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Two qubits in pure nuclear quadrupole resonance

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Abstract

It is shown theoretically that by the use of two radio-frequency fields of the same resonance frequency but with the different phases and directions the degeneracy of the energy spectrum of a spin system with $I = 3/2$ is removed. This leads to four non-degenerate spin states which can be used as a platform for quantum computing. The feasibility of quantum computing based on a pure (without DC magnetic fields) nuclear quadrupole resonance technique is investigated in detail. Various quantum logic gates can be constructed by using different excitation techniques allowing different manipulations with the spin system states. Three realizations of quantum logic gates are considered: the application of an additional magnetic field with the resonance frequency, the amplitude modulation of one of the applied RF fields by the resonance frequency field, and the level-crossing method. It is shown that the probabilities of the resonance transitions depend on the method of excitation and on the direction of the excitation field. Feasibility of quantum computing is demonstrated with the examples of constructing a controlled-NOT logic gate using the resonance excitation technique and SWAP and NOT2 logic gates using the level-crossing method.

1. Introduction

Quantum computing is a new fast developing field that combines together ideas from information theory, computer science, and quantum physics [1]. In recent years, the nuclear magnetic resonance (NMR) technique has received considerable attention as a platform for the practical implementation of a quantum computer (QC) [2–4]. The basic idea for an NMR QC is that two stationary states of spin $\frac{1}{2}$ in an applied magnetic field represent naturally one information quantum bit (qubit).

In contrast to a classical bit, which can be in one of two states, 0 or 1, a qubit can exist in a superposition of two basic quantum states $|0\rangle$ and $|1\rangle$ allowing the QC to perform certain computations more quickly than classical computers do [1–4]. To produce two-qubit gates in a physical system of the same type of nuclei as the spin $\frac{1}{2}$, some interaction between nuclear spins

is required. This interaction forms a strong-coupling network. The strength of the network coupling determines the gate time of the QC [5]. For example, all possible pulse sequences for realization of two-qubit gates in NMR have one feature in common: the evolution time between pulses is of the order of $\frac{1}{2J}$, where J is the spin–spin coupling constant. So, the computation time is the inverse of $2J$ [4]. This constant is in range of 10–200 Hz. Thus the computation time for the two-qubit gates can be quite long: from 100 to 2.5 ms. For example, a C-NOT NMR gate based on cytosine takes about 70 ms to operate [6]. In order to overcome this weak point, using nuclei with an electric quadrupole moment and the nuclear quadrupole resonance (NQR) technique was proposed [7].

It is known that the energy levels of a nucleus with a half-integer spin $I > 1/2$ having an electric quadrupole moment Q are degenerate in an electric field gradient (EFG) according to Kramers' rule [8]. For example, there are two doubly degenerate energy levels for the spin $\frac{3}{2}$ [8] ($\hbar = 1$):

$$\varepsilon_{\pm 3/2} = +\frac{eQq_{ZZ}}{4}\xi, \qquad \varepsilon_{\pm 1/2} = -\frac{eQq_{ZZ}}{4}\xi \tag{1}$$

where $eq_{zz} = \frac{\partial^2 V}{\partial z^2}$ is the ZZ-component of the EFG; V is the electric potential, $\xi = (1 + \eta^2/3)^{1/2}$, and η is the asymmetry parameter of the EFG.

In an applied external DC magnetic field, the degeneracy of the energy levels is removed and four coupled energy levels are obtained for a nucleus [8]. Therefore, any interaction between individual spins of the spatially separated particles is not required to form a two-qubit system [7].

In order to form a non-degenerate energy spectrum, both techniques, NMR and NQR, use high external magnetic fields (1–9 T) and internal interactions: the spin–spin interaction for NMR [2–4] and the interaction of the quadrupole moment with the EFG for NQR [7, 9–11]. Both of these interactions are determined by intrinsic properties of the crystal or liquid crystalline matrix used. The splitting of the energy levels is determined by the magnetic field value.

In the present paper we show that a two-qubit system can be formed using quadrupole nuclei with the spin $\frac{3}{2}$, influenced by two radio-frequency (RF) fields without an external DC magnetic field.

2. Energy spectrum

Let us consider a system of nuclear spins with $I = 3/2$ in zero external magnetic field under the action of two RF fields with the same frequency ω close to the resonance frequency $\omega^0 = \varepsilon_{\pm 3/2} - \varepsilon_{\pm 1/2}$ of the spins but with different amplitudes H_k, directions $\vec{L}_k$, and phases α_k:

$$\vec{H}_k(t) = H_k \vec{L}_k \cos(\omega t + \alpha_k), \tag{2}$$

where $k = 1$ and 2 relate to the first and second RF fields; the $\vec{L}_k$ are given in the principal-axis frame of the EFG by polar (θ_k) and azimuthal (φ_k) angles as $\vec{L}_k = \{\sin\theta_k \cos\varphi_k; \sin\theta_k \sin\varphi_k; \cos\theta_k\}$.

We assume that the spin–spin and spin–lattice interactions are small relative to the quadrupole interaction. In this case the system can be described by the Hamiltonian

$$\mathcal{H}(t) = \mathcal{H}_Q + \mathcal{H}_1(t), \tag{3}$$

where

$$\mathcal{H}_Q = \sum_i \frac{eQq_{zz}}{4I(2I-1)}\left[3I_z^{i2} - \vec{I}^{i2} + \frac{\eta}{2}(I_+^{i2} + I_-^{i2})\right] \tag{4}$$

represents the interaction of the spin system with the EFG; $\vec{I}^i = \{I_x^i, I_y^i, I_z^i\}$ is the operator of spin, $I_\pm^i = I_x^i \pm \mathrm{i}I_y^i$, $\mathrm{i} = \sqrt{-1}$. The summation is over all of the nuclei of the system. $\mathcal{H}_1(t)$ gives the action of two applied RF fields on the spin system:

$$\mathcal{H}_1(t) = \sum_{k=1}^{2} \sum_i \omega_k^1 \vec{L}_k \cdot \vec{I}^i \cos(\omega t + \alpha_k), \tag{5}$$

where $\omega_k^1 = \gamma H_k$; γ is the gyromagnetic nuclear ratio.

Operations with all the spin operators will be performed in the basis in which the Hamiltonian $\mathcal{H}_Q$ has a diagonal form. Using an operator basis $e_{mn} = \sum_i e_{mn}^i$, defined by their matrix elements in the $\mathcal{H}_Q$-representation $\langle m|e_{m'n'}^i|n\rangle = \delta_{mm'}\delta_{nn'}$ and the commutation relation $[e_{mn}^i, e_{m'n'}^j] = \delta_{ij}(\delta_{nm'}e_{mn'}^i - \delta_{n'm}e_{m'n}^i)$ with $m, n = 3/2, 1/2, -1/2 \equiv \overline{1/2}, -3/2 \equiv \overline{3/2}$, the Hamiltonian (3) can be rewritten as

$$\mathcal{H}(t) = \tfrac{1}{2}\omega^0(e_{3/2,3/2} - e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}} + e_{\overline{3/2},\overline{3/2}}) + \sum_{k=1}^{2} \omega_k^1 \cos(\omega t + \alpha_k) \sum_{m,n} (\vec{L}_k \cdot \vec{I})_{mn} e_{mn}, \tag{6}$$

where

$$\begin{aligned}\sum_{m,n} (\vec{L}_k \cdot \vec{I})_{mn} e_{mn} = {} & A_k^{(+)}(e_{3/2,1/2} + e_{\overline{1/2},\overline{3/2}}) + A_k^{(-)}(e_{\overline{3/2},\overline{1/2}} + e_{1/2,3/2}) \\ & - A_k^{(3)}(e_{3/2,\overline{1/2}} + e_{\overline{1/2},3/2} - e_{1/2,\overline{3/2}} - e_{\overline{3/2},1/2}) \\ & + T_{(-)k}e_{3/2,\overline{3/2}} + T_{(-)k}^* e_{\overline{3/2},3/2} + T_{(+)k}e_{\overline{1/2},1/2} + T_{(+)k}^* e_{1/2,\overline{1/2}} \\ & + R_{(+)k}(e_{3/2,3/2} - e_{\overline{3/2},\overline{3/2}}) - R_{(-)k}(e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}})\end{aligned} \tag{7}$$

and

$$\begin{aligned} & T_{(\pm)k} = \tfrac{1}{2}[\sin\theta_k \mp 3^{1/2}\mathrm{e}^{\pm\mathrm{i}\varphi_k} \sin\beta + \mathrm{e}^{\pm\mathrm{i}\varphi_k}(1 \pm \cos\beta)]; \\ & R_{(\pm)k} = \frac{1}{2}\cos\theta_k\left(1 \pm \cos\frac{\beta}{2}\right); \\ & A_k^{(\pm)} = A_k^{(1)} \pm \mathrm{i}A_k^{(2)}; \\ & A_k^{(1)} = \tfrac{1}{2}\sin\theta_k \cos\varphi_k(3^{1/2}\cos\beta + \sin\beta); \\ & A_k^{(2)} = \tfrac{1}{2}\sin\theta_k \sin\varphi_k(3^{1/2}\cos\beta - \sin\beta); \\ & A_k^{(3)} = \cos\theta_k \sin 2\beta; \qquad \tan\beta = \eta(3^{1/2}\xi)^{-1}. \end{aligned}$$

In the vicinity of the resonance, we use the approach developed in [12, 13], which is based on the unitary transformation defined by the operator $U(t) = \exp(\mathrm{i}Dt)$ with

$$D = \tfrac{1}{4}\omega(e_{3/2,3/2} - e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}} + e_{\overline{3/2},\overline{3/2}}). \tag{8}$$

This transformation results in a new representation with the Hamiltonian $\tilde{\mathcal{H}}(t) = U(t)\mathcal{H}(t)U^{-1}(t)$. Using the transformation rule for the operator basis

$$\tilde{e}_{mn} = \tilde{e}_{nm}^* = e_{mn}\mathrm{e}^{\mathrm{i}\omega_{mn}t}, \tag{9}$$

where $\omega_{mn} = 0$ for $m = n, -n$ and $\omega_{mn} = \omega$ otherwise, we find the Hamiltonian $\tilde{\mathcal{H}}(t)$:

$$\begin{aligned}\tilde{\mathcal{H}}(t) = {} & \frac{\Delta}{2}(e_{3/2,3/2} - e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}} + e_{\overline{3/2},\overline{3/2}}) + \\ & + \sum_{k=1}^{2} \omega_k^1 [A_k^{(+)}(e_{3/2,1/2}\mathrm{e}^{\mathrm{i}\omega t} + e_{\overline{1/2},\overline{3/2}}\mathrm{e}^{-\mathrm{i}\omega t}) + A_k^{(-)}(e_{\overline{3/2},\overline{1/2}}\mathrm{e}^{\mathrm{i}\omega t} + e_{1/2,3/2}\mathrm{e}^{-\mathrm{i}\omega t})\end{aligned}$$

$$
\begin{aligned}
&- A_k^{(3)}(e_{3/2,\overline{1/2}}\mathrm{e}^{\mathrm{i}\omega t} + e_{\overline{1/2},3/2}\mathrm{e}^{-\mathrm{i}\omega t} - e_{1/2,\overline{3/2}}\mathrm{e}^{-\mathrm{i}\omega t} - e_{\overline{3/2},1/2}\mathrm{e}^{\mathrm{i}\omega t}) \\
&+ T_{(-)k}e_{3/2,\overline{3/2}} + T^*_{(-)k}e_{\overline{3/2},3/2} + T_{(+)k}e_{\overline{1/2},1/2} + T^*_{(+)k}e_{1/2,\overline{1/2}} \\
&+ R_{(+)k}(e_{3/2,3/2} - e_{\overline{3/2},\overline{3/2}}) - R_{(-)k}(e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}})]\cos(\omega t + \alpha_k), \qquad (10)
\end{aligned}
$$

where $\Delta = \omega^0 - \omega$. The Hamiltonian (10) contains time-independent terms and also terms oscillating with frequencies ω and 2ω. Under real experimental conditions, $\Delta \ll \omega$ and $\omega_k^1 \ll \omega$. Therefore, the role of the rapidly oscillating terms in the evolution of the spin states is negligible and they can be discarded [8]. In this approximation, the effective time-independent Hamiltonian of the system takes the following form:

$$
\begin{aligned}
\mathcal{H}_{eff} = {} & \frac{\Delta}{2}(e_{3/2,3/2} - e_{1/2,1/2} - e_{\overline{1/2},\overline{1/2}} + e_{\overline{3/2},\overline{3/2}}) \\
&+ \sum_{k=1}^{2}\frac{\omega_k^1}{2}[A_k^{(+)}(e_{3/2,1/2}\mathrm{e}^{-\mathrm{i}\alpha_k} + e_{\overline{1/2},\overline{3/2}}\mathrm{e}^{\mathrm{i}\alpha_k}) + A_k^{(-)}(e_{\overline{3/2},\overline{1/2}}\mathrm{e}^{-\mathrm{i}\alpha_k} + e_{1/2,3/2}\mathrm{e}^{\mathrm{i}\alpha_k}) \\
&- A_k^{(3)}(e_{3/2,\overline{1/2}}\mathrm{e}^{-\mathrm{i}\alpha_k} + e_{\overline{1/2},3/2}\mathrm{e}^{\mathrm{i}\alpha_k} - e_{1/2,\overline{3/2}}\mathrm{e}^{\mathrm{i}\alpha_k} - e_{\overline{3/2},1/2}\mathrm{e}^{-\mathrm{i}\alpha_k})]. \qquad (11)
\end{aligned}
$$

Diagonalization of the effective Hamiltonian gives the following energy levels of the spin system in the RF field:

$$
\begin{aligned}
E_3 &= -E_0 = [B_1 + B_2]^{1/2}, \\
E_2 &= -E_1 = [B_1 - B_2]^{1/2},
\end{aligned} \qquad (12)
$$

where

$$
B_1 = \omega_1^1\omega_2^1\left[\frac{1}{4}\frac{\Delta^2}{\omega_1^1\omega_2^1} + \frac{\omega_1^1}{\omega_2^1}\vec{A}_1^2 + \frac{\omega_2^1}{\omega_1^1}\vec{A}_2^2 + 2(\vec{A}_1\cdot\vec{A}_2)\cos(\alpha_1 - \alpha_2)\right], \qquad (13)
$$

$$
B_2 = 2\omega_1^1\omega_2^1|\vec{A}_1 \times \vec{A}_2|\sin(\alpha_1 - \alpha_2), \qquad (14)
$$

$$
\vec{A}_k = \{A_k^{(1)}, A_k^{(2)}, A_k^{(3)}\}. \qquad (15)
$$

Equations (12)–(15) show that the degeneracy of the energy spectrum is removed, without a DC magnetic field, just by application of two RF fields with different phases and directions. The energy levels E_s correspond to the eigenstates of the quantum system described by the effective Hamiltonian $H_{eff}|\zeta_s\rangle = E_s|\zeta_s\rangle$, where the $|\zeta_s\rangle$ are the eigenfunctions with $s = 0, 1, 2, 3$.

According to equations (12)–(15), the splitting between energy levels depends on the phase shift $\alpha_1 - \alpha_2$ and mutual orientations of the RF fields. By variation of these parameters we can change the values of the resonance frequencies $\Omega_{ss'} = E_s - E_{s'}$.

Let us consider in more detail a special case where the EFG has axial symmetry, $\eta = 0$, and both RF fields have equal amplitudes $\omega_1^1 = \omega_2^1 = \omega^1$ and polar angles of the direction vectors $\theta_1 = \theta_2 = \pi/2$. In this case equations (13) and (14) reduce to

$$
B_1 = (\omega^1)^2\left\{\frac{1}{4}\left(\frac{\Delta}{\omega^1}\right)^2 + \frac{3}{2}[1 + \cos(\varphi_1 - \varphi_2)\cos(\alpha_1 - \alpha_2)]\right\}, \qquad (16)
$$

$$
B_2 = \tfrac{3}{2}(\omega^1)^2\sin(\varphi_1 - \varphi_2)\sin(\alpha_1 - \alpha_2). \qquad (17)
$$

The dependence of the energy levels $E_{0,1,2,3}$ on the difference of phases $\alpha_1 - \alpha_2$ according to equations (16) and (17) for $\varphi_1 - \varphi_2 = \pi/2$ and $\frac{1}{6}(\frac{\Delta}{\omega^1})^2 = 0.1$ is shown in figure 1. The energy level dependence on the relative orientation of the RF fields, $\varphi_1 - \varphi_2$, has the same character. By variation of the difference $\alpha_1 - \alpha_2$ we can control the splitting between the energy levels of the spin system. Figure 1 illustrates that there are level-crossing points at $\alpha_1 - \alpha_2 = \pi p$, $p = 0, 1, 2\ldots$. In the case of the exact resonance $\Delta = 0$, the level-crossing points are achieved at the following conditions: $E_0 = E_1$ and $E_2 = E_3$ at $\alpha_1 - \alpha_2 = \pi p$; $E_0 = E_3$ at $\alpha_1 - \alpha_2 = \frac{1}{2}\pi + \pi(2p+1)$; and $E_1 = E_2$ at $\alpha_1 - \alpha_2 = \frac{1}{2}\pi + 2\pi p$; $p = 0, 1, 2\ldots$.

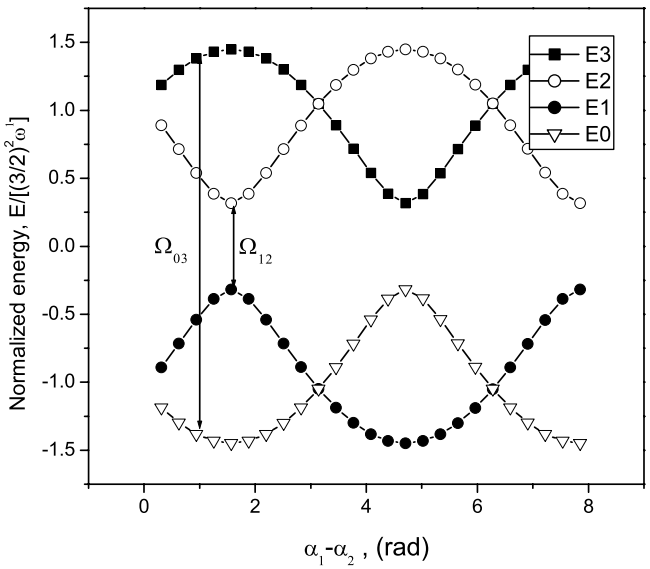

Figure 1. Energy levels, calculated as a function of the difference of phases $\alpha_1 - \alpha_2$.

3. Resonance transitions

The probabilities of the resonance transitions $s \to s'$, $P_{ss'} \sim \langle s|\vec{l}\cdot\vec{I}|s'\rangle^2$ depend on the method of excitation and the direction $\vec{l}$ of the excitation field. We will consider two methods of excitation: the application of an additional magnetic field with the resonance frequency $\Omega_{ss'}$ and the amplitude modulation of one of the applied RF fields.

3.1. Additional magnetic field

One commonly used excitation technique [14–17] consists in the application of an additional magnetic field $\vec{h} = h\vec{l}\cos\Omega t$ with amplitude h and frequency Ω close to $\Omega_{ss'} = E_s - E_{s'}$. This frequency Ω is estimated from the experimental data of [14–17] to be in the range 10–40 kHz. The sensitivity in this method is determined by the large frequency, which is 10 MHz. These are the so-called 'experiments in the rotating frame' [18]. The vector $\vec{l}$ is written in the principal-axis frame of the EFG: $\vec{l} = \{\sin\theta_3\cos\varphi_3; \sin\theta_3\sin\varphi_3; \cos\theta_3\}$. In the case of $\theta_3 = 0$, the probabilities $P_{03} = \frac{1}{4}(1 - \frac{\Delta^2}{4E_0^2})$, $P_{12} = \frac{1}{4}(1 - \frac{\Delta^2}{4E_1^2})$, and $P_{23} = P_{02} = P_{01} = P_{13} = 0$.

In the case of $\theta_3 = \pi/2$, we have another situation. The probabilities of the transitions $2 \to 3$, $0 \to 2$, $0 \to 1$, and $1 \to 3$ are non-zero and determined by

$$\begin{aligned} P_{10} &= \frac{(E_0 + \frac{\Delta}{2})(E_1 + \frac{\Delta}{2})}{4E_0E_1}, \qquad P_{02} = \frac{(E_0 - \frac{\Delta}{2})(E_1 + \frac{\Delta}{2})}{4E_0E_1}, \\ P_{13} &= \frac{(E_0 + \frac{\Delta}{2})(E_1 - \frac{\Delta}{2})}{4E_0E_1}, \qquad P_{23} = \frac{(E_0 - \frac{\Delta}{2})(E_1 - \frac{\Delta}{2})}{4E_0E_1}. \end{aligned} \tag{18}$$

To determine the probabilities P_{03} and P_{12} we use the same method of averaging of rapidly oscillating terms [8]. Both probabilities become proportional to $(\frac{\gamma h}{\omega^0})^2 \ll 1$.

Note that by changing the difference of the phases of the RF fields $\alpha_1 - \alpha_2$, one can control the probabilities of different transitions. As follows from (18), in the case of

$$\varphi_1 - \varphi_2 = \alpha_1 - \alpha_2 = \pi/2 \tag{19}$$

the transition $0 \to 2$ is forbidden, and the transitions $1 \to 3$ and $2 \to 3$ can be excited with the probabilities $P_{13} = \frac{E_0 - E_1}{2E_0}$ and $P_{23} = \frac{E_1 + E_0}{2E_0}$, respectively.

In the case of

$$\varphi_1 - \varphi_2 = -(\alpha_1 - \alpha_2) = \pi/2 \tag{20}$$

the transition $1 \to 3$ is forbidden, and the transitions $0 \to 2$ and $2 \to 3$ can be excited with the probabilities $P_{02} = \frac{E_1 - E_0}{2E_1}$ and $P_{23} = \frac{E_1 + E_0}{2E_1}$, respectively.

In both of these cases the transition $0 \to 1$ is forbidden.

We emphasize that the transitions $0 \to 2$ and $1 \to 3$ have equal resonance frequencies, but they can be excited independently, because of the different excitation conditions.

3.2. Amplitude modulation method

Another technique of excitation is based on the amplitude modulation of an RF field [18]. The amplitude modulation of one of the applied RF fields by the low frequency $\Omega_{ss'}$ (for example, $\vec{H}_2(t) = \frac{\omega^1}{\gamma}\vec{L}_2 \cos(\omega t + \alpha_2) \cos \Omega_{ss'} t$) allows us to operate without an additional coil. The resonance transitions $0 \to 3$ and $1 \to 2$ can be realized with the probabilities

$$P_{03} = \frac{9}{16E_0^2}\left\{\left(\frac{\Delta}{2} + E_0\right)^2 + 12(\omega^1)^2 \cos^2\left[\frac{(\varphi_1 - \varphi_2) + (\alpha_1 - \alpha_2)}{2}\right] \times [\cos(\varphi_1 + \varphi_2 + \alpha_1 + \alpha_2) - \sin(\varphi_1 + \varphi_2 + \alpha_1 + \alpha_2)]\right\} \tag{21}$$

and

$$P_{12} = \frac{9}{16E_1^2}\left\{\left(\frac{\Delta}{2} + E_1\right)^2 + 12(\omega^1)^2 \cos^2\left[\frac{(\varphi_1 - \varphi_2) - (\alpha_1 - \alpha_2)}{2}\right] \times [\cos(\varphi_1 + \varphi_2 - \alpha_1 - \alpha_2) - \sin(\varphi_1 + \varphi_2 - \alpha_1 - \alpha_2)]\right\}. \tag{22}$$

Averaging of rapidly oscillating terms gives for the probabilities of the transitions $2 \to 3$, $0 \to 2$, $1 \to 3$, and $0 \to 1$: $P_{23} \sim P_{02} \sim P_{13} \sim P_{10} \sim (\omega^1/\omega^0)^2 \ll 1$.

3.3. Level-crossing method

Note that there is another interesting method for realization of $s \to s'$ transitions between states, which is similar to the amplitude modulation technique. Let us show how this can be realized. For this purpose we shall consider a nuclear quadrupole spin system under the action of two RF fields (5) with different frequencies, $\omega_1 = \omega_2 + \delta$, and with both frequencies ω_1 and ω_2 close to the resonance one, ω^0. After performing the unitary transformation (8) with $\omega = \omega_1$ and neglecting terms describing fast oscillations with frequencies ω and 2ω [8], the spin system's Hamiltonian can be written in the form

$$\mathcal{H}_e(t) = \mathcal{H}_{eff} + \mathcal{H}_{1e}(t) \tag{23}$$

where $\mathcal{H}_{eff}$ has a time-independent part represented by equation (11) and a time-dependent part:

$$\mathcal{H}_{1e}(t) = \omega_1^1[A_1^{(+)}(e_{3/2,1/2}\mathrm{e}^{-\mathrm{i}\delta t} + e_{\overline{1/2},\overline{3/2}}\mathrm{e}^{\mathrm{i}\delta t}) + A_k^{(-)}(e_{\overline{3/2},\overline{1/2}}\mathrm{e}^{-\mathrm{i}\delta t} + e_{1/2,3/2}\mathrm{e}^{\mathrm{i}\delta t}) - A_k^{(3)}(e_{3/2,\overline{1/2}}\mathrm{e}^{-\mathrm{i}\delta t} + e_{\overline{1/2},3/2}\mathrm{e}^{\mathrm{i}\delta t} - e_{1/2,\overline{3/2}}\mathrm{e}^{\mathrm{i}\delta t} - e_{\overline{3/2},1/2}\mathrm{e}^{-\mathrm{i}\delta t})]. \tag{24}$$

For δ close to $\Omega_{ss'}$, this time-dependent interaction of the spin system can be used to excite the transitions between eigenstates $|\zeta_s\rangle$ of the Hamiltonian $\mathcal{H}_{eff}$.

4. Feasibility of quantum computing

Let us consider the set of the eigenstates obtained for the spin system as a platform for quantum computing. In quantum informatics, a calculation is represented as a sequence of unitary transformations (logic gates) of the states of a quantum system. The basic universal set of quantum logic gates consists of the one-qubit gates and one or more non-trivial two-qubit gates [1–3]. In our case, a one-qubit gate can be designed on the basis of one qubit with the excitation of the resonant transitions between the two eigenstates of the system using one of the excitation techniques described above. 'One qubit' for QC can be defined as an element with two quantum states—for example, $s = 0$ and $s' = 3$ or $s = 1$ and $s' = 2$. The eigenfunctions $|\zeta_s\rangle$ are factorized as is usual in the quantum information theory; for example: $|\zeta_0\rangle = |0\rangle$ and $|\zeta_3\rangle = |1\rangle$.

Two-qubit gates are more complicated: they involve conditional evolution and thus require some interaction between the qubits. The states of the two-qubit system can be factorized in the following way: $|\zeta_0\rangle = |00\rangle, |\zeta_1\rangle = |01\rangle, |\zeta_2\rangle = |10\rangle, |\zeta_3\rangle = |11\rangle$. In NMR QC, any operator acting in the (4×4)-dimensional space can be expressed as a linear combination of the direct product of the two (2×2)-dimensional Hilbert spaces $\mathcal{R} \otimes \mathcal{P}$ [7]. In the case considered, we can also present the basic vectors of the spin system in the form

$$
\begin{aligned}
|00\rangle &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathcal{R}} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathcal{P}}, \qquad |01\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathcal{R}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathcal{P}}, \\
|10\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathcal{R}} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathcal{P}}, \qquad |11\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathcal{R}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathcal{P}}.
\end{aligned} \tag{25}
$$

Representation (25) allows one to use the virtual spin formalism [7, 19] and to apply the algorithms developed for NMR QC.

Two-qubit gates, such as a C-NOT (controlled-NOT gate), are based on the following condition: the evolution of one qubit has to depend on the state of the other qubit. The C-NOT gate can be realized by using a selective pulse which excites the transitions between states 2 and 3 and exchanges the populations on these levels. Pulse excitation of a single resonance transition $m \to n$ can be described by a unitary operator $U_\phi(\Omega_{mn}) = \mathrm{e}^{\mathrm{i}\frac{\phi}{2}\sum_{mn}(\delta_{\Omega_{mn,\Omega}} e'_{mn} + \delta_{\Omega_{nm,\Omega}} e'_{nm})}$ [12] with nutation angle $\phi = \gamma h t_w$ and frequency Ω_{mn} for the transition $m \to n$, where t_w is the duration of the pulse of the additional field and operators e'_{mn} are defined in the basis of eigenfunctions $|\zeta_s\rangle$ of the effective Hamiltonian (11) with $s = 0, 1, 2, 3$. At $\phi = \pi$ the unitary transformation becomes $U_\pi(\Omega_{23}) = \mathrm{i}(e'_{32} + e'_{23} + e'_{11} + e'_{00})$ which is just the C-NOT operation up to the additional phase factor i which has global character and can be completely ignored [20]. The result of the action of the $U_\pi(\Omega_{23})$ pulse on the states follows from the representation (25): $|00\rangle \to |00\rangle, |01\rangle \to |01\rangle, |11\rangle \to |10\rangle, |10\rangle \to |11\rangle$. Here the role of the control qubit is played by the states in the first Hilbert space $\mathcal{R}$ and the target qubit is formed by the states in the second Hilbert space $\mathcal{P}$. The computation time for the two-qubit gates consists of duration of the pulse t_w, which is of the order of 10 μs [17].

Another two-qubit gate can be realized using the level-crossing method [21]. For example, for a SWAP logical gate[11] it is possible to change the difference of the phases of the applied RF fields $\alpha_1 - \alpha_2$ from $\alpha_1 - \alpha_2 < \frac{\pi}{2}$ to $\frac{\pi}{2} < \alpha_1 - \alpha_2 < \pi$ (see figure 1), which leads to $|11\rangle \to |11\rangle, |10\rangle \to |01\rangle, |01\rangle \to |10\rangle, |00\rangle \to |00\rangle$. A NOT2 logical gate [11] can be realized by adiabatic variation of the difference of the phases of the applied RF fields $\alpha_1 - \alpha_2$ from $\frac{\pi}{2} < \alpha_1 - \alpha_2 < \pi$ to $\pi < \alpha_1 - \alpha_2 < \frac{3\pi}{2}$ (see figure 1), for which we

have $|11\rangle \rightarrow |10\rangle, |10\rangle \rightarrow |11\rangle, |01\rangle \rightarrow |00\rangle, |00\rangle \rightarrow |01\rangle$. The first step of a quantum computation is the preparation of a well-defined initial state of the system. The spin system usually used, suitable for NMR and NQR measurements, should consist of $O(10^{20})$ spins. Pure states of such a large system can be realized only at very low temperatures of the order of $\sim$0.1 K, which is a substantial technical problem. To overcome this problem, using an effectively pure (a so-called a 'pseudo-pure') state [2, 3, 22], which is dynamically equivalent to a pure state, was suggested. In our case, the 'pseudo-pure' state $|00\rangle$ can be created by applying two selective pulses: $U_{\pi/2}(\Omega_{23})$ and $U_{\pi}(\Omega_{12})$ [9]. This pulse sequence leads to equal populations of the states 1, 2, and 3, distinct from the population in the state 0.

5. Conclusions

We have shown that by the use of two RF fields with different phases and directions, the degeneracy of the energy spectrum of a spin system with spin $I = 3/2$ is removed without applying a DC magnetic field. The four non-degenerate quantum states obtained can be used as a platform for a QC, which—as distinct from a QC based on NMR [1] and NQR [7]—can be realized without a high external magnetic field and with full dynamical control of the energy spitting. Various logic gates can be constructed by using different excitation techniques allowing different manipulations of the spin system states. The computation time for the two-qubit gates is of the order of 10 μs, which is faster than in NMR QC. Individual addressing of qubits is provided by various conditions of the excitation, instead of distinctions in resonant frequencies, which are usually used in NMR QC. The system considered allows one to apply the level-crossing technique, which opens possibilities for creation of new algorithms. The practical implementation of a pure NQR QC can be realized using solids containing, for example, nuclei of ^{35}Cl or ^{23}Na with spin $\frac{3}{2}$. To increase the number of qubits, the nuclear spin $\frac{7}{2}$ can be used. By exciting the two resonance transitions between quadrupole energy levels with a pair of radio-frequency fields differing in phase and direction, the double degeneracy of the spin energy spectrum in an EFG is removed. This leads to eight states of the nuclear spin which can be used as three qubits. The three-qubit system is useful for the realization of some interesting algorithms—for example, the quantum Fourier transform [23]

The method described above is appropriate for a simple demonstration of QC with small numbers of qubits. Unfortunately, there are several difficulties with increasing the number of qubits [6]. For example, to produce four-qubit gates (without applying a high magnetic field), some interaction between two nuclear spins with $I = \frac{3}{2}$ is required, which leads to increase in the computation time. Moreover, to implement quantum gates one needs to apply special methods to suppress the interaction, which results in complication of the implementation of algorithms. Note that at high temperature, the polarization and signal decrease exponentially with the size of the spin system [6]. The most obvious ways to overcome these difficulties are considered in [4, 6].

References

[1] Steane A 1998 *Rep. Prog. Phys.* **61** 117
[2] Gershenfeld N A and Chuang I L 1997 *Science* **275** 350
[3] Gory D G, Fahmy A F and Havel T F 1997 *Proc. Natl Acad. Sci. USA* **94** 1634
[4] Jones J A 2000 *LANL preprint* quant-ph/0009002
[5] Marjanska M, Chuang I L and Kubinec M G 2000 *J. Chem. Phys.* **112** 5095
[6] Jones J A 2000 *LANL preprint* quant-ph/0002085
[7] Kessel A R and Ermakov V L 1999 *JETP Lett.* **70** 61
[8] Abragam A 1961 *The Principles of Nuclear Magnetism* (Oxford: Clarendon)

[9] Khitrin A K and Fung B M 2000 *J. Chem. Phys.* **112** 6963
[10] Khitrin A K, Song H and Fung B M 2001 *Phys. Rev.* A **63** 020301(R)
[11] Sinha N, Mahesh T S, Ramanathan K V and Kumar A 2001 *J. Chem. Phys.* **114** 4415
[12] Ainbinder N E and Furman G B 1983 *Sov. Phys.–JETP* **58** 575
[13] Furman G B and Kadzhaya I M 1992 *Z. Naturf.* a **47** 235
[14] McArthur D A and Hahn E L 1969 *Phys. Rev.* **188** 609
[15] Mefed A E and Atsarkin V A 1978 *Sov. Phys.–JETP* **47** 378
[16] De Luca F, Nuccetelli C, De Simone B C and Maraviglia B 1989 *Solid State Commun.* **70** 797
[17] Furman G B, Kadzhaya I M, Kibrik G E, Polyakov A Yu and Shaposhnikov I G 1992 *Z. Naturf.* a **409**
[18] Goldman M 1970 *Spin Temperature and Nuclear Magnetic Resonance in Solids* (Oxford: Clarendon)
[19] Kessel A R and Ermakov V L 2000 *JEPT Lett.* **71** 307
[20] Jones J A, Hansen R H and Mosca M 1998 *J. Magn. Reson.* **135** 353
[21] Averin D V 1998 *Solid State Commun.* **105** 659
[22] Knill E, Chuang I and Laflamme R 1998 *Phys. Rev.* A **57** 3348
[23] Weinstein Y S, Pravia M A, Fortunato E M, Lloyd S and Gory D G 2001 *Phys. Rev. Lett.* **86** 1889