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Realization of quantum gates in rotating single crystal

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Abstract：Quantum gates in solid-state nuclear magnetic resonance (NMR) under magic-angle spinning (MAS) was realized. First，all anisotrope interactions of the sample were averaged out under the MAS. Then，the special pulse sequences or conditions were used to recover the interactions used to realize controlled operations. The advantage of this method for them in liquid NMR is that the pulse sequences of controlled operations are simplified，because they do not need complicated decoupling sequences，and the evolution time of the pulse sequences is shorter. Finally，the quantum operations were simulated，and the results are in complete agreement with the theoretical predictions.

Key words：quantum computing；solid state NMR；quantum gate；MAS；recoupling

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旋转单晶体系下的量子门的实现

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摘要：在魔角旋转的固体核磁共振体系中，实现了量子逻辑门. 首先，利用魔角旋转去除掉样品中核间的耦合. 然后，利用特殊的恢复耦合序列或者条件恢复实现量子门需要的耦合. 此方法相比液体中实现量子门有较简单的序列，因为其不需要复杂的去耦序列，另外构成量子门的序列的时间也较短. 最后，模拟了一系列量子门，模拟结果与理论预期一样.

关键词：量子计算；固体核磁共振；量子门；魔角旋转；恢复耦合

0 Introduction

In nuclear magnetic resonance (NMR) quantum computing experiments，quantum gate operations have been realized by eliminating all qubit interactions except the one that is intended to construct a special quantum gate. The Hamiltonian of the liquid NMR system can be easily utilized complete a needed quantum logic gate[1] in high accuracy. But the J couplings in liquid are usually smaller than the dipole-dipole couplings in solid state NMR，so the total time of pulse sequences implementing logical gates in liquid state is longer. If we can use solid state NMR to realize quantum

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logical gates by using the dipole-dipole coupling interactions, the total time will be greatly reduced. Another problem is the usage of the pseudo-pure states because the polarization is much smaller than 1, but recent studies on dynamic nuclear polarization (DNP)[2] have revealed that high nuclear spin polarization close to 1 can be realized in solid state at an appropriate temperature. So we want to realize gates in solid state NMR. But the Hamiltonian form in solid state is much more complicated, as the anisotropic interactions and the couplings between the system and the environment are usually large. To solve these problems, we can first use magic-angle spinning (MAS) to average the anisotropic interactions and the coupling between the system and the environment to zero if the spin rate is large enough. Then, using the recoupling pulse sequences[3-6] to recouple the interactions to be used for completing the desired quantum logical gates. Recently, some Japanese scientists made a preliminary study on this problem[7], and we follow their work to figure out several important conditions to realize the quantum gates, and then simulate these quantum gates with Matlab and SIMPSON[8].

1 Theory

The Hamiltonian in rotating solid-state NMR is time-dependent. Let us consider the simplest system, an isolated two spin-1/2 heteronuclear system, I and S, in the rotating solid. The Hamiltonian of dipolar interaction is[9]

$$H_{IS}(t) = \omega_{IS}(t) \cdot 2S_z I_z \quad (1)$$

Here, $\omega_{IS}(t)$ is time-dependent component due to MAS, and it is written as

$$\omega_{IS}(t) = -\frac{\sqrt{2}}{2} b_{IS} \sin(2\beta)\cos(\omega_r t + \varphi_0 - \gamma) - \frac{1}{2} b_{IS} \sin^2\beta \cos(2\omega_r t + 2\varphi_0 - 2\gamma) \quad (2)$$

where b_{IS} is the dipolar coupling constant

$$b_{IS} = -\frac{\mu_0}{4\pi}\frac{\gamma_I \gamma_S \hbar}{r_{IS}^3}.$$

ω_r is a sample spinning rate, φ_0 is the initial phase of the rotor which is a sample container. α, β, γ are the Euler angles between the dipolar interaction tensor's principal axil frame and the rotor's rotor frame[10]. When the spinning rate of the rotor exceeds the magnitude of the dipolar coupling between spins I and S, according to the average Hamiltonian theory[11], the dipolar interaction does not affect the system in the first order. But if we want to construct a quantum gate in the SI system, we need the coupling between spins S and I, so RF field with intensity ω_1 is shined on spin S or I. When $\omega_1 = \omega_r$, that is, the RF field is at the resonance offset for S or I, the average Hamiltonian in RF interaction frame is

$$\overline{H}_{IS} = \omega_{IS}^{(1)} S_z(I_z - \mathrm{i}I_y) + \omega_{IS}^{(-1)} S_z(I_z + \mathrm{i}I_y) \quad (3)$$

Here,

$$\omega_{IS}^{(1)} = -\frac{\sqrt{2}}{4} b_{IS} \sin(2\beta) \mathrm{e}^{\mathrm{i}(\varphi_0 - \gamma)},$$

$$\omega_{IS}^{(-1)} = -\frac{\sqrt{2}}{4} b_{IS} \sin(2\beta) \mathrm{e}^{-\mathrm{i}(\varphi_0 - \gamma)}.$$

We can make the initial phase of the rotor φ_0 satisfy $\mathrm{e}^{\mathrm{i}(\varphi_0 - \gamma)} = 1$, then the average Hamiltonian is obtained

$$\overline{H} = \frac{G_1}{2} S_z I_z \quad (4)$$

where $G_1 = -\sqrt{2} b_{IS} \sin(2\beta)$. Then, we can use the average Hamiltonian in RF interaction frame to construct quantum gates, such as CNOT, SWAP gate, controlled-Z, controlled-phase, in the SI system. Fig. 1 illustrates the pulse sequences. The controlled-Z gate is a special controlled phase gate when the phase shift θ is π in Fig. 1(c).

Note that the desired average Hamiltonian is in the dipolar interaction frame, but the propagator of period τ_1 here is in RF interaction frame. If we want the correct quantum gate in the labratory the frame or in the rotating frame, the propagator U_{CNOT}^{int} of period τ_1 in the RF interaction frame must be equal to U_{CNOT}^{rot} in the rotating frame. However, the relationship between the propagators in the two frames is[11]

$$U_{CNOT}^{rot} = U_{RF}^{-1}(\tau_1) U_{CNOT}^{int} \quad (5)$$

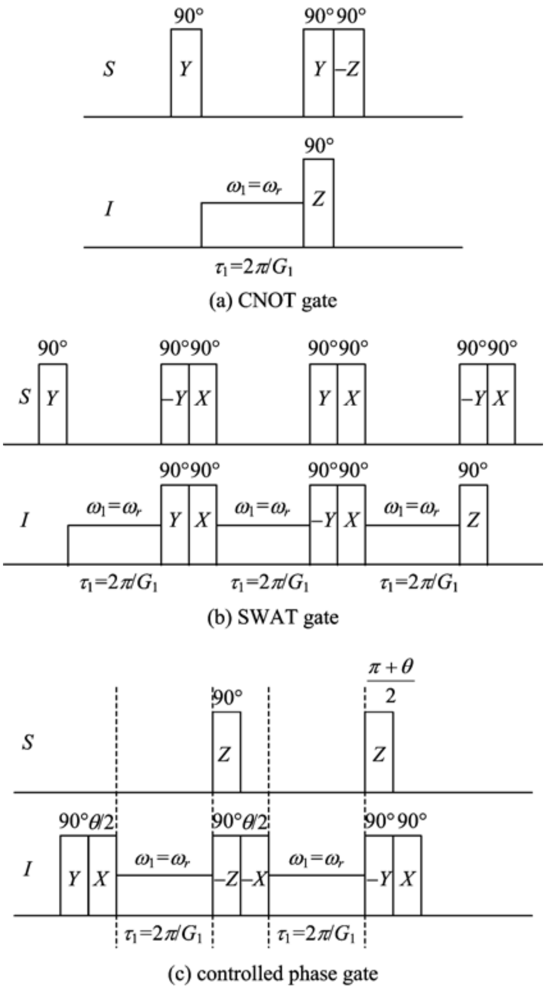


Fig. 1 The pulse sequence of CNOT gate, SWAP gate and controlled phase gate in *IS* heteronuclear system

Here, $U_{\mathrm{RF}}^{-1}(\tau_1)$ and τ_1 is

$$U_{\mathrm{RF}}(t)=\exp\{-\mathrm{i}\omega_1 I_x t\} \tag{6}$$

$$\tau_1=2\pi/G_1 \tag{7}$$

So $U_{\mathrm{RF}}^{-1}(\tau_1)=\hat{1}$. According to Eqs. (6), (7) and $\omega_1=\omega_r$, we have

$$\omega_r\tau_1=4n\pi \tag{8}$$

where n is integer. Then

$$\omega_r=2nG_1 \tag{9}$$

When the system is homonuclear, the internal Hamiltonian of the system is[9]

$$H(t)=\omega_S S_z+\omega_I I_z+ 2\omega_{IS}(t)\left\{I_z S_z-\frac{1}{4}(I_+S_-+I_-S_+)\right\} \tag{10}$$

We use another recoupling method called rotational resonance[5]. The recoupling condition is

$$\omega_r=\omega_S-\omega_I \tag{11}$$

If the rotor's spin rate meets Eq. (11), without any RF field in the delay period. Define

$$U^c(t)=\exp\{-\mathrm{i}(\omega_S S_z+\omega_I I_z)t\},$$

then the interaction frame Hamiltonian is

$$H_{\mathrm{int}}(t)=(U^c(t))^{-1}H_{IS}(t)U^c(t)= D(t)\left\{I_z S_z-\frac{1}{4}(\mathrm{e}^{-\mathrm{i}\Delta\omega t}I_+S_-+\mathrm{e}^{\mathrm{i}\Delta\omega t}I_-S_+)\right\} \tag{12}$$

where $\Delta\omega=\omega_S-\omega_I$. Then we can get an average Hamiltonian with the following form

$$\overline{H}=\frac{G_1}{8}(I_+S_-+I_-S_+) \tag{13}$$

With this average Hamiltonian, the pulse sequences can be designed as shown in Fig. 2 to get the propagator which is the same as that in heteronuclear *SI* system in the rotating frame. So, the pulse sequences of CNOT gate, SWAP gate, controlled phase gate in the homonuclear system is the same as those used in heteronuclear except that the evolution period τ_1 is replaced by Fig. 2.

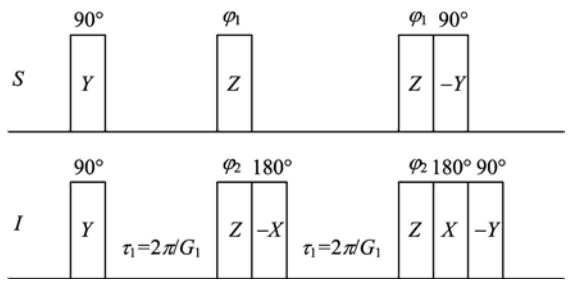


Fig. 2 The component of controlled gates in *SI* homonuclear system

2 Simulation

To verify the theory above, we simulated the pulse sequence using Matlab. In the experiments, if we want to verify the CNOT's pulse sequence and estimate its fidelity, we can't get the propagator directly, but have to use the tomography[12] technique. Here, in the simulation, we directly calculate the propagator of the CNOT pulse sequence given in the program. According to the numerical calculation of the propagator[9]

$$U(t,0) = \prod_{j=0}^{n-1} \exp\{-\mathrm{i}H(j\Delta t)\Delta t\} \qquad (14)$$

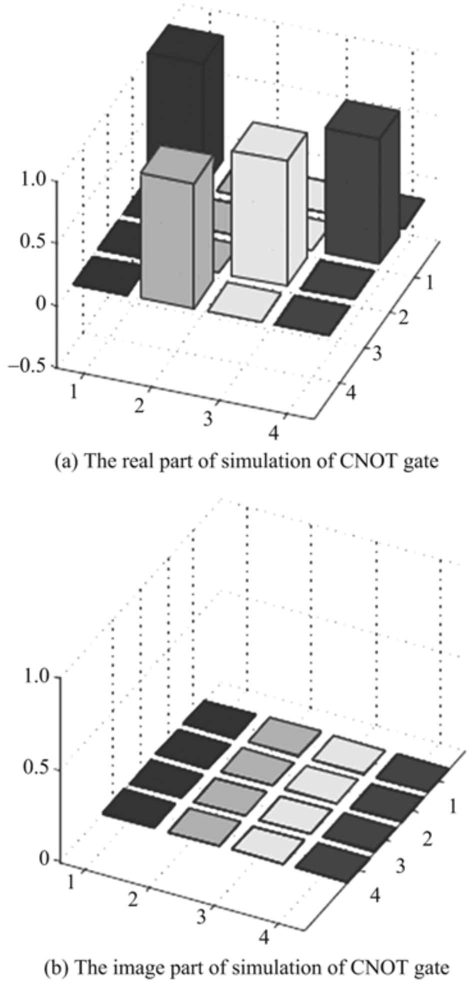
where n is the number of infinitesimal time intervals Δt spanning the full period from 0 to $t = n\Delta t$ over each of which the Hamiltonian may be considered time-independent. $H(t)$ is the Hamiltonian of the system with pulse sequence at time t.

In the Matlab simulation, we consider a CH heteronuclear system, in which the dipolar constant between $S = C^{13}$ and $I = H^1$ is $b_{IS} = -2\pi \times 20\,000$ rad/s, the Euler angle between the dipolar interaction's principal axil frame and rotor frame is $\{\alpha = \text{arbitrary value}, \beta = 45°, \gamma = 0\}$, and the initial phase of rotor φ_0 is 0. The value of β is set at 45° to ensure that $\tau_1 = 2\pi/G_1$ is the shortest. According to Eq. (9), the value of n is 1, and the rotor's spin rate ω_r can be calculated to be 56.569 kHz. Then the last value of the CNOT's propagator of the system under MAS is calculated as shown in Fig. 3. It is a spin I controlling spin S CNOT gate. The ideal propagator of this CNOT is

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

It can be seen from the result in Fig. 3 that the simulation has a high accuracy relative to ideal CNOT matrix. Also, the SWAP, controlled-Z gate is simulated with Matlab, and the result is shown in Figs. 4 and 5 respectively.

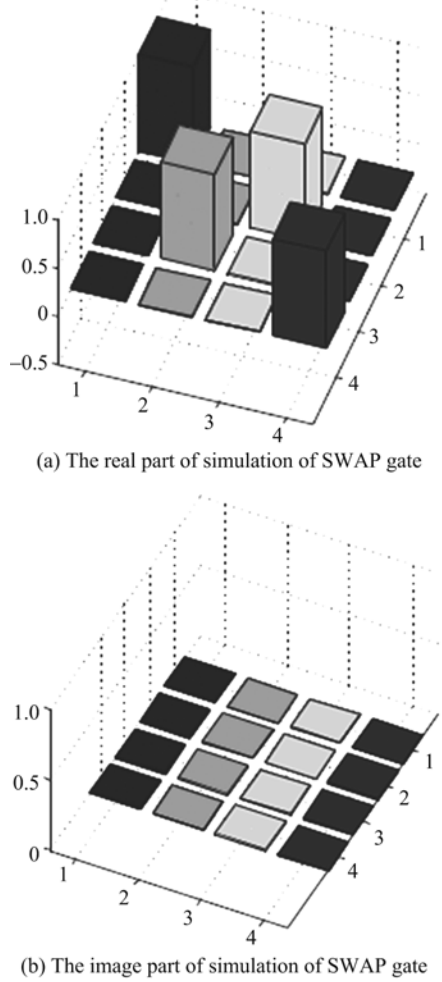
The simulation of CNOT which is closer to real experiments operation is completed by using



(a) The real part of simulation of CNOT gate

(b) The image part of simulation of CNOT gate

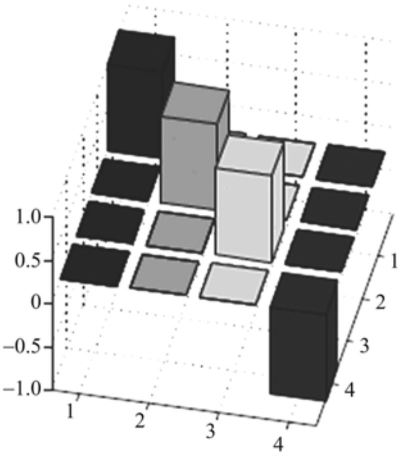
Fig. 3　The results of CNOT gate simulated with Matlab



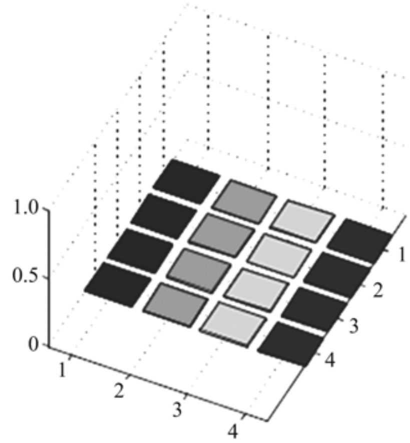
(a) The real part of simulation of SWAP gate

(b) The image part of simulation of SWAP gate

Fig. 4　The results of SWAP gate simulated with Matlab



(a) The real part of simulation of controlled-Z gate



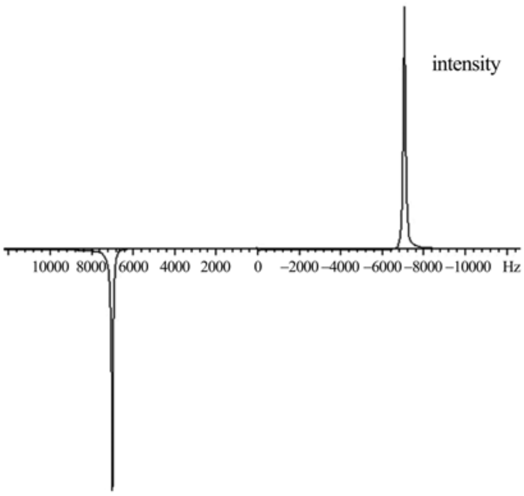
(b) The image part of simulation of controlled-Z gate

Fig. 5 The results of controlled-Z gate simulated with Matlab

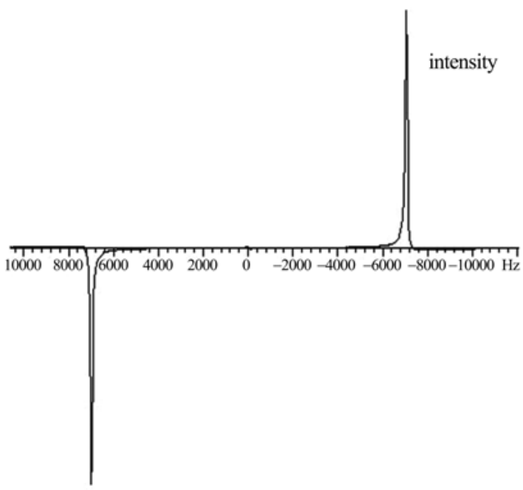
SIMPSON in a CH system. Here, initial states |00〉, |01〉, |10〉, |11〉 are used, and series of FIDs are collected after a 90° pulse and after the pulse sequence of CNOT followed by a 90° pulse. Both FIDs are sampled at the RF field of recoupling on channel C^{13}, and then FIDs are converted into spectra through fast Fourier transformation (FFT).

From Figs. 6～9, we can see that the spectra of initial state |00〉 and |10〉 are almost the same using or without using CNOT, and that the spectra of initial state |01〉 is the same as that of initial state |11〉 and the spectra of initial state |11〉 is the same as that of initial state |01〉. The results are consistent with properties of the CNOT gate, which demonstrates that it is highly feasible to employ the pulse sequence to implement the CNOT gate. To further confirm the result, a full tomography is needed, which will be our future work.

In the case of the homonuclear system, we can use C^{13}-labeled glycine, whose spins S and I are two C^{13} nuclei. The parameters of the sample are set to be $\omega_S = 2\,000$ Hz, $\omega_I = 18\,000$ Hz, which is appropriate for the real condition, $\omega_r = 16\,000$ Hz, and the value of b_{IS} and the Euler angles are the same as those in the heteronuclear case for simplicity. The simulations are done with the pulse sequences, CNOT, SWAP, controlled-Z and controlled phase. The figures of these simulations are not shown here.

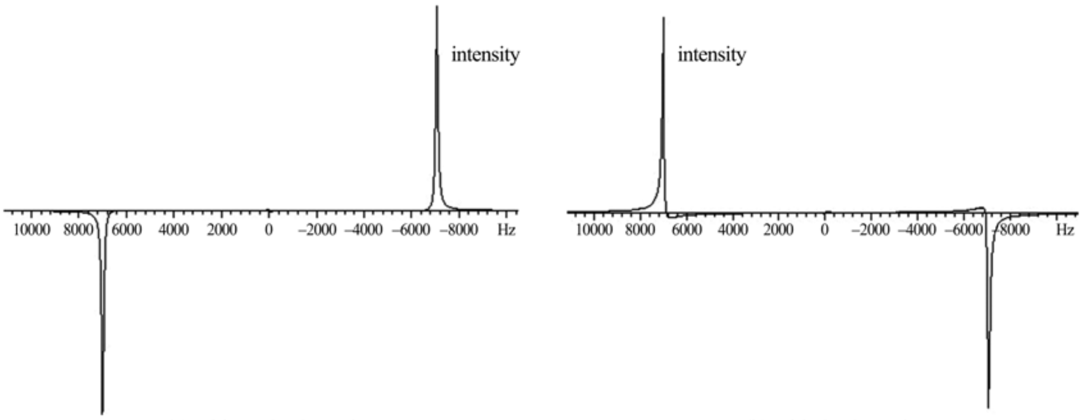


(a) without CNOT pulse



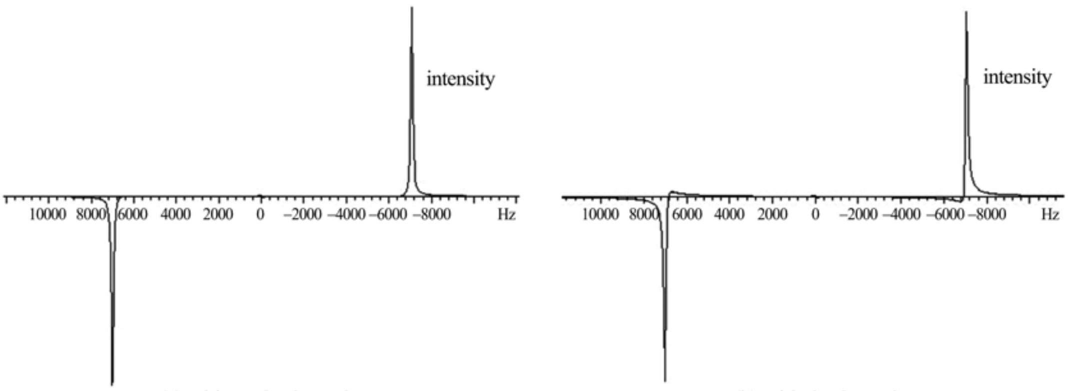
(b) with CNOT pulse

Fig. 6 The spectrums of initial state |00〉



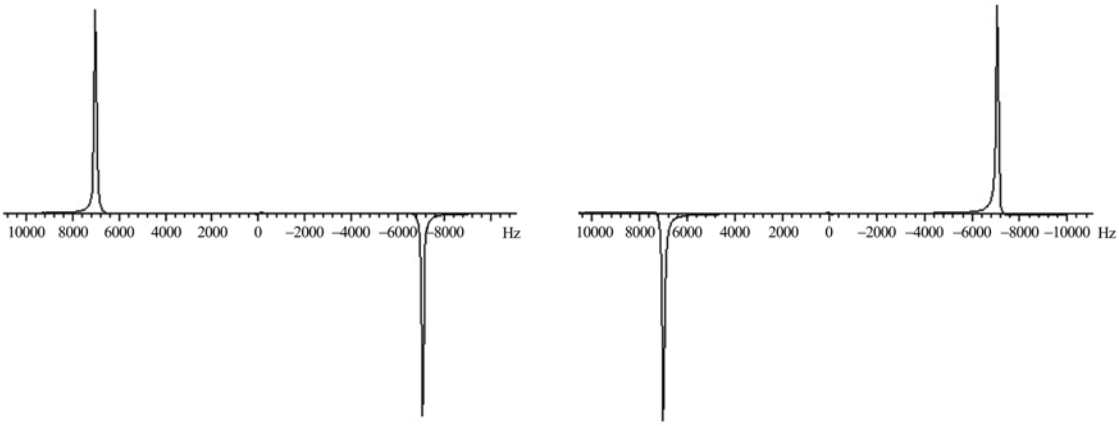
(a) without CNOT pulse (b) with CNOT pulse

Fig. 7 The spectrums of initial state |01⟩



(a) without CNOT pulse (b) with CNOT pulse

Fig. 8 The spectrums of initial state |10⟩



(a) without CNOT pulse (b) with CNOT pulse

Fig. 9 The spectrums of initial state |11⟩

3 Conclusion

In this work, a novel approach has been proposed to realize quantum operations in the solid state NMR, and several important conditions are shown to realize quantum gates in rotating crystal. The advantage of this approach to realizing quantum gates in rotating crystal is that the pulse sequence is simple. For example, C^{13}-labeled glycine which is composed of two C^{13} nuclei with different chemical shift and H^1 nucleus can be seen as a homonulear system when the heteronuclear couplings are decoupled by pulse sequences, whereas, the decoupling pulse squence is not needed when we apply MAS with a large spin rate. On the other hand, the simulations here is a basis of the experiments in solid state NMR to realize controlled gate in the future, such as the tomography experiments in rotating solids.

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