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Journal of Magnetic Resonance 159 (2002) 46–54
JMR Journal of Magnetic Resonance
www.academicpress.com

Implementation of conditional phase-shift gate for quantum information processing by NMR, using transition-selective pulses

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Received 24 April 2002; revised 16 July 2002

Abstract

Experimental realization of quantum information processing in the field of nuclear magnetic resonance (NMR) has been well established. Implementation of conditional phase-shift gate has been a significant step, which has lead to realization of important algorithms such as Grover's search algorithm and quantum Fourier transform. This gate has so far been implemented in NMR by using coupling evolution method. We demonstrate here the implementation of the conditional phase-shift gate using transition selective pulses. As an application of the gate, we demonstrate Grover's search algorithm and quantum Fourier transform by simulations and experiments using transition selective pulses.

1. Introduction

Theoretical possibility of quantum information processing (QIP) has generated a lot of enthusiasm for its experimental realization [1–8]. Nuclear magnetic resonance (NMR) has played a leading role for practical demonstration of quantum algorithms and quantum gates [10–32]. Deutsch-Jozsa algorithm [9–12], Grover's search algorithm [13–15], quantum Fourier transform [16], and the Shor's factorization algorithm [17] have been implemented by liquid-state NMR. The unitary operators needed for implementation of these algorithms by NMR, have mostly been realized using spin selective radio frequency (r.f.) pulses and coupling evolution, utilizing indirect spin–spin (J) or dipolar couplings among the spins. On the other hand, several logic gates and algorithms have also been implemented using transition selective (soft; low power, long duration) r.f. pulses [10,11,20,26,29]. The use of transition selective pulses in quantum information processing is popular for its simplicity of logical operations. For example, a C^2-NOT gate in a three-qubit system using coupling evolution, requires a series of spin (qubit) selective $\pi/2$ and π pulses interspaced with J-evolutions on all three qubits, cascading a series of unitary transforms, while the same gate needs a single transition selective π pulse [10].

Conditional phase-shift gate is an integral part of many algorithms such as Grover's search algorithm and quantum Fourier transform (QFT) [6]. This gate introduces a phase-shift only if a certain condition is fulfilled. This gate has been realized using J-evolution by earlier workers [13,15,16]. In this work, we construct conditional phase-shift gate using transition selective pulses. As an application, we demonstrate Grover's search algorithm and quantum Fourier transform in a three-qubit system by simulations, and Grover's search algorithm in a two-qubit system by experiments, using transition selective pulses.

It may be mentioned that while theoretically the transition selective pulses are attractive since they simplify the logic of an operation, their experimental implementation requires long low power r.f. pulses, which give rise to experimental errors due to relaxation and unwanted evolution under the internal Hamiltonian during long pulses [31]. However, the transition selective

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PII: S1090-7807(02)00009-5

pulse method has yielded experimental results with fidelity comparable to J-evolution method [19]. Recently, use of transition selective pulses for quadrupolar nuclei of spin 3/2 and 7/2 partially oriented in liquid crystal matrices, respectively, as two- and three-qubit systems has been demonstrated [25–27]. Transition selective pulses have also been used to demonstrate the use of oriented dipolar coupled CH_3 and $^{13}CH_3$ groups as two and three qubits, respectively, and work is in progress to use transition selective pulses for quantum information processing in strongly coupled spins [28–30]. In all these cases, the J-evolution method is either not applicable or too complex to implement [32]. In such situations, the use of transition selective pulses method, inspite of its experimental limitations, provides an attractive alternative. It is conceivable that in future the two methods could be combined in order to increase the efficiency or for finding alternate routes for QIP.

2. The conditional phase-shift gate

The conditional phase-shift gate introduces a phase-shift only if a predetermined condition is satisfied. In one-qubit system, the conditional phase-shift gate is an unitary transform of the form [8]:

$$C_1(\phi) = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{pmatrix} \quad \text{or} \quad C_0(\phi) = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix}. \tag{1}$$

The $C_1(\phi)$ introduces a phase-shift if the qubit is in state $|1\rangle$ and $C_0(\phi)$ introduces a phase-shift if the qubit is in state $|0\rangle$. However, these two operations are identical within an overall phase, since $C_0(\phi) = e^{i\phi}C_1(-\phi)$. The phase-shift gate can be realized experimentally by a rotation of the magnetization vector of a spin-1/2 nucleus (qubit) by angle ϕ about z-axis (z-rotation). A ϕ angle pulse about z-axis has the form

$$(\phi)_z = \exp(-i\phi\sigma_z/2) = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}, \tag{2}$$

where σ_z is Pauli's z-matrix. We note that the phase gate $C_1(\phi)$ can be achieved using $(\phi)_z$, since

$$C_1(\phi) = e^{i\phi/2}(\phi)_z. \tag{3}$$

A ϕ angle pulse about z-axis can be experimentally realized by a composite pulse of the form $(\phi)_z = (\pi/2)_y(\phi)_x(\pi/2)_{-y}$, where $(\phi)_y$ means a rotation of magnetization vector by an angle (ϕ) about y-axis. This pulse sequence in widely known in NMR as a composite z-pulse [33,34].

In a two-qubit system, there are four possible conditional phase-shift gates ($C_{00}(\phi)$, $C_{01}(\phi)$, $C_{10}(\phi)$, and $C_{11}(\phi)$). A $C_{11}(\phi)$ gate introduces a phase-shift of ϕ only if both the qubits are $|1\rangle$, whereas a $C_{10}(\phi)$ gate does the same only if first qubit is $|1\rangle$ and second qubit is $|0\rangle$. Similar logic holds for the other two gates. The unitary operator corresponding to $C_{11}(\phi)$ is

$$C_{11}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \tag{4}$$

This gate has been implemented earlier using J-coupling evolution and spin selective pulses [16]. Here, we demonstrate that $C_{11}(\phi)$ can also be constructed using transition selective z-pulses. For this purpose, we first describe phase rotation of a qubit. The unitary operator describing a rotation of angle ϕ about z-axis on the first qubit, when the second qubit is in state $|0\rangle$ has the form

$$(\phi)_{z0} = \exp\left(-i\phi\left(\frac{1}{2}\sigma_z^{(1)} \otimes \sigma_0^{(2)}\right)\right) = \begin{pmatrix} e^{-i\phi/2} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{i\phi/2} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

This is a transition-selective phase rotation by angle ϕ about z-axis. $\sigma_0^{(2)}$ is the polarization operator of the second qubit corresponding to the state $|0\rangle$. The polarization operators of jth qubit when it is in state $|0\rangle$ or $|1\rangle$ are

$$\sigma_0^{(j)} = |0\rangle\langle 0| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \sigma_1^{(j)} = |1\rangle\langle 1| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{6}$$

respectively [34]. Similarly a ϕ angle pulse about z-axis on the first qubit when the second qubit is in state $|1\rangle$ has the matrix form

$$(\phi)_{z1} = \exp\left(-i\phi\left(\frac{1}{2}\sigma_z^{(1)} \otimes \sigma_1^{(2)}\right)\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i\phi/2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi/2} \end{pmatrix}. \tag{7}$$

The ϕ angle z-rotation of second qubit when the first qubit is, respectively, in the state $|0\rangle$ and $|1\rangle$ are

$$(\phi)_{0z} = \exp\left(-i\phi\left(\sigma_0^{(1)} \otimes \frac{1}{2}\sigma_z^{(2)}\right)\right) = \begin{pmatrix} e^{-i\phi/2} & 0 & 0 & 0 \\ 0 & e^{i\phi/2} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{8}$$

$$(\phi)_{1z} = \exp\left(-i\phi\left(\sigma_1^{(1)} \otimes \frac{1}{2}\sigma_z^{(2)}\right)\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & e^{-i\phi/2} & 0 \\ 0 & 0 & 0 & e^{i\phi/2} \end{pmatrix}. \tag{9}$$

The conditional phase-shift gate $C_{11}(\phi)$ can now be realized by the sequence of z-rotations, $[(\phi/2)_{z0}(\phi/2)_{z1}][(\phi)_{1z}]$ with an overall phase of $e^{-i\phi/4}$, as

$$C_{11}(\phi) = [(\phi/2)_{z0}(\phi/2)_{z1}][(\phi)_{1z}] = e^{-i\phi/4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \quad (10)$$

The $C_{11}(\phi)$ gate is also termed as Controlled phase-shift gate [8]. Similarly, the other conditional phase gates in the two-qubit system can be achieved within an overall phase of $e^{-i\phi/4}$ by the pulse sequences

$$C_{10}(\phi) = [(\phi/2)_{z0}(\phi/2)_{z1}][(\phi)_{0(-z)}], \quad (11)$$

$$C_{01}(\phi) = [(\phi/2)_{(-z)0}(\phi/2)_{(-z)1}][(\phi)_{1z}], \quad (12)$$

$$C_{00}(\phi) = [(\phi/2)_{(-z)0}(\phi/2)_{(-z)1}][(\phi)_{0(-z)}]. \quad (13)$$

The pulses in the first bracket are transition selective pulses on the transitions of first qubit, while the second bracket has a transition selective pulse on a transition of second qubit. Each pulse about z-axis is experimentally realized by transition selective composite z-pulses. In a three-qubit system, there are eight conditional phase-shift gates $(C_{000}(\phi), C_{001}(\phi), \ldots, C_{111}(\phi))$. The $C_{111}(\phi)$ gate introduces a phase-shift of ϕ when all the three qubits are in state $|1\rangle$ and does nothing otherwise. The unitary operator of the $C_{111}(\phi)$ gate is

$$C_{111}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \quad (14)$$

With the same logic as applied to one- and two-qubit systems, we realize the phase-shift gate $C_{111}(\phi)$ (with an overall phase factor of $e^{-i\phi/8}$) by a sequence of transition selective z-pulses,

$$C_{111}(\phi) = [(\phi/4)_{z00}(\phi/4)_{z01}(\phi/4)_{z10}(\phi/4)_{z11}] \times [(\phi/2)_{1z0}(\phi/2)_{1z1}][(\phi)_{11z}]. \quad (15)$$

The pulses in the first bracket are on first qubit, second bracket on second qubit and third bracket on third qubit. The other phase-shift gates can be achieved by the same number of transition selective z-rotations, with different pulses on transitions of second and third qubits. For example two other phase gates $C_{000}(\phi)$ and $C_{110}(\phi)$, which will be used later for demonstration of Grover's search algorithm, are

$$C_{110}(\phi) = [(\phi/4)_{z00}(\phi/4)_{z01}(\phi/4)_{z10}(\phi/4)_{z11}] \times [(\phi/2)_{1z0}(\phi/2)_{1z1}][(\phi)_{11(-z)}], \quad (16)$$

$$C_{000}(\phi) = [(\phi/4)_{(-z)00}(\phi/4)_{(-z)01}(\phi/4)_{(-z)10}(\phi/4)_{(-z)11}] \times [(\phi/2)_{0(-z)0}(\phi/2)_{0(-z)1}][(\phi)_{00(-z)}]. \quad (17)$$

Like $C_{111}(\phi)$ case, these pulse sequences also have an overall phase of $e^{-i\phi/8}$.

The above sequences can be easily generalized into a single formula to build an N-qubit conditional phase-shift gate $C_{ijk\cdots mn}(\phi)$ (where the N-qubits are $i,j,k,\ldots,m,n = 0$ or 1), as given below

$$C_{ijk\cdots mn}(\phi) = \left[\prod_{j'k'\cdots m'n'}^{2^{N-1}}\left(\frac{\phi}{2^{N-1}}\right)_{\{(-1)^{i+1}z\}j'k'\cdots m'n'}\right] \times \left[\prod_{k'\cdots m'n'}^{2^{N-2}}\left(\frac{\phi}{2^{N-2}}\right)_{i\{(-1)^{j+1}z\}k'\cdots m'n'}\right]\cdots \left[\prod_{n'}^{2}\left(\frac{\phi}{2}\right)_{ijk\cdots\{(-1)^{m+1}z\}n'}\right]\left[(\phi)_{ijk\cdots m\{(-1)^{n+1}\}z}\right], \quad (18)$$

where $j', k', \ldots, m', n' = 0$ or 1. It is to be noted that the above Eqs. (10)–(18) are not unique. The smallest angle pulse $(\phi/2^{(N-1)})$ need not be applied only on the first qubit but can be applied on any qubit. Similarly pulse $(\phi/2^{(N-2)})$ can be applied on any qubit other than on the qubit on which $(\phi/2^{(N-1)})$ is applied. Hence, different combinations of transition selective z-pulses can create the same gate, but in all pulse sequences the logic of Eq. (18) is maintained. For example, the $C_{111}(\phi)$ given in Eq. (15) can also be created by different pulse sequences such as

$$\begin{aligned} C_{111}(\phi) &= [(\phi/4)_{0z0}(\phi/4)_{1z0}(\phi/4)_{0z1}(\phi/4)_{1z1}] \times [(\phi/2)_{z10}(\phi/2)_{z11}][(\phi)_{11z}] \\ &= [(\phi/4)_{00z}(\phi/4)_{10z}(\phi/4)_{01z}(\phi/4)_{11z}] \times [(\phi/2)_{0z1}(\phi/2)_{1z1}][(\phi)_{z11}] \\ &= [(\phi/4)_{00z}(\phi/4)_{10z}(\phi/4)_{01z}(\phi/4)_{11z}] \times [(\phi/2)_{z01}(\phi/2)_{z11}][(\phi)_{1z1}]. \end{aligned} \quad (19)$$

However, all the sequences require the same number of pulses.

For quantum Fourier transform in a three-qubit system, a reduced conditional phase-shift gate is required where the condition is on two qubits and there is no condition on the third qubit. For example, $C_{11\epsilon}(\phi)$ gate acts according to the states of first and second qubits and introduces a phase-shift only if both the qubits are in state $|1\rangle$ (shown by subscript), and is independent of the state of the third qubit which can be in state $|0\rangle$ or $|1\rangle$ ($\epsilon = 0$ or 1). The unitary operator of $C_{11\epsilon}(\phi)$ gate is

$$C_{11\epsilon}(\phi) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{i\phi} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \quad (20)$$

The pulse sequences of the reduced conditional phase-shift gate can be easily constructed from the pulse sequences of the conditional phase-shift gates. For example,

$$C_{11\epsilon}(\phi) = C_{111}(\phi)C_{110}(\phi). \quad (21)$$

Using Eqs. (15), (16) and (21), this gate can be realized (with an overall phase of $e^{-i\phi/4}$) by a sequence of transition selective z-pulses

$$\begin{aligned} C_{11\epsilon}(\phi) = {} & [(\phi/4)_{z00}(\phi/4)_{z01}(\phi/4)_{z10}(\phi/4)_{z11}] \\ & \times [(\phi/2)_{1z0}(\phi/2)_{1z1}][(\phi)_{11z}] \\ & \times [(\phi/4)_{z00}(\phi/4)_{z01}(\phi/4)_{z10}(\phi/4)_{z11}] \\ & \times [(\phi/2)_{1z0}(\phi/2)_{1z1}][(\phi)_{11(-z)}]. \end{aligned} \quad (22)$$

Since all z-pulses commute Eq. (22) reduces to:

$$\begin{aligned} C_{11\epsilon}(\phi) = {} & [(\phi/4)_{z00}(\phi/4)_{z01}(\phi/4)_{z10}(\phi/4)_{z11}]^2 \\ & \times [(\phi/2)_{1z0}(\phi/2)_{1z1}]^2[(\phi)_{11z}(\phi)_{11(-z)}]. \end{aligned} \quad (23)$$

The last two pulses cancel and the squares of exponential operators double the angle of rotation, yielding,

$$C_{11\epsilon}(\phi) = [(\phi/2)_{z00}(\phi/2)_{z01}(\phi/2)_{z10}(\phi/2)_{z11}][(\phi)_{1z0}(\phi)_{1z1}]. \quad (24)$$

This reduced gate requires one z-pulse less than $C_{111}(\phi)$ or $C_{110}(\phi)$ gate. Other reduced conditional phase-shift gates can also be similarly realized (with an overall phase of $e^{-i\phi/4}$) as:

$$C_{1\epsilon 1}(\phi) = [(\phi/2)_{z00}(\phi/2)_{z01}(\phi/2)_{z10}(\phi/2)_{z11}][(\phi)_{10z}(\phi)_{11z}], \quad (25)$$

$$C_{\epsilon 11}(\phi) = [(\phi/2)_{z00}(\phi/2)_{z01}(\phi/2)_{z10}(\phi/2)_{z11}][(\phi)_{01z}(\phi)_{11z}]. \quad (26)$$

Thus, these gates can also be realized by transition selective pulses. One can extend the composite transition selective z-pulse sequence to construct a 'm'-qubit conditional phase gate in any 'N'-qubit system (with an overall phase of $e^{(-i\phi/2^m)}$). For such a gate, the number of transition selective z-pulse required are $(2N - 2^{N-m})$. The number of pulses decreases as the number of conditional qubits 'm' decrease. Each transition selective z-pulse is experimentally realized by three transition selective r.f. pulses along x and y-axis [35]. As an example the z-pulse on one of the transitions of third qubit in a N-qubit system can be realized as

$$(\phi)_{ijzl\cdots n} = (\pi/2)_{ijyl\cdots n}(\phi)_{ijxl\cdots n}(\pi/2)_{ij-yl\cdots n}, \quad (27)$$

where $i, j, l, \ldots, n = 0$ or 1.

It may be mentioned that for all the gates described above (Eqs. (10)–(27)) the first set of 2^{N-1} transition selective z-pulses act on all transitions of a spin (qubit), and wherever possible (in weakly coupled spin-1/2 systems), can be experimentally implemented by using a spin (qubit) selective z-pulse, thus reducing the number of transition selective pulses by 2^{N-1} pulses. For example, the $C_{11\epsilon}$ type gates (Eqs. (24)–(26)) require one spin selective and two transition selective pulses.

3. Simulations

3.1. Grover's search algorithm

Grover's search algorithm can search (with high probability) any state of an N-qubit system in $O(\sqrt{2^N})$ iterations [5]. Each iteration has two steps, namely 'conditional sign-flip' and 'inversion about average.' These can be implemented by using the conditional phase-shift gate. We demonstrate here the implementation of Grover's search algorithm by simulation using transition selective pulses on a three-qubit system. In a three-qubit system, the algorithm requires two iterations. The algorithm starts with an initial pseudo-pure state, say $|000\rangle$. A Hadamard gate 'H' is applied on this state. The Hadamard gate rotates each qubit from $|0\rangle$ state to an uniform superposition $(|0\rangle + |1\rangle)/\sqrt{2}$. The unitary transform of Hadamard gate for jth qubit is [6]

$$H_j = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (28)$$

and when applied on all three qubits, it is of the form

$$\begin{aligned} H &= H_1 \otimes H_2 \otimes H_3 \\ &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \\ &\quad \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \end{aligned} \quad (29)$$

The Hadamard gate on all qubits, applied on a pseudo-pure state, creates an uniform superposition of all possible states,

$$|\psi_1\rangle = H|000\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix} \times \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}. \quad (30)$$

H gate is realized experimentally by the pulse sequence $(\pi/2)_{-y}(\pi)_x$ (hard pulses, applied on all qubits). Grover's iteration starts from this point by the application of 'conditional sign-flip.' In the 'conditional sign-flip' step, the state which is being searched is inverted; that is a phase-shift of $\phi = \pi$ is introduced in that particular state. This can be achieved by a conditional phase-shift gate with $\phi = \pi$ corresponding to that state. For example, for the search of $|110\rangle$ state, the conditional sign-flip is the conditional phase-shift gate $C_{110}(\pi)$. The same logic holds for searches of other states.

The second step of Grover's iteration is 'inversion about average,' in which all the states are inverted about their average amplitude. The unitary operator (Λ) of this step for a three-qubit system is of the form [5]

$$\Lambda = \frac{1}{4}\begin{pmatrix} -3 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -3 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -3 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & -3 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -3 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -3 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -3 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & -3 \end{pmatrix}. \quad (31)$$

This step can be realized by applying a Hadamard gate 'H' (on all qubits) before and after a conditional phase-shift $C_{000}(\pi)$ gate, hence $\Lambda = HC_{000}(\pi)H$ [5,13]. It may be noted that the $C_{000}(\pi)$ gate is required because we started with $|000\rangle$ pseudo-pure state, whereas if one starts with another pseudo-pure state, say $|001\rangle$, then the corresponding phase-shift gate $C_{001}(\pi)$ will be required. After one full Grover's iteration (starting from $|000\rangle$ pseudo-pure state and searching for $|110\rangle$ state), the state of the system is

$$|\psi_2\rangle = (\Lambda)(C_{110}(\pi))|\psi_1\rangle = (HC_{000}(\pi)H)(C_{110}(\pi))|\psi_1\rangle = \frac{1}{4\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 5 \\ 1 \end{pmatrix}. \quad (32)$$

After the second Grover's iteration (conditional sign-flip and inversion about average), we find the final state to be

$$|\psi_3\rangle = [\Lambda C_{110}(\pi)]|\psi_2\rangle = [\Lambda C_{110}(\pi)][\Lambda C_{110}(\pi)]|\psi_1\rangle = [HC_{000}(\pi)HC_{110}(\pi)]^2 H|000\rangle = \frac{1}{8\sqrt{2}}\begin{pmatrix} -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \\ 11 \\ -1 \end{pmatrix}. \quad (33)$$

The result of measurement on the final state will give the searched state $|110\rangle$ with high probability. The entire sequence for two iterations after pseudo-pure state is $HC_{000}(\pi)HC_{110}(\pi)HC_{000}(\pi)HC_{110}(\pi)H$. The pulse sequence for the required phase-shift gates C_{110} and C_{000} are as in Eqs. (16) and (17), which use transition selective pulses. This demonstrates that the Grover's search algorithm can be implemented using transition selective pulses complementing the coupling evolution method proposed earlier [15]. Fig. 1 shows the density matrices of the system at (a) initial pseudo-pure state, followed by (b) state of uniform superposition (Eq. (30)), (c) after conditional sign-flip, (d) inversion about average (Eq. (32)), (e) after conditional sign-flip of second iteration, and (f) after inversion about average of second iteration which is the final result (Eq. (33)). The searched state is clearly identified in Fig. 1f.

3.2. Quantum Fourier transform

Just as classical Fourier transform extracts periodicity in functions, quantum Fourier transform (QFT) extracts periodicity of wave functions. It is defined as follows:

$$\mathrm{QFT}_q|x\rangle = \frac{1}{\sqrt{q}}\sum_{x'=0}^{q-1} e^{2\pi i x x'/q}|x'\rangle, \quad (34)$$

where $q = 2^n$ is the dimension of Hilbert space for a n-qubit system. If $f(x)$ is periodic with periodicity r, then

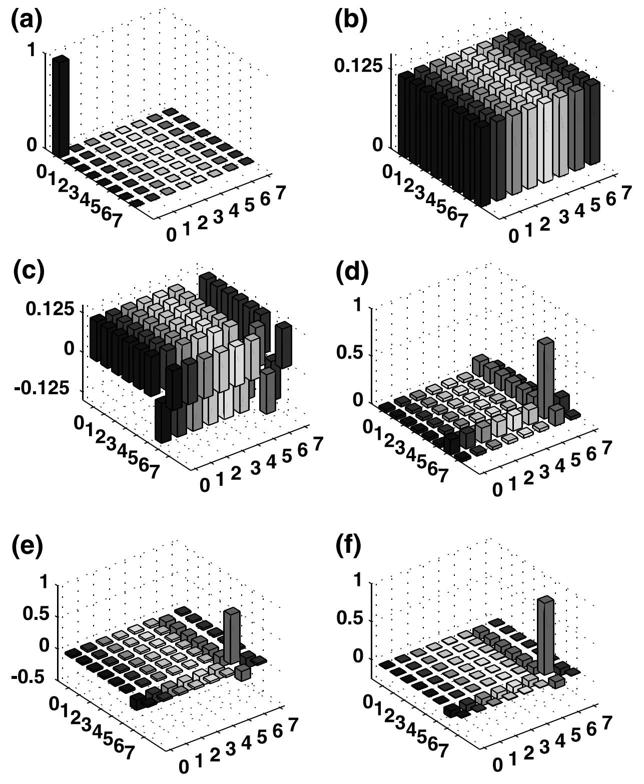

Fig. 1. Implementation of three-qubit Grover's search algorithm is shown by simulations. The state $|1\,1\,0\rangle$ is searched. The density matrices at different stages of the algorithm are shown. (a) Pseudopure $|0\,0\,0\rangle$ state, (b) uniform superposition, (c) conditional sign-flip, (d) inversion about average, (e) conditional sign-flip of second iteration, and (f) inversion about average of the second iteration. The high probablity of $|1\,1\,0\rangle$ state is reflected in the final density matrix. The x- and y-axis labels correspond to different states as: $0 \rightarrow |000\rangle$, $1 \rightarrow |001\rangle$, $2 \rightarrow |010\rangle$, $3 \rightarrow |011\rangle$, $4 \rightarrow |100\rangle$, $5 \rightarrow |101\rangle$, $6 \rightarrow |110\rangle$, and $7 \rightarrow |111\rangle$.

the corresponding quantum Fourier transformed function $f(p)$ will give a peak at $p = q/r$. The quantum circuit for three-qubit QFT [8] is given in Fig. 2.

Quantum Fourier transform has been demonstrated using J-coupling evolution by Weinstein et al. [16]. Here, we demonstrate quantum Fourier transform using transition selective pulses. From quantum circuit, Fig. 2, one can infer the QFT gate sequence in three-qubit system as

$$\mathrm{QFT}_8 = \mathrm{SWAP}_{13} H_3 C_{\epsilon 11}(\pi/2) H_2 C_{1\epsilon 1}(\pi/4) C_{11\epsilon}(\pi/2) H_1. \quad (35)$$

H_j is the Hadamard gate operated on jth qubit. Here the operation are applied in the sequence from right to left such that the SWAP_{13} is the last operation. The pulse sequence of $C_{11\epsilon}$, $C_{1\epsilon 1}$, and $C_{\epsilon 11}$ gates are given in Eqs. (24)–(26). The SWAP_{13} gate performs a swap between qubits 1 and 3, and is realized by a cascade of transition selective π pulses [12].

$$\mathrm{SWAP}_{13} : [(\pi)_{00x}(\pi)_{x00}(\pi)_{00x}][(\pi)_{11x}(\pi)_{x11}(\pi)_{11x}]. \quad (36)$$

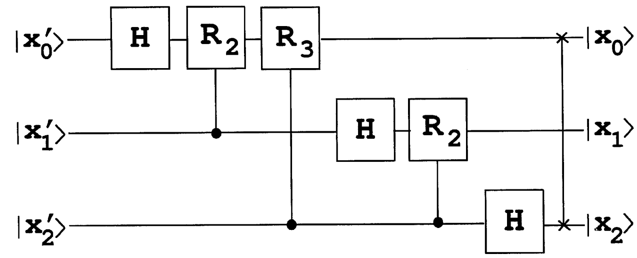

Fig. 2. Efficient quantum circuit for quantum Fourier transform in a three-qubit system. x'_0, x'_1, and x'_2 are states of the three-qubits in the input, and, x_0, x_1, and x_2 are the corresponding states in the output. The last operation is a swap gate between qubits 1 and 3. The unitary transformation R_k is the phase-gate $R_k = \begin{pmatrix} 1 & 0 \\ 0 & e^{2\pi i/2^k} \end{pmatrix}$.

It may be noted that in Eq. (36) the first set of three pulses taken together commute with the last set of three pulses taken together, and can be applied in any order. QFT sequence will extract the periodicity of an input state of any periodicity r. We demonstrate QFT for two different inputs. First input has state periodicity $r = 4$, and is created by a $(\pi/2)_y$ qubit selective hard pulse on the first qubit, Fig. 3a. The output state obtained by applying sequence of Eq. (35) shows a periodicity of $q/r = 2^3/4 = 2$, as is evident from the density matrix of output state, shown in Fig. 3b. The second input state has periodicity 2, and is created by a $(\pi/2)_y$ qubit selective hard pulse on the first and second qubits, Fig. 3c. The output state obtained by applying sequence of Eq. (35), has expected periodicity of $q/r = 4$ as shown in Fig. 3d.

4. Experiments

Grover's two-qubit search has also been carried out experimentally using transition selective pulses on a two-qubit system formed by the carbon-13 and proton of the molecule $^{13}CHCl_3$. Experiment have been performed at room temperature in DRX 500 spectrometer. The coherence times were; $T_1 = 20$ s and $T_2 = 0.4$ s for the proton, $T_1 = 21$ s and $T_2 = 0.3$ s for the carbon. The proton resonance frequency on the DRX 500 MHz spectrometer is 500.13 MHz, and that of carbon-13 is 125.76 MHz. The spin–spin (J) coupling in this system is 209 Hz. Gaussian shaped pulses of duration 20 ms were used as transition selective pulses. The initial pseudo-pure state were also prepared using transition selective pulses. A pulse sequence $[(70.5°)_{x1}(90°)_{1x}-$grad] equalizes the populations of the states $|01\rangle$, $|10\rangle$, and $|11\rangle$, keeping the population of $|00\rangle$ state undisturbed, different from the equalized population of other states; hence establishing $|00\rangle$ pseudo-pure state [22,30]. An inhomogeneous magnetic field gradient pulse along z-direction destroys any created coherence. This state is shown in Fig. 4a.

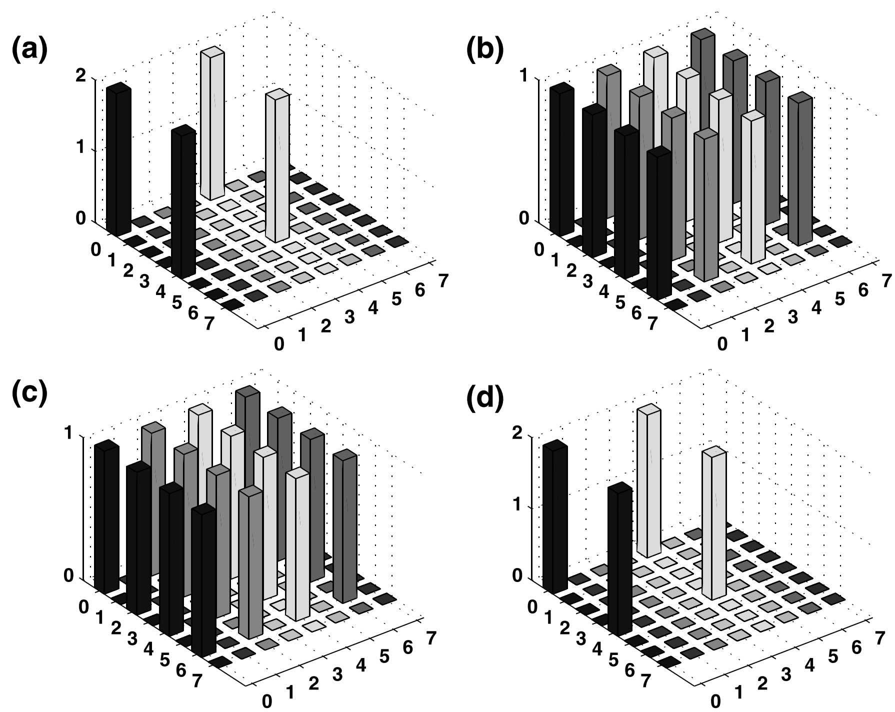

Fig. 3. Quantum Fourier transform in three-qubits is shown by simulations. The dimension of the Hilbert's space of the system is 8. (a) and (c) are two different input states with periodicity (r) 4 and 2, respectively. The density matrices of the corresponding output states (b) and (d), show periodicities (q/r) as 2 and 4, respectively. This shows QFT extracted the periodicity of the input state. The x- and y-axis labels correspond to different states as: $0 \to |000\rangle$, $1 \to |001\rangle$, $2 \to |010\rangle$, $3 \to |011\rangle$, $4 \to |100\rangle$, $5 \to |101\rangle$, $6 \to |110\rangle$, and $7 \to |111\rangle$.

Grover's algorithm for two-qubit system requires only one iteration. The gate sequence (after pseudo-pure state) for two-qubit search is $HC_{ij}(\pi)HC_{00}(\pi)H$, where $ij = 00, 01, 10$, and 11 for searching the states $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$, respectively. The first Hadamard H gate is applied to create uniform superposition state, the C_{ij} phase gate is for 'conditional sign-flip step,' and $HC_{00}(\pi)H$ performs the 'inversion about average.' The pulse sequence used for different C_{ij} phase gates are as in Eqs. (10)–(13). Each C_{ij} requires three z-pulses. The first two z-pulses are to be applied on both the transitions of first qubit, hence making it a qubit selective z-rotation

$$(\phi/2)_{z0}(\phi/2)_{z1} = (\phi/2)_z^{(1)}, \tag{37}$$

where the superscript shows that it is a z-rotation of qubit 1. The large Larmor frequency difference between two qubits (^{13}C and ^1H) allows one to achieve the first two z-pulses by qubit selective hard pulses on the first qubit. For example, in the case of $C_{11}(\phi)$ gate

$$\begin{aligned}[(\phi/2)_{z0}][(\phi/2)_{z1}] &= [(\pi/2)_{y0}(\phi)_{x0}(\pi/2)_{(-y)0}] \\ &\quad \times [(\pi/2)_{y1}(\phi)_{x1}(\pi/2)_{(-y)1}] \\ &= (\pi/2)_y^{(1)}(\phi)_x^{(1)}(\pi/2)_{(-y)}^{(1)}. \end{aligned} \tag{38}$$

The third z-pulse ϕ_{1z} was achieved by three transition selective pulses on a transition of the second qubit, as in case of $C_{11}(\phi)$, $(\phi)_{1z} = (\pi/2)_{1y}(\phi)_{1x}(\pi/2)_{1(-y)}$. Hence, each conditional phase-shift gate required three-qubit selective and three-transition selective pulses.

We have experimentally determined the search of all the states $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$ in four different experiments, the results being shown in Fig. 4.

The pseudo-pure state and the final states were tomographed by efficient quantum state tomography using two-dimensional Fourier transform technique [21,35]. The diagonal elements were measured using a one-dimensional experiment. In this experiment, all off-diagonal elements were dephased by a gradient pulse along the z-direction, and then a small angle (15°) pulse was used for detection. The detected signal yielded all the diagonal elements. The off-diagonal elements were measured using a two-dimensional experiment. Here, the density matrix was allowed to evolve for a time t_1, then a (90°) hard pulse (on all qubits) transforms every element of density matrix into all other elements including diagonal elements. A gradient pulse retains only diagonal elements, and a (45°) hard pulse (on all qubits) is applied and the signal is detected as a function of time t_2. The detected signal is Fourier transformed with respect to t_1 and t_2, yielding a two-dimensional frequency domain spectrum $S(\omega_1, \omega_2)$. The intensities of various peaks in $S(\omega_1, \omega_2)$ yields all the off-diagonal elements of the initial density matrix. The above procedure of measuring off-diagonal elements requires ideal (90°) and (45°) pulse. Therefore, we also performed another one-dimensional experiment without applying any pulses, which allows us to directly measure the single quantum elements of the initial density matrix. These intensities

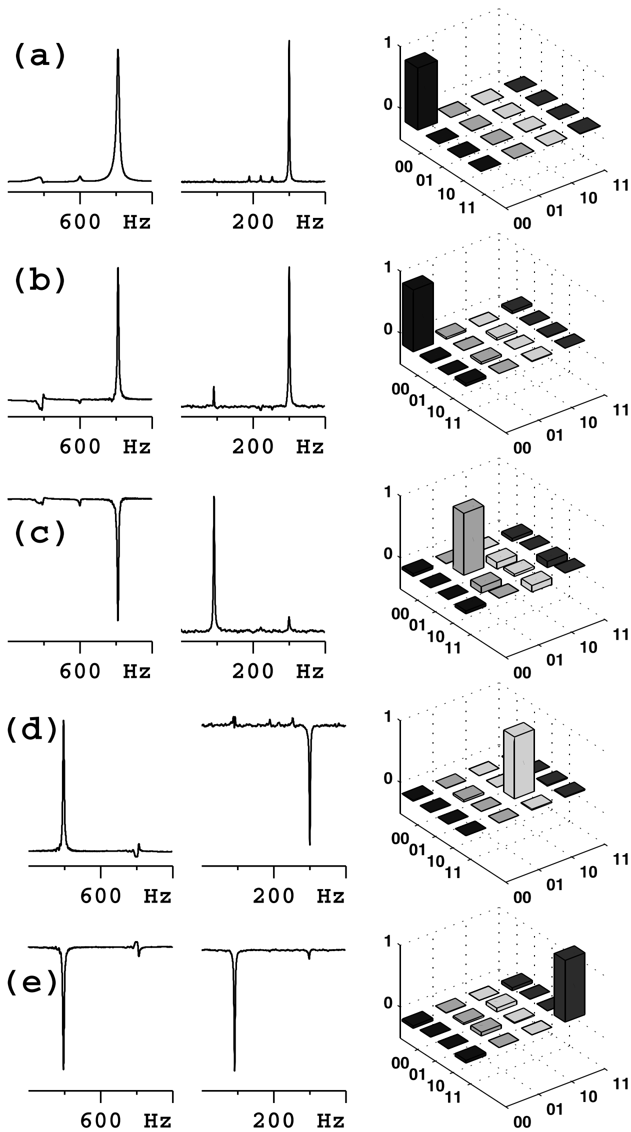

Fig. 4. Experimental implementation of Grover's search algorithm on a two-qubit system using transition selective pulses (a) is the initial pseudopure state $|00\rangle$, (b) is the search of $|00\rangle$ state, (c) of $|01\rangle$ state, (d) of $|10\rangle$ state and (e) is of $|11\rangle$ state. The left-hand side figures show the spectra for mapping of the diagonal elements. An inhomogenous magnetic field along z-direction kills all unwanted off-diagonal elements created by pulse imperfections, and then a small angle (15°) pulse yielded the above spectra. The real part of the complete tomographed density matrices are shown in the right-hand side.

were compared with the single quantum elements measured by the two-dimensional experiment and were used to normalize the remaining off-diagonal elements. The errors in the diagonal elements were less than 5%. The errors in the off-diagonal elements were less than 15%. The errors are mainly due to errors in long low power r.f. pulses (transition selective), during which relaxation and evolution adds to the errors. However, the errors in the present experiment are comparable to those performed earlier using J-evolution [13].

5. Conclusion

In this work, we suggest transition selective pulses as candidate for implementation of phase-shift gates for quantum information processing. The implementation of unitary operators by J-evolution requires refocusing pulse schemes for removal of evolution under chemical shifts and unwanted couplings [23]. The use of transition selective pulses do not need such pulse schemes. The search of more qubits has led researchers to use molecules oriented in liquid crystalline matrices as computers [24,25,28,29]. In these systems, one often encounters spins which are strongly coupled, and in such cases evolution under J-coupling or dipolar coupling becomes too complex for quantum information processing [32]. The use of transition selective pulses for quantum information processing is especially useful in such systems [30]. The use of low power, long duration r.f. pulses, gives rise to experimental errors due to relaxation and unwanted evolution under the internal Hamiltonian during long pulses. The experimental error may be reduced by using strongly modulating selective pulses of shorter duration, developed recently [36].

Acknowledgments

Useful discussions with Prof. K.V. Ramanathan and Mr. Neeraj Sinha are gratefully acknowledged. The use of DRX-500 NMR spectrometer of the Sophisticated Instruments Facility, Indian Institute of Science, Bangalore, funded by the Department of Science and Technology, New Delhi, is also gratefully acknowledged.

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