Implementing unitary operators in quantum computation

Jaehyun Kim, Jae-Seung Lee, and Soonchil Lee
Department of Physics, Korea Advanced Institute of Science and Technology, Taejon 305-701, Korea
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We present a general method which expresses a unitary operator by the product of operators allowed by the Hamiltonian of spin-1/2 systems. In this method, the generator of an operator is found first, and then the generator is expanded by the base operators of the product operator formalism. Finally, the base operators disallowed by the Hamiltonian, including more than two-body interaction operators, are replaced by allowed ones by the axes transformation and coupling order reduction technique. This method directly provides pulse sequences for the nuclear magnetic resonance quantum computer, and can be generally applied to other systems.

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I. INTRODUCTION

In 1973, Bennett [1] proposed a reversible Turing machine that is as efficient as an irreversible one, and this led to the idea of using a quantum system as a computer because the time evolution of a quantum system is reversible. Feynman [2] introduced the concept of a quantum computer, and its theoretical model was given by Deutsch [3]. On the other hand, Fredkin and Toffoli [4] proved that an arbitrary computation can be performed by a reversible Turing machine by showing that AND, OR, and NOT gates can be generated by reversible three-bit gates, among which a Toffoli gate [5] is most frequently used nowadays. In quantum computation, a three-bit gate cannot be implemented directly because it requires a simultaneous interaction of three particles. Thus there have been efforts to find two-bit universal gates [6–12]. In particular, Barenco *et al.* showed that a combination of two-bit *c*-NOT gates and one-bit gates can replace a Toffoli gate, and proposed a method to make general *n*-bit controlled gates [13]. Therefore, it is proved that an arbitrary computation can be performed by a quantum computer, and the implementation of these universal gates became the basic requirement for any quantum system to be a quantum computer.

However, the proof that an arbitrary computation can be done by a quantum computer does not necessarily mean that we know a general implementation procedure. If a unitary operator U, equivalent to a combination of gates, is related to the Hamiltonian $\mathcal{H}$ of a certain quantum system by $U=\exp(-\imath\mathcal{H}t/\hbar)$, it can be realized by the time evolution of the system during time t. But there are only a few operations that can be implemented in this way by the limited Hamiltonians of nature. Therefore, it is very necessary to find a general method to implement an arbitrary operation using only the given Hamiltonians. Feynman proposed a way to construct an artificial Hamiltonian when U is given by $U=U_k\cdots U_3U_2U_1$ and all $\mathcal{H}_i$'s corresponding to U_i's exist in nature [14], but it is impractical to construct artificial Hamiltonians. It will be more practical to partially control a Hamiltonian by turning perturbations ''on'' and ''off'' if U can be expressed as a product of operators corresponding to the perturbation terms. Whether Feynman's artificial Hamiltonians or switchable perturbations are used, an operator of interest must be expressed as a product of the operators allowed by Hamiltonians. This is equivalent to finding the combination of universal gates, or a quantum network, and generally is a very difficult problem having several solutions.

In this work, we propose a general method of expressing a unitary operator as a product of the operators allowed by the Hamiltonian of the spin-$\frac{1}{2}$ systems, including the nuclear magnetic resonance (NMR) quantum computer. This method makes use of the fact that a unitary operator U is always given by $U=\exp[-\imath G]$, where G is a Hermitian operator. Once the generator of an operator, G, is found, it is expanded by suitable base operators. Then U is expressed as a product of operators having only one base operator as a generator, and, finally, each operator in the product is replaced by the allowed ones. Compared to a previous report [15], only the operators of physical variables were used in each transformation procedure. This helps to understand the physical meaning of operations done by a quantum computer.

II. DECOMPOSITION

The first step of implementation is to find the generator of a given operator. Since the only way to implement an operator is to use the time evolution of a state under a suitable Hamiltonian, a generator, which is the product of Hamiltonian and time, gives the physical information necessary for implementation. A unitary operator is represented by a normal matrix and always diagonalized by unitary transformation. The matrix T that diagonalizes U also diagonalizes G as

$$U'=TUT^{\dagger}=e^{-\imath TGT^{\dagger}}=e^{-\imath G'}, \tag{1}$$

where U' and G' are diagonalized matrices of U and G, respectively. Once the operator and its generator become diagonal, G' is easily obtained from

$$U'_{kk}=e^{-\imath G'_{kk}}, \tag{2}$$

and G is obtained by inverse transformation $G=T^{\dagger}G'T$. Since G is Hermitian, G'_{kk}, the eigenvalues of G, are real,

and U'_{kk} are complex with absolute value of unity. It is worthwhile to note that the mapping from U'_{kk} to G'_{kk} is not unique.

To relate the generator G with Hamiltonians, consider the following operators of the product operator formalism for N spin-$\frac{1}{2}$ particles [16–18]:

$$B_s = 2^{(q-1)}(I_{\alpha_1} \otimes I_{\alpha_2} \otimes \cdots \otimes I_{\alpha_N}), \tag{3}$$

where $s=\{\alpha_1,\alpha_2,\ldots,\alpha_N\}$ and α_i is 0, x,y, or z. I_0 is E, i.e., a 2×2 unity matrix, I_{α_i} is a spin angular momentum operator for $\alpha_i \neq 0$, and q is the number of nonzero α_i's. For example, $\{B_s\}$ for $N=2$ is given by

$$\begin{aligned} &q=0; \quad E/2, \\ &q=1; \quad I_{1x}, I_{1y}, I_{1z}, I_{2x}, I_{2y}, I_{2z}, \\ &q=2; \quad 2I_{1x}I_{2x}, 2I_{1x}I_{2y}, 2I_{1x}I_{2z}, \ldots, \end{aligned} \tag{4}$$

which are 16 Dirac matrices except the factor of $\frac{1}{2}$. In Eq. (4), unity matrices are not shown and spin indices are added for convenience. $\{B_s\}$, consisting of 4^N elements, makes a complete set and, therefore, an arbitrary $2^N \times 2^N$ matrix can be expanded by the linear combination of B_s's. Since G and B_s's are Hermitian, coefficients of the linear expansion are real numbers and obtained by applying the inner product of G and B_s's.

A unitary operator is now expressed as $U=\exp(-\imath\Sigma_s b_s B_s)$, of which the generator is related to physical observables. In general, there exists no Hamiltonian that corresponds to a linear combination of B_s's. Therefore, our next step is to express U as a product of *single operators*, which have only one B_s as a generator like $\exp[-\imath b_s B_s]$. Sometimes this decomposition is the most difficult step, and it has not yet been proven whether the decomposition is generally possible even for spin operators. Fortunately, many useful gates can be easily decomposed by using the commutation relations of B_s's. B_s's are either commuting or anticommuting with each other. If G is expanded with only commuting B_s's, U can be easily represented by a product of single operators as

$$U=\exp\left[-\imath\sum_s b_s B_s\right] \rightarrow \prod_s \exp[-\imath b_s B_s]. \tag{5}$$

A swap gate and an f-controlled phase shift gate used in Grover's search algorithm belong to this case.

Even though a generator has noncommuting B_s's, there are cases where decomposition is straightforward. Suppose two base operators B_{s1} and B_{s2} satisfy the relation ($\hbar=1$):

$$[B_{s1}, B_{s2}] = \imath B_{s3}; \tag{6}$$

then B_{s3} also belongs to $\{B_s\}$. This commutation relation makes the three operators B_{s1}, B_{s2}, and B_{s3} transform like Cartesian coordinates under rotation, meaning that

$$\exp[-\imath\phi B_{s3}]B_{s1}(\exp[-\imath\phi B_{s3}])^\dagger = B_{s1}\cos\phi + B_{s2}\sin\phi \tag{7}$$

for cyclic permutations of $s1$, $s2$, and $s3$. If a generator has only these operators, it can be decomposed using Euler rotations. For example, $\exp[-\imath\phi(B_{s1}+B_{s2})]$ is understood to be the rotation with the angle of $\sqrt{2}\phi$ about the axis 45° off the ''B_{s1} axis'' on the plane of B_{s1} and B_{s2} axes. Therefore, this operation is equivalent to the successive rotations about B_{s1} and B_{s3} axes as follows:

$$e^{-\imath\phi(B_{s1}+B_{s2})} = e^{-\imath(\pi/4)B_{s3}} e^{-\imath\sqrt{2}\phi B_{s1}} e^{\imath(\pi/4)B_{s3}}. \tag{8}$$

This decomposition technique by Euler rotations is also applicable when an operator has a generator in the factorized form as follows:

$$U=\exp\left[-\imath\prod_{i=1}^{N}\left(\sum_{\alpha_i}\phi_{i\alpha_i}I_{i\alpha_i}\right)\right], \tag{9}$$

where $\phi_{i\alpha_i}$ are real numbers. Since I_{1x}, I_{1y}, and I_{1z} satisfy the commutation relation in Eq. (6), and commute with any other spin operators with $i\neq 1$, spin-1 components are decomposed as

$$U_1 \exp\left[-\imath(\phi_{10}E+\phi_1 I_{1\alpha_1})\prod_{i=2}^{N}\left(\sum_{\alpha_i}\phi_{i\alpha_i}I_{i\alpha_i}\right)\right]U_1^\dagger, \tag{10}$$

where U_1 is the product of the single operators of which the generators have only spin-1 components, corresponding to Euler rotations. Repeated applications of this process to successive spins give

$$U = U_N \cdots U_1 e^{-\imath G} U_1^\dagger \cdots U_N^\dagger, \tag{11}$$

where

$$G=\prod_{i=1}^{N}(\phi_{i0}E+\phi_i I_{i\alpha_i}). \tag{12}$$

Then decomposition is finished because all terms in Eq. (12) commute with each other. All the controlled gates belong to this case. If none of the above methods are applicable, U can be approximately expanded as a product of single operators to any desired accuracy [19].

III. REDUCTION

Although B_s is a product of spin operators that are physical quantities, not all B_s's exist in Hamiltonians that nature allows. The next step of implementation is to replace disallowed single operators in the product by allowed ones. The Hamiltonian of a spin-$\frac{1}{2}$ system used for implementation of a quantum computer allows only the following single operators in general:

$$\begin{aligned} R_{i\alpha}(\phi) &= e^{-\imath\phi I_{i\alpha}}, \\ J_{ij\alpha}(\phi) &= e^{-\imath\phi 2 I_{i\alpha}I_{j\alpha}}. \end{aligned} \tag{13}$$

The first term is a rotation operator that rotates spin i about the α axis by the angle of ϕ, and the second one is a spin-

spin interaction operator between spins i and j. The angle ϕ in the second term is proportional to the spin-spin coupling constant and evolution time, but we denote it as a rotation angle because the effect of spin-spin interaction can be understood as a rotation of one spin due to the magnetic field of the other. Before going further, we assume the following more restricted set of operators as allowed ones in this study:

$$R_{i\alpha}(\phi)=e^{-\imath\phi I_{i\alpha}} \quad (\alpha=x \text{ or } y),$$
$$J_{ij}(\phi)=J_{ijz}(\phi)=e^{-\imath\phi 2I_{iz}I_{jz}}. \tag{14}$$

In this set, only x and y axes are used for single-spin rotations, and a spin-spin interaction is limited to the Ising type. Needless to say, the greater the number of single operators allowed, the easier it is to implement an algorithm. However, Eq. (14) is a sufficient set to realize any unitary operators as shown below, and in fact these are the only operators allowed by an NMR quantum computer. Single-spin rotations are implemented by selective rf pulses and spin-spin interactions by Hamiltonian evolution with intermediate refocusing pulses [20]. These two rotation operators can generate any single bit operation and the interaction operator can make a *c*-NOT gate in combination with rotation operators [20,21]. Therefore, these three operators consist of the minimum set to implement universal gates.

Now, we are to show that the minimum set in Eq. (14) can generate all the other single operators. First, the single-bit operation excluded in Eq. (14), $R_{iz}(\phi)$, can be transformed from $R_{ix}(\phi)$ as

$$R_{iz}(\phi)=R_{iy}\left(-\frac{\pi}{2}\right)R_{ix}(\phi)R_{iy}\left(\frac{\pi}{2}\right). \tag{15}$$

This is the composite pulse technique well-known in the NMR experiments [17]. Any rotation about one axis can be replaced by the composite of rotations about the other two. All the second-order operators, where the nth-order operator means the single operator that has a generator B_s with $q=n$, can be transformed into the Ising-type operator in Eq. (14) by this technique [22,23]. For example, $\exp[-\imath\phi 2I_{ix}I_{jz}]$ is transformed as

$$\exp[-\imath\phi 2I_{ix}I_{jz}]=R_{iy}\left(\frac{\pi}{2}\right)\exp[-\imath\phi 2I_{iz}I_{jz}]R_{iy}\left(-\frac{\pi}{2}\right). \tag{16}$$

In the same way, any nth-order operator can be transformed into the product of single operators and the nth-order coupling operator that is defined as the nth-order operator with all $\alpha_i=z$.

After all the spin coordinates are changed to z using this technique, the operators with more than two-body interaction can be reduced to an Ising type two-body interaction operator as discussed below. The key idea of the coupling order reduction is that the nth-order coupling operator can be thought as the $(n-1)$th-order one controlled by one spin state. For example, the third-order coupling operator [24], $\exp[-\imath\phi 4I_{iz}I_{jz}I_{kz}]$ is represented by

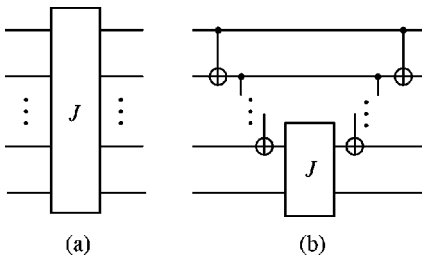

FIG. 1. Quantum network for the nth-order coupling operator (a) and its equivalent network consisting of allowed operators (b).

$$\begin{aligned}
&\exp[-\imath\phi 4I_{iz}I_{jz}I_{kz}]\\
&=\exp\left[-\imath\phi\begin{pmatrix}2(I_z\otimes I_z) & 0\\ 0 & -2(I_z\otimes I_z)\end{pmatrix}\right]\\
&=\begin{pmatrix}\exp[-\imath\phi 2(I_z\otimes I_z)] & 0\\ 0 & \exp[\imath\phi 2(I_z\otimes I_z)]\end{pmatrix}\\
&=\begin{pmatrix}J_{jk}(\phi) & 0\\ 0 & J_{jk}(-\phi)\end{pmatrix}
\end{aligned} \tag{17}$$

in the subspace of spin i. The final form of Eq. (17) implies that the third-order coupling operator can be understood as a second order one with coupling between spin j and k, but its rotation direction depends on the state of spin i. We note that if one spin is flipped during the evolution of the spin-spin interaction, then the sign of the interaction changes and this has the effect of time reversal. This means that the rotation direction changes [17,20] and, therefore, we can implement Eq. (17) with the second-order coupling operator by flipping spin j or k depending on the state of spin i. It is a well-known CNOT(XOR) gate that flips one spin depending on the state of the other spin. A CNOT gate is given by

$$U_{\text{CNOT}}=R_{iz}\left(\frac{\pi}{2}\right)R_{jx}\left(\frac{\pi}{2}\right)R_{jy}\left(\frac{\pi}{2}\right)J_{ij}\left(-\frac{\pi}{2}\right)R_{jy}\left(-\frac{\pi}{2}\right) \tag{18}$$

up to an overall phase, and this is the product of allowed operators in Eq. (14).

In the same way, an nth-order coupling operator can be reduced to an $(n-1)$th-order one by conditionally flipping odd number of spins except the spin i. Repeated applications of this process obviously reduce an nth-order coupling operator to a second-order one. Figure 1 shows the quantum networks of the nth-order coupling operator and its equivalent combination of the allowed operators. In Fig. 1(b), the CNOT gates after the second-order coupling operator are inserted to flip spins to their original states. Instead of the CNOT gates before and after the second-order coupling operator, a pseudo-CNOT gate $U_{ij}=R_{jx}(\pi/2)J_{ij}(\pi/2)R_{jy}(\pi/2)$ and $U_{ij}^{\dagger}$ can be used, respectively.

As an example, we apply this general implementation procedure to a Toffoli gate [25]. The generator of a Toffoli

gate obtained after the processes of diagonalization and inverse unitary transformation is expanded by base operators as

$$G=\pi\left(-\frac{1}{8}E+\frac{1}{4}I_{1z}+\frac{1}{4}I_{2z}-\frac{1}{4}2I_{1z}I_{2z}+\frac{1}{4}I_{3x}-\frac{1}{4}2I_{1z}I_{3x}-\frac{1}{4}2I_{2z}I_{3x}+\frac{1}{4}4I_{1z}I_{2z}I_{3x}\right). \quad (19)$$

Since all terms in this generator commute with each other, the corresponding operator is easily expressed by the product of single operators. After replacing disallowed operators, $I_{1z}I_{3x}$ and $I_{1z}I_{2z}I_{3x}$ in this case, by allowed ones by axes transformation and coupling order reduction, the gate is finally expressed as

$$R_{1z}\left(\frac{\pi}{4}\right)R_{2z}\left(\frac{\pi}{4}\right)J_{12}\left(-\frac{\pi}{4}\right)R_{3x}\left(\frac{\pi}{4}\right)R_{3y}\left(\frac{\pi}{2}\right)\times J_{13}\left(-\frac{\pi}{4}\right)J_{23}\left(-\frac{\pi}{4}\right)U_{12}J_{23}\left(\frac{\pi}{4}\right)U_{12}^{\dagger}R_{3y}\left(-\frac{\pi}{2}\right) \quad (20)$$

up to an overall phase.

IV. CONCLUSION

Our method is applicable to any quantum computers that use spin-$\frac{1}{2}$ states as qubits, because the operators of Eq. (14) make the minimum set required to those quantum computers. This method can be generalized for other quantum computer systems that should provide a complete set of operators similar to those of Eq. (14). Since our method uses generators that are closely related to Hamiltonians, this method helps us to see the physical meaning of an operation. Operators with generators disallowed by Hamiltonians are replaced by allowed ones using axes transformation and order reduction techniques. Therefore, it is possible to simulate an Hamiltonian that does not exist in nature using this method, including more than two-body interactions.

This method does not necessarily give either optimal or unique solutions to implementation. As the number of spins increases, the number of base operators grows exponentially, and a generator could have too many terms. Therefore, it is impractical to apply this method to a system with many spins, but our method still provides a good guide to implement an operator of interest.

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