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Preparation of subspace effective-pure state for NMR QIP by means of strongly modulating pulses

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Abstract: An alternative method for preparing an effective-pure state in a subsystem of a three-spin system for quantum information processing (QIP) in liquid-state nuclear magnetic resonance (NMR) was demonstrated experimentally. With the aid of numerical search methods, strongly modulating pulses (SMP) scheme was obtained and can perform accurate, arbitrary, selective gates on a three-qubit system. Compared with low-power (nuclear-selective) pulse scheme, the number of shaped pulses and the width of each pulse were both reduced. A pair of two-qubit subspace effective-pure states within a three-spin system was acquired simultaneously. The tomography for the spin system agreed with theoretical predictions, which shows that the experiments were successfully implemented. The short pulse-width of SMP substantially reduced the effects of relaxation within the period of pulse. This is very useful for NMR QIP involving larger numbers of qubits.

Key words: NMR; effective-pure state; strong modulating pulses; QIP

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强调制脉冲方法制备 NMR 子空间有效纯态

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摘要: 使用强调制脉冲方法在核磁共振系统中实验制备出量子计算所需的有效纯态. 在数值搜索方法的辅助下优化参数获得的强调制脉冲辐照能准确地执行三量子位系统中的核选幺正演化操作. 与低功率的核选脉冲相比, 强调制脉冲方案不仅减少实验脉冲序列中的脉冲数目, 而且降低了脉冲(时间)宽度. 还在实验上同时制备出了一对两量子位子空间有效纯态, 由 NMR 频谱重构出的自旋量子系统状态与理论预期吻合. 整个实验方案中所用到的强调制脉冲宽度都明显比执行同一幺正操作的低功率(核选)脉冲的宽度短, 因此

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减少了脉冲操作时间段内系统弛豫以及环境噪声下的量子系统退相干对量子计算的影响. 量子计算向更多的量子位扩展必然需要数目更多的脉冲操作,这时强调制脉冲的优势就会明显体现.

关键词:核磁共振;有效纯态;强调制脉冲;量子信息处理

0 Introduction

Quantum computation devices[1~3] under the principle of quantum mechanics have more advantages over classical ones in certain cases. Quantum computation can be divided into three stages consisting of the preparation of initial states, computation, and the readout of the final states. The proper preparation of a initial pure state is very important in the process. It is not only the starting point of the quantum computation, but also the foundation of quantum error correction[4,5].

In liquid-state NMR ensemble quantum computation[6~9], effective-pure states[10], in fact a highly mixed states, provide a faithful representation for the dynamical evolution of pure states.

There are mainly three methods to obtain an effective-pure state for NMR QIP. Among them, logical labeling method[6] works by selecting subspace states from a set of spin states arising from a larger spin-system[11]. With a careful choice of states it is possible to find 2^k levels whose relative populations correspond to those of $|00\cdots0\rangle_k\langle00\cdots0|$ and these levels can be used as an effective-pure state of a k-spin system. The subspace effective-pure state can be prepared from the thermal equilibrium state. The details can be found in Ref. [12].

As the number of qubits increases, the experimental complexity increases exponentially. In NMR quantum computation, if the duration of the whole experiment approaches the relaxation time of a spin system, quantum computation is no longer in force because of decoherence of qubits (quantum bits). So we hope that radio-frequency (RF) pulses which can perform arbitrary unitary evolution would be as short as possible in experimental sequences. Strong modulating pulse method provides an approach to this subject. Here we present an experimental demonstration using the strong modulating pulse technique to prepare a pair of 2-qubit subspace effective-pure states simultaneously within a 3-spin molecule. In addition, we compare SMP experiment with common low-power (nuclear-selective) pulses experiment.

1 Strong modulating pulses

The experiments of NMR QIP use many well established spectroscopic techniques developed for decades, such as using low-power shaped radio-frequency pulses to obtain selective operations. Low-power pulses, including nuclear-selective pulses, have better selectivity than hard pulses, but they take much longer to acquire the same nutation angle. This disadvantage not only introduces errors due to relaxation, or decoherence, but also allows significant evolution under the action of the internal Hamiltonian. How to improve selectivity and reduce the duration of control pulses simultaneously is an interesting research subject. To address this problem, Fortunato et al[13] proposed strongly modulating pulses methods which can average out unwanted evolution by the use of strong control fields. The method is to find high-power pulses that strongly modulate a system's dynamics to produce precisely a desired spin-selective unitary propagator. These strongly modulating pulse operations allow arbitrary rotations of each spin around independent single-spin axes, while refocusing the internal evolution. The method has been applied in some QIP experiments to demonstrate algorithms, study notions of measurement, and test new methods for quantum control[14~16].

Quantum computation can be expressed as a

series of unitary operations. The physical implementation of quantum computation requires the use of a quantum system with a Hamiltonian that contains a sufficient set of externally controlled parameters to allow for the generation of a universal set of gates[17,18]. Given a control sequence, solving the effective Hamiltonian is straightforward. On the contrary, to find an RF waveform that produces a propagator with desired properties is much more difficult. With the aid of computer, a more efficient and accurate solution can be found.

The nuclear spins in a NMR system are subjected to a strong static magnetic field. The external control of the NMR system can be realized via RF pulse operations and periods of free evolution. The internal Hamiltonian of a weakly coupled nuclear spin system in solution is[19]

$$H_{\text{int}} = \sum_{k=1}^{n} \omega_k I_z^k + 2\pi \sum_{j>k}^{n} \sum_{k=1}^{n} J_{kj} I^k I^j, \qquad (1)$$

where ω_k is the chemical shift of the spins, J_{kj} is the coupling constant between spins k and j, and n is the number of spins. The Hamiltonian describing an external oscillating RF field is

$$H_{\text{ext}}(\omega_{\text{RF}}, \phi, \omega, t) = \sum_{k=1}^{n} \mathrm{e}^{-\mathrm{i}(\omega_{\text{RF}} t + \phi) I_z^k} (-\omega I_x^k) \mathrm{e}^{\mathrm{i}(\omega_{\text{RF}} t + \phi) I_z^k}, \qquad (2)$$

where ω_{RF} is irradiation frequency of RF field, ϕ is the initial phase, and ω is RF power. The RF pulses can be parameterized with fixed power, irradiation frequency, initial phase, and pulse duration (τ). The total Hamiltonian $H_{\text{tot}} = H_{\text{int}} + H_{\text{ext}}$ can be made time independent by transforming the frame into one that rotates at the frequency of the transmitter. Initially, the starting density matrix is the same in both frames, $\tilde{\rho}(0) = \rho(0)$. After the pulse is executed, the density matrix in the new frame is given by

$$\tilde{\rho}(\tau) = \mathrm{e}^{-\mathrm{i}H_{\text{eff}}\tau} \rho(0) \mathrm{e}^{\mathrm{i}H_{\text{eff}}\tau}, \qquad (3)$$

where H_{eff} is the effective Hamiltonian in the new frame[19]. Transforming this density matrix back to the original rotating frame gives

$$\rho = U_z(\tau)^{-1} \mathrm{e}^{-\mathrm{i}H_{\text{eff}}\tau} \rho(0) \mathrm{e}^{\mathrm{i}H_{\text{eff}}\tau} U_z(\tau), \qquad (4)$$

where

$$U_z(\tau) = (\mathrm{e}^{\mathrm{i}\omega_{\text{RF}} \sum_{k=1}^{n} I_z^k \tau}). \qquad (5)$$

Therefore, in the original rotating frame, the transformation is given by

$$U_{\text{period}}(\tau) = U_z^{-1}(\tau) \mathrm{e}^{-\mathrm{i}H_{\text{eff}}\tau}. \qquad (6)$$

Because the evolution under the whole sequence is given in the original rotating frame, no additional resources are required to concatenate pulses, nor is any mathematical correction required at the end of an experiment.

Cascading these periods yields the net transformation

$$U_{\text{net}} = \prod_{m=1}^{N} U_z^{-1}(\tau_m) \mathrm{e}^{-\mathrm{i}H_{\text{eff}}^m(\omega^m, \omega_{\text{RF}}^m, \phi^m)\tau_m}, \qquad (7)$$

where the control sequence is composed of a cascade of RF pulses, the index m refers to the m^{th} period, each square pulse in the sequence having a corresponding set of four parameters. The task is to find proper sets of parameter values to get the maxima of the operation's fidelity F[13]. Here, a quality factor $Q = 1 - \sqrt{F}$ is minimized by searching through the mathematical parameter space using the Nelder-Mead Simplex algorithm[20].

2 Experimental implementation

Our experiments were carried out on Bruker AVANCE-400 spectrometer at Instruments' Center for Physical Science, University of Science and Technology of China. We utilize the three ^{13}C labeled nuclei of alanine ($CH_3CH(NH_2)COOH$) dissolved in deuterated water as quantum bits. The internal Hamiltonian of the spin system is written as ($\hbar = 1$)

$$H = \sum_{i=1}^{3} \omega_i I_z^i + 2\pi \sum_{i<j}^{3} J_{ij} I_z^i I_z^j. \qquad (8)$$

Molecular structure and Hamiltonian parameters for alanine is shown in Fig. 1. Three nuclear spins of alpha-carbon, carboxyl-carbon, and methyl-carbon are denoted as A, B, and C, respectively.

The initial state of the ensemble is the equilibrium state $\rho_{\text{eq}} = I_z^A + I_z^B + I_z^C$. The pulse

A	*B*	*C*	
5 124.7	54.0	34.9	*A*
	17 725.1	−1.3	*B*
		1 662.3	*C*

Fig. 1 Molecular structure and Hamiltonian parameters (in Hz) for alanine. The chemical shift of each of the carbon nuclei is given by the corresponding diagonal elements while the coupling constants are given by the each of the different off-diagonal elements

sequence to prepare a subspace effective-pure state $|00\rangle_{BC}$ is

$$[\pi/2]_y^A - \tau 1 - [\pi]_x^B - \tau 2 - [\pi/2]_y^A[\pi]_x^B, \quad (9)$$

where $\tau 1+\tau 2=\frac{1}{2J_{AC}}$, $\tau 1-\tau 2=\frac{1}{2J_{AB}}$, in our case $\tau 1$ takes about 11.77 ms, and $\tau 2$ takes about 2.51 ms. $[\theta]_\alpha^i$ represents spin i rotating at an angle of θ about the axis α. After this operation, the system evolves from thermal equilibrium into BC subspace effective-pure state, i. e.

$$\rho_s = P\rho_{eq}P^\dagger = 4I_z^A I_z^B I_z^C + I_B^2 + I_z^C.$$

Tab. 1 Parameters of three strong modulating pulses

parameter	t/μs	ω/Hz
$[\pi/2]_y^A$	289.6	4 257.0
$[\pi]_x^B$	297.3	5 379.7
$[\pi/2]_y^A[\pi]_x^B$	288.3	5 829.3

By computer-aided numerical searching, the optimal parameters (listed in Tab. 1) for three selective operations was acquired. There were three selective operations and two periods of free evolution in the sequence (9). According to the experiments of low-power (nuclear-selective) pulses in Ref. [12], the nuclear-selective pulse width of the first operation $[\pi/2]_y^A$ is about 0.8 ms, while that of the second operation $[\pi]_x^B$ is also about 0.8 ms. The last operation $[\pi/2]_y^A[\pi]_x^B$ implemented by two nuclear-selective pulses takes about 1.7 ms in total. The widths of the strongly modulating pulses are on the order of 0.3 ms, significantly shorter than the widths of low-power pulses. The fidelities of all the pulses in Tab. 1 are above 0.99. The detailed wave forms of three strong modulating pulses are shown in Figs. 2～4 respectively. The vertical axes of top figures are amplitudes and those of bottom figures are phases, the horizontal axes are time.

In the experiment, we applied RF pulse

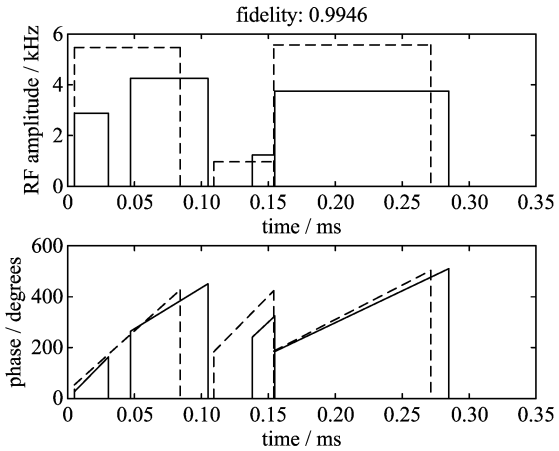

Fig. 2 Wave form for $[\pi/2]_y^A$

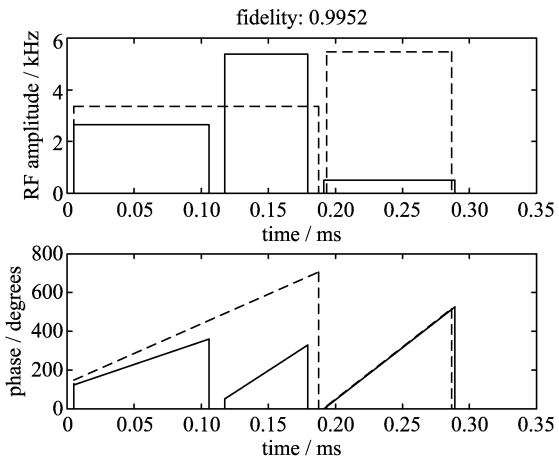

Fig. 3 Wave form for $[\pi]_x^B$

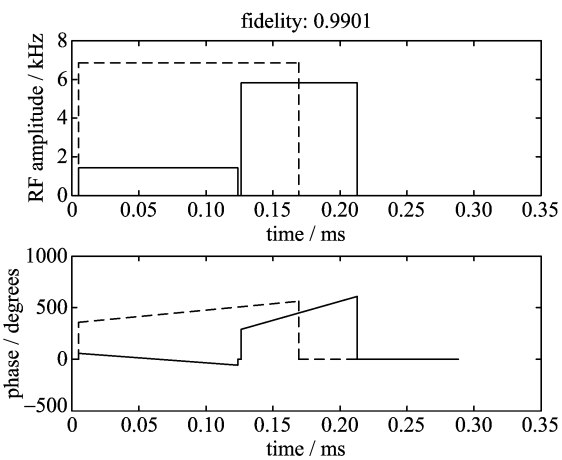

Fig. 4 Wave form for $[\pi/2]_y^A[\pi]_x^B$

sequence (9) to the thermal equilibrium ρ_{eq}. Protons were decoupled during the whole process. After the pulse sequence, we performed the following measurements: *EEE*, *EEX*, *EXE*, *XEE*, *EEY*, *YEE*, *XEY*, *YEX*, *EXX* to reconstruct the density matrix of ρ_s[8,21]. Here *E*, *X* and *Y* represent the identity operation, a 90° rotation with respect to the *x* axis, and a 90° rotation with respect to the *y* axis, respectively. We normalized the deviation density matrix by $\rho_{nor}=\frac{I}{8}+\frac{\rho}{12}$. The tomography result is shown in Fig. 5. The imaginary part of theoretical normalized density matrix equals zero, and the imaginary part of experimental normalized density matrix is below 0.02. The fidelity $F(\rho_{s_{nor}}^{exp}, \rho_{s_{nor}})$ equals 0.982. This proves that a subspace effective-pure state has been prepared successfully. In the low-power (nuclear-selective) pulse scheme in Ref. [12], the fidelity equals 0.993. This indicates that the quaity of strongly modulating pulse schemes are comparable with that of nuclear-selective pulse schemes. It should be noted that there are two longer periods of free evolution in the pulse sequence, the total time of which is about 14 ms. We expect that reasonably the fewer periods of free evolution in the experimental scheme, the more advantage strongly modulating pulse will have.

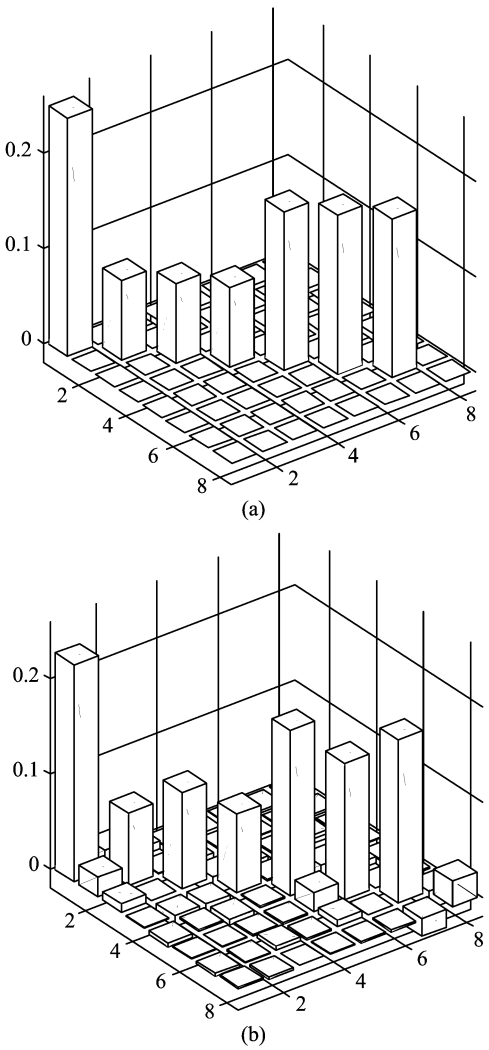

Fig. 5　Theoretical density matrix $\rho_{s_{nor}}$ (a) and real experimental density matrix $\rho_{s_{nor}}^{exp}$ (b) after completion of whole pulse sequence, all the imaginary components are small

3　Conclusion

In summary, we made use of strong modulating pulse techniques and prepared a pair of 2-qubit subspace effective-pure states embedded in a 3-spin system. And we compared this method with the lower-power (nuclear-selective) pulses method. The application of strong modulating pulses makes our pulse scheme keep selectivity and reduce the durations of control pulses by a half of magnitude, thus significantly reducing the effects of relaxation and quantum decoherence within the durations of pulses. Furthermore, this pulse scheme requires no additional corrections after experiments. They can be placed back to back in longer sequences, which is increasingly useful in NMR QIP experiments which need larger numbers of qubits[6]. On the other hand, the embedding computation of subsystem may be helpful for us to study Berry phase[22], error tolerant quantum computation[23] and quantum process tomography[24] in NMR.

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