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Realization of the Three-Qubit Toffoli Gate in Molecules *

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We present the experimental realization of this gate with a solution of chlorostyrene molecules. Our method does not depend heavily on the two-qubit controlled operation, which used to serve as the basic quantum operation in quantum computing. At present, we use transition operator that can be applied to all qubits in one operation. It appears that no experimental realization has yet been reported up to now regarding the implementation of quantum Toffoli gate using transition pulse on three-qubit nuclear magnetic resonance quantum computers. In addition, our method is experimentally convenient to be extended to more qubits.

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The research of quantum computing begins with the academic question concerning the minimum amount of heat produced in one computational step. Landauer has shown that only logical operations which require dissipation of energy are irreversible.[1] This leads Bennett to the discovery of the possibility of reversible dissipationless computation.[2] Then Toffoli suggests the existence of the famous reversible logic gate, which is named as Toffolli-gate now.[3] In 1989, David Deutsch has proved that all the computational capabilities of any finite machine obeying the laws of quantum computation are contained in a single machine called a universal quantum computer. Such a computer can be built from the quantum equivalence of the Toffoli gate by adding a few extra operations for linear superposition of 0 and 1 states. The universal quantum computer is complete.[4]

On the one hand, because any unitary transformation can be build up from combinations of the two-qubit quantum controlled-not (CNOT) operation and the single-qubit operations,[5] several schemes have been proposed to realize Toffoli gate by these fundamental quantum logic gates. For example, a best known implementation of Toffoli gate is a six two-bit-gate proposed by Coppersmith. Barenco *et al.* have also presented a five two-bit-gate implementation.[6] Smolin and Devincenzo have indicated that Toffoli gate can be obtained with not less than five two-bit-gate of any type.[7] In addition, Margolus demonstrated the implementation of a slightly modified Toffoli gate with only three two-bit gates.[5] Many studies concerned about how to decrease the numbers of the reversible two-bit CNOT gates used.

It is recognized that the reversible computation could be executed within a quantum-mechanical physical system. The methods to realize the universal three-qubit Toffoli gate within various quantum-mechanical physical systems (such as trapped ions,[8] quantum dots,[9] cavity quantum electronic dynamics[10] (QED)) are proposed. Until recent, it is only of theoretical interest, as it is extremely difficult to build a quantum computer. In the last few years, however, there has been substantial progress in the construction of small quantum computers based on nuclear magnetic resonance (NMR) studies of the nuclei of small molecules in solution.[11−13] Some actual experimental realizations have been carried out.[14−22]

In this paper, we present a new approach and implement Toffoli gate in our chlorostyrene three-qubits NMR quantum computer from the thermal equilibrium state,

$$\begin{aligned}\rho_{\rm eq} &= \frac{1}{2^3} I_{8\times 8} + \varepsilon (I_z^1 + I_z^2 + I_z^3) \\ &= \frac{1}{2^3} I_{8\times 8} + \varepsilon [3|000\rangle\langle 000| + |001\rangle\langle 001| \\ &\quad + |010\rangle\langle 010| - |011\rangle\langle 011| + |100\rangle\langle 100| \\ &\quad - |101\rangle\langle 101| - |110\rangle\langle 110| - 3|111\rangle\langle 111|], \end{aligned} \tag{1}$$

where $I_\alpha^k (k = \{1,2,3\}, \alpha = \{x,y,z\})$ is the usual matrix for the α-component of the angular momentum of the spin-k, the relation between I_α^k and Pauli matrix σ_α^k is $I_\alpha^k = \sigma_\alpha^k/2$. Through the unitary transformation with high-selectivity radio-frequency pulses designed to perturb transverse magnetization one line in NMR, we get the final state

$$\begin{aligned}\rho_{\rm out} &= \frac{1}{2^3} I_{8\times 8} + \varepsilon (I_z^1 + I_z^2 + \frac{1}{2} I_z^3 + I_z^1 I_z^3 + I_z^2 I_z^3 - 2 I_z^1 I_z^2 I_z^3) \\ &= \frac{1}{2^3} I_{8\times 8} + \varepsilon [3|000\rangle\langle 000| + |001\rangle\langle 001| \\ &\quad + |010\rangle\langle 010| - |011\rangle\langle 011| + |100\rangle\langle 100| \\ &\quad - |101\rangle\langle 101| - 3|110\rangle\langle 110| - |111\rangle\langle 111|], \end{aligned} \tag{2}$$

It appears, however, that no experimental realization has yet been reported up to now regarding the implementation of quantum Toffoli gate using transition pulse on three-qubit NMR quantum computers. It seems that our method is experimentally convenient to be extended to more qubits.

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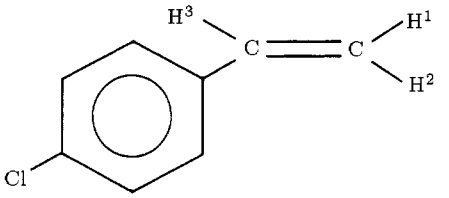

Fig. 1. Chemical structure of the chlorostyrene molecule, the three weakly coupled spin 1/2 hydrogen nuclei denoting the three qubits.

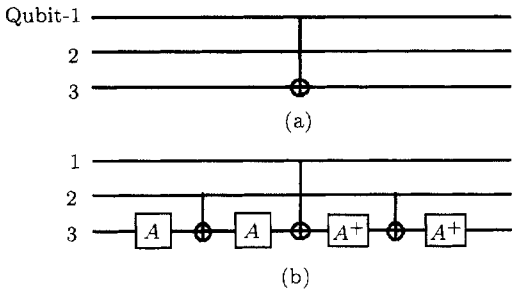

Fig. 2. (a) Quantum circuit symbol for Toffoli gate. (b) Margolus's simplified Toffoli gate construction, just three two-bit-gate and four one-bit-gate.

Toffoli gate is a three-qubit gate shown in Fig. 2. Let qubit-1, qubit-2 and qubit-3 be the first, second, and third labels. Toffoli gate can be described by the following operator

$$\begin{aligned} U_{\mathrm{TOF}} \equiv & |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| \\ & + |011\rangle\langle 011| + |100\rangle\langle 100| + |101\rangle\langle 101| \\ & + |110\rangle\langle 111| + |111\rangle\langle 110|]. \end{aligned} \tag{3}$$

where the first two qubits are the control qubits and the third qubit is the target qubit. If any one of the two control qubits is in the ground state $|0\rangle$, the target qubit does not change its value after the action of Toffoli gate. This situation is described by the first six terms in Eq. (3). Otherwise, if the two control qubits are both in state $|1\rangle$, the target qubit flips its state. This case corresponds to the seventh and eighth terms in Eq. (3).

One possible way to implement Toffoli gate would be to make use of the fact that any unitary transformation can be built up from combinations of the controlled-not (CNOT) operation and operations on a single qubit. For example, Margolus showed the creation of three-qubit Toffoli gate that can be performed as shown in Fig. 2.[5] In the circuits, there are four single-qubit operations (A denotes that gate A is applied to qubit-3, A^+ is the conjugate operator of A) and three two-qubit controlled-not gates (from qubit-1 to qubit-3 written as CN_{13}, from qubit-2 to qubit-3 written as CN_{23}). The matrix representation of the circuit in Fig. 2 is:

$$\begin{aligned} U_{\mathrm{example}} \equiv & A^+ \cdot CN_{23} \cdot A^+ \cdot CN_{13} \cdot A \cdot CN_{23} \cdot A \\ = & |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| \\ & + |011\rangle\langle 011| - |100\rangle\langle 100| + |101\rangle\langle 101| \\ & + |110\rangle\langle 111| + |111\rangle\langle 110|]. \end{aligned} \tag{4}$$

The above method to realize Toffoli gate depends heavily on using the fundamental two qubit quantum controlled-not gate which is experimentally realized in our two-qubit NMR quantum computer.[16] However, the extension of this procedure to more than two coupled spins is complicated and not easy to implement. As in NMR, doing nothing (suspending evolution) in one part of a system while doing something in another part of the system is nontrivial. For example, it is much more complicated to apply two-qubit quantum controlled-not gate CN_{13} (Fig. 2) on qubit-1 and qubit-3 while doing nothing on qubit-2 in three-qubit system than to apply the same two-qubit controlled-not gate in our two-qubit NMR quantum computer. That is to say, "given a unitary transformation of the quantum logic operation, what is the shortest sequence of pulses and evolutions which generates it? " Clearly this can be viewed as a problem in Lie algebra theory (but note that the answer depends on the molecule being used!).

Further more, we try to realize Toffoli gate in our three-qubit NMR system according to the theoretical schemes.[5-7] Although each gate in these schemes can be implemented by appropriately refocused evolutions in NMR, we find that the approach is not efficient in general. There are two main reasons. One is that in these schemes the two-qubit operation is considered as the basic operation. This may not be a physically reasonable choice in NMR quantum computing, but for the moment this should be considered as just a mathematical convenience which will permit us to address some general questions. The other is that NMR quantum operations depends heavily on the molecule being used. The fact that the chemical shift and coupling constant is small in our chlorostyrene molecule leads to the requirement of the highly frequency selectivity which is important in quantum operation.

A more direct approach, which we employ successfully in our work, is the use of single transition operator designed to perturb transverse magnetization one line.[14] For example we apply the high-selectivity π pulse ($\beta = \pi$) with the form[13]

$$\begin{aligned} U_{\mathrm{transition}} = & \exp[-\mathrm{i}\beta\frac{1}{4}(I_x^3 - 2I_z^1 I_x^3 - 2I_z^2 I_x^3 + 4I_z^1 I_z^2 I_x^3)] \\ = & |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| \\ & + |011\rangle\langle 011| + |100\rangle\langle 100| + |101\rangle\langle 101| \\ & + \mathrm{i}|110\rangle\langle 111| + \mathrm{i}|111\rangle\langle 110|. \end{aligned} \tag{5}$$

All NMR experiments are performed at room temperature and pressure on Bruker Avance DMX 500 spectrometer using chlorostyrene in Laboratory of Structure Biology, University of Science and Technology of China.

In our NMR approach to realize three-qubit Toffoli gate we need three nuclei. A convenient system is the liquid consisting of identical chlorostyrene molecules, whose chemical structure is shown in Fig. 1. The three weakly coupled spin 1/2 hydrogen nuclei, which are distinguished by their different resonance frequencies, i.e. $\omega_1/(2\pi)$, $\omega_2/(2\pi)$ and $\omega_3/(2\pi)$, can be regarded

as the isolated qubits. Because the energy level differences are small at room temperature and scalar coupling is weak, the initial state in this three-qubit system is the thermal equilibrium state, which is shown in Eq. (1). To implement the quantum Toffoli gate in our three-qubit system, we use the high-selectivity π Gaussian soft pulse with the form in Eq. (5) to perturb transverse magnetization one line at a time. The transmitter frequency of the π Gaussian soft pulse is set at $\omega_1/(2\pi) + J_{23}/2 + J_{13}/2$, and the duration of the transition-pulse t_p is adjusted to optimize the frequency selectivity ($t_p = 250\,\mathrm{ms}$). Therefore we can get the output state $\rho_{out} = U\rho_{in}U^+$, which is shown in Eq. (2), by applying this operator on the equilibrium state ρ_{in} shown in Eq. (1).

The measured quantity in NMR experiments is the free induction decay (FID) induced in a pick-up coil in the xy-plane:

$$V(t) \propto iV_0T_r[(e^{-i\hat{H}t} \cdot \rho \cdot e^{i\hat{H}t}) \times ((\sigma_x + i\sigma_y) \otimes I + I \otimes (\sigma_x + i\sigma_y))]. \quad (6)$$

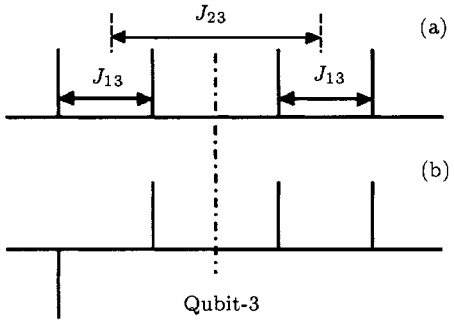

Fig. 3. Schematic NMR spectra of the target qubit-3 obtained by acting selective readout pulse on the qubit-3 (a) the input thermal equilibrium state ρ_{eq} (b) the output value ρ_{out} obtained with $U_{transition}$ acting on ρ_{eq}.

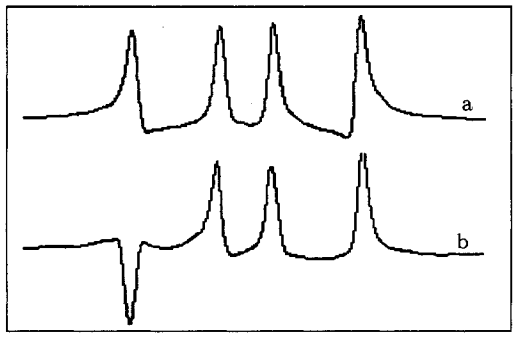

Fig. 4. Experimental NMR spectra of the target qubit-3 obtained by acting selective readout pulse on the qubit-3 (*a*) the input thermal equilibrium state ρ_{eq} (*b*) the output value ρ_{out} obtained with $U_{transition}$ acting on ρ_{eq}.

In Fig. 3, we show the schematical spectrum corresponding to the state of $\rho_{in}(\rho_{out})$ in NMR by applying $R_y^3(90)$ readout pulses on them. All four lines arise from the target qubit-3, and the intensity of each line is proportional to the total population difference between the corresponding states, which correspond to the left-to-right processes (from '4' to '1') in the following transitions $|1\rangle_1|1\rangle_2(|0\rangle_3 \leftrightarrow |1\rangle_3)$, $|0\rangle_1|1\rangle_2(|0\rangle_3 \leftrightarrow |1\rangle_3)$, $|1\rangle_1|0\rangle_2(|0\rangle_3 \leftrightarrow |1\rangle_3)$ and $|0\rangle_1|0\rangle_2(|0\rangle_3 \leftrightarrow |1\rangle_3)$. The experimental spectrum of the state of $\rho_{in}(\rho_{out})$ in NMR after readout pulses $R_y^3(90)$ is shown in Fig. 4. In this experiment, the difference frequencies of the three spins are 471.8 Hz between qubit-2 and qubit-3, 228.5 Hz between qubit-1 and qubit-2, and 700.3 Hz between qubit-1 and qubit-3, respectively, and the corresponding coupling constant between the two qubits are $J_{23} = 17.6$, $J_{12} = 0.65$ and $J_{13} = 10.9\,\mathrm{Hz}$. The real part of the Fourier transform of the resulting signal gives an NMR spectrum containing four peaks at frequencies $\omega_1/(2\pi) \pm J_{23}/2 \pm J_{13}/2$. It is clear that our implementation of the quantum logic gate leaves the computer in a final result as expected in Fig. 3.

We can see the small but significant distortions in the final spectra the difficulty of implementing perfect selective pulses and inhomogeneity of the magnetic field. The experimental task is to shape the radio-frequency pulse envelope so as to achieve sufficient selectivity in the frequency domain that there is negligible perturbation of the next nearest neighbor of the spin multiplet.

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