Pure NQR Quantum Computing

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It is shown that pure NQR can be utilized as a platform for quantum computing without applying a high external magnetic field. By exciting each resonance transition between quadrupole energy levels with two radio-frequency fields differing in phase and direction, the double degeneracy of the spin energy spectrum in an electric field gradient is removed. As an example, in the case of $I = 7/2$ (nuclei ^{133}Cs or ^{123}Sb) the energy spectrum has eight levels which can be used as three qubits.

Key words: NQR; Quantum Computing; Zeeman Effect.

1. Introduction

Use of the nuclear magnetic resonance (NMR) spectrometer as a device for quantum computations [1 - 4] becomes a fast developing new field. The basic idea of an NMR quantum computer(QC) is that i) two stationary states of spin 1/2 in a high external magnetic field represent one information quantum bit (qubit), and ii) conventional tools of pulse NMR can be used to construct a quantum logical gate. A simple logic gate can be designed by using a one spin system (a single qubit) with two eigenstates, $|1/2\rangle$ and $|-1/2\rangle$, or its linear superposition, and the nuclear spin states are manipulated by applying resonant radiofrequency (RF) fields in pulses of controlled duration [6, 7]. To perform more interesting computations, however, more complex gates, such as two or three qubits, are needed, which use two and three coupling spins 1/2. This requires some form of interactions (such as dipole-dipole, scalar or exchange) between nuclear spins. The strength of the coupling determines the relaxation time. Short relaxation times limit possible calculation times or gate time of the QC [6, 7]. In order to overcome this weak point, use of spins greater then 1/2 has been proposed [8]. It is known that the spin energy levels of nuclei with spin > 1/2 located in an electric field gradient (EFG) are doubly degenerated (we mean half-integer spin). In a constant external magnetic field the degeneracy of the energy levels is removed. This is the well known Zeeman effect. So spins greater than 1/2 with a complicated energy spectrum can be used as a basis for a multiqubit device for QC [8].

In order to form a non-degenerated energy spectrum, both techniques, NMR and NQR, use high external magnetic fields and some kind of internal interaction: the spin-spin interaction for NMR [2, 3, 6] and the interaction of the quadrupole moment with the EFG for NQR [8 - 10]. Both these interactions are determined by the internal properties of the used crystal. The splitting of energy levels in an external magnetic field is determined by the magnetic field and the internal interactions.

In the present paper we consider the case where the degeneration of the energy levels is removed only in the rotating frame (the so-called Zeeman effect in RF), while in the laboratory frame (LR) the degeneration remains. The Zeeman effect in RF can be considered as a platform for quantum computing using NMR methods without applying high magnetic fields. By exciting each resonance transition between quadrupole energy levels with two radio-frequency fields differing in phase and direction the double degeneracy of the spin energy spectrum in an EFG is removed. As an example in the case of $I = 7/2$, the energy spectrum has eight levels which can be used as three qubits.

2. Zeeman effect in rotating frame

Let us consider a spin system with spin $I = 7/2$ in an EFG with arbitrary symmetry and retain only those terms in the system's Hamiltonian $H(t)$ which are necessary for calculation of the energy spectrum of the spin system. In this case the system's Hamiltonian in the laboratory frame (LF) is

$$\mathcal{H}(t) = \mathcal{H}_Q + \mathcal{H}_1(t), \quad (1)$$

where

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

represents the interaction of the spin system with the EFG, eQq_{zz} is the quadrupole interaction constant and η the asymmetry parameter. $H_1(t)$ gives the action of the three pairs of radiofrequency fields $\vec{H}_{k_{mn}}(t) = \vec{H}_{k_{mn}} \cos\left(\omega_{mn}^{rf} t + \phi_{k_{mn}}\right)$ with $m, n = \pm 1/2, \pm 3/2, \pm 5/2, \pm 7/2$ $(m \neq n)$ on the spin system:

$$\mathcal{H}_1(t) = \sum_{k=1}^{2} \sum_{mn} \gamma \vec{I} \vec{H}_{k_{mn}} \cos\left(\omega_{mn}^{rf} t + \phi_{k_{mn}}\right), \quad (3)$$

where $k = 1, 2$ marks the two RF fields acting on each resonance transition $m \to n$ (and $-m \to -n$) of the spin system, γ is the gyromagnetic nuclear ratio, $\vec{I} = \sum_i \vec{I}^i$, $\left|\vec{H}_{k_{mn}}\right| = H_{k_{mn}}$, ω_{mn}^{rf}, and $\phi_{k_{mn}}$ are the amplitude, frequency and phase of the two RF fields differing in phase and direction applying on the double degenerated transition $m \to n$ (and $-m \to -n$), respectively. All spin operators will be considered in a basis in which the Hamiltonian $\mathcal{H}_Q$ is diagonal.

Using the projection operators $e_{mn} = \sum_i e_{mn}^i$, defined
by their matrix elements in the $\mathcal{H}_Q$-representation $\left\langle m \left| e_{m'n'}^i \right| n \right\rangle = \delta_{mm'} \delta_{nn'}$ and the commutation relation $\left[e_{mn}^i, e_{m'n'}^j\right] = \delta_{ij}\left(\delta_{nm'} e_{mn'}^i - \delta_{n'm} e_{m'n}^i\right)$ with $-m = \bar{m}, -n = \bar{n}$, the Hamiltonian (1) can be rewritten as

$$\mathcal{H}(t) = (2I+1)^{-1} \sum_{m,n} \omega_{mn}^0 e_{mm} \quad (4)$$

$$+ \sum_{k=1}^{2} \sum_{m,n} \omega_{k_{mn}} (\vec{I} \vec{l}_{k_{mn}})_{mn} \cos\left(\omega_{mn}^{rf} t + \phi_{k_{mn}}\right) e_{mn},$$

where $\omega_{mn}^0 = \lambda_m - \lambda_n, \lambda_m$ are the eigenvalues of $\mathcal{H}_Q : \mathcal{H}_Q \mid m\rangle = \lambda_m \mid m\rangle$, $\omega_{k_{mn}} = \gamma H_{k_{mn}}$, $\vec{l}_{k_{mn}}$ are unit vectors of the RF fields $\vec{H}_{k_{mn}}(t)$, given in the principle axes system of the EFG by polar θ_{k_m} and assimilate φ_{k_m} angles as $\vec{l}_{k_{mn}} = \left\{\sin\theta_{k_{mn}} \cos\varphi_{k_{mn}}; \sin\theta_{k_{mn}} \sin\varphi_{k_{mn}}; \cos\theta_{k_{mn}}\right\}$.

In order to correctly taking into account the time dependence terms of the Hamiltonian it proves to be profitable to carry out the unitary transformation [11, 12] of the operators used by means of the operator $U(t) = \exp(iAt)$ with

$$A = (2I+1)^{-1} \sum_{m,n} \omega_{mn} e_{mm}, \quad (5)$$

where $\omega_{mn} = \omega_{mn}^{rf}$ if ω_{mn}^{rf} is close to resonance frequencies ω_{mn}^0, and $\omega_{mn} = \omega_{mn}^0$ otherwise. After performing the transformation we obtain the system's Hamiltonian in rotating frame representation (RFR)

$$\mathcal{H}(t) = (2I+1)^{-1} \sum_{m,n} \Delta_{mn} e_{mm} + \sum_{k=1}^{2} \sum_{m,n} \omega_{k_{mn}} \quad (6)$$

$$\cdot (\vec{I} \vec{l}_{k_{mn}})_{mn} e^{i\omega_{mn} t} \cos\left(\omega_{mn}^{rf} t + \phi_{k_{mn}}\right) e_{mn},$$

where $\Delta_{mn} = \omega_{mn}^0 - \omega_{mn}$ are resonant offsets. Taking into account that under the condition $\omega_{k_{mn}} \ll \omega_{mn}^0$ (which is experimentally realizable) it is possible to neglect the influence of rapid, oscillations with frequency $\sim 2\omega_{mn}^0$, components, the effective time-independent Hamiltonian of the system in RFR takes the form

$$\mathcal{H}_{\text{eff}} = (2I+1)^{-1} \sum_{m,n} \Delta_{mn} e_{mm}$$

$$+ \sum_{k=1}^{2} \sum_{m,n} \omega_{k_{mn}} (\vec{I} \vec{l}_{k_{mn}})_{mn} \quad (7)$$

$$\cdot \left(\delta_{\omega_{mn}, \omega_{mn}^{rf}} e^{-i\phi_{k_{mn}}} + \delta_{\omega_{nm}, \omega_{mn}^{rf}} e^{i\phi_{k_{mn}}}\right) e_{mn}.$$

Diagonalization of the effective Hamiltonian gives eight energy levels of the spin system in the RF. So, in the case of spin 7/2 the spectrum consists of the eight energy levels which can be explored as the platform for quantum computing as three qubits without using a high external magnetic field.

As example, let us consider the simplest case of the excitation of the nuclear spin system with $I = 7/2$, when the nuclear spin system is localized in an axially symmetric EFG and only two resonance transitions $\pm 1/2 \to \pm 3/2$ and $\pm 5/2 \to \pm 7/2$ are excited exactly in resonance (all resonance offsets $\varDelta_{mn} = 0$) by two RF fields differing in direction and phase and equal in amplitude. Furthermore, we suppose that the first RF field in each pair lies along the X-axis $\left(\theta_{1_{\frac{1}{2}\frac{3}{2}}} = \theta_{1_{\frac{5}{2}\frac{7}{2}}} = \frac{\pi}{2};\ \varphi_{1_{\frac{1}{2}\frac{3}{2}}} = \varphi_{1_{\frac{5}{2}\frac{7}{2}}} = 0\right)$ and the second one along the Y-axis $\left(\theta_{2_{\frac{1}{2}\frac{3}{2}}} = \theta_{2_{\frac{5}{2}\frac{7}{2}}} = \frac{\pi}{2};\ \varphi_{2_{\frac{1}{2}\frac{3}{2}}} = \varphi_{2_{\frac{5}{2}\frac{7}{2}}} = \frac{\pi}{2}\right)$ in the principle axes system of the EFG. In this case the effective Hamiltonian takes the form

$$\mathcal{H}_{\text{eff}} = \frac{\omega_k}{2}\Big[\sqrt{7}\big(1 - ie^{-i\phi_1}\big)e_{\frac{7}{2}\frac{5}{2}} + \sqrt{7}\big(1 + ie^{i\phi_1}\big)e_{\frac{5}{2}\frac{7}{2}} + \sqrt{7}\big(1 - ie^{i\phi_1}\big)e_{-\frac{5}{2}-\frac{7}{2}} + \sqrt{7}\big(1 + ie^{-i\phi_1}\big)e_{-\frac{7}{2}-\frac{5}{2}} + \sqrt{15}\big(1 - ie^{-i\phi_2}\big)e_{\frac{3}{2}\frac{1}{2}} + \sqrt{15}\big(1 + ie^{i\phi_2}\big)e_{\frac{1}{2}\frac{3}{2}} + \sqrt{15}\big(1 - ie^{i\phi_2}\big)e_{-\frac{1}{2}-\frac{3}{2}} + \sqrt{15}\big(1 + ie^{-i\phi_2}\big)e_{-\frac{3}{2}-\frac{1}{2}}\Big], \tag{8}$$

where $\phi_1 = \phi_{2_{\frac{7}{2}\frac{5}{2}}}$ and $\phi_2 = \phi_{2_{\frac{3}{2}\frac{1}{2}}}$ are the differences in phases between the first and second RF field for $\pm 5/2 \to \pm 7/2$ and $\pm 1/2 \to \pm 3/2$, respectively.

Diagonalization of the effective Hamiltonian (8) gives the next expression for the eight energy levels of the spin system in the RF:

$$E_{0,1,2,3} = \pm\frac{\omega_k}{\sqrt{2}}\sqrt{7\,(1 \pm \sin\phi_1)}, \tag{9}$$

$$E_{4,5,6,7} = \pm\frac{\omega_k}{\sqrt{2}}\sqrt{15\,(1 \pm \sin\phi_2)}. \tag{10}$$

As follows from (9) and (10) the degeneracy of the energy spectrum is removed in the RF only under the action of two RF fields with different phase and direction. Under the action of an additional alternating magnetic field, the frequency of which is equal or close to the difference between the energy levels (9) and (10), it is possible to excite resonance transitions between states $|\zeta_b\rangle$, where $|\zeta_s\rangle$ are eigenfunctions of the effective Hamiltonian

$$H_{\text{eff}}\,|\zeta_a\rangle = E_s\,|\zeta_a\rangle \tag{11}$$

with $a = 0, 1, 2, 3,4,5,6,7$.

3. Quantum Computing

The basic element of the QC is a qubit. The qubit represents any two states of quantum systems. Thus, as one-qubit we can choose the quantum states corresponding to $|\zeta_a\rangle$ with a =0 and $a' = 1$. The eigenfunctions $|\zeta_a\rangle$ can be factorized in the form adopted in the quantum information theory: $|\zeta_0\rangle = |0\rangle$ and $|\zeta_1\rangle = |1\rangle$.

Different sets of logical gates are based on all possible one qubit gates. A one qubit gate can be designed on the basis of one qubit with the help of excitation of the resonant transitions between the two states $|0\rangle$ and $|1\rangle$. The resonance can be excited by applying the oscillating magnetic field, whose audiofrequency $\varOmega$ corresponds to $\varOmega_{01} = E_0 - E_1$. The value of the frequency $\varOmega$ is determined by the amplitudes and orientation of the RF fields, and their phase shift. Applying the resonance audiofrequency magnetic fields in form of the pulse $U_\phi\,(\varOmega_{01})$, the populations of the energy levels E_0 and E_1 can be changed. Here we use the following notations for the excitation pulse: $U_\phi\,(\varOmega)$ is a selective pulse with nutation angle ϕ and frequency $\varOmega$.

The two-qubit system is more complex since it should include the connection between the two qubits. As those we can choose the states $|\zeta_0\rangle$ and $|\zeta_3\rangle$ as the first qubit and the states $|\zeta_1\rangle$ and $|\zeta_2\rangle$ as the second qubit of the two qubit system. The resonance frequencies of the transitions between the chosen states are different, which causes the two qubit to be individually addressable. At the same a time the chosen qubits may be coupled by applying an additional oscillating magnetic field whose frequency $\varOmega$ equals the resonance frequency $\varOmega_{23}$ corresponding to the transition $2 \to 3$.

The states of the two qubit system can be factorized in the form: $|\zeta_0\rangle = |00\rangle, |\zeta_1\rangle = |01\rangle, |\zeta_2\rangle = |10\rangle, |\zeta_3\rangle = |11\rangle$.This factorization can be considered as a direct product of the two 2×2 dimensional Hilbert space $\mathcal{R} \otimes \mathcal{P}$[8] . Thus the basis vectors of the spin system under consideration in 2×2 dimensional Hilbert space are given by

$$|00\rangle = (0,0,0,1)^{\mathrm{T}} = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix},$$

$$|01\rangle = (0,0,1,0)^{\mathrm{T}} = \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix},$$

$$|10\rangle = (0,1,0,0)^{\mathrm{T}} = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix},$$

$$|11\rangle = (1,0,0,0)^{\mathrm{T}} = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}. \qquad (12)$$

Any operator $\mathcal{A}$ acting in the 4×4 dimensional space can be expressed as a linear combination of the direct product $\mathcal{R} \otimes \mathcal{P}$. Using this approach, the methods are developed in NMR QC can be directly applied to the system under consideration.

Two qubit gates, such as a controlled-NOT gate (CNOT), involve conditional evolution: the evolution of one qubit has to depend on the state of the other qubit. For constructing two qubit gates, the two resonance transitions between the states $|\zeta_0\rangle \ \rightarrow |\zeta_3\rangle$ and $|\zeta_1\rangle \ \rightarrow |\zeta_2\rangle$ with resonance frequencies Ω_{03} and Ω_{12} can be used.

The initial step in QC is to prepare the quantum system in the pure state. It was proposed to use the "pseudo-pure" state whose dynamic is equivalent to that of the pure state. It is possible to create the "pseudo-pure" state $|00\rangle$ by using two selective pulses: $U_{\pi/2}(\Omega_{23})$ and $U_{\pi}(\Omega_{12})$[9]. The first pulse changes the populations of states $|\zeta_2\rangle$ and $|\zeta_3\rangle$, and the second pulse changes the populations of states $|\zeta_2\rangle$ and $|\zeta_1\rangle$. As a result, the "pseudo-pure" state with equal populations of energy levels E_3, E_2, and E_1 is obtained.

Combination of an arbitrary one-qubit gate together with the C-NOT gates makes it possible to construct a universal logic gate[2]. In our case the C-NOT gate can be realized by using the selective pulse $U_{\pi}(\Omega_{23})$. As the result of the $U_{\pi}(\Omega_{23})$-pulse action on the states (12) we obtain

$$U_{\pi}(\Omega_{23})\,|00\rangle = |00\rangle\,, U_{\pi}(\Omega_{23})\,|11\rangle = |11\rangle\,,$$

$$U_{\pi}(\Omega_{23})\,|01\rangle = |10\rangle\,, U_{\pi}(\Omega_{23})\,|10\rangle = |01\rangle\,. \qquad (13)$$

The role of the target qubit plays the first qubit with the states $|\zeta_0\rangle = |00\rangle$ and $|\zeta_3\rangle = |11\rangle$ and the role of the controlled one plays the second qubit with the states $|\zeta_1\rangle = |01\rangle$ and $|\zeta_2\rangle = |10\rangle$.

Other interesting computations require further qubits. For example, the AND operation is achieved by use of the three qubit "controlled-controlled-NOT" gate, in which the third qubit experiences NOT if and only if both the others are in the appointed state [7]. In order to permit the whole operation to be unitary the use of three qubits is necessary. Recently, a quantum Fourier transform has been implemented on a three qubit NMR quantum computer to extract the periodicity of an input state[14].

As three qubit system we can choose the eight states $|\zeta_a\rangle$ (11) which can be factorized in the form adopted in the quantum information theory$|\ \zeta_0\rangle =|\ 000\rangle$, $|\ \zeta_1\rangle =|\ 001\rangle$, $|\ \zeta_2\rangle =|\ 010\rangle$, $|\ \zeta_3\rangle =|\ 011\rangle$, $|\ \zeta_4\rangle =|\ 100\rangle$, $|\ \zeta_5\rangle =|\ 101\rangle$, $|\ \zeta_6\rangle =|\ 110\rangle$, $|\ \zeta_7\rangle =|\ 111\rangle$.

The control of the splitting between energy levels of the spin system by variation of the amplitudes or/and phases of the RF fields results in an additional possible realization of the quantum logic gates which is based on the method of adiabatic crossing levels [15] without applying the audiofrequency magnetic fields. From (8) and (9) follows that manipulation of the spin states may be performed by adiabatically varying the phases. The populations of the energy levels are equilibrated when they are crossed.

The main advantage of the proposed method is that quantum computing can be performed i) by means of a separate particle, which does not require any interaction between the spatially separated particles, ii) without high external magnetic field, and iii) with full and independent control of all differences between the resonance transitions and of the coupling between various qubits. The proposed technique possesses long relaxation times and great flexibility. That the linewidth of the audio resonance is sufficiently narrow resulted from the partial averaging of the sources of line broadening by the RF field in both NMR [16, 17] and NQR [11] spectroscopies. This was the influence of rapidly oscillating external irradiations leads to a well resolved spectrum and to a long decay of the signal. Using a pair of coupled spins with $I = 7/2$, a system with four qubits can be created.

4. Conclusion

It was shown that pure NQR can be used as a platform for quantum computing without applying a high external magnetic field. In was shown that the energy levels are spat by two RF fields. Thus states of an $I = 7/2$ system can be used as a platform for three qubit quantum computing with the following advantages of the proposed technique: i) by using of the a single particle, which needs not in any interaction between the spatially separated particles, ii) without high external magnetic field, and iii) by independent control of the differences between energy levels and control of coupling between qubits. This technique possess relatively long relaxation times and large flexibility. Solids containing nuclei with spin $7/2$, for example ^{133}Cs or ^{123}Sb, can be utilized for this goal.

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