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Quantum data bus in dipolar coupled nuclear spin qubits

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We implement an iterative quantum state transfer exploiting the natural dipolar couplings in a spin chain of a liquid-crystal NMR system. During each iteration, a finite part of the amplitude of the state is transferred and, by applying an external operation on only the last two spins, the transferred state is made to accumulate on the spin at the end point. The transfer fidelity reaches one asymptotically through increasing the number of iterations. We also implement the inverted version of the scheme which can transfer an arbitrary state from the end point to any other position of the chain and entangle any pair of spins in the chain, acting as a full quantum data bus.

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I. INTRODUCTION

In quantum computation and quantum communication, the transfer of an arbitrary quantum state from one qubit to another is a fundamental element. The most obvious method to implement the quantum state transfer (QST) on an array of qubits is based on a sequence of SWAP gates for neighboring spins. In spin qubit systems, the SWAP gate (up to a known phase factor) can be implemented through the evolution of the dipolar coupling between the neighboring spins for $1/2D$ time by decoupling the other spins, where D denotes the dipolar coupling strength. In experiments, however, the required decoupling operations are hard to implement if the spins cannot be individually addressed by spectral selectivity, e.g., in large-size solid-state NMR systems. This makes the direct implementation of such gates in a large spin system challenging.

To overcome this problem, schemes based on “always on” spin systems were proposed [1,2]. The state can be transferred with unit fidelity in engineered spin chains or networks with XY interactions [3]. However, the required fine-tuned XY couplings are not found in natural spin systems [4]. In other schemes based on spin chains with Heisenberg interactions [1,5] or with a double-quantum Hamiltonian [4], the fidelity of the QST cannot approach unity in scalable systems.

The above limitations can be relaxed significantly by applying gate operations to receive and store the transferred state [6,7]. The gates are only applied to two spins at one end of a spin chain. In this paper, we experimentally implement the QST in a liquid-crystal NMR system based on this scheme. Opposed to previous experimental implementations [7] where the required XY interactions were engineered by radio-frequency pulses and scalar couplings, the dipolar couplings exist naturally in the system and are directly exploited for the QST. The dipolar couplings are much stronger (up to 2 to 3 orders of magnitude) than the scalar couplings and therefore can significantly speed up the implementation of the logical gates for quantum information processing [8]. The transfer with high fidelity is achieved in an iterative

manner. Each iteration transfers a finite part of the input amplitude to the target spin at the end of the chain. The fidelity of the transfer asymptotically approaches unity by increasing the number of iterations. We also experimentally demonstrate the time-inverted version of [6]. Through this, a full *quantum data bus* is implemented, where arbitrary unknown quantum states can be steered to *any* position of the chain. This is also useful for the selective excitation of one spin, which is addressed by the two-spin gates, rather than by its individual properties, e.g., chemical shift in NMR. As opposed to previous schemes [9], global control is not required. Surprisingly, the reversal operation can also be used to *entangle* any pair of spins in the chain by operations at its end only. We demonstrate the entangling operation in the qubits at the end points of the chain.

The QST and its reversal operations mean that the chain is really used as a wire with an input, an output, and no gates in the middle; the many-body Hamiltonian of the chain is responsible for the transport. Only two spins at the end are required to address. The fidelity of transfer converges exponentially fast to unity with respect to the number of iterations. The required number of iterations to achieve a good fidelity (e.g., larger than 0.999) scales roughly linearly with the system size [6]. Moreover, this method is stable when the engineered Hamiltonian in implementation deviates the required Hamiltonian [10]. Hence, our method scales favorably with the size of the spin chains and suitable for large-size systems, such as solid- or liquid-crystal NMR systems, where the differences of the chemical shifts are too small to address all the spins individually.

II. ITERATIVE TRANSFER ALGORITHM IN A SPIN CHAIN

Our first goal is to transfer the state $\alpha|0\rangle + \beta|1\rangle$ from spins j to N in an N -spin chain. The Hamiltonian for spins 1 to $N-1$ is represented as

$$H = \frac{1}{2} \pi \sum_{j,k=1,k>j}^{N-1} D_{jk} (2\sigma_z^j \sigma_z^k - \sigma_x^j \sigma_x^k - \sigma_y^j \sigma_y^k), \quad (1)$$

where σ_x^j , σ_y^j , and σ_z^j denote the Pauli matrices with j indicating the affected spin. Noting that H preserves the total number of excited spins [1,3], we have

$$U_\tau |\mathbf{0}\rangle = e^{i\theta} |\mathbf{0}\rangle, \quad (2)$$

$$U_\tau |\mathbf{j}\rangle = \sum_{k=1}^{N-1} a_k |\mathbf{k}\rangle, \quad (3)$$

where $U_\tau = e^{-i\tau H}$ and $e^{i\theta}$ is the (1,1) matrix element of U_τ . The state $|\mathbf{0}\rangle$ denotes all spins pointing up, and $|\mathbf{j}\rangle$ denotes all spins up except the spin j pointing down.

The main operation is the two-spin gate applied only on spins $N-1$ and N , and, in iteration n , the gate is denoted as

$$W(c_n, d_n) = I_{1,2,\dots,N-2} \otimes \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & d_n^* & c_n^* & 0 \\ 0 & -c_n & d_n & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{N-1,N}, \quad (4)$$

where $I_{1,\dots,N-2}$ denotes the unit operator for spins 1 to $N-2$. The basis order for spins $N-1$ and N is $|00\rangle$, $|01\rangle$, $|10\rangle$, and $|11\rangle$. Noting $|c_n|^2 + |d_n|^2 = 1$, one finds

$$W(c_n, d_n)(c_n |\mathbf{N}-1\rangle + d_n |\mathbf{N}\rangle) = |\mathbf{N}\rangle. \quad (5)$$

The N spin system is initialized into the input state $\alpha|\mathbf{0}\rangle + \beta|\mathbf{j}\rangle$ by setting spin j in the system to state $\alpha|0\rangle + \beta|1\rangle$. Here, j is the location of the sender (receiver) of the QST for the (inverse) protocol, which is on some arbitrary spin of the quantum data bus. It is sufficient to only discuss the transfer of $|\mathbf{j}\rangle$ because U_τ only introduces a known phase factor before $|\mathbf{0}\rangle$ [see Eq. (2)] and $W(c_n, d_n)$ does not change $|\mathbf{0}\rangle$ [see Eq. (4)]. Iteration n is represented as

$$Q_{j,n} = [I_{1,\dots,N-2} \otimes W(c_n, d_n)] [U_\tau \otimes I_N]. \quad (6)$$

After n iterations, one obtains

$$|\psi_n\rangle = T_{j,n} |\mathbf{j}\rangle = \sum_{k=1}^N A_{k,n} |\mathbf{k}\rangle, \quad (7)$$

using Eqs. (3)–(6). Here $T_{j,n} = Q_{j,n} \dots Q_{j,2} Q_{j,1}$, $A_{N-1,n} = 0$, and

$$A_{N,n} = \sqrt{p_n}, \quad (8)$$

where

$$p_n = p_{n-1} + |\langle \mathbf{N}-1 | U_\tau \otimes I_N | \psi_{n-1} \rangle|^2, \quad (9)$$

with $p_0 = 0$ and $|\psi_0\rangle = |\mathbf{j}\rangle$. $W(c_n, d_n)$ is obtained by setting

$$d_n = e^{i\theta} \sqrt{p_{n-1}} / \sqrt{p_n}, \quad (10)$$

$$c_n = \langle \mathbf{N}-1 | U_\tau \otimes I_N | \psi_{n-1} \rangle / \sqrt{p_n}. \quad (11)$$

In strict nearest-neighbor chains, it can be shown [6] that p_n converges to unity by increasing the number of iterations. In the present case, we have also non-nearest-neighbor interac-

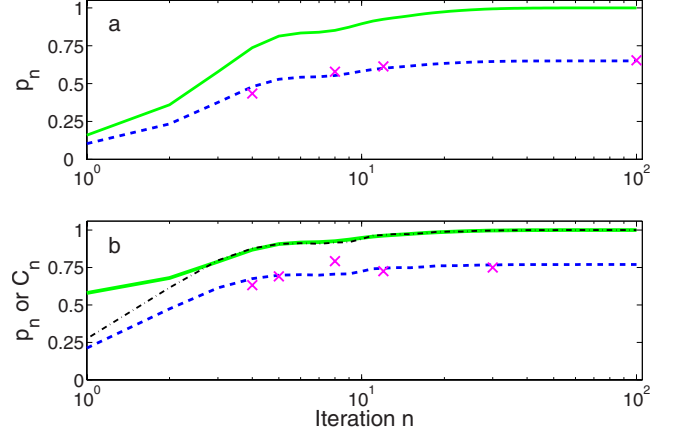


FIG. 1. (Color online) The numerical simulation (solid) and experimental results (data marked by \times) for the probability p_n of the QST as a function of iterations in the four spin system used in experiments (see text for dipolar couplings) for transferring a state from spins 1 to 4 (a) and entangling the two spins (b) when $\tau = 2.1$ ms. In (b), p_n can be approximated as the observable coherence C_n [dot dashed, see Eq. (19)] where $|C_n - p_n| \leq 0.0175$ when $n > 2$. The experimental data can be fitted as $0.65p_n$ and $0.77C_n$ shown as the dashed curves, respectively.

tions, but numerical results show p_n still approaches unity, with a convergence speed which depends on the evolution time τ [see Fig. 1(a)]. The process of QST after a large number of iterations can be presented as

$$T_{j,n}(\alpha|\mathbf{0}\rangle + \beta|\mathbf{j}\rangle) \rightarrow \alpha e^{in\theta} |\mathbf{0}\rangle + \beta |\mathbf{N}\rangle, \quad (12)$$

i.e., spin N ends with the state $\alpha e^{in\theta} |\mathbf{0}\rangle + \beta |\mathbf{1}\rangle$ and $e^{in\theta}$ is known.

We can exploit the inversion of $T_{j,n}$ to implement the QST from spin N to spin j , i.e., without applying the external operation directly on the spin j to evolve it into state $\alpha|0\rangle + \beta|1\rangle$. Hence, the spin chain functions as a quantum data bus, which can transfer arbitrary unknown states to any qubit. This method also allows to create a selective excitation that does not require spectral selectivity, e.g., chemical shift in NMR, to address spin j . The external operations are only applied to spins $N-1$ and N . By taking the inner product of Eq. (7) with $\langle \mathbf{N} |$ and using Eq. (8) one obtains

$$p_n = |\langle \mathbf{j} | T_{j,n}^{-1} | \mathbf{N} \rangle|^2, \quad (13)$$

i.e., p_n is the fidelity for generating $|\mathbf{j}\rangle$ by applying $T_{j,n}^{-1}$ to $|\mathbf{N}\rangle$. The creation of the selective excitation for spin j is represented as

$$T_{j,n}^{-1}(\alpha|\mathbf{0}\rangle + \beta|\mathbf{N}\rangle) \rightarrow \alpha e^{-in\theta} |\mathbf{0}\rangle + \beta |\mathbf{j}\rangle. \quad (14)$$

By modifying the input state, one can obtain $T_{j,n}^{-1}(\alpha e^{in\theta} |\mathbf{0}\rangle + \beta |\mathbf{N}\rangle) \rightarrow \alpha |\mathbf{0}\rangle + \beta |\mathbf{j}\rangle$ [11].

The method of the inverse QST, furthermore, can be used to entangle arbitrary spins j, k indirectly by acting at spins $N-1$ and N only. This can be done by designing a pulse analogously to Eq. (6), and the required pulse sequence is very similar to the inverse QST. For this purpose, we set the input state as an entangled state of a pair of spins j and k represented as

$$|\psi_{jk}\rangle = (|j\rangle + |k\rangle)/\sqrt{2}. \quad (15)$$

Iteration n can still be represented as Eq. (6), where $Q_{j,n}$ is rewritten as $Q_{j,k,n}$, noting that it depends on the input state. $W(c_n, d_n)$ is obtained in a similar way by changing $p_0 = |\langle \mathbf{N} | \psi_{jk} \rangle|^2$ and $|\psi_0\rangle = |\psi_{jk}\rangle$. After a large number of iterations, we obtain

$$T_{j,k,n}|\psi_{jk}\rangle \rightarrow |\mathbf{N}\rangle, \quad (16)$$

where $T_{j,k,n} = Q_{j,k,n} \dots Q_{j,k,2} Q_{j,k,1}$. From Eq. (16) one can entangle spins j and k with high fidelity by applying $T_{j,k,n}^{-1}$ on $|\mathbf{N}\rangle$, represented as

$$T_{j,k,n}^{-1}|\mathbf{N}\rangle \rightarrow |\psi_{jk}\rangle. \quad (17)$$

The fidelity for generating $|\psi_{jk}\rangle$ is also represented by Eq. (13) through replacing $T_{j,n}^{-1}$ by $T_{j,k,n}^{-1}$ and $|j\rangle$ by $|\psi_{jk}\rangle$. The numerical simulation for p_n is illustrated as Fig. 1(b).

III. EXPERIMENTAL RESULTS

We use the four protons in orthochlorobromobenzene (C_6H_4ClBr) dissolved in the liquid-crystal solvent ZLI-1132 as four qubits to implement the experiments. The Hamiltonian is represented as

$$H_{\text{NMR}} = -\pi \sum_{i=1}^4 \nu_i \sigma_z^i + \frac{1}{2} \pi \sum_{k=2, j < k}^4 D_{jk} (2\sigma_z^j \sigma_z^k - \sigma_x^j \sigma_x^k - \sigma_y^j \sigma_y^k). \quad (18)$$

Through fitting the spectra [12] obtained by Cory48 [13] and one-dimensional MREV-8 pulse sequences and referring to the spectra of molecules with similar structures [8,14], we measure $\nu_1 = 106.2$, $\nu_2 = -187.7$, $\nu_3 = -58.6$, and $\nu_4 = 91.3$ with respect to the transmitter frequency, $D_{12} = -1233.7$, $D_{13} = -149.4$, $D_{14} = -93.2$, $D_{23} = -716.0$, $D_{24} = -236.6$, $D_{34} = -1677.5$ Hz, and the effective transverse relaxation times (T_2^*) as 91, 87, 88, and 82 ms [15]. The NMR spectrum obtained by Cory48 from the thermal equilibrium state $\rho_{th} = \sum_{i=1}^4 \sigma_z^i$ is shown in Fig. 2(a).

All experiments start with the deviation density matrix $\rho_{ini} = |0000\rangle\langle 0000| - |1111\rangle\langle 1111|$, which can be prepared by the double-quantum coherence Hamiltonian [16] $H_d = \frac{1}{2} \pi \sum_{k=2, j < k}^4 D_{jk}^d (\sigma_x^j \sigma_x^k - \sigma_y^j \sigma_y^k)$ in a molecule with C_{2v} symmetry [17]. However, we choose to generate the effective H_d using a gradient ascent pulse engineering pulse [18]. Using temporal averaging, we prepare ρ_{ini} by summing the three states $U_d \rho_{th} U_d^\dagger$, $U_d \rho_{th} U_d^\dagger$, $2\rho_{th}$, where $U_d = e^{-it_d H_d}$ by choosing $t_d = 8.00/D_{12}^d$ [17]. In the numerical simulation, we prepare ρ_{ini} with fidelity of 99.97%. Figure 2(b) shows the NMR spectrum obtained by a collective $\pi/2$ pulse in the experiment when the system lies in ρ_{ini} . The NMR peaks marked by “+” indicate the single-quantum transitions between magnetic quantum numbers 2 and 1.

We demonstrate the QST by transferring ρ_0 from spins 1 to 4 by choosing $\rho_0 = \sigma_x$, σ_y , σ_z , and I , respectively. Because $T_{j,n}$ is spin preserving, the transitions marked by + in Fig. 2(b) can represent the QST starting with the input state $\rho_0 |000\rangle\langle 000|$. We therefore can ignore $|1111\rangle\langle 1111|$ in ρ_{ini}

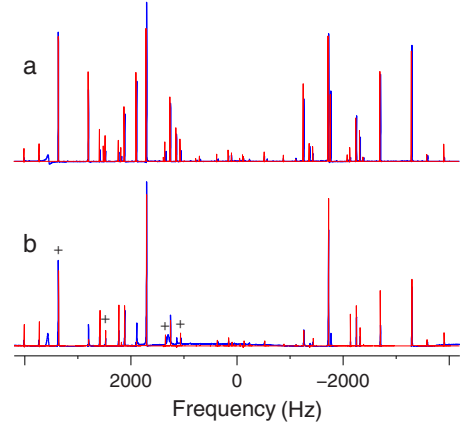


FIG. 2. (Color online) NMR spectra (thick) obtained by Cory48 pulse sequence from the (a) thermal equilibrium state and by a (b) collective $\pi/2$ pulse from ρ_{ini} . The thin spectra show the results by simulation. The plot's vertical axes have arbitrary units. The NMR peaks marked by + indicate the single-quantum transitions between magnetic quantum numbers 2 and 1.

and omit the negative frequency spectral region.

The input state is prepared by applying an operation U_{ini} to ρ_{ini} . With increasing n , $T_{1,n}$ transforms $\rho_0 |000\rangle\langle 000|$ to $|000\rangle\langle 000| \rho$ asymptotically, where $\rho = e^{in\theta\sigma_z/2} \rho_0 e^{-in\theta\sigma_z/2}$. In experiments, we removed the phase factor between ρ and ρ_0 by phase correction. For a fixed n , we implement the unitary $T_{1,n} U_{ini}$ using one GRAPE pulse. The experimental results of the QST after 100 iterations for the various input states are shown as Figs. 3(a)–3(d), respectively.

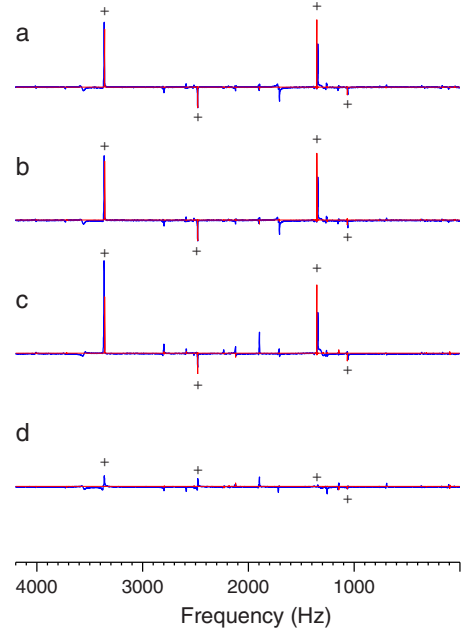


FIG. 3. (Color online) (a)–(d) NMR spectra for implementing the QST from spins 1 to 4 after 100 iterations, when the input states are chosen as $\sigma_x |000\rangle\langle 000|$, $\sigma_y |000\rangle\langle 000|$, $\sigma_z |000\rangle\langle 000|$, and $I |000\rangle\langle 000|$, respectively, where the readout operation $e^{i\pi\sigma_y^4/4}$ is applied to obtain observable signals in (c) or (d). The plot's vertical axes have the same scale.

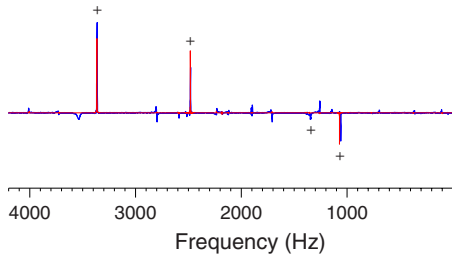


FIG. 4. (Color online) NMR spectra for implementing the selective excitation and quantum data bus for spin 2.

Exploiting the transformation between the computational basis and energy eigenbasis and ignoring the difference of T_2^* of the four protons, we can approximately obtain $A_{k,n}$ in Eq. (7) through measuring the amplitudes of the peaks marked by + in Figs. 3(a)–3(c) by choosing the signals in Fig. 2(b) as the reference. Therefore, we obtain $p_n = |A_{4,n}|^2$. For the input states $\sigma_x|000\rangle\langle 000|$, $\sigma_y|000\rangle\langle 000|$, and $\sigma_z|000\rangle\langle 000|$, p_{100} is measured as 0.654 ± 0.046 , 0.660 ± 0.052 , and 0.693 ± 0.037 , respectively. All other $|A_{k,100}|^2$ are below 0.02.

To observe p_n increasing with n , we also implement the QST by choosing various n when the input state is $\sigma_x|000\rangle\langle 000|$. The measured p_n is shown in Fig. 1(a) as the data marked by “×,” which can be fitted as $0.65p_n$.

Next we implement the selective excitation or quantum data bus for spin 2. The reverse QST starts with the input state $|000\rangle\langle 000|\sigma_x$ obtained by applying $R_y^4 = e^{-i\sigma_y^4\pi/4}$ to ρ_{ini} . When $n=100$, $T_{2,n}^{-1}$ transforms $|000\rangle\langle 000|\sigma_x$ to $|0\rangle\langle 0|\rho|00\rangle\langle 00|$ with a probability close to 1, where $\rho = e^{-in\theta\sigma_z/2}\sigma_x e^{in\theta\sigma_z/2}$. The experimental results are shown in Fig. 4. The fidelity of excitation is measured as 0.744 ± 0.036 .

We choose $|\psi_{14}\rangle = (|1\rangle + |4\rangle)/\sqrt{2}$ as the target to demonstrate the entangling operation in spins 1 and 4. To measure the fidelity, we rewrite Eq. (13) as $p_n = |\langle 0000|\Psi_n\rangle|^2$ [19] by replacing $|j\rangle$ by $|\psi_{14}\rangle$. Here $|\Psi_n\rangle = P^\dagger T_{1,4,n}^{-1}|4\rangle$ where P denotes the operation to prepare $|\psi_{14}\rangle$ from $|0000\rangle$ (e.g., see [20]). When p_n is close to 1, we can obtain p_n approximately by applying a readout operation $e^{i\pi\sigma_y^1/4}$ to $|\Psi_n\rangle$. Noting that $|1111\rangle\langle 1111|$ in ρ_{ini} does not contribute observable signals for measuring p_n , we approximate p_n as the coherence

$$C_n = |\text{Tr}(2|0000\rangle\langle 1000|\rho_n)|, \quad (19)$$

where $\rho_n = U_{tot,n}\rho_{ini}U_{tot,n}^\dagger$ with $U_{tot,n} = e^{i\pi\sigma_y^1/4}P^\dagger T_{1,4,n}^{-1}e^{i\pi\sigma_x^4/2}$. The simulated and measured C_n is shown in Fig. 1(b). The

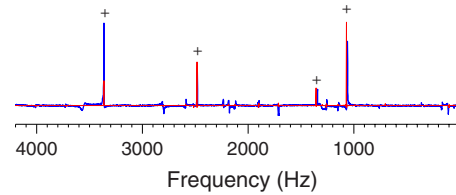


FIG. 5. (Color online) NMR spectra for measuring the fidelity of the generation of $(|1\rangle + |4\rangle)/\sqrt{2}$.

experimental data can be fitted as $0.77C_n$. Figure 5 illustrates the NMR spectra when $n=8$.

The operations U_d , U_d^\dagger , R_y^4 , $T_{1,n}U_{ini}$, $T_{2,n}^{-1}R_y^4$, and $U_{tot,n}$ are experimentally implemented using the GRAPE pulses with fidelities in theory larger than 0.99, respectively. The pulse lengths are 10 ms for U_d and U_d^\dagger , 20 ms for the other pulses. The experimental errors could mainly result from the inhomogeneities of the magnetic field, imperfect implementation of GRAPE pulses, and decoherence. In order to estimate the quality of the experimental spectra, we also list the ideal ones in simulation shown as the red thin curves in Figs. 2–5.

IV. CONCLUSION

We have given an NMR implementation for various important tasks of quantum control that, in principle, can be achieved *indirectly* by controlling the end of a spin chain. The dipolar couplings naturally existing in the liquid-crystal NMR system are directly exploited for the QST. The experimental results demonstrate the successful control of the spin system with dipolar couplings by the GRAPE pulses. First, we implemented the transfer of an arbitrary quantum state. Second, by implementing the reverse QST, we have created a full quantum data bus which is controlled by the two-qubit end gates. Finally, as another application of the reverse QST, we proposed and demonstrated a different method to implement an entangling operation.

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