Original Article

A Realization Scheme for Half-adder at Room Temperature by Two Transition Pulses in NMR Quantum Information Processing

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ABSTRACT

In quantum information processing, realization of 3-qubit quantum operation is challenging especially when multiple logic operations are required to build non-trivial quantum circuits. Quantum half-adder is a 3-qubit circuit and in this work, a simple realization scheme for quantum half-adder operation is proposed. The 3-qubit quantum circuit is composed of a Toffoli operation and a controlled-NOT operation in succession. These two operations are shown to be achievable only by two transition pulses in nuclear magnetic resonance based quantum computing at room temperature. In our proposed scheme, three weakly coupled spin 1/2 nuclei of a molecule serve as three qubits. The time-independent internal Hamiltonian of the system allows us to obtain the desired multi-qubit operation. The simple structure of the spin 1/2 systems of our scheme make it easy to be implemented in experiments. Simulation on fidelity estimation reveals that more than 96% fidelity is achievable in worst case scenario.

Keywords: NMR-based quantum computing, Quantum circuit, Quantum half-adder, Quantum information processing.

INTRODUCTION

In information processing, the limits of classical computation, and promise of exponential speedups together with minimum heat generation from quantum mechanical effects recently brought a new dimensional attention to build up a quantum computer. The realization of reversible arithmetic and logical operation using quantum mechanical phenomenon is one of the most challenging problems in modern science. Quantum information processing requires controllable quantum phenomenon and in this regard several physical architectures have been demonstrated recently. The majority of these architectures involve implementation of quantum gates using optics, ion trap, nuclear magnetic resonance (NMR), superconductivity etc.[1-5] A serious barrier to a full-scale implementation is the requirement of large number of gates to realize even small quantum circuits.

Universal quantum logic gates and quantum arithmetic operations are the basic building blocks of a quantum computer. Realization of the universal quantum logic gates such as Fredkin and Toffoli[6-11] motivates the implementation of quantum arithmetic operations such as addition, subtraction etc.[12,13] A half-adder operation is a 3-qubit operation and it is the basis of full adder and quantum multiplication operations. Commonly, a multi-qubit operation (when the number of qubit is more than two) is divided into combinations of 2- and 1-qubit operations. The 3-qubit arithmetic operation such as half-adder is demonstrated and realized using optics and NMR based architectures[12-13]. In the NMR based scheme, it is shown that at least three transition pulses (selective RF π-pulses) are required to obtain the quantum half-adder operation[13]. Obtaining the same functionality with the reduction in number of transition pulses definitely reduces the experimental complexity and possible errors.

In this paper, we have proposed a NMR based scheme to realize half-adder operation only by two transition pulses at room temperature (note that the NMR-based scheme proposed in Ref. 13 requires low temperature during actual operation). The quantum half-adder circuit is shown in the Fig. 1. It can be seen from Fig. 1 that a half-adder operation can be achieved by sequential operation of a Toffoli gate and controlled-NOT (CNOT) gate. First, the Toffoli operation is performed with *a*, *b* as control bits and *c* as the target bit. Second, a CNOT operation is performed with *a* as control bit and *b* as target bit (see Fig. 1). The first operation provides $c \oplus (a \wedge b)$ (at the output port of the bit *c*) which is equal to *c*+*carry*, where, $\oplus$ indicates addition modulo-2 and $\wedge$ indicates AND operation. On the other hand, the second operation provides $a \oplus b$ (at the output port of the bit *b*) which is the '*sum*' of the bit *a* and *b*. The classical truth table of half-adder operation is given in Table 1. However, the quantum operators are unitary operators and they are reversible. The reversibility is achieved using an ancillary bit (bit *c* in Fig. 1). If Toffoli and CNOT each of these two operations are possible to achieve by applying single transition pulse, then by applying only two transition pulses we can obtain the half-adder operation and such an optimum half-adder scheme is our proposal.

REALIZATION SCHEME

The half-adder operation

A half-adder operation is composed of a Toffoli gate and a CNOT gate. The Toffoli operation is described by the operator

$$U_{TOF} = |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011| + |100\rangle\langle 100| + |101\rangle\langle 101| + |110\rangle\langle 111| + |111\rangle\langle 110|$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad (1)$$

On the other hand, the CNOT operation (which a is two-bit operation) in a three-bit system (any two bits take part in the operation without effecting the third bit) is realized by the operator

$$U_{CNOT} = |000\rangle\langle 000| + |001\rangle\langle 001| + |010\rangle\langle 010| + |011\rangle\langle 011| + |100\rangle\langle 110| + |101\rangle\langle 111| + |110\rangle\langle 100| + |111\rangle\langle 101|$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (2)$$

The half-adder operator is the product of the above two operators and which is given by

$$U_{ADD} = U_{CNOT} . U_{TOF}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (3)$$

The system Hamiltonian

To obtain half-adder operation by applying minimum number of transition pulses, we propose a heteronuclear system with three spin 1/2 nuclei and the nuclei of the system are weakly coupled to each other. For such a system the internal time-independent Hamiltonian is expressed as[14-15]:

$$\mathcal{H}_{int} = \frac{\hbar}{2}\left[\sum_{i=a,b,c} \omega_i \sigma_z^i + \pi \sum_{i \neq j} J_{ij} \sigma_z^i \sigma_z^j\right] \quad (4)$$

Where σ_z is the Pauli spin matrix, ω is the Larmor precession frequency (in radians) and *J* (in Hertz) is the scalar coupling. The second order term in the expression (4) clearly dictates that every possible combination of couplings amongst all pairs of spins within the system may be achievable in NMR experiment[14-15]. The coupling between the nuclei is schematically shown in Fig. 2.

Transition pulse and decoherence time

It is shown that the Hamiltonian for a molecular system expressed by Eq. (4) can be employed to achieve controlled operation with more than one qubit as control bits by a single transition pulse at room temperature[14-15]. In fact Toffoli operation (which is a 3-qubit operation with two control bits and one target bit) is experimentally realized by applying a properly selected single transition pulse in chlorostyrene molecule at room temperature[8]. A similar Toffoli operation is also experimentally realized (as part of Fredkin operation) by a single transition pulse in alanine molecule[7].

However, alanine and chlorostyrene molecules are not suitable for half-adder operation by applying minimum number of transition pulses. As one of the coupling is very small (compared to the other two), it is virtually inaccessible directly (though same can be made accessible indirectly by at least three transition pulses and such studies are not the scope of this work)[14,16]. As a result, all possible combination of couplings for a given system (for which the Hamiltonian is expressed by Eq. (4)) cannot be utilized in circuit operation. The main reason for the said inaccessibility (in alanine and chlorostyrene molecules) is because of the time spent for the lowest coupling ($1/2J_{lowest}$) is comparable to the smallest decoherence time (T_2) of the molecular system.

In order to implement our half-adder scheme by applying two transition pulses, we propose molecules with three weakly coupled spin ½ nuclei such as (a) Diethyl-fluoromalonate[17-18], (b) (2,3)-dibromo-propanoic acid[19], (c) Bromotrifluoro-ethylene[20] etc. for which NMR based quantum computing is well known. The structures of these molecules are shown in Fig. 3 and their important NMR parameters are given in Table 2. From these parameters, one can check that every possible combination of couplings of spins within a given molecular system is achievable and

hence, the bits (*a*, *b* and *c*) can be assigned arbitrarily for a given molecule.

The large decoherence time of these molecules allow multiple transition pulses for sequential operations[17-20]. It is to be noted that the chemical shift differences are small for (2,3)-dibromopropanoic acid, placing heavy demands on the selectivity of the soft π pulses, the uniformity of excitation across a chosen spin multiplet, and the effectiveness of the suppression off-resonance[19]. Hence, (2,3)-dibromopropanoic acid it is not the best choice among the proposed molecules for half-adder operation. Apart from these proposed molecules, there are other molecules which are being studied for 3-bit quantum computation. A list of such molecules can be found in somewhere else[21]. However, we restrict our study to the above mentioned three molecules for which half-adder operation is possible to achieve at room temperature.

In experiments, the Toffoli operation given in Eq. (1) can be realized by applying a π-transition pulse of frequency $\omega_c/(2\pi)+J_{ac}/2+J_{bc}/2$ and the corresponding operator is expressed as,

$$U_{TOF}^{E} = exp\left[-i\pi\frac{1}{8}(1-\sigma_z^a)(1-\sigma_z^b)\sigma_x^c\right] \quad (5)$$

In a similar manner, the CNOT operation given in Eq. (2) can be realized by applying a π-transition pulse of frequency $\omega_b/(2\pi) + J_{ab}/2$ and the corresponding operator of which is expressed as (the third bit remains unaffected),

$$U_{CNOT}^{E} = exp\left[-i\pi\frac{1}{4}(1-\sigma_z^a)\sigma_y^b\right] \quad (6)$$

Therefore, the experimental realization yields the half-adder operator as,

$$U_{ADD}^{E} = U_{CNOT}^{E}.U_{TOF}^{E}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix} \quad (7)$$

In contrast to the half-adder operator given by Eq. (3), an expected phase term appears in the operator given by Eq. (7) and can be ignored. The sequence of the above operations to obtain the half-adder operator is schematically shown in Fig. 4. Note that for proper operation of the circuit, the input qubit $|c\rangle$ is to be maintained in the state of $|0\rangle$ and this can be done during the initial state preparation[17,18,21]. The output states are then verified with all possible input states and expected half-adder operation is obtained.

FIDELITY SIMULATION

Fidelity is one of the important aspects in the implementation of a quantum scheme. In order to estimate the fidelity, computer simulation is performed. By computer simulation, it is possible to predict the error that may arise in the practical implementation of the scheme. As an example, consider implementation of a 180°_{x} pulse using a naive pulse with a fractional pulse length error ofε, the actual flip angle of the pulse is 180°×(1+ε). The quality can be assessed by calculating the propagator fidelity F between the desired propagator U and the actual propagator V by[21],

$$F = |Tr(VU^{-1})/Tr(UU^{-1})| \quad (8)$$

Based on the expression given by Eq. (8), simulation is performed to estimate the resultant fidelity of the two operations involved in our proposed half-adder scheme and the result of the fidelity estimation is shown in Fig. 5.

Our simulation result reveals that, in a worst case scenario (defined by 20% error in each pulse length), more than 96% fidelity is achievable for the proposed quantum half-adder scheme (for simplicity only the main component of error i.e. the error in pulse length is considered here).

CONCLUSIONS

In this work, we have demonstrated the possibility of obtaining quantum half-adder operation by applying only two transition pulses in NMR based quantum computing. A heteronuclear system of three spin ½ nuclei with weakly scalar coupling between the spins is proposed to realize the scheme. The Hamiltonian of such system allows all possible combination of scalar coupling amongst all pairs of spins within the system and hence provides flexibility in quantum circuit design. Molecules like Diethyl-fluoromalonate, (2,3)-dibromo-propanoic acid, Bromotrifluoro-ethylene etc. are proposed to implement the scheme. Promising result is obtained by simulation on fidelity estimation.

ACKNOWLEDGEMENTS

The authors would like to thank to Mr. Jyotirmay Maiti (Ph.D. student, Dept. of Chemistry, West Bengal State University) for his assistance in preparing the images of molecular structure presented in this article.

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Table 1: Classical truth table of a half-adder

Input		Output	
a	*b*	*sum*	*carry*
0	0	0	0
0	1	1	0
1	0	1	0
1	1	0	1

Table 2: Important parameters of the proposed molecules

Molecule	Differences in chemical shifts (in Hz)	Couplings (in Hz)	Smallest decoherence time ($T_2^{Smalltes}$ in sec)	Refs
Diethyl-fluoromalonate	–6380.28 82514.66 76134.34	160.06 –194.67 48.35	1.1	[18, 17]
(2,3)-dibromopropanoic acid	1379.16 320.44 1184.38	–10.1 4.3 11.3	1.8	[19]
Bromotrifluoroethylene	82938.05 23247.79 59690.26	–122.1 53.8 75.0	4	[20]

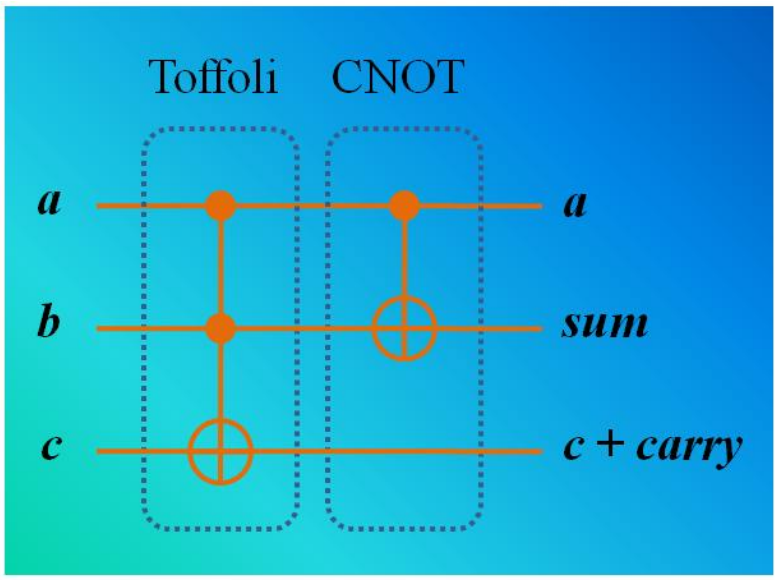

Fig. 1. Quantum half-adder circuit. The initial state of the qubit $|c\rangle = |0\rangle$ should be maintained to obtain the half-adder operation.

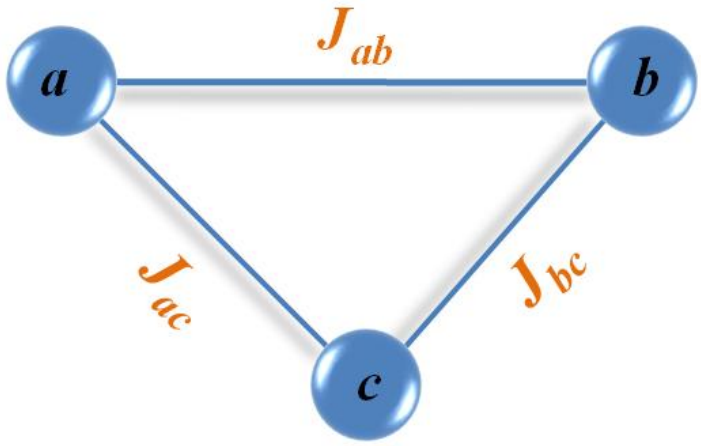

Fig. 2. Schematic of the three spin ½ nuclei system. The three nuclei are labelled by 'a', 'b' and 'c'. The couplings between the nuclei are J_{ab}, J_{bc}, J_{ac}.

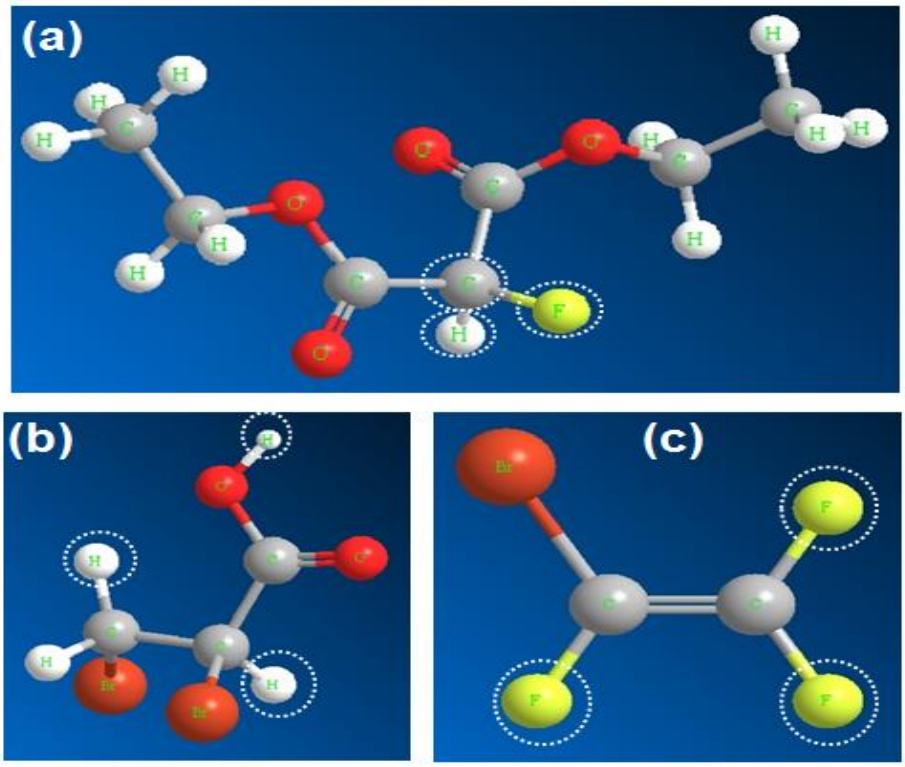

Fig. 3. Molecular structures. (a) Diethyl-fluoromalonate, (b) (2,3)-dibromopropanoic acid, (c) Bromotrifluoroethylene. The participating nuclei in NMR are by dotted circle.

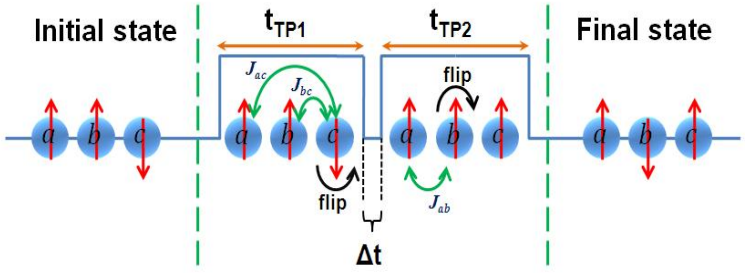

Fig. 4. Schematic representation of the pulse sequence on the molecular system. The joint state of the three spin $|110\rangle$ is considered as the initial state. t_{TP1} and t_{TP2} represent the two selective π-transition pulses correspond to Toffoli and CNOT operation respectively. Δt is the time gap between the two transition pulses and which is to be minimized in the experimental implementation..

 ISSN 2349-3917

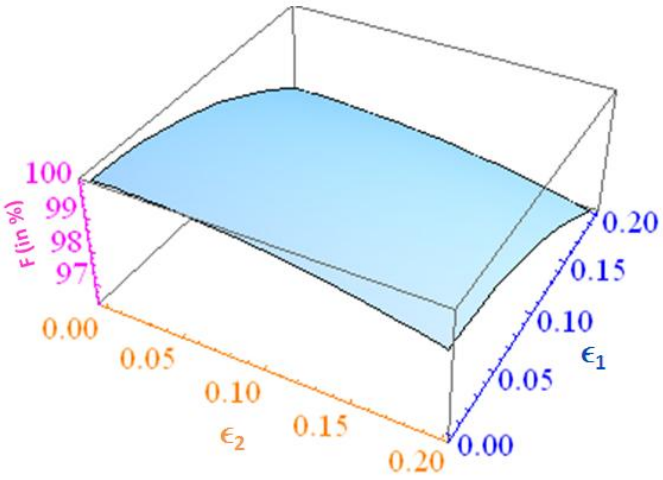

Fig. 5. Fidelity estimation of the proposed half-adder. Here, ε_1 and ε_2 represent the fractional pulse length error in Toffoli and CNOT operation respectively.