Optimal two-qubit quantum circuits using exchange interactions

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We give the optimal decomposition of a universal two-qubit circuit using Heisenberg exchange interactions and single qubit rotations. Tuning the strength and duration of the Heisenberg exchange allows one to implement $(\mathrm{SWAP})^\alpha$ gates. Our optimal circuit is constructed from only *three* $(\mathrm{SWAP})^\alpha$ gates and *six* single qubit gates. We show that three $(\mathrm{SWAP})^\alpha$ gates are not only sufficient, but necessary. Since six single-qubit gates are already known to be necessary, our implementation is optimal in gate count.

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I. INTRODUCTION

In several general solid-state quantum computation appoaches [1–6], two-qubit interactions are generated by a tunable exchange interaction. For example, the Heisenberg exchange between two electron spin qubits results in a $(\mathrm{SWAP})^\alpha$ gate, where the exponent α is controlled by adjusting the strength and duration of Heisenberg exchange. Single-qubit rotations have also been proposed for solid-state computation; notable mechanisms for rotating spin qubits being g-tensor resonance [7,8] and localized magnetic resonance [9]. In general, it is desirable to optimize quantum circuits with respect to the number of physical operations required, which for most solid-state quantum computation proposals implies that circuits should be optimized with respect to the number of $(\mathrm{SWAP})^\alpha$ operations and single-qubit rotations.

The problem of optimizing quantum circuits for executing general n-qubit operations is computationally intractable. Hence, just as in the classical computation case, one needs to develop techniques for optimizing only few-qubit circuits and then assemble these circuits together in a modular fashion. Toward this end, circuit optimization results have mostly dealt with the case where controlled-NOT (CNOT) gates and single-qubit rotations are the basic building blocks. For example, for a general two-qubit unitary operation, it has been recently shown that three CNOT gates and additional single-qubit rotations are sufficient and necessary [10,11]. Now, it is known that one CNOT gate can be realized by two $(\mathrm{SWAP})^{1/2}$ gates and single-qubit unitary gates [1]. Hence, six $(\mathrm{SWAP})^{1/2}$ gates are sufficient to implement any two-qubit operation. The question is whether this strategy of simple substitution is optimal? Or, are $(\mathrm{SWAP})^\alpha$ gates just as efficient as CNOT gates (in terms of gate count) in performing two-qubit operations? Our answer to the latter is in the affirmative: The $(\mathrm{SWAP})^\alpha$ *gates and CNOT gates are both equally efficient* at realizing any two-qubit quantum operation (when measured in terms of number of gates), and that, in order to achieve optimal realizations *each type of circuit requires its own optimization scheme*.

The primary results of our paper are as follows. An arbitrary two-qubit operation can be implemented using only three $(\mathrm{SWAP})^\alpha$ gates and six single-qubit rotations. We augment this result with a number of lower bounds. First, we show that, by considering entanglement power alone, a CNOT gate requires at least two $(\mathrm{SWAP})^\alpha$ gates. Next, we prove that three $(\mathrm{SWAP})^\alpha$ gates are not only sufficient, but in fact necessary, to implement an arbitrary two-qubit operation. Our universal two-qubit circuit is optimal in the number of both $(\mathrm{SWAP})^\alpha$ and single qubit gates.

II. HEISENBERG INTERACTION

Let us first fix some notation; the four Bell states are written as $|\Phi^\pm\rangle=(1/\sqrt{2})(|00\rangle\pm|11\rangle)$, $|\Psi^\pm\rangle=(1/\sqrt{2})\times(|01\rangle\pm|10\rangle)$. The SWAP gate is defined as $\mathrm{SWAP}|\psi\rangle|\phi\rangle=|\phi\rangle|\psi\rangle$. For a $\mathcal{C}^2\otimes\mathcal{C}^2$ system, it can be written explicitly as

$$\mathrm{SWAP}=|\Phi^+\rangle\langle\Phi^+|+|\Phi^-\rangle\langle\Phi^-|+|\Psi^+\rangle\langle\Psi^+|+e^{i\pi}|\Psi^-\rangle\langle\Psi^-|. \tag{1}$$

In this paper, our basic two-qubit gate is $(\mathrm{SWAP})^\alpha$; it can be written as

$$(\mathrm{SWAP})^\alpha=|\Phi^+\rangle\langle\Phi^+|+|\Phi^-\rangle\langle\Phi^-|+|\Psi^+\rangle\langle\Psi^+|+e^{i\pi\alpha}|\Psi^-\rangle\langle\Psi^-| = \begin{pmatrix} 1 & 0 & 0 & 0\\ 0 & \frac{1+e^{i\pi\alpha}}{2} & \frac{1-e^{i\pi\alpha}}{2} & 0\\ 0 & \frac{1-e^{i\pi\alpha}}{2} & \frac{1+e^{i\pi\alpha}}{2} & 0\\ 0 & 0 & 0 & 1\end{pmatrix}. \tag{2}$$

The Hamiltonian of the isotropic Heisenberg exchange interaction between electron spins $\vec{S}_1$ and $\vec{S}_2$ is

$$\mathcal{H}=J(t)\vec{S}_1\cdot\vec{S}_2, \tag{3}$$

where $\vec{S}=\{\sigma_x,\sigma_y,\sigma_z\}$ is a vector of Pauli matrices

$$\sigma_x=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},\quad \sigma_z=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{4}$$

The coupling constant $J(t)$ can in principal be tuned for confined electrons [1]. The unitary operator generated by this Hamiltonian is

$$U_{12} = \exp\left(-\frac{i}{\hbar}\vec{S}_1 \cdot \vec{S}_2 \int J(t)dt\right). \quad (5)$$

By adjusting the integrated coupling $\int J(t)dt$, the unitary operator U_{12} can naturally realize the gate $(\mathrm{SWAP})^\alpha$ where $\alpha = \int J(t)dt/h$. In this paper, we will use the $(\mathrm{SWAP})^\alpha$ gate as the two-qubit gate. It was proposed to use the Heisenberg interaction *alone* to implement quantum computing [4–6]. This scheme encodes one logical qubit as three physical qubits. Additionally, one CNOT gate requires 19 Heisenberg interactions among the six physical qubits. We consider the scheme where *both Heisenberg interaction*, as well as, *single-qubit rotations* are available.

III. CNOT GATE REQUIRES TWO $(\mathrm{SWAP})^\alpha$ GATES

We know that one CNOT gate can be realized by two square root of SWAP gates, $\sqrt{\mathrm{SWAP}}$. If we use a more general gate, $(\mathrm{SWAP})^\alpha$, can we realize the CNOT by only one $(\mathrm{SWAP})^\alpha$ gate and a certain number of single-qubit rotations? By studying the nonlocal invariants of the quantum gates, Makhlin showed that the CNOT gate cannot be constructed by applying the Heisenberg interaction $\mathcal{H}$ only once, i.e., two $(\mathrm{SWAP})^\alpha$ gates are necessary to construct one CNOT [12]. In this section, we give a different proof, using entanglement power, to show that the CNOT gate requires at least two $(\mathrm{SWAP})^\alpha$ gates.

The entanglement power of a unitary operator $U \in \mathrm{SU}(4)$ is defined as

$$E_p(U) = \mathrm{average}_{|\psi_1\rangle\otimes|\psi_2\rangle}[E(U|\psi_1\rangle \otimes |\psi_2\rangle)], \quad (6)$$

where the average is over all product states $|\psi_1\rangle\otimes|\psi_2\rangle \in \mathcal{C}^2 \otimes \mathcal{C}^2$ in uniform distribution, see [13], and E is the linear entropy which is also the concurrence [14]. Note that for arbitrary $U_1\otimes U_2 \in \mathrm{SU}(2)\otimes\mathrm{SU}(2)$, $E_p(U)=E_p(U_1\otimes U_2 U)$. So, the entanglement power of $(u_1\otimes v_1)(\mathrm{SWAP})^\alpha(u_2\otimes v_2)$ is actually the entanglement power of $(\mathrm{SWAP})^\alpha$.

A simple formula can be used to calculate the entanglement power [11,13]

$$E_p(U) = \frac{5}{9} - \frac{1}{36}[\langle U^{\otimes 2}, T_{1,3}U^{\otimes 2}T_{1,3}\rangle + \langle(\mathrm{SWAP}\cdot U)^{\otimes 2}, T_{1,3}(\mathrm{SWAP}\cdot U)^{\otimes 2}T_{1,3}\rangle], \quad (7)$$

where $T_{1,3}$ acting on $\mathcal{C}^2\otimes\mathcal{C}^2\otimes\mathcal{C}^2\otimes\mathcal{C}^2$ is the transposition operator: $T_{1,3}|a,b,c,d\rangle = |c,b,a,c\rangle$. By tedious but straightforward calculations we can show that

$$E_p[(\mathrm{SWAP})^\alpha] = \frac{1}{12} - \frac{1}{12}\cos(2\pi\alpha). \quad (8)$$

For detailed calculations, see Appendix A in Ref. [18]. When $\alpha=1/2$, $(\mathrm{SWAP})^\alpha$ has a maximum entanglement power of 1/6. Since the entanglement power of CNOT is 2/9 [11], which is strictly larger than 1/6, one $(\mathrm{SWAP})^\alpha$ operator with the help of single-qubit gates is not sufficient to realize the CNOT. Hence, at least two $(\mathrm{SWAP})^\alpha$ gates are necessary to realize a general SU(4) operator.

IV. GENERAL TWO-QUBIT OPERATION

Kraus and Cirac [15] gave the following result (see also [16]): an arbitrary unitary transformation $U \in \mathrm{SU}(4)$ has the decomposition

$$U = (u_4' \otimes v_4')e^{-iH}(u_1 \otimes v_1), \quad (9)$$

where $u_1, v_1, u_4', v_4' \in \mathrm{SU}(2)$, and

$$H \equiv h_x\sigma_x \otimes \sigma_x + h_y\sigma_y \otimes \sigma_y + h_z\sigma_z \otimes \sigma_z, \quad (10)$$

where $\pi/4 \geqslant h_x \geqslant h_y \geqslant h_z \geqslant 0$. Then H in (10) can be written as

$$H = \lambda_{00}|\Phi^+\rangle\langle\Phi^+| + \lambda_{01}|\Psi^+\rangle\langle\Psi^+| + \lambda_{10}|\Phi^-\rangle\langle\Phi^-| + \lambda_{11}|\Psi^-\rangle\langle\Psi^-|, \quad (11)$$

with

$$\lambda_{00} = h_x - h_y + h_z, \quad \lambda_{01} = h_x + h_y - h_z,$$

$$\lambda_{10} = -h_x + h_y + h_z, \quad \lambda_{11} = -h_x - h_y - h_z. \quad (12)$$

The diagonal form of H thus gives

$$e^{-iH} = e^{-i\lambda_{00}}|\Phi^+\rangle\langle\Phi^+| + e^{-i\lambda_{01}}|\Psi^+\rangle\langle\Psi^+| + e^{-i\lambda_{10}}|\Phi^-\rangle\langle\Phi^-| + e^{-i\lambda_{11}}|\Psi^-\rangle\langle\Psi^-|. \quad (13)$$

Vidal and Dawson [10] and Vatan and Williams [11] have shown that the operator e^{-iH} can be realized by only three CNOT gates and some single-qubit rotation gates. Thus an arbitrary $U \in \mathrm{SU}(4)$ can be realized by three CNOT gates and additional single-qubit gates; see also the Appendix B in Ref. [18].

V. ARBITRARY TWO-QUBIT UNITARY OPERATIONS REQUIRE ONLY THREE $(\mathrm{SWAP})^\alpha$ GATES AND SIX SINGLE QUBIT GATES

Recall that a CNOT gate can be realized by two $(\mathrm{SWAP})^{1/2}$ gates and a few extra single qubit operations. We know the optimal circuit for a general $U \in \mathrm{SU}(4)$ needs three CNOT gates, so six $(\mathrm{SWAP})^\alpha$ gates are needed if we simply substitute SWAP circuits for CNOT gates. Our aim is to find a circuit to realize $U \in \mathrm{SU}(4)$ optimal in the number of $(\mathrm{SWAP})^\alpha$ gates.

From the result of Kraus and Cirac [Eq. (13)] [15], we need to create arbitrary phases on four Bell states by $(\mathrm{SWAP})^\alpha$ gates. But we already know that $(\mathrm{SWAP})^\alpha$ applies a phase to the Bell state $|\Psi^-\rangle$ while leaving the other three Bell states invariant. Also, by Pauli rotations on one particle of the bipartite state, we can transform the Bell states among each other. Thus, it is straightforward to create four independent phases on the Bell states. We can rewrite the operator $\exp(-iH)$ as

$$e^{-iH} = e^{i(h_z-h_x-h_y)}(|\Psi^+\rangle\langle\Psi^+| + e^{2i(h_x+h_y)}|\Psi^-\rangle\langle\Psi^-| + e^{2i(h_y-h_z)}|\Phi^+\rangle\langle\Phi^+| + e^{2i(h_x-h_z)}|\Phi^-\rangle\langle\Phi^-|). \quad (14)$$

This operator can be constructed by $(\mathrm{SWAP})^\alpha$ operators as

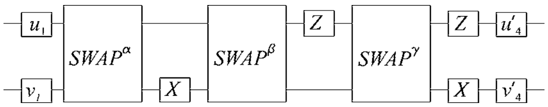

FIG. 1. Circuit for arbitrary unitary transformation $U \in \mathrm{SU}(4)$ as decomposed in Eqs. (9) and (16). Three SWAP gates and six local unitaries (upon combination of u'_4 and v'_4 with Z and X, respectively) are required.

$$e^{-iH} = e^{i(h_z-h_x-h_y)}[(I \otimes \sigma_x\sigma_z)(\mathrm{SWAP})^{2(h_y-h_z)/\pi}(I \otimes \sigma_z\sigma_x)][(I \otimes \sigma_x)(\mathrm{SWAP})^{2(h_x-h_z)/\pi}(I \otimes \sigma_x)][(\mathrm{SWAP})^{2(h_x+h_y)/\pi}]. \quad (15)$$

This circuit just involves three $(\mathrm{SWAP})^{\alpha}$ operators and single-qubit gates which are Pauli matrices. So as a whole, we can construct any $U \in \mathrm{SU}(4)$ by only three SWAP gates and single-qubit rotations. Note that besides Pauli matrices, general single-qubit rotations are also necessary to transform e^{-iH} to U.

Up to an overall phase, we can rewrite e^{-iH}

$$e^{-iH} = (\sigma_z \otimes \sigma_x)(\mathrm{SWAP})^{\gamma}(\sigma_z \otimes I)(\mathrm{SWAP})^{\beta}(I \otimes \sigma_x)\times(\mathrm{SWAP})^{\alpha}, \quad (16)$$

where $\alpha=2(h_x+h_y)/\pi$, $\beta=2(h_x-h_z)/\pi$, $\gamma=2(h_y-h_z)/\pi$. The corresponding circuit for U is illustrated in Fig. 1.

In any implementation, single-qubit rotations as well as two-qubit operations will require physical resources such as time and hardware. Hence, it is helpful to consider the number of single-qubit gates involved in each circuit as well. In the circuit of Vidal and Dawson [10], eight single-qubit gates are used to construct the general $U \in \mathrm{SU}(4)$, while in our circuit, six single-qubit gates are used. It is known that this is the least possible number of single-qubit rotations [17]. If we assume that each single-qubit rotation is as expensive as a two-qubit operation, then our circuit is potentially *cheaper*.

We next show that our circuit is optimal in the number of $(\mathrm{SWAP})^{\alpha}$ gates used, i.e., three $(\mathrm{SWAP})^{\alpha}$ gates are *necessary* to construct a general circuit. Let us write out a general unitary operator which contains just two $(\mathrm{SWAP})^{\alpha}$ gates

$$U = (U_1 \otimes V_1)(\mathrm{SWAP})^{\alpha}(U_2 \otimes V_2)(\mathrm{SWAP})^{\beta}(U_3 \otimes V_3), \quad (17)$$

where U_j, V_j, and $j=1,2,3$ are single-qubit operations.

One can group single-qubit unitaries about the $(\mathrm{SWAP})^{\alpha}$ operators as follows:

$$U = (U_1 \otimes V_1)(\mathrm{SWAP})^{\alpha}(U_1^{\dagger} \otimes V_1^{\dagger})(\widetilde{U}_2 \otimes \widetilde{V}_2)(\mathrm{SWAP})^{\beta}(\widetilde{U}_2^{\dagger} \otimes \widetilde{V}_2^{\dagger})(\widetilde{U}_3 \otimes \widetilde{V}_3), \quad (18)$$

where $\widetilde{U}_2=U_1U_2$, $\widetilde{V}_2=V_1V_2$, $\widetilde{U}_3=U_1U_2U_3$, and $\widetilde{V}_3=V_1V_2V_3$. Here we notice that operators $(U_1 \otimes V_1)(\mathrm{SWAP})^{\alpha}(U_1^{\dagger} \otimes V_1^{\dagger})$ and $(\widetilde{U}_2 \otimes \widetilde{V}_2)(\mathrm{SWAP})^{\beta}(\widetilde{U}_2^{\dagger} \otimes \widetilde{V}_2^{\dagger})$ are just SWAP gates in some different basis. So we can write this relation as

$$U = (\mathrm{SWAP})^{\alpha}(\widetilde{\mathrm{SWAP}})^{\beta}(u \otimes v). \quad (19)$$

A single $(\mathrm{SWAP})^{\alpha}$ gate can create one phase in one maximally entangled state, with the orthogonal three-dimensional space left invariant. So for two $(\mathrm{SWAP})^{\alpha}$ gates, there exist two maximally entangled orthogonal states, $|\chi_1\rangle$ and $|\chi_2\rangle$, simultaneously orthogonal to $|\Psi^-\rangle$ and $|\widetilde{\Psi}^-\rangle$. From the symmetry of the $(\mathrm{SWAP})^{\alpha}$ operation, it follows that for every two-$(\mathrm{SWAP})^{\alpha}$-gate circuit there exists at least two orthogonal and maximally entangled states such that they cannot be assigned a relative phase by the circuit. That is, the unitary operator corresponding to the two-$(\mathrm{SWAP})^{\alpha}$-gate circuit must satisfy $U|\chi_j\rangle=(u\otimes v)|\chi_j\rangle$, $j=1,2$. Note that local unitary operations cannot add a relative phase to two maximally entangled states. However, since a general two-qubit operation can assign independent phases to three maximally entangled states, one can find $U \in \mathrm{SU}(4)$ such that it will never satisfy the preceding constraint. Hence, two $(\mathrm{SWAP})^{\alpha}$ gates and single-qubit rotations are not sufficient to construct an arbitrary $U \in \mathrm{SU}(4)$.

VI. SPIN-BASED QUANTUM COMPUTATION BY SWAP CIRCUIT

In this section, we will estimate the real time required to implement our $(\mathrm{SWAP})^{\alpha}$ circuit. We consider both the GaAs and Si semiconductor systems; for review see Ref. [19]. A reasonable effective resonant magnetic field is $B=1$ mT, giving a Rabi frequency for an electron in GaAs (Si) of approximately 6.2 MHz (28 MHz), so that a single-qubit π rotation requires approximately 80 ns (18 ns). The effective resonant magnetic field could be generated by localized magnetic excitation [9] or through g-tensor modulation [7,8]. A SWAP gate needs about 50 ps for $J\approx 0.1$ meV Eq. (3), and hence 50 ps is the maximum time required for performing a $(\mathrm{SWAP})^{\alpha}$ gate.

From the point of view of operating time (and hence qubit storage errors), reducing the number of single qubit gates becomes the overwhelming consideration in designing a circuit. Our circuit is formed by at most three $(\mathrm{SWAP})^{\alpha}$ gates and six single qubit rotations. Considering that single-qubit rotations can in principle be performed on individual qubits simultaneously, the total time to implement a general $(\mathrm{SWAP})^{\alpha}$ circuit is at most the time required for three single-qubit rotations. The optimal CNOT circuit given by Ref. [10] contains three CNOT gates and eight single-qubit rotations. If we assume that a CNOT gate takes almost the same time as a SWAP gate, we find that the time to implement the CNOT circuit is also at most the time to implement three single-qubit rotations [distinct from the single-qubit rotations of the $(\mathrm{SWAP})^{\alpha}$ circuit]. In practice, one would like to implement specific instances of $U \in \mathrm{SU}(4)$, so that gate counts and timings depend on the target operation U. The self-evident example is that it is best to implement $U=$CNOT with a CNOT circuit, and similarly $U=$SWAP with a $(\mathrm{SWAP})^{\alpha}$ circuit. The essential point is that given the physical means to implement single-qubit rotations and $(\mathrm{SWAP})^{\alpha}$, we can arrive at the most efficient decomposition (in terms of operating time and gate count) of a target $U \in \mathrm{SU}(4)$ that might be specified using a network of CNOT's, controlled phase gates, or other logically convenient gates. This optimization is essential for minimizing both storage and gate errors introduced by performing the operation U.

The entanglement power of the $(\mathrm{SWAP})^{\alpha}$ gate is strictly less than the CNOT gate, but the $(\mathrm{SWAP})^{\alpha}$ gate is as efficient as the CNOT gate (in terms of gate count) in performing two-qubit operations. From the point of view of operating time, we also showed that both the $(\mathrm{SWAP})^{\alpha}$ circuit and the CNOT circuit are the same for a general two-qubit unitary operation. So the optimal $(\mathrm{SWAP})^{\alpha}$ circuit is as good as the optimal CNOT circuit if the complexity of physical implementation of two-qubit gates [CNOT gate and $(\mathrm{SWAP})^{\alpha}$ gate] and single-qubit gates are the same. However, if we directly replace a CNOT gate by two $(\mathrm{SWAP})^{1/2}$ gates and some single-qubit gates to implement a general two-qubit operation, we need six $(\mathrm{SWAP})^{1/2}$ gates and the operating time will be at least doubled compared with the optimal $(\mathrm{SWAP})^{\alpha}$ circuit. In this sense the optimizition of a $(\mathrm{SWAP})^{\alpha}$ circuit is necessary; the advantages of the optimization are, first, that the number of two-qubit gates is reduced by half, and second, the operating time is reduced to one-half to one-third due to the reduction of the number of single qubit gates.

Our circuit realizes the three free parameters in Eq. (12) by adjusting the α in the $(\mathrm{SWAP})^{\alpha}$ gate. So the SWAP circuit generally involves three different $(\mathrm{SWAP})^{\alpha}$ gates with fixed single-qubit rotations. This is in contrast with the CNOT circuit, in which the two-qubit operation, the CNOT gate, is fixed, and the single-qubit rotations are tuned according to the free parameters in Eq. (12). This is a trade off in designing a circuit, which do we prefer: tuning $(\mathrm{SWAP})^{\alpha}$ gates or tuning single qubit rotations? As is generally accepted, in solid state with Heisenberg exchange interaction, the $(\mathrm{SWAP})^{\alpha}$ gate can be realized by simply controlling the interaction time as presented in Eq. (5). An arbitrary single-qubit rotation is potentially more difficult to realize and may take up to 100 ns [20] to process. For example, one can apply magnetic time varying magnetic fields. Since the single-qubit rotations are fixed in the SWAP circuit of Ref. [16] (the single-qubit rotations at the front and back of the circuit still need be adjusted according to the specified operations), the directions, gradients, pulse time, etc., of the magnetic field can be fixed. In this sense, for spin-based quantum computation, tuning the $(\mathrm{SWAP})^{\alpha}$ gate in our circuit could be advantageous compared to using a fixed $(\mathrm{SWAP})^{\alpha}$ circuit, such as $(\mathrm{SWAP})^{1/2}$, and tuning the single-qubit rotations.

VII. SUMMARY AND DISCUSSION

When it comes to solid state implementations, the exchange interaction has emerged as the primary mechanism for constructing nonlocal quantum gates, and the $(\mathrm{SWAP})^{\alpha}$ gate is the cheapest and the most natural two-qubit gate that can be realized using this technology. We have shown that simply replacing individual CNOT gates with its SWAP circuit is not an efficient implementation technique for exchange-interaction-based quantum computing systems. We have presented an alternate optimization technique and have derived the optimal circuit for an arbitary two-qubit unitary operator using SWAP gates and single-qubit rotations.

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