Minimum Construction of Two-Qubit Quantum Operations

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Optimal construction of quantum operations is a fundamental problem in the realization of quantum computation. We here introduce a newly discovered quantum gate, B, that can implement any arbitrary two-qubit quantum operation with minimal number of both two- and single-qubit gates. We show this by giving an analytic circuit that implements a generic nonlocal two-qubit operation from just two applications of the B gate. Realization of the B gate is illustrated with an example of charge-coupled superconducting qubits for which the B gate is seen to be generated in shorter time than the CNOT gate.

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Quantum computation requires achieving unitary operations on arrays of coupled qubits in order to realize the speedup associated with quantum algorithms. It is usually described in the quantum circuit model with combinations of single- and two-qubit operations [1]. While the algorithmic complexity is independent of the efficiency of these circuits, which are known to be interchangeable with a polynomial overhead [2], the performance of any physical realization of a quantum circuit may be highly dependent on minimal switchings of control fields and interaction Hamiltonians and achieving a minimal time of gate operations, due to the introduction of decoherence arising from unwanted interactions between qubits and/or with the external environment. Efficient construction of any arbitrary two-qubit quantum operation is thus of high priority in the search for a realizable quantum information processor. The current standard paradigm is based on a combination of quantum controlled-NOT (CNOT) gates between pairs of qubits and single-qubit gates [1]. Recent work shows that the CNOT gate is also one of the most efficient quantum gates known, in that just three applications supplemented with local gates can implement any arbitrary two-qubit operation [3–6]. In this Letter, we introduce a minimum construction from a newly discovered quantum gate B to implement any arbitrary two-qubit quantum operation with two applications of B together with six single-qubit gates, both of which are the least possible.

The single-qubit operations are generally easily implemented by a local Hamiltonian or external field and can be finitely generated by any convenient basis on su(2) [7]. In contrast, two-qubit operations are highly dependent on the physical implementation, and it is in general much more difficult to implement an *arbitrary* two-qubit operation. The number of single-qubit gates can be independently optimized from a carefully chosen library [4] once the intrinsic quantum circuit structure of two-qubit gates is determined. It is therefore advantageous to employ the concept of *locally equivalent* two-qubit gates, namely, $U = k_1 U_1 k_2$, where k_1, k_2 are local unitary gates, in order to obtain the minimal total circuit length. We denote the local equivalence relation by $U \sim U_1$. It has been shown that two gates are locally equivalent if and only if they have identical values of three invariants [8]. Classification of two-qubit gates based on these invariants was given an intuitive geometric interpretation in [9], which is summarized in Fig. 1. Each point in the tetrahedron (also known as the Weyl chamber, from the specific group symmetries used in its construction) represents a local

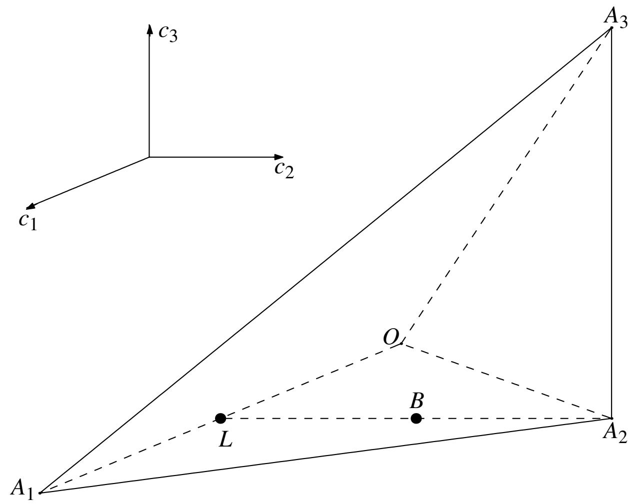

FIG. 1. Tetrahedron $OA_1A_2A_3$ contains all the local equivalence classes of nonlocal gates [9], where $O([0,0,0])$ and $A_1([\pi,0,0])$ both correspond to local gates, $L([\frac{\pi}{2},0,0])$ to the CNOT gate, $A_2([\frac{\pi}{2},\frac{\pi}{2},0])$ to the double-CNOT gate, $A_3([\frac{\pi}{2},\frac{\pi}{2},\frac{\pi}{2}])$ to the SWAP gate, and $B([\frac{\pi}{2},\frac{\pi}{4},0])$ to the new gate we introduce in this Letter. From the Cartan decomposition on su(4), any two-qubit unitary operation $U \in \mathrm{SU}(4)$ can be written as $U = k_1 A k_2 = k_1 e^{c_1(i/2)\sigma_x^1\sigma_x^2} e^{c_2(i/2)\sigma_y^1\sigma_y^2} e^{c_3(i/2)\sigma_z^1\sigma_z^2} k_2$, where $\sigma_\alpha^1\sigma_\alpha^2 = \sigma_\alpha \otimes \sigma_\alpha$, σ_α are the Pauli matrices, and $k_1, k_2 \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$ are local gates [9–11]. Since the local gates are fully accessible, it is evident that we need to construct a circuit for only the nonlocal block A in terms of the available entangling gates (or Hamiltonians).

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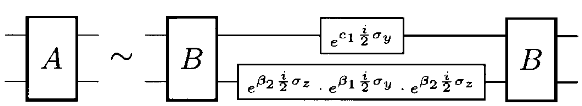
equivalence class of nonlocal gate U, with the exception of vertices O and A_1 which are local gates. The special status of CNOT was demonstrated by an analysis of circuit optimality within the geometric approach, which showed that it is indeed the most efficient controlled-unitary operation and requires only three applications to construct any arbitrary two-qubit quantum operation [6]. These and related [3–5] investigations of optimality with CNOT motivate the enquiry as to the existence of two-qubit gates that may be even more efficient than CNOT. The demonstration of at least one gate [the double-CNOT (DCNOT) gate] that is *equally efficient* as CNOT, requiring also just three applications together with at most eight single-qubit gates to construct any two-qubit operation, is one step in this direction [6].

We have now discovered a new quantum gate that possesses greater efficiency than both the CNOT and double-CNOT gates and that provides the desired minimal number of gate switchings to simulate an arbitrary two-qubit quantum operation. The new gate, which we term the B gate, is the following: $B = e^{(\pi/2)(i/2)\sigma_x^1\sigma_x^2} e^{(\pi/4)(i/2)\sigma_y^1\sigma_y^2}$. In the geometric representation illustrated in Fig. 1, this gate is located at point B on the base of the tetrahedron $OA_1A_2A_3$. This is a point of high symmetry, lying in the center of the region of gates on the base that can generate the maximum amount of entanglement [9] when no local ancillas are allowed [12,10]. This gate has the remarkable quality that only *two* applications together with at most *six* single-qubit gates can simulate any arbitrary two-qubit unitary. We show this by giving an analytic circuit that implements a generic nonlocal operation from B. Such a generic nonlocal operation is $A = e^{c_1(i/2)\sigma_x^1\sigma_x^2} e^{c_2(i/2)\sigma_y^1\sigma_y^2} e^{c_3(i/2)\sigma_z^1\sigma_z^2}$ [9–11]. As discussed in Ref. [9], the local invariants of A can be completely defined in terms of the coefficients $[c_1, c_2, c_3]$, which correspond to the Cartesian coordinates in Fig. 1. The values of these coordinates for points in the tetrahedron therefore provide a complete parametrization of all possible nonlocal gates.

Simulation of this generic nonlocal operation can be done with the following quantum circuit:



where the parameters β_1 and β_2 satisfy

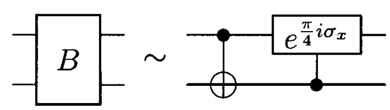
$$\cos\beta_1 = 1 - 4\sin^2\frac{c_2}{2}\cos^2\frac{c_3}{2}, \qquad \sin\beta_2 = \sqrt{\frac{\cos c_2 \cos c_3}{1 - 2\sin^2(c_2/2)\cos^2(c_3/2)}}. \tag{1}$$

To prove that the above quantum circuit is indeed locally equivalent to A, we follow the procedure of Refs. [8,9] to calculate the local invariants of this quantum circuit as

$$g_1 = 4\cos c_1 \cos^2\frac{\beta_1}{2}\sin^2\beta_2, \qquad g_2 = 4\sin c_1 \sin\beta_1 \cos\beta_2,$$
$$g_3 = 2[\cos^4\beta_2(\cos\beta_1 + 1)^2 + 2\cos^2\beta_2(\cos^2\beta_1 - 2\cos\beta_1 - 3) + 4\cos^2 c_1 + \cos^2\beta_1 + 2\cos\beta_1 - 1]. \tag{2}$$

Substituting Eq. (1) into Eq. (2), with some subsequent simplifications, leads to the demonstration that the local invariants of this quantum circuit are identical to those of the generic nonlocal operation A [see Eq. (25) in Ref. [9]]. Hence, this quantum circuit provides an analytic construction for realization of any arbitrary two-qubit operation. Note that in this circuit, at most six single-qubit gates are needed.

The new B gate is not a controlled-unitary gate. These lie on the line OA_1 in Fig. 1 (note that OL is equivalent to A_1L [9]). B is instead a completely new gate with a different character from the CNOT gate and any other familiar quantum gate. It is locally equivalent to a gate that performs the operation $|m\rangle \otimes |n\rangle \rightarrow e^{(\pi/4)i\sigma_x(m\oplus n)}|m\rangle \otimes |m \oplus n\rangle$ on the computational basis. We can thus describe gate B by a simple circuit in terms of commonly used quantum gates as follows:



This quantum circuit consists of a CNOT gate with the control qubit on the top wire following a controlled-$e^{(\pi/4)i\sigma_x}$ gate with the control qubit on the bottom wire. The local equivalence between gate B and this quantum circuit can be proved by showing that they both have local invariants $g_1 = g_2 = g_3 = 0$. Given the greater efficiency of the B gate relative to the standard CNOT for constructing arbitrary two-qubit unitaries, it will be interesting to explore the use of this new gate for construction of quantum compilers and quantum algorithms [13,14], and in quantum error correction [15,16].

We now consider how the new B gate may be realized in experiments. Since the B gate is optimal in constructing a quantum circuit, this suggests that one might always prefer to implement B as the elementary two-qubit gate for any given physical system. However, the ease and efficiency of constructing the elementary gates for quantum computation from an available Hamiltonian is also a critical issue for realization of quantum circuits [17–19]. Optimally efficient construction of quantum operations is realized by the quantum circuit which contains a minimal number of single- and two-qubit gates, where *each* gate is itself also implemented with a minimal application time. From a physical perspective, there are therefore two aspects to optimality, namely, the circuit gate count and the cost (e.g., in time) for physical generation of individual gates from the physical Hamiltonian. Our result above shows that the B gate is optimal for the former. Concerning the second question of cost in constructing gates from a given Hamiltonian, we find that this depends on the form of the Hamiltonian, with the B gate easier to implement than the CNOT (or DCNOT) gate in some situations while the CNOT (or DCNOT) gate may be easier to achieve in other situations. As a simple example, we can consider pure nonlocal Hamiltonians, i.e., those containing no single-qubit terms. From the geometric theory [9], it is straightforward to prove that when the physical Hamiltonians are $\sigma_z^1\sigma_z^2$ (Ising interaction), $\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2$ (XY interaction), and $2\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2$, it requires only one switching to implement the CNOT, the DCNOT, and the B gate, respectively. The overall circuit optimality is thus implicitly linked to the particular choice of physical implementation.

We now illustrate physical generation of the B gate with an example where B is seen to be implemented with a shorter application time than CNOT and hence provides an overall optimal circuit. We consider charge-based Josephson qubits that are inductively coupled [20]. The elementary two-qubit operations are generated by the interaction Hamiltonian $H_J = -\frac{1}{2}E_J(\sigma_x^1 + \sigma_x^2) + (E_J^2/E_L)\sigma_y^1\sigma_y^2$, where E_J is the single-qubit Josephson energy and E_L is a scale factor. Without loss of generality we can set $E_J = \alpha E_L$, so that $H_J = -\frac{1}{2}\alpha E_L(\sigma_x^1 + \sigma_x^2) + \alpha^2 E_L\sigma_y^1\sigma_y^2$, and consider $E_L = 1$. Estimates based on current circuit capabilities suggest that values $0.01 \leq \alpha \simeq 1$ are feasible [21]. Application of this two-qubit Hamiltonian generates a unitary evolution $U = e^{iH_J t}$ (with $\hbar = 1$) that is characterized by the three local invariants [9]

$$g_1 = \frac{4}{1+\alpha^2}[\alpha^2(x^2+y^2-1)+x^2], \quad g_2 = 0,$$
$$g_3 = \frac{4}{1+\alpha^2}(3\alpha^2 - 1 - 4y^2\alpha^2 + 8\alpha^2x^2y^2 + 4x^2 - 4x^2\alpha^2), \tag{3}$$

where $x = \cos\alpha^2 t$ and $y = \cos\sqrt{(\alpha^2+1)}\alpha t$. The geometric theory provides us with the means to translate the time-dependent values of these invariants to a trajectory of points in the tetrahedron of Fig. 1 and hence to the specific nonlocal two-qubit gates that are naturally implemented as a function of this time evolution. From the second invariant, $g_2 = 0$, we obtain the Cartesian coordinate $c_3 = 0$ in Fig. 1, which implies that all nonlocal operations that are generated by one application of H_J must be located on the base of the tetrahedron $OA_1A_2A_3$. The CNOT gate is located at the point L in Fig. 1, whereas the B gate is located in the middle of the triangular base (see also Fig. 2). Each of these gates represents a different local equivalence class and is characterized by its own set of values (g_1, g_2, g_3). For CNOT $(g_1, g_2, g_3) = (0, 0, 4)$ [9], whereas for the B gate $(g_1, g_2, g_3) = (0, 0, 0)$. Thus to find conditions such that the Hamiltonian H_J exactly achieves either of these gates in one application, we need to both tune the Hamiltonian parameter α and also to find the time duration t that solves Eq. (3) for the corresponding values of g_1 and g_3. Whenever there is no solution, at least two switchings of the Hamiltonian will be required to reach the target gate.

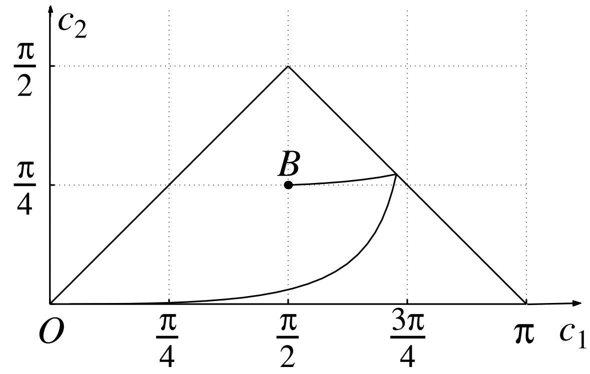


FIG. 2. Trajectory of inductively coupled Josephson junction qubits that generates gate B from the Hamiltonian H_J. Shown here is the minimum time solution, which is obtained for the Hamiltonian parameters $E_L = 1$, $\alpha = 1.1436$ with minimal time duration $t = 1.5014$. The trajectory is confined to the c_1, c_2 basal plane of the tetrahedron $OA_1A_2A_3$ of Fig. 1.

In [9], we have shown that the time optimal solution to reach CNOT in a single application is achieved when $\alpha = 1.1992$, with application time $t = 2.7309$. In contrast, the new B gate is found to be reached with a shorter single application time of H_J for its optimal solution, which has a similar value of α. After some algebraic work, we find that the solutions to Eq. (3) for $g_1 = g_3 = 0$ must satisfy

$$x = \cos\frac{2n+1}{8}\pi, \qquad y^2 = 1 - \frac{1+\alpha^2}{\alpha^2}x^2, \tag{4}$$

where n is an integer. Hence the time t at which B is achieved is $t = (2n+1)\pi/8\alpha^2$, where α satisfies

$$\sin^2\sqrt{1+\alpha^{-2}}\frac{2n+1}{8}\pi = \frac{1+\alpha^2}{\alpha^2}\cos^2\frac{2n+1}{8}\pi. \tag{5}$$

The numerical solution indicates that the allowable values of α constitute an infinite set. The minimum time solution is obtained for $\alpha = 1.1436$, with corresponding minimum application time $t = 1.5014$. The trajectory representing this time evolution through the nonlocal gate space to the target gate B is shown in Fig. 2. Thus, in this physical system the dual savings of shorter application time of the B gate over CNOT will add to the smaller number of gate applications required to implement an arbitrary operation, resulting in significantly less introduction of decoherence in experimental implementations of quantum logic and simulations that are based on the B gate.

In summary, we have presented a new quantum gate B that provides a direct analytic recipe to efficiently implement any arbitrary two-qubit quantum operation with just two applications. This is more efficient than the standard CNOT gate and the double-CNOT gate, both of which require three applications to realize an arbitrary two-qubit unitary. The B gate indeed achieves the minimum number possible, as is easily seen by recognizing that a circuit consisting of just one application of a given two-qubit gate together with local unitaries can produce only quantum operations that are locally equivalent to that given gate. To simulate an arbitrary two-qubit operation with this B gate, we need only to determine two parameters in a simple quantum circuit. An explicit expression for these two parameters is given here. Taken together with at most six single-qubit gates accompanying this minimal two-qubit gate count, this provides a new paradigm for optimally efficient construction of quantum operations.

We have illustrated the physical generation of B with the example of inductively coupled Josephson junction qubits, for which generation of B is also seen to be more efficient than generation of CNOT in that it requires less application time. In this situation, the new gate provides an optimal route from the Hamiltonian to any arbitrary two-qubit quantum operation, thereby providing an efficient realization of one of the basic requirements for quantum circuit construction. A similar analysis can be made for other physical implementations using the time evolution approach described above and in Ref. [9]. Given these advantages of the new B gate, we expect it will be very useful for the further development of quantum computation.

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