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Synthesizing NMR analogs of Einstein-Podolsky-Rosen states using the generalized Grover's algorithm

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By designing a proper unitary operator U, we synthesize nuclear-magnetic-resonance (NMR) analogs of Einstein-Podolsky-Rosen (EPR) states (pseudo-EPR states) using the generalized Grover's algorithm on a NMR quantum computer. Experiments also demonstrate the generalized Grover's algorithm for the case in which there are multiple marked states.

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Since the quantum searching algorithm was first proposed by Grover [1], several generalizations of the original algorithm have been developed [2–4]. One of the generalized algorithms can be posed as follows. For a system with a total of N basis states, a composite operator Q is defined as $Q \equiv -I_s U^{-1} I_t U$. U can be almost any valid quantum-mechanical unitary operator. I_s is defined as $I_s \equiv I - 2|s\rangle\langle s|$, where I denotes unit matrix. $|s\rangle$ denotes a predefined basis state that is used as an initial state in our experiments. I_s is a diagonal matrix with all diagonal elements equal to 1 except the ssth elements which are -1. Similarly, I_t can be written as $I_t \equiv I - \Sigma_t 2|t\rangle\langle t|$, where $|t\rangle$ denote the marked states, and there are r marked states. For any $|t\rangle$, $I_t|t\rangle = -|t\rangle$. u is defined as $u = \sqrt{\Sigma_t |U_{ts}|^2}$, where $U_{ts} = \langle t|U|s\rangle$. It has been proved that $\pi/4u$ applications of Q transform the system from $|s\rangle$ into a superposition denoted as $|\psi\rangle = (1/u)\Sigma_t U_{ts} U^{-1}|t\rangle$ if $u \ll 1$. By 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 generalized algorithm [5]. Nevertheless, we find that some useful superpositions, such as nuclear-magnetic-resonance (NMR) analogs of Einstein-Podolsky-Rosen (EPR) states (pseudo-EPR states) [6–8], can be synthesized using the algorithm without an ancilla qubit. Such superpositions can be represented as $|\psi_{su}\rangle = (1/\sqrt{r})\Sigma_t e^{i\phi_t}|t\rangle$ (su for superposition), where ϕ_t denote the phases of $|t\rangle$. By designing a proper U, we make $|U_{ts}|$ identical, and let $U_{ts}/|U_{ts}| = e^{i\phi_t}$, so that $|\psi\rangle$ can be represented as $|\psi\rangle = (1/\sqrt{r})\Sigma_t e^{i\phi_t} U^{-1}|t\rangle$. After the application of U, the system lies in $|\psi_{su}\rangle$, where an irrelevant overall phase factor can be ignored.

In our previous work, we have realized the generalized Grover's searching algorithm for the case in which there is one marked state on a two-qubit NMR quantum computer [9]. In this paper, we will synthesize the pseudo-EPR states using the algorithm.

Our experiments use a sample of carbon-13 labeled chloroform dissolved in $d6$ acetone. Data are taken at room temperature with a Bruker DRX 500-MHz spectrometer. 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 $\hat{z}$ axis, by setting $\hbar = 1$, the Hamiltonian of this system is represented as

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

where $I_z^k (k=1,2)$ are the matrices for $\hat{z}$ component of the angular momentum of the spins [10]. In the rotating frame of spin k, the evolution caused by a radiofrequency (rf) pulse on resonance along $\hat{x}$ or $-\hat{y}$ axis 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 $\varphi_k = B_1\gamma_k t_p$, with k specifying the affected spin. B_1, γ_k, and t_p represent the strength of the rf pulse, gyromagnetic ratio, 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

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

where τ is evolution time. The initial pseudopure state

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

is prepared by using spatial averaging [11], 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 $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. Pseudo-EPR states are denoted as $|\psi_1\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$, $|\psi_2\rangle = (|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$, $|\psi_3\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, and $|\psi_4\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. EPR (or pseudo-EPR) states are very useful in quantum information and have been implemented in experiments [12,13]. We will synthesize pseudo-EPR states using the generalized Grover's algorithm.

U is chosen as $U = Y_1(\varphi_1)Y_2(\varphi_2)$, represented as

$$U = \begin{pmatrix} c_1c_2 & c_1s_2 & s_1c_2 & s_1s_2 \\ -c_1s_2 & c_1c_2 & -s_1s_2 & s_1c_2 \\ -s_1c_2 & -s_1s_2 & c_1c_2 & c_1s_2 \\ s_1s_2 & -s_1c_2 & -c_1s_2 & c_1c_2 \end{pmatrix}, \tag{4}$$

where $c_k \equiv \cos(\varphi_k/2)$, $s_k \equiv \sin(\varphi_k/2)$. According to the first column of U, we design φ_1 and φ_2 for synthesizing pseudo-EPR states. U is chosen as $U_1 = Y_1(\pi/4)Y_2(3\pi/4)$, U_2

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$=Y_1(\pi/4)Y_2(-3\pi/4)$, $U_3=Y_1(\pi/4)Y_2(\pi/4)$, and $U_4=Y_1(-\pi/4)Y_2(\pi/4)$ for $|\psi_1\rangle$, $|\psi_2\rangle$, $|\psi_3\rangle$, and $|\psi_4\rangle$, respectively. One can prove that $u_j=\sqrt{\Sigma_t|U_{jts}|^2}=1/2$, where $j=1$, 2, 3, or 4. The following discussion will show that the condition $u\ll 1$ is not necessary. If the system starts with other basis states, U is chosen as other forms. For example, if $I_s=|\uparrow\downarrow\rangle$, according to the second column of U, U is chosen as $U_1=Y_1(-\pi/4)Y_2(\pi/4)$, $U_2=Y_1(\pi/4)Y_2(\pi/4)$, $U_3=Y_1(\pi/4)Y_2(-3\pi/4)$, and $U_4=Y_1(\pi/4)Y_2(3\pi/4)$. If U is chosen as $U_1=X_1(\pi/4)Y_2(3\pi/4)$, $U_2=X_1(\pi/4)Y_2(-3\pi/4)$, $U_3=X_1(\pi/4)Y_2(\pi/4)$, and $U_4=X_1(\pi/4)Y_2(-\pi/4)$, pseudoentangled states $(|\uparrow\uparrow\rangle-i|\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\uparrow\rangle+i|\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\downarrow\rangle-i|\downarrow\uparrow\rangle)/\sqrt{2}$, and $(|\uparrow\downarrow\rangle+i|\downarrow\uparrow\rangle)/\sqrt{2}$ can be obtained, respectively. If $|s\rangle=|\uparrow\uparrow\rangle$, I_s is chosen as I_0, represented as

$$I_0=\begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{5}$$

Because $r=N/2$, the conditional sign-flip operators for $|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$, and for $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ can be chosen in the same form represented as

$$I_t=\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{6}$$

Q is represented as $Q_j\equiv -I_sU_j^{-1}I_tU_j$ for $|\psi_j\rangle$. The operator $G_j^{(n)}$ is defined as $G_j^{(n)}\equiv U_jQ_j^n$, which means that operation Q_j is repeated n times, and then U_j is applied. It is easy to prove that $G_1^{(1)}|\uparrow\uparrow\rangle=-|\psi_1\rangle$, $G_2^{(1)}|\uparrow\uparrow\rangle=-|\psi_2\rangle$, $G_3^{(1)}|\uparrow\uparrow\rangle=-|\psi_3\rangle$, and $G_4^{(1)}|\uparrow\uparrow\rangle=-|\psi_4\rangle$. The required n to synthesize a target state displays a period of 3. For example, $G_3^{(4)}|\uparrow\uparrow\rangle=|\psi_3\rangle$ and $G_3^{(7)}|\uparrow\uparrow\rangle=-|\psi_3\rangle$.

The following rf and gradient pulse sequence $[\alpha]_x^2-[\text{grad}]_z-[\pi/4]_x^1-1/4J-[\pi]_x^{1,2}-1/4J-[-\pi]_x^{1,2}-[-\pi/4]_y^1-[\text{grad}]_z$ transforms the system from the equilibrium state represented as

$$\rho_{eq}=\gamma_1 I_z^1+\gamma_2 I_z^2 \tag{7}$$

to the initial state represented as

$$\rho_0=I_z^1/2+I_z^2/2+I_z^1I_z^2, \tag{8}$$

which can be used as the pseudopure state $|\uparrow\uparrow\rangle$ [14]. $\alpha=\arccos(\gamma_1/2\gamma_2)$, $[\text{grad}]_z$ denotes gradient pulse along the $\hat{z}$ axis, and the symbol $1/4J$ means that the system evolutes under the Hamitonian H for $1/4J$ time when pulses are switched off. The pulses are applied from left to right. $[\pi]_x^{1,2}$ denotes a nonselective 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. (2) [15]. $[\pi]_x^{1,2}$ pulses are applied in pairs, each of which take opposite phases in order to reduce the error accumulation caused by imperfect calibration of the $[\pi]$ pulses [16].

U_1, U_2, U_3, and U_4 are realized by $[\pi/4]_y^1-[3\pi/4]_y^2$, $[\pi/4]_y^1-[-3\pi/4]_y^2$, $[\pi/4]_y^1-[\pi/4]_y^2$, and $[-\pi/4]_y^1-[\pi/4]_y^2$, respectively. $I_t=[1/J]$, which realized by $1/2J-[\pi]_x^{1,2}-1/2J-[-\pi]_x^{1,2}$. According to Ref. [17], I_0 is realized by $1/4J-[\pi]_x^{1,2}-1/4J-[-\pi]_x^{1,2}-[-\pi/2]_y^{1,2}-[-\pi/2]_x^{1,2}-[\pi/2]_y^{1,2}$. $G_j^{(1)}$ transforms the system from the initial state into the corresponding target state. For example, $G_3^{(1)}$ transforms the system from ρ_0 into ρ_3, represented as

$$\rho_3=I_x^1I_x^2+I_y^1I_y^2-I_z^1I_z^2, \tag{9}$$

which is equivalent to $|\psi_3\rangle\langle\psi_3|$. A readout pulse $[\pi/2]_y^1$ transforms ρ_3 to $I_z^1I_x^2+I_y^1I_y^2+I_x^1I_z^2$, which is equivalent to

$$\rho_{3r}=\frac{1}{4}\begin{pmatrix} 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{pmatrix}. \tag{10}$$

The information on matrix elements (1,3) and (2,4) in Eq. (10) 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 $|\psi_1\rangle$, $|\psi_2\rangle$, or $|\psi_4\rangle$, through the readout pulse $[\pi/2]_y^1$, the system lies in the state described as

$$\rho_{1r}=\frac{1}{4}\begin{pmatrix} 1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 \\ -1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 \end{pmatrix}, \tag{11}$$

$$\rho_{2r}=\frac{1}{4}\begin{pmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 \end{pmatrix}, \tag{12}$$

or

$$\rho_{4r}=\frac{1}{4}\begin{pmatrix} 1 & -1 & 1 & 1 \\ -1 & 1 & -1 & -1 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & 1 \end{pmatrix}. \tag{13}$$

Through observing the matrix elements (1,3), (2,4), (1,2), and (3,4) in Eqs. (10)–(13), one can distinguish the pseudo-EPR states.

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

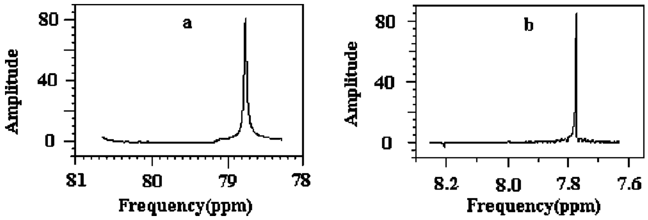

FIG. 1. The carbon spectrum (a) obtained through selective readout pulse for ^{13}C $[\pi/2]_y^1$ and the proton spectrum (b) obtained through selective readout pulse for ^{1}H $[\pi/2]_y^2$ when the two-spin system lies in the pseudopure state $|\uparrow\uparrow\rangle$. The amplitude has arbitrary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

phases of the signals are meaningful [18]. When the system lies in the initial pseudopure state described as Eq. (8), the readout pulses $[\pi/2]_y^1$ and $[\pi/2]_y^2$ transform it into states represented as

$$\rho_{sr1}=\frac{1}{4}\begin{pmatrix} 1 & 0 & -2 & 0 \\ 0 & -1 & 0 & 0 \\ -2 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{14}$$

and

$$\rho_{sr2}=\frac{1}{4}\begin{pmatrix} 1 & -2 & 0 & 0 \\ -2 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{15}$$

respectively. In the carbon spectrum or proton spectrum, there is only one NMR peak corresponding to element (1,3) in ρ_{sr1} or to 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 as 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. (14) and (15) correspond to the positive peaks in Figs. 1(a) and 1(b).

Experiments start with pseudopure state $|\uparrow\uparrow\rangle$. $G_j^{(1)}$ transforms $|\uparrow\uparrow\rangle$ into $|\psi_j\rangle$. If no readout pulse is applied, the amplitudes of peaks is so small that they can be ignored. By applying the spin-selective readout pulse $[\pi/2]_y^1$, we obtain carbon spectra shown in Figs. 2(a–d), and proton spectra 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. (11), respectively. Similarly, in Fig. 2(e), the two peaks correspond to the matrix elements (1,2) and (3,4) in Eq. (11). The phases of the signals corroborate the synthesis of pseudo-EPR states.

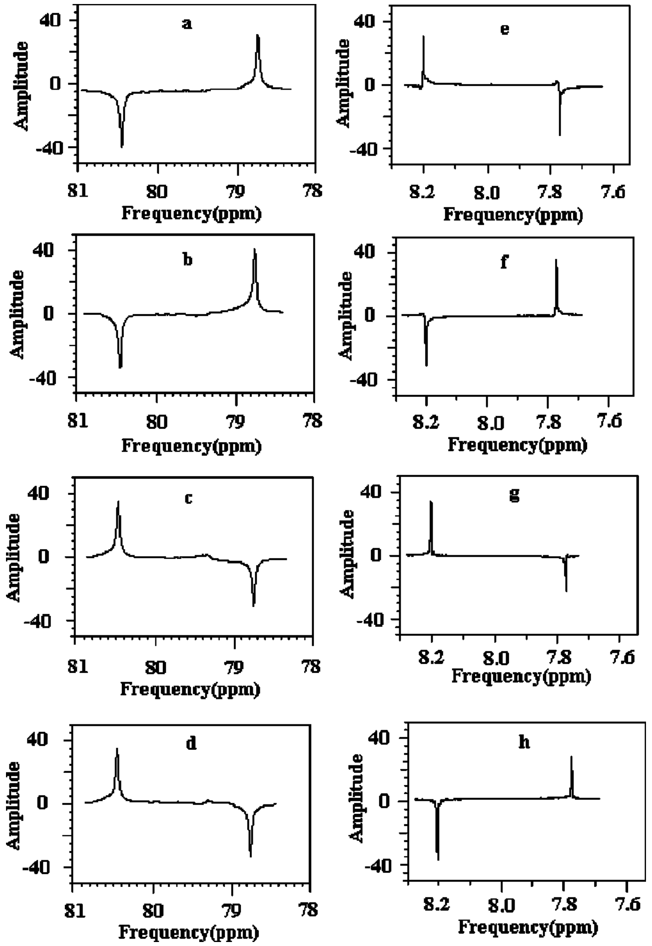

FIG. 2. Carbon spectra (shown by the left column) and proton spectra (shown by the right column) obtained through $[\pi/2]_y^1$ after pseudo-EPR states are synthesized. (a)–(d) and (e)–(h) correspond to states $(|\uparrow\uparrow\rangle+|\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\uparrow\rangle-|\downarrow\downarrow\rangle)/\sqrt{2}$, $(|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle)/\sqrt{2}$, and $(|\uparrow\downarrow\rangle-|\downarrow\uparrow\rangle)/\sqrt{2}$, respectively.

In conclusion, we synthesize pseudo-EPR states using the generalized Grover's algorithm by choosing a proper U. Although the ancilla qubit is not used, our experimental scheme shows the essential meaning of Grover's original idea. The experiments also demonstrate the generalized Grover's algorithm for the case in which there are $N/2$ marked states.

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