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Dynamics of nuclear spin-1/2 system in a strong bichromatic RF-field

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Abstract Based on calculating the influence of RF-field with various physical parameters on the dynamics of the spin 1/2 system, it was found that the spin state could be changed up and down by choosing appropriate RF pulses, and the coherent control of the RF pulses could substantially modify the behavior of spin dynamics: quicker change of two states could be produced even for small pulse duration. In addition, the oscillatory structures around the resonant frequency and the propagation features of the pulses depend on the relative phase of the bichromatic RF pulses.

Key words Nuclear spin-1/2 system, RF-field, Coherent control

1 Introduction

To study the response of finite quantization systems, such as nuclear spin systems, the method of periodic RF (radio frequency)-pulses has attracted considerable interests both theoretically and experimentally. In NMR, nicely designed RF-pulses are used to bring about a controlled evolution of the nuclear spin systems that are of heteronuclear spin-spin decoupling[1,2], and independent of homonuclear spin-spin couplings[3].

On the other hand, in nanotechnology and the development of semiconductor and metal devices, as the quantum size is approaching its limit, researchers are trying to find solutions to the size limit problem. Consequently, the idea of quantum computations and quantum computers, in which the elements that carry quantum bits of the information are atoms or nuclear spin, has attracted the attention of many scientists[4-7]. Generally, we assume that a minimal system for carrying a qubit of information is a two-state atom (spin). The atom (spin) can be populated either in the ground state, or in the excited state. Information can then be represented by a set of atoms (spins), some of which are in the ground state |0> and others in the excited state |1>.

To pave ways for technological applications of quantum computing and quantum information processing, it is necessary to control the electron or nuclear spin dynamics of the quantum system. And considerable research efforts have been paid by many groups[8-10].

2 Models and methods

The present paper is concerned with the nuclear spin-1/2 dynamics in a sub-microsecond bichromatic RF-pulses. For this fast dynamics, the time scale is much shorter than that of the usual spin-lattice relaxation process and even than that of the spin-spin relaxation. Moreover, it is clear that the system ought to obey the rule of quantum mechanism. Based on the time-dependent Schrödinger equation and by virtue of the time-dependent density operation of spin 1/2 system, we study the possibility of coherent control in dynamics and, in particular, influences of variations of the RF-pulse parameters and the coherent effects for bichromatic RF-pulses propagating in a nuclear spin medium.

We assume that a spin-1/2 system is placed in a static magnetic field B_0 in the Z-direction and polarized RF-field $B_1(t)$ in the X-Y plane. The spin-1/2 system has two quantum states: the spin up state |↑> and the spin down state |↓>. The energy difference $\Delta E_{\uparrow\downarrow}$ between the two states is $\hbar\omega_0$, where $\omega_0=-\gamma B_0$. The Hamiltonian $H(x,t)$ of a spin-1/2 particle in magnetic fields is given as

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$$H(x,t) = H_0 + H_{\rm int}(x,t) = -\gamma\hbar B_0 S_z - \frac{1}{2}\gamma\hbar(B_1(t)S^+ + B_1(t)^* S^-) \quad (1)$$

$$S_Z = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, S^+ = \begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}, S^- = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix} \quad (2)$$

where H_0 is the time-independent Hamiltonian of the system. The parameter γ designates the gyromagnetic ratio of the spin-1/2 under discussion and is assumed to be positive. $H_{\rm int}(x, t)$ is the interaction of the spin system with the RF-field, and B_1 is the magnetic-field strength induced by the RF-pulse fields.

In this paper, the bichromatic RF-pulses are turned on and off adiabatically, i.e.

$$B_1(t) = B_{11}\exp[-t^2/\tau_1^2 - {\rm i}\omega_1 t) + B_{12}\exp(-t^2/\tau_1^2 - {\rm i}(\omega_2 t + \varphi)] \quad (3)$$

where B_{11} and B_{12} are amplitude of the magnetic-field strength of the fundamental field and $n^{\rm th}$ harmonic field with the frequency ω_1 and ω_2, respectively; and φ is the relative phase between the fundamental and the $n^{\rm th}$ harmonic field. At the same time, we choose the RF-field with the Gaussian shaped $[\exp(-t^2/\tau^2)]$.

For studying a spin 1/2 particle in pulse fields, solving the time-dependent Schrödinger equation is necessary. Here, we use the time-dependent density operator $\rho(t)$ of the system, which evolves in time according to

$$\rho(t) = U(t,0)\rho(0)U^+(t,0) \quad (4)$$

where $\rho(0)=\begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$ and U^+ denotes the adjoint of U, which is the time-evolution operator. From Eqs.(1) and (4), $\rho(t)$ can be expressed as

$$\rho(t) = \begin{pmatrix}\cos^2\eta & -\exp({\rm i}\xi)\sin\eta\cos\eta\\ -\exp(-{\rm i}\xi)\sin\eta\cos\eta & \sin^2\eta\end{pmatrix} \quad (5)$$

where ξ and η obey Eq.(6)

$$\begin{cases}\dot{\xi}=\omega_0+\dfrac{ctg\eta - tg\eta}{\hbar}[\dfrac{1}{2}\gamma B_{11}\exp(-\dfrac{t^2}{\tau_1^2})\cos(\xi+\omega_1 t)+\\ \dfrac{1}{2}\gamma B_{12}\exp(-\dfrac{t^2}{\tau_1^2})\cos(\xi+\omega_2 t+\varphi)]\\ \dot{\eta}=\dfrac{-1}{\hbar}[\dfrac{1}{2}\gamma B_{11}\exp(-\dfrac{t^2}{\tau_1^2})\sin(\xi+\omega_1 t)+\\ \dfrac{1}{2}\gamma B_{12}\exp(-\dfrac{t^2}{\tau_1^2})\sin(\xi+\omega_2 t+\varphi)]\end{cases}. \quad (6)$$

In addition, being interested in the response of the system to the application of sequential RF-pulses, we simulate RF-field by a periodically applied pulse. To calculate the periodical operator $\rho(kT+t)$, where T is the time of a pulse period and k=0, 1, 2…represents period numbers of RF-pulses, a direct time-domain integration in one period can be performed [10,11]. Accordingly, one obtains

$$\rho(kT+t) = [U(T)]^k U(t)\rho(0)U^+(t)[U(T)]^{k+} \quad (7)$$

3 Results and discussion

In order to compute conveniently, we assume the energy difference $\Delta E_{\uparrow\downarrow}$ is 0.28×10^{-7} eV. The $|\uparrow>$ state occupation reaches a maximum, when the main frequency ω_1 ($\omega_2=2\omega_1$) of the pulse is in resonance with the energy difference $\Delta E_{\uparrow\downarrow}$ between the two spin states. Fig.1 shows the dependence of the $|\uparrow>$ state occupation (shading, here φ=0, $\omega_2=2\omega_1$) on both the γB_1(y axis) and the pulse duration τ(x axis), for a fundamental frequency resonant with the level splitting.

In Fig.1a, which is the density graphics, alternate zones of high (black) and low (white) occupation depending on either γB_1 or τ can be observed. The black zones express that the $|\uparrow>$ state occupation is the maximum(i.e.:1.00), and the white zones express that the $|\uparrow>$ state occupation is the minimum(i.e.: 0), while the alternate zones from black to white express that the $|\uparrow>$ state occupation is from 1.00 down to 0 gradually. It is clear that this result is the quantity that must be tuned to obtain the complete transition to the $|\uparrow>$ state.

Fig.1b shows a horizontal cut of Fig.1a at different values of γB_1.The oscillatory behavior is clearly visible and the oscillatory frequency difference factor among four graphs is due to differences of the maximum magnetic-field amplitude. The value of γB_1 and frequency are bigger, i.e. the period time of circulations become small and small.

Fig.2 is the density graph of the $|\uparrow>$ occupation (shading, here B_{11}= B_{11}= 2.0 T) ($\omega_2=2\omega_1$) on both the relative phase of the bichromatic RF-field (y axis) and the pulse duration (x axis), for a main frequency resonant with the level splitting. Alternate zones of high (black) and low (white) occupation for both φ or τ can be observed.

Compared with monochromatic RF-field, the relative phase φ of the bichromatic RF-field is an inherent and controllable parameter; it is convenient and effortless to modulate it in experiments. Based on the above study, it is no doubt that we can only choose the parameter φ to finish the expected quantum control by changing other parameters in monochromatic RF-field. It is also a possible choice using the relative phase to control quantum state while the monochromatic RF pulse reaches to its limit in the present experiments.

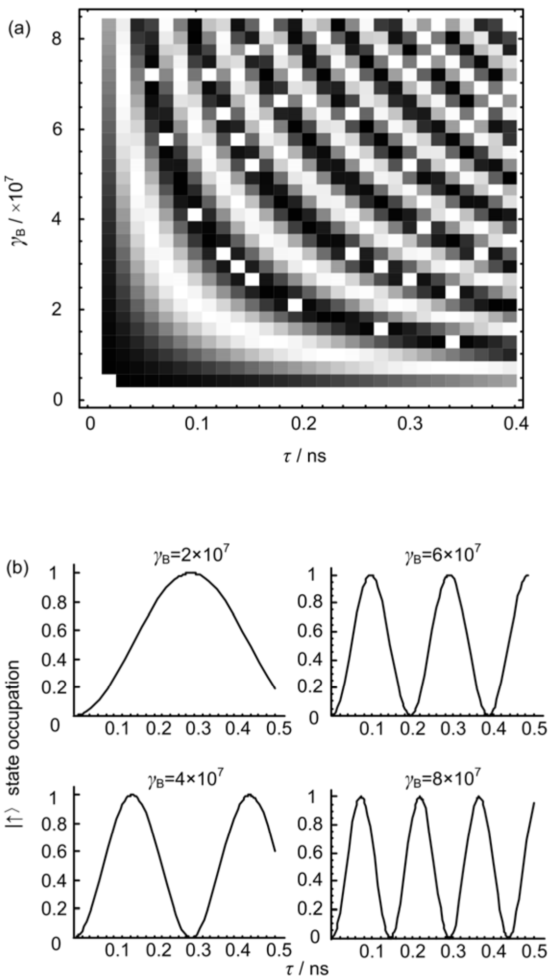

Fig.1 Dependences of the |↑>state occupation on both the magnetic field amplitude and pulse duration. (a) The density graphics. (b) The horizontal cut.

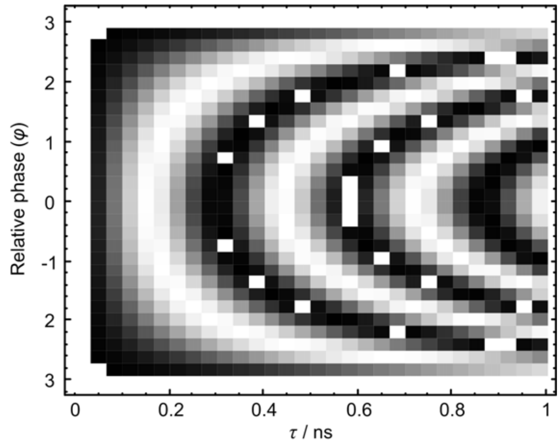

Fig.2 Dependences of the |↑> state occupation on both the relative phase and pulse duration.

Fig.3 shows the time evolution of the state occupation for a Gaussian pulse. When the conditions for a complete transition are fulfilled, that is, the duration of the pulse, relative phase, frequency, and amplitude is properly tuned (such as $\omega_2=2\omega_1, \varphi=0$, $\tau_1=\tau_2=0.008$ μs and $B_{11}=B_{12}=$ 2.93 *T*), the expected quantum control can be achieved, as shown in Fig.3b.

The cases shown in Fig.3a ($\tau_1=\tau_2=0.01$ μs) and Fig.3c ($\tau_1=\tau_2=0.006$ μs) correspond to durations of the pulses being too long or too short, respectively. In the first case, the pulse is still on when the complete transition is obtained thus generating stimulated emission that begins to take the system again to its |↓> state, while in the second, the excitation is turned off before the system reaches a transition probability equal to one. As can be seen in Fig.3d, the successive application of pulses makes the system go from the |↓> state to the |↑> state and back, so that in this system it may control the state of the system and make it work as a read/write unit.

Monochromatic RF-field is also used to study effect on spin 1/2 field, so as to compare the results with the present work. It was found that the chosen pulse width τ of the bichromatic RF-field is shorter than the monochromatic RF-field's in the case of the same other parameters. Therefore, the time of quantum control may be shorter in the bimonochromatic RF-field.

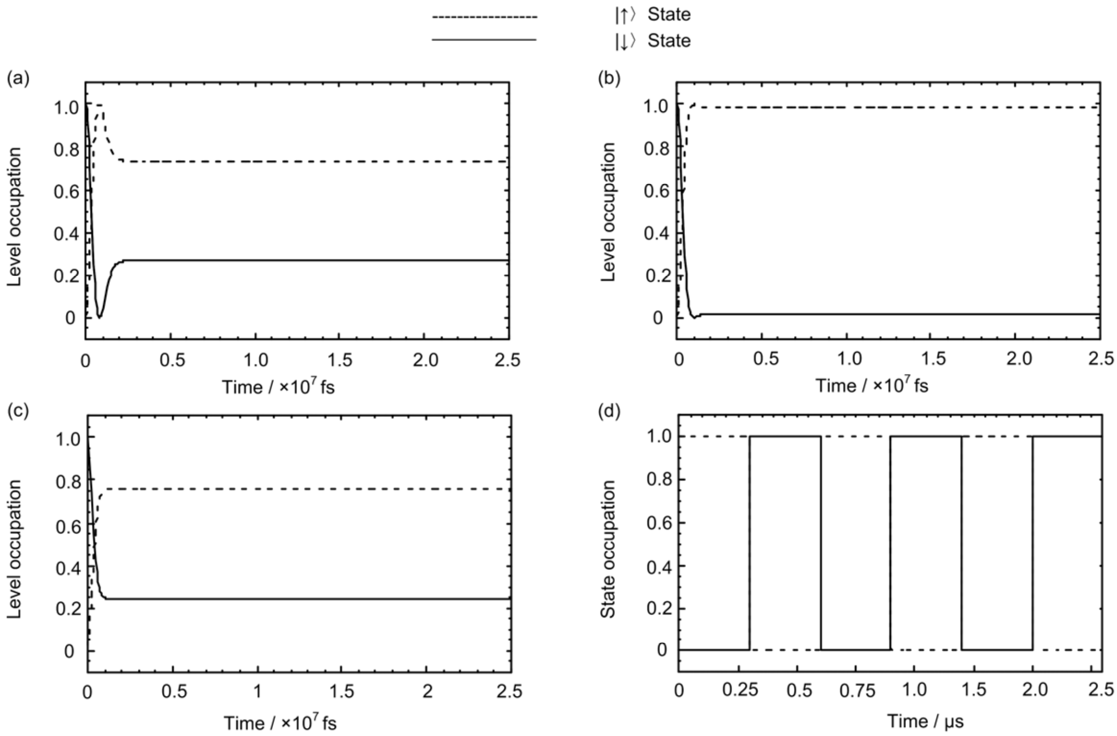

Fig.3 Time evolution of the state occupation for a 1/2 spin system in a bichromatic RF-field. (a) Over excitation. (b) Complete transition. (c) Under excitation. (d) Several pulses tuned to complete transition.

4 Conclusion

The quantum control is essential to the quantum information processing and the quantum computing as well as for raising the signal to noise ratio of the NMR. In this paper, we have investigated the coherent effects of RF-pulses propagating in the nuclear spin-1/2 medium. The influences of the variations of RF-pulse duration, intensity, relative phase between the fundamental field and n^{th} harmonic field, and n^{th} harmonic frequency have been studied. From the theoretical results, it is clear that the control of the transitions from one state to another and back can be obtained, even for the complete transitions as shown in Fig. 3d. It is also found that the coherent control of the two RF-pulses can substantially modify the behavior of the spin dynamics: quicker change of two states can be produced even for small pulse durations. Moreover, the oscillatory structures around the resonant frequency and the propagation features of the RF-pulses depend on the relative phase φ of the two pulses.

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