NMR experimental realization of seventh-order coupling transformations and the seven-qubit modified Deutsch-Jozsa algorithm

Daxiu Wei, Jun Luo, Xiaodong Yang, Xianping Sun, Xizhi Zeng, Maili Liu, Shangwu Ding, and Mingsheng Zhan

State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics,
Wuhan Institute of Physics and Mathematics,
Chinese Academy of Sciences, Wuhan 430071, People’s Republic of China

Abstract

We propose a scalable method on the basis of nth-order coupling operators to construct f-dependent phase transformations in the n-qubit modified Deutsch-Jozsa (D-J) quantum algorithm. The novel n-qubit entangling transformations are easily implemented via J-couplings between neighboring spins. The seven-qubit modified D-J quantum algorithm and seventh-order coupling transformations are then experimentally demonstrated with liquid state nuclear magnetic resonance (NMR) techniques. The method may offer the possibility of creating generally entangled states of n qubits and simulating n-body interactions on n-qubit NMR quantum computers.

PACS numbers: 03.67.Lx, 76.60.-k, 75.10.Jm
By using the characteristics of quantum mechanics, quantum computers (QC) are faster than their classical counterparts when performing certain computational tasks such as factorizing a large number [1], searching unsorted database [2], and especially when simulating quantum systems themselves [3]. Among all quantum algorithms, Deutsch’s algorithm [4, 5] was not only the first to be proposed, but also the first to be demonstrated [6] using liquid state nuclear magnetic resonance (NMR) techniques [7, 8]. An experimental realization of Deutsch-Jozsa (D-J) algorithm has not only demonstrated that QCs have an information-processing capability much greater than that of their classical counterparts, but also provided crucial insight into more impressive quantum algorithms [9]. Based on the Cleve version [5], two-, three- or five-qubit D-J algorithm has been implemented with NMR spectroscopy [6]. All of the previous D-J algorithms required n+1 qubit quantum systems to realize the n-bit D-J algorithm. However, Collins et al. [10] proposed a modified version of the D-J algorithm, which allowed an implementation of the n-qubit D-J algorithm by using n qubits. Up to now, the modified D-J algorithm has been implemented only on three-qubit spin systems [10].

Extending qubit number in quantum computation has been a subject of much recent interest [11]. Currently only NMR technique is used to experimentally demonstrate quantum information processing with more than four qubits. Such progresses [12] include seven-qubit “cat”-state [13] and Shor’s algorithm [14], five-qubit D-J algorithm [6], five-qubit order finding algorithm [15] and five-qubit error correction benchmark [16]. However, experimentally it is a technical challenge to extend to more qubits because of the low signal-to-noise ratio (SNR) in NMR experiments and furthermore, the SNR’s exponential decrease with the increase of qubit number [17]. In the way to get more qubits, there are two obstacles. First, although efficient methods have been developed to refocus the interaction of single-spin and two spins [18], it is not easy to control the coherent evolution between two specific spins. This is because the coupling network becomes more complex when more qubits are involved. Second, it is difficult to find any molecule that has appreciable J-coupling configuration between any pair of spins. Fortunately, Mádi et al. [19] have used quantum swap gates to surmount the second difficulty.

In this letter, we propose a simple method to construct n-qubit entangling transformations on the basis of nth-order coupling operators. The method we present is general and scalable. The key to the method is only to use the J-couplings between neighbouring spins to
implement nth-order coupling transformations. With this method, we can construct n-qubit entangling transformations for balanced functions in the modified D-J algorithm. And then we experimentally demonstrate the seven-qubit modified D-J algorithm and seventh-order coupling transformations using NMR.

The modified D-J algorithm.—A D-J problem \[4, 5\] is: given Boolean function \( f(x) : \{0, 1\}^n \rightarrow \{0, 1\} \), how many evaluations are necessary to determine \( f(x) \) being constant or balanced—constant functions \( f(x) \) always give the same output (all 0 or all 1) for all input values, but balanced functions \( f(x) \) have an equal number of 0 outputs as 1s. In a modified version of the D-J algorithm \[10\], the key to the scheme is to perform an f-controlled gate \[10\], whose transformation on the basis elements \( |x> \equiv |x_{n-1} \cdots x_0> [x_i \in (0, 1)] \) is defined as \[10\]:

\[
U_f|x> := (-1)^{f(x)}|x> .
\] (1)

The unitary transformation \( U_f \) is an f-dependent phase operation on \( 2^n \) eigenstates of an n-qubit quantum computer. For example, the number of functions for the seven-bit D-J problem is \( \binom{128}{64} + 2 \), which is a large number. In general, it is difficult to express the unitary transformation \( U_f \) as the product of operators allowed by the Ising-type Hamiltonian of spin-1/2 systems. Fortunately, we can classify the \( U_f \) s as seven representative types of unitary transformations namely, non-entangling, and from two-qubit entangling to seven-qubit entangling.

Constructing n-qubit f-dependent phase transformations via nth-order coupling operators.—We consider 9 explicit transformations, as shown in table 1. The transformations \( U_{f4} - U_{f9} \) in table 1 correspond to the two-qubit to seven-qubit entangling operators, respectively. From the transformations \( U_{f4} - U_{f9} \), we can easily extend the entangling transformations to an n-qubit case. For example, an f-dependent phase transformation for any balanced function in the n-bit D-J algorithm can read:

\[
U_{n-bit-f} = \frac{1}{2} \left( E^{(1)} \otimes \cdots \otimes E^{(n-2)} \otimes \sigma_z^{(n-1)} \otimes E^{(n)} + E^{(1)} \otimes \cdots \otimes E^{(n-2)} \otimes \sigma_z^{(n-1)} \otimes \sigma_z^{(n)} \right) \\
+ \frac{1}{2} \left( \sigma_z^{(1)} \otimes \cdots \otimes \sigma_z^{(n-1)} \otimes E^{(n)} - \sigma_z^{(1)} \otimes \cdots \otimes \sigma_z^{(n)} \right), \quad (2)
\]
where $\sigma_z$ is the Pauli matrix, $E$ is a $2 \times 2$ unit matrix, and superscripts label the qubits involved. The transformation $U_{n\text{-bit-}f}$ is diagonal in the $2^n$ eigenbasis vectors. It is interesting to note that the transformation $U_{n\text{-bit-}f}$ cannot be decomposed as direct products of single-spin operators and is hence an entangling operation. The n-qubit entangling transformation $U_{n\text{-bit-}f}$ in the modified D-J algorithm can be constructed on the basis of second, nth, and (n-1)th-order coupling operators. In order to realize the n-qubit entangling transformation $U_{n\text{-bit-}f}$ experimentally, $U_{n\text{-bit-}f}$ can be decomposed with the product operator basis set:

$$U_{n\text{-bit-}f} = \exp[i\pi] \left\{ \exp \left[ -i \frac{\pi}{2} \sigma_z^{(1)} \cdot \cdot \cdot \sigma_z^{(n-1)} \right] \otimes E^{(n)} \right\} \exp \left[ i \frac{\pi}{2} \sigma_z^{(1)} \cdot \cdot \cdot \sigma_z^{(n)} \right]$$

(3)

Following a procedure similar to that given in Ref. [20], we perform the nth-order coupling operation $\exp \left[ i \frac{\pi}{2} \sigma_z^{(1)} \cdot \cdot \cdot \sigma_z^{(n)} \right]$ in terms of the operators allowed by the Hamiltonian of spin-1/2 systems, i.e., with radio frequency pulses and scalar J-couplings between two neighboring spins. For example, a quantum circuit for performing a seven-qubit entangling transformation $(U_{f9})$ is demonstrated in Fig. 1(a).

**Experimental realization.**—A quantum circuit shown in Fig. 1(b) can be used to implement the seven-qubit modified D-J algorithm. This circuit begins with an initial state $|0000000\rangle$. In fact, however, the statistical mixture of pure states can be used as input states, since the D-J algorithm can accept the thermal equilibrium state as an input [6, 10, 21]. There are two important operations in Fig. 1(b), namely pseudo-Hadamard and f-dependant phase gates. $h$ and $h^{-1}$ are pseudo-Hadamard gates, which can be implemented by 90 degree pulses along $\pm y$ axes, respectively. The key to this approach is to realize seven-qubit f-dependant phase transformations shown in table 1 and Fig. 1(a).

In order to read out results, it is necessary to apply a selective $(\pi/2)_y$ pulse to the corresponding spin. According to phases (absorption or emission) of the $^{13}$C and $^1$H NMR signals, NMR spectra clearly indicate where the system is. Therefore we can determine the constant or balanced nature of the function (Fig. 1(b)). Fortunately, we can cancel the final pseudo-Hadamard transformations by the $(\pi/2)_y$ read-out pulse used in NMR experiments. In
order to improve experimental results, we have used the first-order phase correction methods [22], and acquired NMR spectra with 96 scans.

We have selected a seven-qubit spin system [U-13C4-labeled crotonic acid (13C1H3 13C2H1=13C3H2 13C4O2H, Cambridge Isotope Laboratories Inc. Cat. No. CLM-6118), where right superscripts label the qubits] [13]. The sample of 20mg crotonic acid was dissolved in deuterated acetone, degassed and flame-sealed in a standard 5mm NMR test tube, the coupling constants of which can be found in Ref. [13]. We began the experiment from a thermal equilibrium state. We have used four carbons and three protons as the seven qubits. We carried out the experiment with a Varian INOVA 600 NMR spectrometer. All NMR experiments were conducted at 25 °C. The shape of the soft pulse was Gaussian. The J-coupling interactions in NMR spin systems have been used to implement entangling transformations required for the seven-qubit modified D-J algorithm.

Results and discussion.—Typical experimental results are shown in figures 2 and 3. The experimental spectra in figure 2 correspond to the constant function (Uf1), which is directly obtained after applying a 90 degree pulse to the thermal equilibrium state. The spectra in Fig. 2 served as reference spectra. The phase of the reference spectra was adjusted so that signals from all the seven spins appear in absorption (positive phase). The experimental spectra in Fig. 3 correspond to the balanced functions (Uf2, Uf4, Uf5, and Uf9), respectively. Compared with the reference spectra in Fig. 2, the spectra in Fig. 3 show that there is at least one line with a π phase difference (in emission). By determining the relative phase of the signals from the seven spins, we can determine that the functions corresponding to Fig. 3 are balanced. It should be noticed that only a single function call is used.

Fig. 2 shows that the spectra of C1 contain 128 peaks. This indicates that spin C1 interacts with 7 neighbors. This results from the J-couplings of the three other 13C, the two protons (H1, H2) and the three methyl protons (H3). It should be noted that the J-coupling effect of the methyl protons on the spin C1 is the same as that of two protons.

As for the thermal equilibrium state used as an input state in our experiments, the investigations [6, 10, 21] have shown that the D-J algorithm can be implemented by starting with thermal rather than pure initial states. The reason is that the thermal equilibrium state has similar effect as the effective pure state.

There are imperfect phases in the experimental results. The signals do not exhibit pure absorption or pure emission lineshapes. The phase errors mainly come from (a) the im-
perfection of the selective pulses, (b) the inaccuracy of the 90 and 180 degree pulses, (c) inaccurate refocusing of chemical shifts during the J-coupling delays, and (d) J-coupling evolution during long selective pulses.

It should be noted that n-qubit entangling transformations in the modified D-J algorithm can be performed with radio frequency pulses and scalar J-couplings between two neighboring spins. The scheme may be used to create generally entangled states with n qubits on the basis of the interactions between neighboring spins. This is very important for demonstrating the role of quantum entanglement in quantum information processing.

We used seventh-order coupling operators to construct a seven-qubit entangling transformation. We have successfully realized the seven-qubit entangling transformation in the context of the modified D-J algorithm. Therefore we have experimentally performed the seventh-order coupling operator. In fact, there is no seventh-order coupling in liquid state NMR systems. Our experimental results show that seven-body interactions can be simulated with such an experimental method. This will be useful in simulating many-body interactions in other quantum systems.

The NMR experimental realization of multi-qubit quantum algorithms is a difficult proposition. In a multi-qubit NMR QC, it is necessary to suppress the interactions coming from the other qubits when realizing the quantum logic gate between two given spins. Our experimental results have demonstrated that the control of multi-qubit’s evolution is successful.

Conclusions.—On the basis of constructing f-dependent phase transformations in the modified D-J quantum algorithm with nth-order coupling operators, we have experimentally tested the modified D-J algorithm for seven qubits and performed seventh-order coupling transformations. This may open a way to experimentally simulate n-body interactions and to realize n-qubit entangling transformations on NMR quantum computers.

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Table 1. The transformations $U_f$ and their definitions. $E^{(A,B,C,...)}$ and $\sigma_z^{(A,B,C,...)}$ mean $E^{(A)} \otimes E^{(B)} \otimes E^{(C)} \otimes \ldots$, and $\sigma_z^{(A)} \otimes \sigma_z^{(B)} \otimes \sigma_z^{(C)} \otimes \ldots$, respectively. $C_i$ (i=1,2,3, and 4) and $H^j$ (j=1,2, and 3) are carbon and hydrogen nuclei used in experiments.

| $U_f$       | Definitions                                                                 |
|------------|-----------------------------------------------------------------------------|
| Constant:  | $E(C^1,C^2,C^3,C^4,H^1,H^2,H^3)$                                           |
| $U_{f1}$   | $\sigma_z^{(C^2,C^3)} \otimes E(C^1,C^4,H^1,H^2,H^3)$                      |
| Balanced:  | $\sigma_z^{(C^1,C^2,C^3,H^1,H^2,H^3)}$                                     |
| $U_{f2}$   | $\frac{1}{2} \left( E(C^3) + \sigma_z^{(C^3)} \otimes E(C^4) + E(C^3) \otimes \sigma_z^{(C^4)} - \sigma_z^{(C^3,C^4)} \right) \otimes \sigma_z^{(C^2)} \otimes E(C^1,H^1,H^2,H^3)$ |
| $U_{f3}$   | $\frac{1}{2} \left( E(C^2) \otimes \sigma_z^{(C^1)} \otimes E(H^3) + E(C^2) \otimes \sigma_z^{(C^1,H^3)} + \sigma_z^{(C^2,C^1)} \otimes E(H^3) - \sigma_z^{(C^2,C^3,H^3)} \right)$ |
| $U_{f4}$   | $\frac{1}{2} \left( E(C^1,C^2,C^3) \otimes \sigma_z^{(C^3)} \otimes E(H^1) + E(C^1,C^2,C^3) \otimes \sigma_z^{(C^4)} \otimes \sigma_z^{(H^1)} \right) \otimes E(H^2,H^3)$ |
| $U_{f5}$   | $\frac{1}{2} \left( E(C^1,C^2,C^3) \otimes \sigma_z^{(C^3)} \otimes E(H^1) + E(C^1,C^2,C^3) \otimes \sigma_z^{(C^4)} \otimes \sigma_z^{(H^1)} \right) \otimes E(H^2,H^3)$ |
| $U_{f6}$   | $\frac{1}{2} \left( E(C^1,C^2,C^3) \otimes \sigma_z^{(C^3)} \otimes E(H^1) + E(C^1,C^2,C^3) \otimes \sigma_z^{(C^4)} \otimes \sigma_z^{(H^1)} \right) \otimes E(H^2,H^3)$ |
| $U_{f7}$   | $\frac{1}{2} \left( E(C^1,C^2,C^3) \otimes \sigma_z^{(C^3)} \otimes E(H^1) + E(C^1,C^2,C^3) \otimes \sigma_z^{(C^4)} \otimes \sigma_z^{(H^1)} \right) \otimes E(H^2,H^3)$ |
| $U_{f8}$   | $\frac{1}{2} \left( E(C^1,C^2,C^3) \otimes \sigma_z^{(C^3)} \otimes E(H^1) + E(C^1,C^2,C^3) \otimes \sigma_z^{(C^4)} \otimes \sigma_z^{(H^1)} \right) \otimes E(H^2,H^3)$ |
| $U_{f9}$   | $\frac{1}{2} \left( E(C^3,H^1,H^2,H^3) \otimes \sigma_z^{(C^1)} \otimes E(C^2) + E(C^3,H^1,H^2,H^3) \otimes \sigma_z^{(C^2,C^3)} \right)$ |
**Figure captions**

FIG. 1. (a) A quantum network for realizing the seven-qubit entangling transformation $U_{f_9}$. Refocusing and decoupling pulses are not included. Vertical bars denote J-coupling gates, which are given by the unitary transformation $\exp\{ -i\sigma_z^{(k)}\sigma_z^{(l)} \pi/4 \}$ on spins k and l. (b) A quantum circuit for implementing the seven-qubit modified D-J algorithm. A function $f$ is constant if and only if the output state for every qubit is in all the $|0\rangle$ state, otherwise a function is balanced.

FIG. 2. The experimental spectra corresponding to the transformation $(U_{f_1})$ for the constant function $f_1$ from seven spins. Horizontal axes, relative frequency (ppm); vertical axes, intensity (arbitrary units).

FIG. 3. Same as Fig. 2, but (a), (b), (c), and (d) corresponding to the balanced function transformations $U_{f_2}, U_{f_4}, U_{f_5},$ and $U_{f_9}$, respectively.
Fig. 2
Fig. 3