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NMR analogue of the generalized Grover's algorithm of multiple marked states and its application*

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The generalized Grover's algorithm for the case in which there are multiple marked states is demonstrated on a nuclear magnetic resonance (NMR) quantum computer. The Walsh–Hadamard transform and the phase inversion are all replaced. NMR analogues of Einstein–Podolsky–Rosen states (pseudo-EPR states) are synthesized using the above algorithm.

Keywords: generalized Grover's algorithm, nuclear magnetic resonance, Einstein–Podolsky–Rosen states

PACC: 0365, 4250, 3325

1. Introduction

Since the quantum searching algorithm was first proposed by Grover,[1] several generalizations of the original algorithm have been developed.[2−4] The generalized algorithm that we will realize can be posed as follows. Let N basis states of a system constitute a set D. A function F is defined as $F : D \to \{0, 1\}$. The states satisfying $F(x) = 1$ are defined as marked states, which constitute the set M with a total of r states. The other states in D, satisfying $F(x) = 0$, constitute the set $\overline{M}$ with a total of $N - r$ states. The states in M and $\overline{M}$ have amplitudes k_i, $|i\rangle \in M$ and l_i, $|i\rangle \in \overline{M}$, respectively. A unitary operator U transforms a predefined basis state $|s\rangle$ into a superposition denoted as $|g(0)\rangle = U|s\rangle$. U can be almost any valid quantum mechanical unitary operator. $|g(0)\rangle$ is the initial state for the algorithm. The phase rotation of the marked states is described by $I_t^\gamma = \sum_x \mathrm{e}^{\mathrm{i}\gamma F(x)}|x\rangle\langle x|$. Obviously, if $|x\rangle \in M$, $I_t^\gamma|x\rangle = \mathrm{e}^{\mathrm{i}\gamma}|x\rangle$; if $|x\rangle \in \overline{M}$, $I_t^\gamma|x\rangle = |x\rangle$. A composite operator is defined as $G \equiv -UI_s^\beta U^\dagger$. I_s^β is defined as $I_s^\beta \equiv I - (1 - \mathrm{e}^{\mathrm{i}\beta})|s\rangle\langle s|$, where I denotes unit matrix. The problem is to transform $|g(0)\rangle$ to a target state denoted as $|\psi_t\rangle = \sum_{i\in M} k_i|i\rangle$ by repeating Grover iteration GI_t^γ. When the system lies in $|\psi_t\rangle$, measurement yields $|k_i|^2$, the probability of the system being in the marked state $|i\rangle$. When $\beta = \pi$, $\gamma = \pi$, $|s\rangle = |\overline{0}\rangle$, and U is chosen as the Walsh–Hadamard (W-H) transform, the generalized algorithm becomes the original Grover's algorithm, where $|\overline{0}\rangle$ denotes all qubits in the 0 state.

Biham *et al*[3] have analysed the generalized Grover's algorithm using recursion equations. Through introducing an ancilla qubit and choosing a proper U, Grover proposed a theoretical scheme to synthesize a specified quantum superposition on N states in $O(\sqrt{N})$ steps using the above algorithm.[5] We find that some special superpositions, such as Einstein–Podolsky–Rosen states (EPR states),[6−8] can be synthesized using the generalized algorithm without an ancilla qubit.

NMR is an important experimental tool to study quantum computation or simulate quantum systems.[9−13] Using NMR, Long *et al*[14] realized the algorithm of one marked state by choosing the phase rotation as $I_t^{\frac{\pi}{2}}$, while the W-H transform is retained. In our previous work, we realized the algorithm by replacing the W-H transform by another unitary operator, while the phase inversion was unaltered.[15] Moreover, we synthesized the NMR analogues of Einstein–Podolsky–Rosen states (pseudo-EPR states) using the

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algorithm.[16] In this paper, we realize the generalized algorithm of multiple marked states. The W-H transform is replaced by another unitary operator and the phase rotation is chosen as $I_t^{\frac{\pi}{2}}$ or $I_t^{-\frac{\pi}{2}}$. We will synthesize pseudo-EPR states to demonstrate an application of the algorithm.

2. The generalized Grover's algorithm

In this section, we use the recursion equations[3] to express the principle of our experiments.

n applications of GI_t^{γ} transform $|g(0)\rangle$ to $|g(n)\rangle$ which are described by

$$|g(n)\rangle = \sum_{i\in M} k_i(n)|i\rangle + \sum_{i\in \overline{M}} l_i(n)|i\rangle. \tag{1}$$

When $n = 0$, the system lies in the initial state

$$|g(0)\rangle = U|s\rangle. \tag{2}$$

Obviously, $k_i(0) = U_{is}$, and $l_i(0) = U_{is}$, where $U_{is} = \langle i|U|s\rangle$. GI_t^{γ} transforms $k_j(n)$, $|j\rangle \in M$ to $k_j(n+1) = \langle j|GI_t^{\gamma}|g(n)\rangle$ and $l_j(n)$, $|j\rangle \in \overline{M}$, to $l_j(n+1) = \langle j|GI_t^{\gamma}|g(n)\rangle$. The recursion equations describing such an iteration are expressed as

$$\begin{aligned} k_j(n+1) =& e^{i\gamma}(1-e^{i\beta})U_{js}\sum_{i\in M} k_i(n)U_{is}^* \\ &+ (1-e^{i\beta})U_{js}\sum_{i\in \overline{M}} l_i(n)U_{is}^* - e^{i\gamma}k_j(n), \end{aligned} \tag{3}$$

$$\begin{aligned} l_j(n+1) =& e^{i\gamma}(1-e^{i\beta})U_{js}\sum_{i\in M} k_i(n)U_{is}^* \\ &+ (1-e^{i\beta})U_{js}\sum_{i\in \overline{M}} l_i(n)U_{is}^* - l_j(n). \end{aligned} \tag{4}$$

In our experiments, $U_{is} \neq 0$, $i = 1, 2, \cdots$. Variable $k_i'(n)$ and $l_i'(n)$ are defined as

$$k_i'(n) = \frac{k_i(n)}{U_{is}}, \tag{5}$$

$$l_i'(n) = \frac{l_i(n)}{U_{is}}. \tag{6}$$

One can easily find that $k_i'(0) = 1$, $l_i'(0) = 1$. The weighted averages are defined as

$$\overline{k'}(n) = \frac{1}{W_k}\sum_{i\in M} |U_{is}|^2 k_i'(n), \tag{7}$$

$$\overline{l'}(n) = \frac{1}{W_l}\sum_{i\in \overline{M}} |U_{is}|^2 l_i'(n), \tag{8}$$

where $W_k = \sum_{i\in M} |U_{is}|^2$, and $W_l = \sum_{i\in \overline{M}} |U_{is}|^2$. With these variables, the recursion equations can be rewritten as

$$\begin{aligned} k_j'(n+1) =& e^{i\gamma}(1-e^{i\beta})W_k\overline{k'}(n) \\ &+ (1-e^{i\beta})W_l\overline{l'}(n) - e^{i\gamma}k_j'(n), \end{aligned} \tag{9}$$

$$\begin{aligned} l_j'(n+1) =& e^{i\gamma}(1-e^{i\beta})W_k\overline{k'}(n) \\ &+ (1-e^{i\beta})W_l\overline{l'}(n) - l_j'(n). \end{aligned} \tag{10}$$

By averaging over all the marked states in Eq.(9) and over all the unmarked states in Eq.(10), we obtain the two recursion equations for $\overline{k'}(n)$ and $\overline{l'}(n)$, which are expressed as

$$\begin{pmatrix} \overline{k'}(n+1) \\ \overline{l'}(n+1) \end{pmatrix} = A \begin{pmatrix} \overline{k'}(n) \\ \overline{l'}(n) \end{pmatrix}, \tag{11}$$

where

$$A = \begin{pmatrix} e^{i\gamma}(1-e^{i\beta})W_k - e^{i\gamma} & (1-e^{i\beta})W_l \\ e^{i\gamma}(1-e^{i\beta})W_k & (1-e^{i\beta})W_l - 1 \end{pmatrix}. \tag{12}$$

Using Eqs.(9)–(12), we obtain

$$k_i'(n) = \overline{k'}(n), \tag{13}$$

$$l_i'(n) = \overline{l'}(n), \tag{14}$$

noting that the subscript has been denoted by i.

From the above discussion, for any U, $\overline{k'}(n)$ and $\overline{l'}(n)$ can be solved from Eq.(11). Through Eqs.(13), (14), (5), and (6), the explicit expressions for $k_i(n)$ and $l_i(n)$ can be obtained. Equation (11) shows that $\overline{k'}(n)$ and $\overline{l'}(n)$ are dependent on γ, β, and $|U_{is}|$. If U is replaced by a different U' where $|U_{is}'| = |U_{is}|$, the analytic forms of $\overline{k'}(n)$ and $\overline{l'}(n)$ are unaltered. If $l_i(n)$ approach 0 when $n = n_0$, the system lies in

$$|\psi_t\rangle = \sum_{i\in M} U_{is}\overline{k'}(n_0)|i\rangle. \tag{15}$$

Generally, the state is not the equally weighted superposition of marked states. By choosing a proper U, some superpositions can be synthesized using the generalized Grover's algorithm. We will solve Eq.(11) in the following section.

3. Experimental scheme

In experiments, we use a sample of carbon-13 labelled chloroform dissolved in d6-acetone. Data are taken at room temperature with a Bruker DRX 500 MHz spectrometer. The resonance frequencies $\nu_1 = 125.76$ 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 $\hat{z}$-axis, by setting $\hbar = 1$, the Hamiltonian of this system is described by

$$H = -2\pi\nu_1 I_z^1 - 2\pi\nu_2 I_z^2 + 2\pi J I_z^1 I_z^2, \qquad (16)$$

where $I_z^k (k = 1, 2)$ are the matrices for $\hat{z}$-component of the angular momentum of the spins.[17] In the rotating frame of spin k, the evolution caused by a radio-frequency(rf) pulse on resonance along $\hat{x}$ or $-\hat{y}$-axis is denoted as $X_k(\varphi_k) = \mathrm{e}^{\mathrm{i}\varphi_k I_x^k}$ or $Y_k(-\varphi_k) = \mathrm{e}^{-\mathrm{i}\varphi_k I_y^k}$, where $\varphi_k = B_1\gamma_k t_p$ with k specifying the affected spin. B_1, γ_k and t_p represent the strength of rf pulse, gyromagnetic ratio and the width of rf pulse, respectively. The pulse used above is denoted as $[\varphi]_x^k$ or $[-\varphi]_y^k$. The coupled-spin evolution is denoted as

$$[\tau] = \mathrm{e}^{-\mathrm{i}2\pi J I_z^1 I_z^2 \tau}, \qquad (17)$$

where τ is evolution time. The predefined pseudo-pure state

$$|s\rangle = |\uparrow\rangle_1 |\uparrow\rangle_2 = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} \qquad (18)$$

is prepared by using spatial averaging,[18] where $|\uparrow\rangle_k$ denotes the state of spin k. For convenience, the notation $|\uparrow\rangle_1 |\uparrow\rangle_2$ is simplified as $|\uparrow\uparrow\rangle$. The basis states are arrayed as $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. U is chosen as $U = Y_1(\varphi_1)Y_2(\varphi_2)$ represented as

$$U = \begin{pmatrix} c_1c_2 & c_1s_2 & s_1c_2 & s_1s_2 \\ -c_1s_2 & c_1c_2 & -s_1s_2 & s_1c_2 \\ -s_1c_2 & -s_1s_2 & c_1c_2 & c_1s_2 \\ s_1s_2 & -s_1c_2 & -c_1s_2 & c_1c_2 \end{pmatrix}, \qquad (19)$$

where $c_k \equiv \cos(\varphi_k/2)$, $s_k \equiv \sin(\varphi_k/2)$.

When $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$ are the two marked states, U is chosen as $U = Y_1(\pi/2)Y_2(\pi/2)$ described by

$$U = \frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}. \qquad (20)$$

I_t^γ and I_s^β are chosen as

$$I_{14}^{-\frac{\pi}{2}} = \begin{pmatrix} -\mathrm{i} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \end{pmatrix}, \qquad (21)$$

$$I_s^{-\frac{\pi}{2}} = \begin{pmatrix} -\mathrm{i} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad (22)$$

where $\gamma = \beta = -\pi/2$. We rewrite Eq.(12) as

$$A = \frac{1}{2}\begin{pmatrix} 1+\mathrm{i} & 1+\mathrm{i} \\ 1-\mathrm{i} & \mathrm{i}-1 \end{pmatrix}, \qquad (23)$$

noting $W_k = W_l = 1/2$. We introduce the diagonal matrix

$$A_{\mathrm{D}} = S^{-1}AS \equiv \begin{pmatrix} \lambda_+ & 0 \\ 0 & \lambda_- \end{pmatrix} \qquad (24)$$

to obtain the explicit expressions for $\overline{k'}(n)$ and $\overline{l'}(n)$. The eigenvalues of matrix A are the solutions of $\det(A - \lambda I) = 0$, and they are $\lambda_+ = \mathrm{e}^{\mathrm{i}\frac{\pi}{6}}$, $\lambda_- = \mathrm{e}^{\mathrm{i}\frac{5\pi}{6}}$. S and S^{-1} are expressed as

$$S = \begin{pmatrix} 1 & 1 \\ \dfrac{\sqrt{3}-1}{1+\mathrm{i}} & -\dfrac{\sqrt{3}+1}{1+\mathrm{i}} \end{pmatrix}, \qquad (25)$$

$$S^{-1} = \begin{pmatrix} \dfrac{\sqrt{3}+1}{2\sqrt{3}} & \dfrac{1+\mathrm{i}}{2\sqrt{3}} \\ \dfrac{\sqrt{3}-1}{2\sqrt{3}} & -\dfrac{1+\mathrm{i}}{2\sqrt{3}} \end{pmatrix}. \qquad (26)$$

The solution of Eq.(11) can be expressed as

$$\begin{pmatrix} \overline{k'}(n) \\ \overline{l'}(n) \end{pmatrix} = A^n \begin{pmatrix} \overline{k'}(0) \\ \overline{l'}(0) \end{pmatrix}, \qquad (27)$$

where $A^n = SA_{\rm D}^n S^{-1}$, expressed as

$$A^n = \frac{1}{2\sqrt{3}} \begin{pmatrix} (\sqrt{3}+1)e^{i\frac{n\pi}{6}} + (\sqrt{3}-1)e^{i\frac{5n\pi}{6}} & (1+i)(e^{i\frac{n\pi}{6}} - e^{i\frac{5n\pi}{6}}) \\ (1-i)(e^{i\frac{n\pi}{6}} - e^{i\frac{5n\pi}{6}}) & (\sqrt{3}-1)e^{i\frac{n\pi}{6}} + (\sqrt{3}+1)e^{i\frac{5n\pi}{6}} \end{pmatrix}. \tag{28}$$

When $n = 1$, we obtain $\overline{k'}(1) = \sqrt{2}e^{i\frac{\pi}{4}}$, and $\overline{l'}(1) = 0$. Using $U_{11} = 1/2$, $U_{41} = 1/2$, we obtain $k_1(1) = e^{i\frac{\pi}{4}}/\sqrt{2}$, and $k_4(1) = e^{i\frac{\pi}{4}}/\sqrt{2}$. The system lies in the state

$$|\psi_1\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)e^{i\frac{\pi}{4}}/\sqrt{2}. \tag{29}$$

The overall phase can be ignored.

When $U = Y_1(-\pi/2)Y_2(\pi/2)$, Eq.(28) is unaltered, so that $\overline{k'}(1) = \sqrt{2}e^{i\frac{\pi}{4}}$, and $\overline{l'}(1) = 0$. We obtain that $k_1(1) = e^{i\frac{\pi}{4}}/\sqrt{2}$, and $k_4(1) = -e^{i\frac{\pi}{4}}/\sqrt{2}$, using $U_{11} = 1/2$, and $U_{41} = -1/2$. The system lies in the state

$$|\psi_2\rangle = (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)e^{i\frac{\pi}{4}}/\sqrt{2}. \tag{30}$$

Considering the experimental convenience, when the marked states are $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$, we choose I_t^γ as $I_{23}^\gamma = iI_{14}^{-\frac{\pi}{2}}$, where $\gamma = \pi/2$. In matrix notation, I_{23}^γ is represented as

$$I_{23}^{\frac{\pi}{2}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{31}$$

I_s^β is chosen as

$$I_s^{\frac{\pi}{2}} = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \tag{32}$$

where $\beta = \pi/2$ to satisfy phase matching.[19] When $\gamma = \beta = \pi/2$, and $U = Y_1(\pi/2)Y_2(\pi/2)$, or $U = Y_1(-\pi/2)Y_2(\pi/2)$, the solution of Eq.(11) can be obtained by replacing i in Eqs.(23)–(28) by $-i$. We obtain $\overline{k'}(1) = \sqrt{2}e^{-i\frac{\pi}{4}}$, and $\overline{l'}(1) = 0$. When $U = Y_1(\pi/2)Y_2(\pi/2)$, we obtain $k_2(1) = -e^{-i\frac{\pi}{4}}/\sqrt{2}$, and $k_3(1) = -e^{-i\frac{\pi}{4}}/\sqrt{2}$, using $U_{21} = -1/2$, and $U_{31} = -1/2$. The system lies in the state

$$|\psi_3\rangle = -(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)e^{-i\frac{\pi}{4}}/\sqrt{2}. \tag{33}$$

Similarly, when $U = Y_1(-\pi/2)Y_2(\pi/2)$, we obtain $k_2(1) = -e^{-i\frac{\pi}{4}}/\sqrt{2}$, and $k_3(1) = e^{-i\frac{\pi}{4}}/\sqrt{2}$, using $U_{21} = -1/2$, and $U_{31} = 1/2$. The system lies in the state

$$|\psi_4\rangle = -(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)e^{-i\frac{\pi}{4}}/\sqrt{2}. \tag{34}$$

$|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$ and $|\psi_4\rangle$ are the four pseudo-EPR states. EPR (or pseudo-EPR) states are very useful in quantum information and have been implemented in experiments.[20–24] Based on the above discussion, they can be synthesized by the generalized Grover's algorithm. The analogues of other entangled states can be obtained by changing U. For example, if U is chosen as

$$U = X_1(\pi/2)Y_2(\pi/2) = \frac{1}{2}\begin{pmatrix} 1 & 1 & i & i \\ -1 & 1 & -i & i \\ i & i & 1 & 1 \\ -i & i & -1 & 1 \end{pmatrix}, \tag{35}$$

and $\gamma = \beta = -\pi/2$, pseudo-entangled state $(|\uparrow\downarrow\rangle - i|\downarrow\uparrow\rangle)e^{-i\frac{\pi}{4}}/\sqrt{2}$ is obtained after one iteration. The target states, such as $|\psi_1\rangle$ and $|\psi_2\rangle$, can also be obtained by matrix multiplication. One can find $A^{n+3} = iA^n$. This fact shows that $\overline{k'}(n)$ and $\overline{l'}(n)$ both have a period of 3.

4. Experimental procedure

The equilibrium density matrix can be represented as

$$\rho_{eq} = \gamma_1 I_z^1 + \gamma_2 I_z^2. \tag{36}$$

The rf and gradient pulse sequence $[\alpha]_x^2 - [\mathrm{grad}]_z - [\pi/4]_x^1 - 1/4J - [\pi]_x^{1,2} - 1/4J - [-\pi]_x^{1,2} - [-\pi/4]_y^1 - [\mathrm{grad}]_z$ transforms ρ_{eq} to

$$\rho_s = I_z^1/2 + I_z^2/2 + I_z^1 I_z^2 = \frac{1}{4}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{37}$$

which can be used as the pseudo-pure state $|\uparrow\uparrow\rangle$;[25] $\alpha = \arccos(\gamma_1/2\gamma_2)$; $[\mathrm{grad}]_z$ denotes the gradient pulse along $\hat{z}$-axis, and the symbol $1/4J$ means that the system evolves under H described in Eq.(16) for $1/4J$ time when pulses are switched off. The pulses are applied from left to right. $[\pi]_x^{1,2}$ denotes a non-selective pulse (hard pulse). The evolution caused by the pulse sequence $1/4J - [\pi]_x^{1,2} - 1/4J - [-\pi]_x^{1,2}$ is equivalent to the coupled-spin evolution $[1/2J]$ described in Eq.(17).[26] π pulses are applied in pairs, each of which takes opposite phases in order to reduce the error accumulation caused by imperfect calibration of $[\pi]$ pulses.[27] $Y_1(\pi/2)Y_2(\pi/2)$ and $Y_1(-\pi/2)Y_2(\pi/2)$ are realized by $[\pi/2]_y^1 - [\pi/2]_y^2$ and $[-\pi/2]_y^1 - [\pi/2]_y^2$, respectively. $I_{23}^{\frac{\pi}{2}}$ and $I_{14}^{-\frac{\pi}{2}}$ are realized by the same sequence $1/4J - [\pi]_x^{1,2} - 1/4J - [-\pi]_x^{1,2}$. By modifying the pulses used in Refs.[14,28], we realize $I_s^{-\frac{\pi}{2}}$ by $1/8J - [\pi]_x^{1,2} - 1/8J - [-\pi]_x^{1,2} - [-\pi/2]_y^{1,2} - [-\pi/4]_x^{1,2} - [\pi/2]_y^{1,2}$, and $I_s^{\frac{\pi}{2}}$ by $15/8J - [\pi]_x^{1,2} - 15/8J - [-\pi]_x^{1,2} - [-\pi/2]_y^{1,2} - [\pi/4]_x^{1,2} - [\pi/2]_y^{1,2}$. U transforms the pseudo-pure state $|\uparrow\uparrow\rangle$ into the initial state $|g(0)\rangle$, and GI_t^γ transforms $|g(0)\rangle$ into the target state. When $U = Y_1(\pi/2)Y_2(\pi/2)$, $(-UI_s^{-\frac{\pi}{2}}U^\dagger I_{14}^{-\frac{\pi}{2}})U$ transforms $|\uparrow\uparrow\rangle$ into $|\psi_1\rangle$, and $(-UI_s^{\frac{\pi}{2}}U^\dagger I_{23}^{\frac{\pi}{2}})U$ transforms $|\uparrow\uparrow\rangle$ into $|\psi_3\rangle$, where "()" indicates Grover iteration. When $U = Y_1(-\pi/2)Y_2(\pi/2)$, $(-UI_s^{-\frac{\pi}{2}}U^\dagger I_{14}^{-\frac{\pi}{2}})U$ transforms $|\uparrow\uparrow\rangle$ into $|\psi_2\rangle$, and $(-UI_s^{\frac{\pi}{2}}U^\dagger I_{23}^{\frac{\pi}{2}})U$ transforms $|\uparrow\uparrow\rangle$ into $|\psi_4\rangle$. The target states are expressed by density matrices. For example, the density matrix corresponding to $|\psi_1\rangle$ is represented as

$$\rho_1 = I_x^1 I_x^2 - I_y^1 I_y^2 + I_z^1 I_z^2$$

$$= \begin{pmatrix} 0.25 & 0 & 0 & 0.5 \\ 0 & -0.25 & 0 & 0 \\ 0 & 0 & -0.25 & 0 \\ 0.5 & 0 & 0 & 0.25 \end{pmatrix}, \tag{38}$$

which is equivalent to $|\psi_1\rangle\langle\psi_1|$. A readout pulse $[\pi/2]_y^2$ transforms ρ_1 to

$$\rho_{1r} = \frac{1}{4}\begin{pmatrix} 0 & -1 & 1 & 1 \\ -1 & 0 & -1 & -1 \\ 1 & -1 & 0 & 1 \\ 1 & -1 & 1 & 0 \end{pmatrix}. \tag{39}$$

The information on matrix elements (1,3) and (2,4) in Eq.(39) can be directly obtained in the carbon spectrum, and the information on elements (1,2) and (3,4) can be directly obtained in the proton spectrum. Similarly, when the system lies in $|\psi_2\rangle$, $|\psi_3\rangle$, or $|\psi_4\rangle$, the readout pulse $[\pi/2]_y^2$ transforms the system into the state represented as

$$\rho_{2r} = \frac{1}{4}\begin{pmatrix} 0 & -1 & -1 & -1 \\ -1 & 0 & 1 & 1 \\ -1 & 1 & 0 & 1 \\ -1 & 1 & 1 & 0 \end{pmatrix}, \tag{40}$$

$$\rho_{3r} = \frac{1}{4}\begin{pmatrix} 0 & 1 & 1 & -1 \\ 1 & 0 & 1 & -1 \\ 1 & 1 & 0 & -1 \\ -1 & -1 & -1 & 0 \end{pmatrix}, \tag{41}$$

or

$$\rho_{4r} = \frac{1}{4}\begin{pmatrix} 0 & 1 & -1 & 1 \\ 1 & 0 & -1 & 1 \\ -1 & -1 & 0 & -1 \\ 1 & 1 & -1 & 0 \end{pmatrix}. \tag{42}$$

Through observing the matrix elements (1,3), (2,4), (1,2) and (3,4) in Eqs.(39)–(42), one can distinguish the four pseudo-EPR states.

5. Results

In experiments, for each target state, the carbon spectrum and proton spectrum are recorded in two experiments. For different target states, carbon spectra or proton spectra are recorded in an identical fashion. Because the absolute phase of an NMR signal is not meaningful, we must use reference signals to adjust carbon spectra and proton spectra so that the relative phases of the signals are meaningful.[29] When the system lies in the pseudo-pure state described as Eq.(37), the readout pulses $[\pi/2]_y^1$ and $[\pi/2]_y^2$ transform it into states represented as

$$\rho_{sr1} = \frac{1}{4}\begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & -1 & 0 & 0 \\ -2 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad (43)$$

and

$$\rho_{sr2} = \frac{1}{4}\begin{pmatrix} 1 & -2 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \qquad (44)$$

respectively. In the carbon spectrum or proton spectrum, there is only one NMR peak corresponding to the element (1,3) in ρ_{sr1} or to the element (1,2) in ρ_{sr2}. Through calibrating the phases of the two signals, the two peaks are adjusted into absorption shapes which are shown in Fig.1(a) for carbon spectrum and Fig.1(b) for proton spectrum. The two signals are used as reference signals, of which phases are recorded to calibrate the phases of signals in other carbon spectra and proton spectra, respectively. One should note that the minus elements in Eqs.(43) and (44) correspond to the positive peaks in Figs.1(a) and (b).

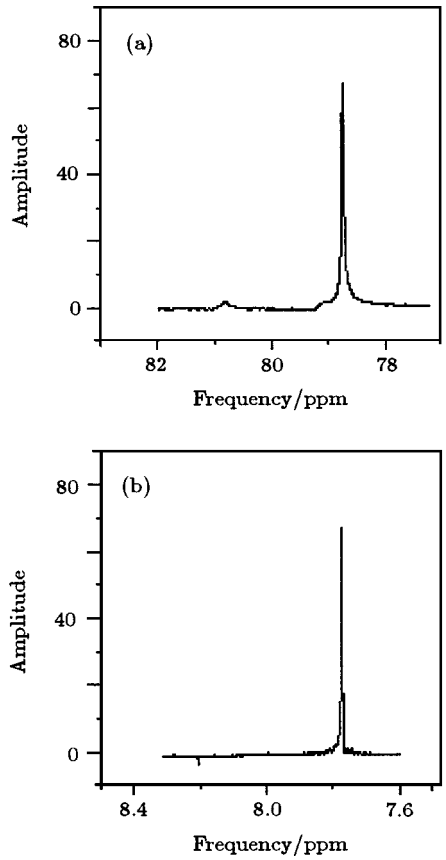


Fig.1. The carbon spectrum (a) obtained through selective readout pulse for ^{13}C $[\pi/2]_y^1$ and the proton spectrum (b) obtained through selective readout pulse for ^{1}H $[\pi/2]_y^2$ when the two-spin system lies in a pseudo-pure state $|\uparrow\uparrow\rangle$. The amplitude has arbitrary units. The two peaks are adjusted into absorption shapes. The two signals are used as reference signals to adjust other spectra.

We implement the generalized Grover's algorithm, starting with the initial state $|g(0)\rangle$. GI_t^γ transforms $|g(0)\rangle$ into one of the pseudo-EPR states. If no readout pulse is applied, the amplitudes of the peaks are so small that they can be ignored. By applying the spin-selective readout pulse $[\pi/2]_y^2$, we obtain the carbon spectra as shown in Figs.2(a)–(d), and the proton spectra as shown in Figs.2(e)–(h), corresponding to $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$, and $|\psi_4\rangle$, respectively. In Fig.2(a), for example, the right and left peaks correspond to the matrix elements (1,3) and (2,4) in Eq.(39), respectively. Similarly, in Fig.2(e), the two peaks correspond to the matrix elements (1,2) and (3,4) in Eq.(39). The phases of the signals corroborate the synthesis of pseudo-EPR states.

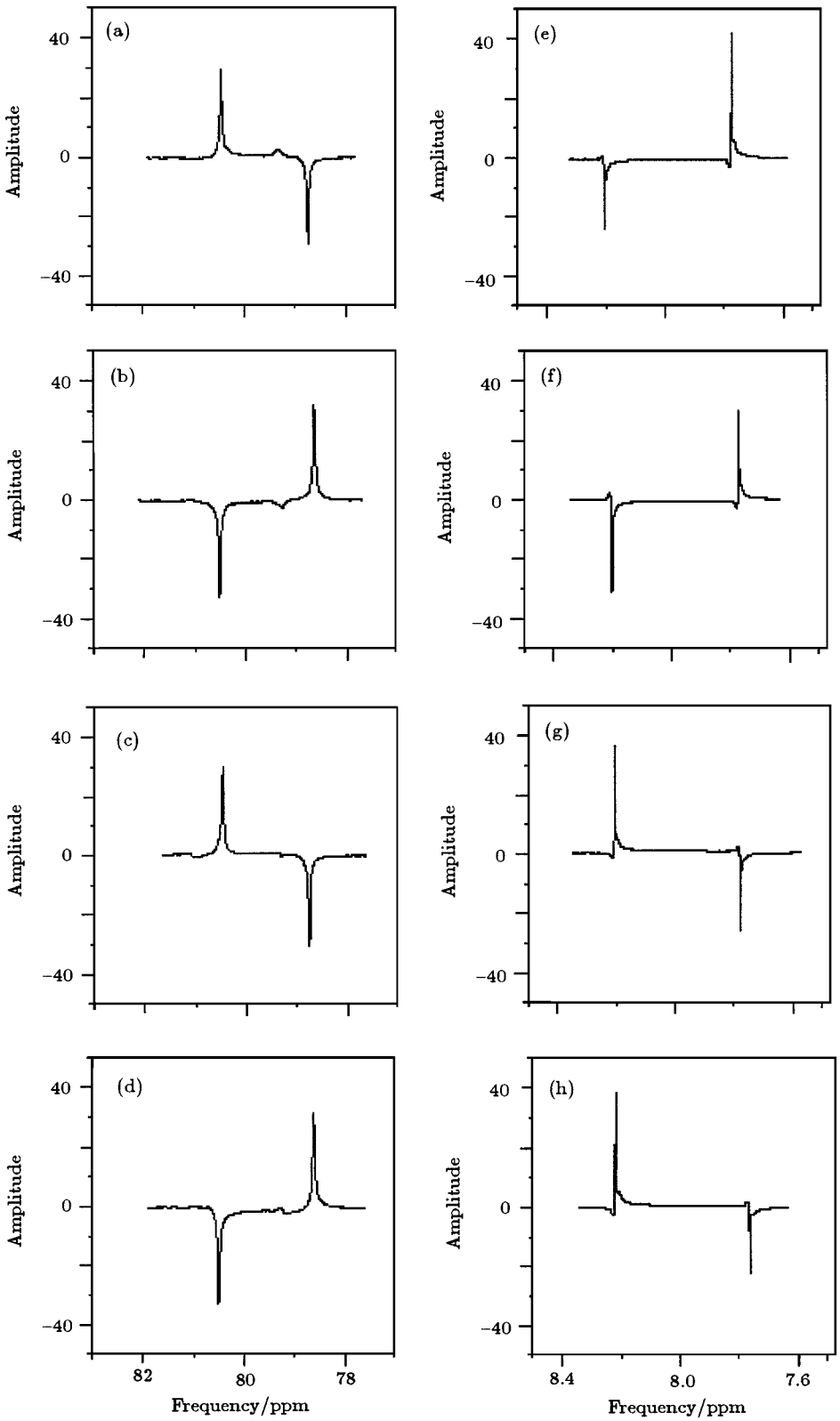


Fig.2. carbon spectra (shown by the left column) and proton spectra (shown by the right column) obtained through $[\pi/2]_y^2$ after pseudo-EPR states are synthesized. (a)–(d) and (e)–(h) correspond to states $(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, and $(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, respectively.

6. Conclusion

In experiments, we demonstrate the generalized Grover's algorithm of two marked states. As its application, pseudo-EPR states are synthesized. The results show that the generalized Grover's algorithm is efficient for the case of $N/2$ marked states. The original Grover's algorithm, however, does not work for this case.[30] For the case of multiple marked states, the final signal is an average over all the marked states. It is difficult or impossible to deduce anything about individual marked states from the ensemble average.[31] In our work, however, the generalized Grover's algorithm is viewed as a technique for synthesizing a particular kind of superposition of marked states.[5] The superposition is described as a density matrix of which the elements can be obtained in the NMR spectrum by readout pulses.[32]

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