Realization of generalized quantum searching using nuclear magnetic resonance

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According to the theoretical results, the quantum searching algorithm can be generalized by replacing the Walsh-Hadamard transform by almost any quantum-mechanical operation. We have implemented the generalized algorithm using nuclear magnetic resonance techniques with a solution of chloroform molecules. Experimental results show a good agreement between the theory and experiment.

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The quantum-searching algorithm was first proposed by Grover [1]. It can speed up some search applications over unsorted data and has become a hot topic in quantum information [2–5]. The surprising result of the algorithm is that searching a particular item in an unsorted list of N elements only requires $O(\sqrt{N})$ attempts [2]. The algorithm needs the properties of the Walsh-Hadamard(W-H) transform and has been implemented using nuclear magnetic resonance (NMR) techniques [6]. Grover generalized the algorithm in theory, in which the Walsh-Hadmamard transform can be replaced by almost any quantum operation [7].

The generalized algorithm can be posed as follows. If a unitary operator U is applied to a quantum system in an initial basis state $|\gamma\rangle$, the system lies in a superposition $\Sigma_i a_i|i\rangle$, where $a_i=\langle i|U|\gamma\rangle=U_{i\gamma}$. The amplitude of reaching the target state $|\tau\rangle$ is $U_{\tau\gamma}$, and the probability of getting the system in state $|\tau\rangle$ is $|U_{\tau\gamma}|^2$ if a measurement is made. Therefore, it will take at least $O(1/|U_{\tau\gamma}|^2)$ repetitions of U and the measurement to get state $|\tau\rangle$ for one time. On the contrary, according to the generalized searching algorithm, in $O(1/|U_{\tau\gamma}|)$ applications, operator Q transforms $|\gamma\rangle$ into $U^{-1}|\tau\rangle$. After U is applied, the system lies in state $|\tau\rangle$. Q is defined as $Q\equiv -I_\gamma U^{-1} I_\tau U$, where $I_i\equiv I-2|i\rangle\langle i|$, and I denotes unit matrix. If I_i is applied to a superposition of states, it only inverts the amplitude in state $|i\rangle$, and leaves the other states unaltered. It has been shown in theory that the number of repetitions of Q required to transform $|\gamma\rangle$ into $|\tau\rangle$ is $\pi/4|U_{\tau\gamma}|$ if $|U_{\tau\gamma}|\ll 1$.

It can be proved that for a two-qubit system, the number of repetitions of Q is also $O(1/|U_{\tau\gamma}|)$ without the condition that $|U_{\tau\gamma}|\ll 1$. Particularly, if $|U_{\tau\gamma}|=1/2$, the number of repetitions is 1, and the probability of getting the target state is 1. In this paper, we will implement the generalized quantum algorithm in this case on a two-qubit NMR quantum computer [8].

Our experiments use a sample of carbon-13 labeled chloroform (Cambridge Isotopes) dissolved in d6-acetone. Data are taken at a controlled temperature (22 °C) with a Bruker DRX 500 MHz spectrometer (Beijing Normal University). The resonance frequencies are $\nu_1=125.76$ MHz for ^{13}C and $\nu_2=500.13$ MHz for ^{1}H. The coupling constant J is measured to be 215 Hz. If the magnetic field is along the $\hat{z}$ axis, and one lets $\hbar=1$, the Hamitonian of this system is

$$H=-2\pi\nu_1 I_z^1-2\pi\nu_2 I_z^2+2\pi J I_z^1 I_z^2, \tag{1}$$

where $I_z^k(k=1,2)$ are the matrices for the $\hat{z}$ component of the angular momentum of the spins [9]. In the rotating frame of spin k, the evolution caused by a radio-frequency (rf) pulse along the $\hat{x}$ or $\hat{y}$ axes is denoted as $X_k(\varphi_k)=e^{i\varphi_k I_x^k}$ or $Y_k(-\varphi_k)=e^{-i\varphi_k I_y^k}$, where $\varphi_k=B_1\gamma_k t_p$. B_1, γ_k, and t_p represent the strength of the magnetic field, gyromagnetic ratio of spin k, and the width of the rf pulse, respectively. The pulse used above is denoted as $[\varphi]_x^k$ or $[-\varphi]_y^k$. The coupled-spin evolution is denoted as

$$t=e^{-i2\pi J I_z^1 I_z^2}, \tag{2}$$

where t is the evolution time. The pseudopure initial state

$$|\gamma\rangle=|\uparrow\rangle_1|\uparrow\rangle_2=\begin{pmatrix}1\\0\\0\\0\end{pmatrix} \tag{3}$$

is prepared by using spatial averaging [10], where $|\uparrow\rangle_k$ denotes the state of spin k. For convenience, the notion $|\uparrow\rangle_1|\uparrow\rangle_2$ is merged into $|\uparrow\uparrow\rangle$ and the subscripts 1 and 2 are omitted. The basis states are arrayed as $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$. In matrix notion, I_i is a diagonal matrix with all diagonal terms equal to 1 except the ii term which is -1. For example, if $|i\rangle=|\downarrow\downarrow\rangle$, I_i is expressed as

$$I_3=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}. \tag{4}$$

U is chosen as three forms

$$U_1=1/2\begin{pmatrix}-1&-1&-1&-1\\-1&1&-1&1\\-1&-1&1&1\\-1&1&1&-1\end{pmatrix}, \tag{5}$$

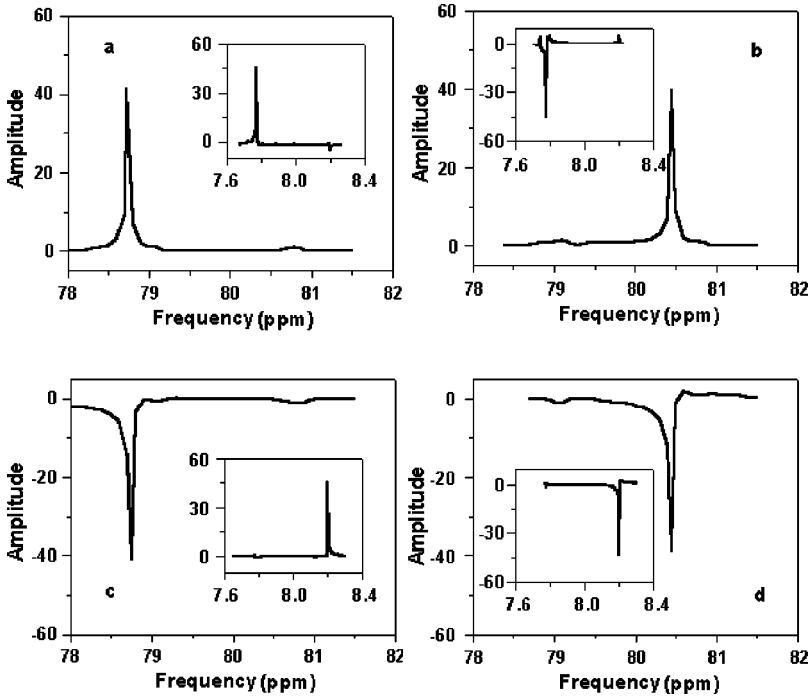

FIG. 1. NMR spectra of ^{13}C (main figures) and ^{1}H (smaller insets), when the two-spin system lies in various pseudopure states via readout pulses selective for ^{13}C (main figures) and ^{1}H (smaller insets). The amplitude has arbitrary units. When the system lies in a pseudopure state, only one NMR peak appears in the spectrum of spin k if a readout pulse $[-\pi/2]_y^k$ is applied. (a)–(d) are spectra corresponding to pseudopure states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, respectively.

$$U_2 = 1/2 \begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \tag{6}$$

and

$$U_3 = 1/2 \begin{pmatrix} 1 & i & i & -1 \\ i & 1 & -1 & i \\ i & -1 & 1 & i \\ -1 & i & i & 1 \end{pmatrix}, \tag{7}$$

where U_1 is the W-H transform used in Ref. [6] (up to a phase factor). It is easily proved that UQ can transform state $|\gamma\rangle$ into state $|\tau\rangle$. The irrelevant overall phase factors are ignored.

The evolution of the system can be represented by its deviation density matrix ρ_Δ [11]. For the heteronuclear system, the following rf and gradient pulse sequence $[\alpha]_x^2 - [\mathrm{grad}]_z - [\pi/4]_x^1 - 1/4J - [\pi]_x^1 - [\pi]_x^2 - 1/4J - [-\pi/4]_y^1 - [\mathrm{grad}]_z$ transforms the system from the equilibrium state

$$\rho_{\Delta eq} = \gamma_1 I_z^1 + \gamma_2 I_z^2 \tag{8}$$

to the initial state required in experiments

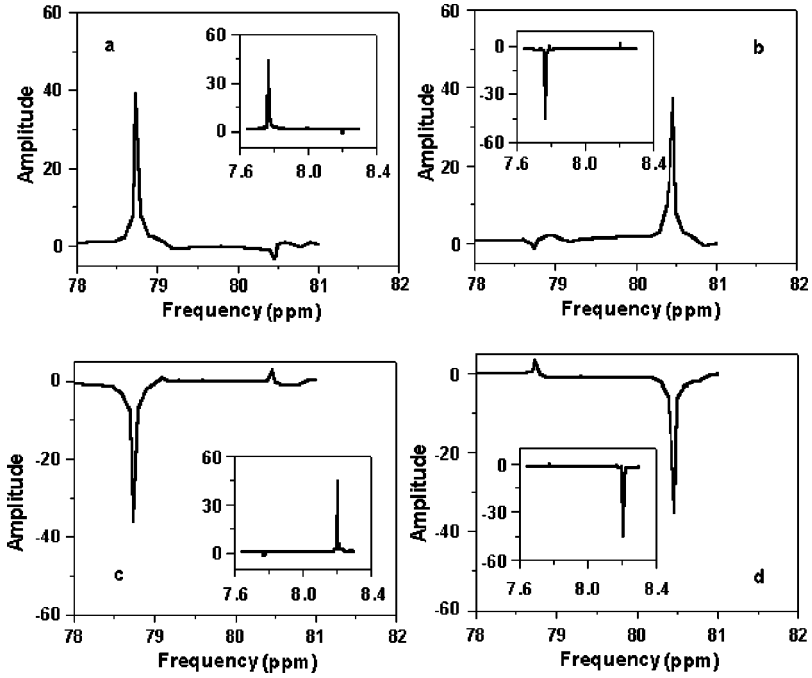

FIG. 2. Spectra of ^{13}C (main figures) and ^{1}H (smaller insets) after completion of the generalized searching algorithm and readout pulses selective for ^{13}C (main figures) and ^{1}H (smaller insets). U is chosen as U_3, and the target state $|\tau\rangle$ is $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, or $|\downarrow\downarrow\rangle$. The corresponding searching results are shown by (a)–(d). By comparing (a)–(d) with Figs. 1(a)–(d), respectively, we confirm that the system is truly in the target state.

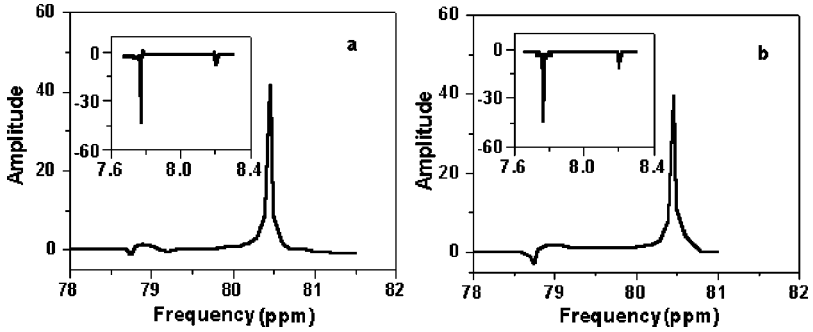

FIG. 3. Spectra of ^{13}C (main figures) and ^{1}H (smaller insets) after completion of the generalized searching algorithm and readout pulses selective for ^{13}C (main figures) and ^{1}H (smaller insets) on condition that $|\tau\rangle=|\uparrow\downarrow\rangle$, and $U=U_1$ shown by (a) or $U=U_2$ shown by (b).

$$\rho_{\Delta 0}=-(I_z^1/2+I_z^2/2+I_z^1I_z^2)=-1/4\begin{pmatrix}3&0&0&0\\0&-1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}, \tag{9}$$

where $\alpha=\arccos(\gamma_1/2\gamma_2)$, and $[\mathrm{grad}]_z$ denotes gradient pulse along $\hat{z}$ axis. The pulses are applied from left to right. The symbol $1/4J$ denotes the evolution caused by the Hamitonian H for $1/4J$ without pulses. The initial state can be used as the pseudopure state $|\uparrow\uparrow\rangle$ in NMR quantum computation [12]. By applying pulse $[\pi]_x^2$, $[\pi]_x^1$ or $[\pi]_x^1[\pi]_x^2$, the pseudopure states corresponding to states $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$ or $|\downarrow\downarrow\rangle$ can be obtained. They are written as

$$\rho_{\Delta 1}=-(I_z^1/2-I_z^2/2-I_z^1I_z^2), \tag{10}$$

$$\rho_{\Delta 2}=-(-I_z^1/2+I_z^2/2-I_z^1I_z^2), \tag{11}$$

$$\rho_{\Delta 3}=-(-I_z^1/2-I_z^2/2+I_z^1I_z^2). \tag{12}$$

We also represent the above four pseudopure states as $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, respectively. According to Ref. [6], we find that

$$I_0=Y_1(\pi/2)Y_2(\pi/2)X_1(-\pi/2)X_2(-\pi/2)Y_1(-\pi/2)Y_2\times(-\pi/2)[1/2J],$$

$$I_1=Y_1(\pi/2)Y_2(\pi/2)X_1(\pi/2)X_2(-\pi/2)Y_1(-\pi/2)Y_2\times(-\pi/2)[1/2J],$$

$$I_2=Y_1(\pi/2)Y_2(\pi/2)X_1(-\pi/2)X_2(\pi/2)Y_1(-\pi/2)Y_2\times(-\pi/2)[1/2J],$$

$$I_3=Y_1(\pi/2)Y_2(\pi/2)X_1(\pi/2)X_2(\pi/2)Y_1(-\pi/2)Y_2(-\pi/2)\times[1/2J].$$

The time order is from right to left. It is easy to prove that

$$U_1=X_1(\pi)X_2(\pi)Y_1(-\pi/2)Y_2(-\pi/2),$$

$$U_2=Y_1(\pi/2)Y_2(\pi/2),$$

$$U_3=X_1(\pi/2)X_2(\pi/2).$$

In our experiments, each NMR spectrum of spin k is obtained by a spin-selective readout pulse $[-\pi/2]_y^k$. The relative phases of signals are meaningful because all experiments are acquired in an identical fashion [13]. At first, we prepare the four pseudopure states described in Eqs. (9)–(12). For the system in a pseudopure state, only one NMR peak appears in a spectrum if a selective readout pulse is applied. Figure 1 shows the experimental MNR spectra when the system lies in various pseudopure states. Figures 1(a)–(d) are spectra when the system lies in pseudopure states $|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, and $|\downarrow\downarrow\rangle$, respectively. In each figure, the main spectrum represents the spectrum of ^{13}C and the ^{1}H spectrum is shown in a smaller inset. For each experiment, the initial state $|\gamma\rangle$ is pseudopure state $|\uparrow\uparrow\rangle$. U is selected as U_1, U_2, or U_3. The searching state $|\tau\rangle$ can be any pseudopure state. UQ transforms state $|\gamma\rangle$ into state $|\tau\rangle$. Therefore, the number of application of Q is 1. The searching results on condition that $U=U_3$ and $|\tau\rangle=|\uparrow\uparrow\rangle$, $|\uparrow\downarrow\rangle$, $|\downarrow\uparrow\rangle$, or $|\downarrow\downarrow\rangle$ are shown in Fig. 2. Comparing Figs. 2(a)–2(d) with Figs. 1(a)–1(d), respectively, we confirm that the system truly lies in the target state. In order to illustrate that the searching results for U_3 are the same as U_1 or U_2, Fig. 3 shows the searching results on condition that $|\tau\rangle=|\uparrow\downarrow\rangle$, and $U=U_1$ [shown by Fig. 3(a)] or U_2 [shown by Fig. 3(b)]. It can be found from various spectra that the experimental errors are not larger than 5% barring the two ^{1}H spectra. The errors mainly result from the imperfection of pulses, inhomogeneity of magnetic field, and effect of decoherence. We find that if each $[\pi/2]_\phi^k$ ($\phi=x$ or y) in I_i is replaced by $[-\pi/2]_\phi^k$, and each $[-\pi/2]_\phi^k$ is replaced by $[\pi/2]_\phi^k$, the results remain the same. This fact can be used to simplify pulse sequences and reduce experimental errors.

In conclusion, we demonstrate the generalized quantum-searching algorithm by replacing W-H transform by different transformations. Because the number of repetition of operator Q is determined by the element $|U_{\tau\gamma}|$ and these three U transformations have the same $|U_{\tau\gamma}|$, it is not surprising that the numbers of repetitions of Q are all 1. Compared with

temporal labeling, the spatial averaging used to prepare initial state shortens the experiment time. It only takes about 2 min to finish one experiment. The searching results can be directly read out from spectra, so that the steps of recording areas of peaks are avoided. These facts simplify the process of experiments and make the searching results easy to observe.

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