.

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