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# Time-optimal control of quantum dynamics of a quadrupole nucleus by NMR techniques

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We apply a gradient ascent pulse engineering (GRAPE) algorithm to the optimal control of a quadrupole nucleus used as a qudit. For spin  $I = 1$  and  $I = 3/2$ , we calculate the time dependence of rf field amplitudes and estimate the minimal time for implementing selective rotation gates and a quantum Fourier transformation (*QFT*) gate. We compare the numerical results with the pulse sequences obtained previously. We show that the straightforward optimization of control field parameters for *QFT* allows to decrease the duration of the gate.

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## 1. Introduction

The development of general rules for controlling quantum systems is one of the problems of modern physics. The most rapid increase in interest to this problem is associated with its applications for controlling chemical reactions and quantum information processing [1]. Particularly, the time-optimal control of spin systems plays an important role for implementing quantum computation by means of nuclear magnetic resonance (NMR) techniques. Because of a number of limitations, the NMR is not promising for the development of a large-scale quantum computer. Nevertheless, NMR remains a main test bed for developing various methods to control quantum systems. Moreover, NMR has been used to realize many of the first demonstrations of quantum algorithms [2, 3].

In addition to two-level systems (qubits) [1–3],  $d$ -level quantum systems (qudits) [4], which are more widespread in nature, are recently discussed as elements for a quantum computer. The quantum computation on qudits has a number of advantages in comparison with qubits, but there are few papers devoted to the qudit control.

Let us consider the problem of time-optimal control for implementing one-qudit gates on a multi-level quantum system. As a quantum system, we have chosen a quadrupole nucleus with spin  $I > 1/2$  in a static magnetic field and controlled by an external radiofrequency (rf) magnetic field. In a reference frame rotating with rf frequency  $\omega_{\text{rf}}$  which equal to the Larmor frequency  $\omega_0$ , the Hamiltonian [5] of this system is

$$H = q(I_z^2 - I(I + 1)) + u_x(t)I_x + u_y(t)I_y. \quad (1)$$

Here  $I_\alpha$  is the spin projection operator onto the  $\alpha$  axis,  $q$  is the constant of quadrupole interaction with the axially symmetric electric field gradient and  $u_\alpha(t)$  is the amplitude of control rf field along the  $\alpha$  axis. Because of a quadrupole interaction the quantum system has a  $d = 2I + 1$  nonequidistant energy levels. We take the quantum states that correspond

to these levels as a basis states for qudit, e.g.  $I_z = +1, 0, -1$  corresponds to the  $|0\rangle$ ,  $|1\rangle$  and  $|2\rangle$  basis states for  $I = 1$ . Note that unlike the work [6] where the frequency of the external rf field  $\omega_{\text{rf}}$  was resonant with the single transition of three-level system (selective excitation), we set  $\omega_{\text{rf}} = \omega_0$  (nonselective excitation).

In order to realize the quantum computation on our system it is necessary to find such control field  $u_\alpha(t)$  that the evolution operator

$$U = \hat{T} \exp\left(-i \int_0^T H dt\right), \quad (2)$$

has taken the fixed form during specified time  $T$ . Thus, it has executed some a logical operation for an arbitrary initial state of the qudit. In (2)  $\hat{T}$  is the time-ordering operator.

At first, we consider the implementation of simplest one-qudit logical gate, selective rotation gate. We denote this gate as  $R_\alpha^{m-n}(\theta)$ . The selective rotation of the two states corresponding to levels  $m$  and  $n$  through an angle  $\theta$  is represented by a  $d \times d$  matrix (we consider the selective rotation only between neighboring states)

$$R_\alpha^{m-n}(\theta) = \begin{bmatrix} E_m & 0 & 0 & 0 \\ 0 & \cos \frac{\theta}{2} & -ie^{-i\varphi} \sin \frac{\theta}{2} & 0 \\ 0 & -ie^{i\varphi} \sin \frac{\theta}{2} & \cos \frac{\theta}{2} & 0 \\ 0 & 0 & 0 & E_{d-n-1} \end{bmatrix}. \quad (3)$$

Here  $E_k$  is the unit matrix of dimension  $k$  and the phase  $\varphi$  defines the axis of rotation  $\alpha$ . In the simplest case of two levels system (qubit), the selective rotation gate can be represented as the rotation of vector on Bloch sphere [1, 5].

In this work, for the NMR implementation of selective rotation gate (3), the time dependence of control field amplitude  $u_\alpha(t)$  was found by numerical optimization at the different durations of the rf field. We use the results of these calculations to estimate the optimal time required for implementing the gate (3) in case of spins  $I = 1$  and  $I = 3/2$  and compare with the results obtained in our previous work [7]. In addition, optimization is performed straightforwardly for a quantum Fourier transformation gate in case of  $I = 3/2$ . Note that these calculations for a quadrupole nucleus are executed for the first time. In the literature previously only the nuclei with spin  $I = 1/2$  were considered.

## 2. Time-optimal control of quadrupole nucleus

The simplest way to realize the selective rotation gate is single selective pulse with frequency, which is equal to resonant frequency of transition between respective energy states [5]. For example, in the case of spin  $I = 3/2$  the selective rotation between  $|0\rangle$  and  $|1\rangle$  states about an  $x$ -axis is implemented by single pulse with frequency  $\omega^{0-1} = \omega_0 - 2q$  and amplitude  $\Omega$ . The pulse duration is

$$t_p = \frac{\theta}{2\Omega I_{x,mn}} = \frac{\theta}{\Omega\sqrt{3}}, \quad (4)$$

where  $I_{x,mn}$  is the matrix element of  $I_x$  operator coupling the  $m$  and  $n$  states. To obtain the selective rotation gate (3) with high precision, the field amplitude should be much less than  $q$ . It is so-called selectivity requirement. The low field amplitude leads to long pulse duration and therefore to increasing of gate error because relaxation processes.

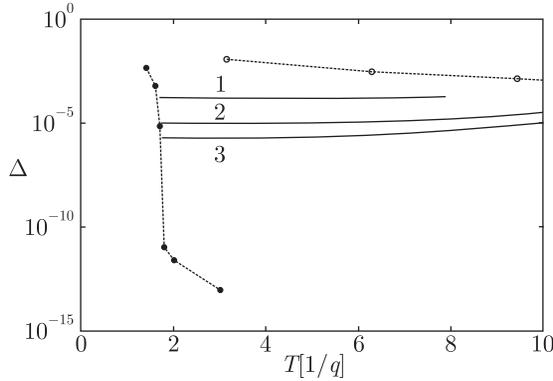


Fig. 1. The error versus the time of implementation for selective rotation  $R_y^{0-1}(\pi/2)$  in case of spin  $I = 1$  at different ways of realization: solid curves is the pulse sequence from the work [7] (number of cycles is given as the digits near the lines), solid circles is the values found by numerical optimization, open circles is the realization by the single selective rectangular pulse.

Another way to implement the selective rotation is using the sequence of nonselective pulse with high amplitude. For two levels system, qubits, this technique is known [8], but for multilevel systems, we have found the pulse sequences more recently [7]. The sequences consist of the nonselective rf pulses which separated by the intervals of free evolution. If we set the amplitude of pulses very high, we can estimate the minimum time  $T_\infty$ , which required for implementing selective rotation gate, as total duration of the intervals of free evolution. However, we have not shown whether the time  $T_\infty$  is optimal. Therefore, we address the following question: is it possible to obtain the same gate in a shorter time?

There are three main methods, which used to find the optimal time, as well as the control parameters  $u_\alpha(t)$ . First, the task of quantum system control can be reduced to the problem of search of the shortest path (geodesic) between two points on the surface of the sphere in a Hilbert space (the problem of quantum brachistochrone) [9]. The second method consist of in the search of the optimal values of time and control parameters by means of mathematical tool of group theory, in particular, the Cartan decomposition [10]. These two approaches are very general and allow obtaining the analytical solutions for control tasks in simple cases. However, the finding solutions are more difficult for complex systems. In this regard, the other direction of research gaining popularity recently is to find the control parameters with aids of different numerical optimization methods [11–14]. The computer simulation of a quantum system control allows to take into account the properties of real physical systems and obtain the parameter values of control fields for the specific experimental equipment.

### 3. Numerical optimization and results

We realized the search of optimal control field using the gradient ascent pulse engineering algorithm (GRAPE) [12]. The advantage of GRAPE over other algorithms is its toler-

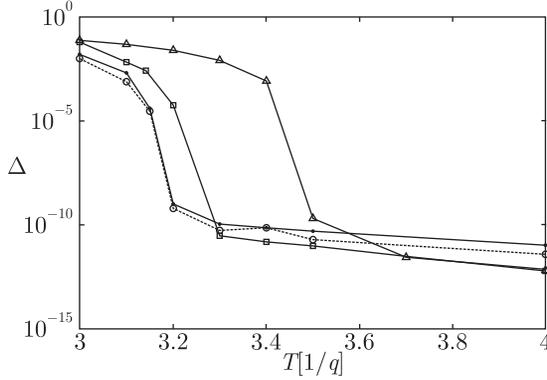


Fig. 2. The error versus the time of implementation for selective rotation  $R_y^{0-1}(\pi/2)$  in case of spin  $I = 3/2$  at the different angle of rotation:  $\theta = \pi/4$  (solid circles),  $\theta = \pi/2$  (open squares),  $\theta = \pi$  (open triangles). For comparison, the dependence for the operator  $R_y^{1-2}(\pi/2)$  is given (open circles).

ance to computational resources that allows to find numerical solutions in a short time for complex systems. GRAPE algorithm changes the shape of control field iteratively, maximizing the performance function

$$\Phi = |\langle U_0 | U \rangle|^2 / D, \quad (5)$$

and respectively minimizing the error of gate

$$\Delta = 1 - \Phi. \quad (6)$$

Here  $U$  is the operator of the evolution of the system (2) during the time  $T$ ,  $U_0$  is the operator of ideal transformation required and  $D$  is the dimension of Hilbert space. We evaluate  $\frac{\delta\Phi}{\delta u_\alpha(t_j)}$  and update all control amplitudes  $u_\alpha(t)$  according to

$$u_\alpha(t_j) \rightarrow u_\alpha(t_j) + \varepsilon \frac{\delta\Phi}{\delta u_\alpha(t_j)}, \quad (7)$$

where  $u_\alpha(t_j)$  is the constant amplitude in  $j$ -th step of time  $T$  discretized in  $N$  equal steps of duration  $\Delta t = T/N$ ,  $\varepsilon$  is a small step size. The calculation of the amplitudes  $u_\alpha(t)$  and the corresponding errors (6) for the different values of  $T$  allows to estimate the optimal time  $T_{\text{opt}}$  in our model.

We use the base form of GRAPE algorithm [12] without any modifications and limitations on the field amplitude or the pulse shape. We set the small constant value  $\sim 10^{-5}$  as initial amplitudes for  $u_\alpha(t)$  and  $N = 30$ .

We perform the optimization for the operator  $R_y^{0-1}(\theta)$ . In the case of  $I = 3/2$  the operator  $R_y^{1-2}(\theta)$  has also been considered because the realization of selective rotation gate on central transition of the four-level system has some peculiarities in [7]. The numerical calculations for the spin  $I = 1$  and  $I = 3/2$  shows the clear boundaries on

time scale, that is fully consistent with the theory. The comparison with analytic pulse sequences [7] shows a close values for times  $T_{\text{opt}}$  and  $T_{\infty} = 3\theta/2\sqrt{2}q$  for the three-level system,  $I = 1$  (Fig. 1). In addition, there are a close values of optimal time for rotation  $R_y^{1-2}(\theta)$  (central transition) in the case of  $I = 3/2$  ( $T_{\infty} = \pi/q$ ). However, for rotation  $R_y^{0-1}(\theta)$  (or  $R_y^{2-3}(\theta)$ , noncentral transitions) on four-level system the analytically obtained minimal time of the operation ( $T_{\infty} = (3\theta/2\sqrt{2} + \pi)/q$ ) is overpriced compared with the numerically found value (Fig. 2). Thus, the shorter sequences can be found for these rotations than previously obtained by us in [7].

The numerically obtained time dependence of rf field (Fig. 3, 4 and 5) are more preferable for the experimental realization than the analytical pulse sequences [7], because we can execute the same operation with less error at the small field amplitudes. The pulse shape is smoothly varying, reducing the transient effects at switching the pulses. Besides the flexible configuration of GRAPE algorithm, as already noted, it allows to take into account the peculiarities of specific experimental equipment at calculating the control field shape. Our results of numerical calculations will be important for experimentalists in the field of quantum system control.

#### 4. Optimal time for $QFT$ gate implementation

There is other important one-qudit gate in quantum computation on qudit [4]. This is the quantum Fourier transformation gate ( $QFT$ ). In general case of  $d$ -level system, the matrix of this gate has a form [1]

$$QFT_d = \frac{1}{\sqrt{d}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \delta & \delta^2 & \cdots & \delta^{d-1} \\ 1 & \delta^2 & \delta^4 & \cdots & \delta^{2(d-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \delta^{d-1} & \delta^{2(d-1)} & \cdots & \delta^{(d-1)^2} \end{bmatrix}; \quad (8)$$

$$\delta = \exp\left(\frac{2\pi i}{d}\right).$$

There are two ways for the realization of  $QFT$  gate on a qudit. First, we can decompose  $QFT$  to the sequence of selective rotation gates. These decompositions for  $d = 3 - 10$  in [15, 16] has been found. In case of  $I = 1$  and  $I = 3/2$  the sequences of gates is

$$QFT_3 = i \cdot R_y^{1-2}(-\pi/2) \cdot R_y^{0-1}(-2 \arctg \sqrt{2}) \cdot R_z^{0-1}(\pi) \cdot R_y^{1-2}(\pi/2); \quad (9)$$

$$QFT_4 = R_y^{2-3}(-\pi/2) \cdot R_y^{1-2}(-2 \arctg \sqrt{2}) \cdot R_y^{2-3}(2\pi/3) \cdot R_y^{0-1}(-2\pi/3) \cdot U_z \cdot R_y^{2-3}(-2\pi/3) \cdot R_y^{1-2}(2 \arctg \sqrt{2}) \cdot R_y^{2-3}(\pi/2); \quad (10)$$

respectively, where  $U_z = R_z^{0-1}(3\pi/4) \cdot R_z^{1-2}(-\pi/2) \cdot R_z^{2-3}(\pi/4)$  is the diagonal matrix of rotations about  $Z$ -axis. We can realize the selective rotations in decomposition by any techniques including the GRAPE optimization as it is performed above. Second, we can obtain the  $QFT$  gate straightforwardly by GRAPE algorithm e.g. we can find

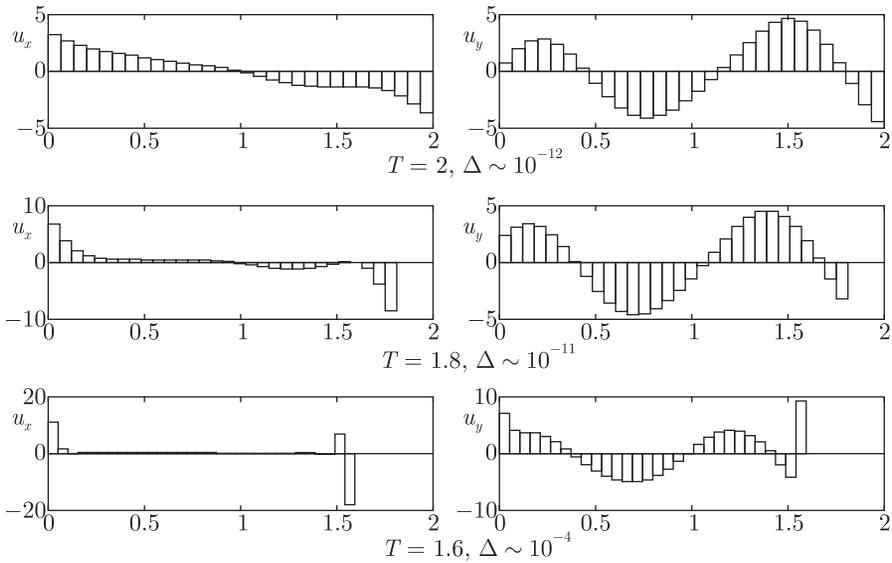


Fig. 3. The numerically calculated time dependence of the amplitudes of rf fields for implementation of the operator  $R_y^{0-1}(\pi/2)$  for the spin  $I = 1$  at different duration of fields  $T$ .  $\Delta$  is error of output operator.

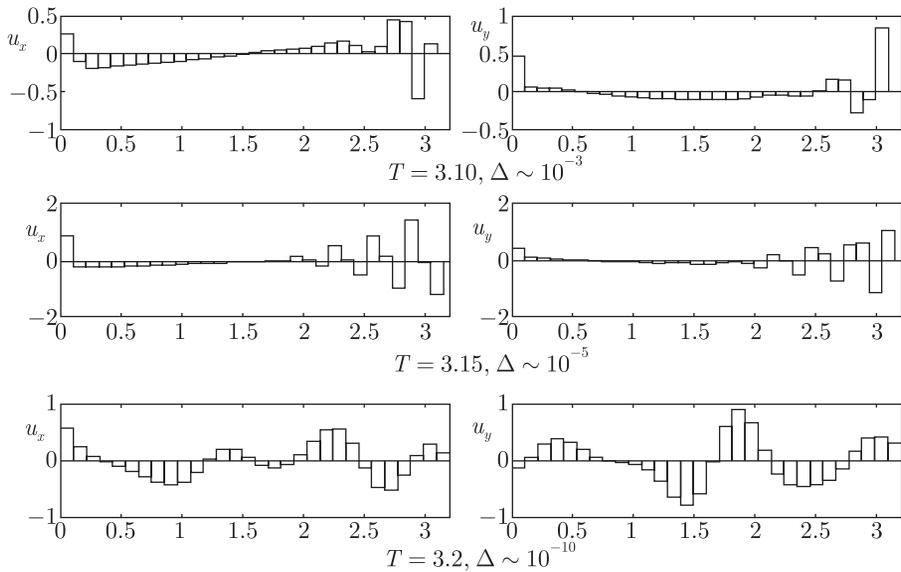


Fig. 4. The numerically calculated time dependence of the amplitudes of rf fields for implementation of the operator  $R_y^{0-1}(\pi/4)$  for the spin  $I = 3/2$  at different duration of fields  $T$ .  $\Delta$  is error of output operator.

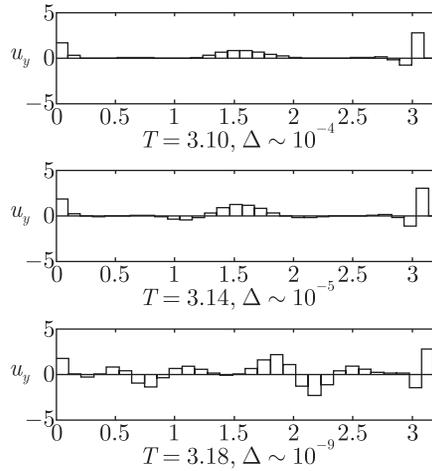


Fig. 5. The numerically calculated time dependence of the amplitude of rf fields for implementation of the operator  $R_y^{1-2}(\pi/2)$  for the spin  $I = 3/2$  at different duration of fields.  $\Delta$  is error of output operator. In this case, it is sufficient to use only the rf field along the Y-axis.

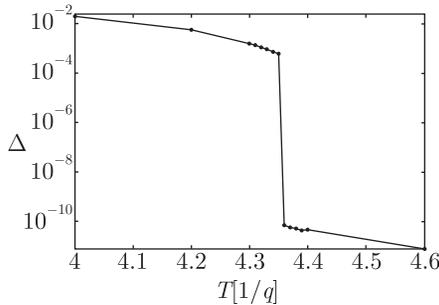


Fig. 6. The error versus the time of implementation for QFT gate in case of spin  $I = 3/2$ . This calculations is performed at  $N = 50$ .

the control field that minimize error (6) with  $U_0 = QFT_d$ . Fig. 6 shows the results of straightforward computation for  $QFT$  gate by the GRAPE algorithm. For  $QFT$  gate, the optimal time obtained by GRAPE is about  $4.4/q$  time units. The time at the realization by the sequence of selective rotation from [15, 16] is approximately  $22.8/q$  time units in case when all rotations are obtained by the GRAPE algorithm. Thus, at the direct optimization of  $QFT$  gate the saving of time is about 5 times. Note that the time  $22.8/q$  for the sequence of selective rotations is the rough approximation for the lower time bound, because we disregard duration of  $z$ -rotations  $U_z$  in sequence (8) and the durations of remaining rotations is estimated by Fig. 2.

## 5. Conclusion

In this work we have shown that the GRAPE algorithm can be successfully applied for calculation of control rf fields on a quadrupole nucleus used as a qudit. The amplitude of resulted fields is less than in the case of composite pulse [7] at the same values of gate error and pulse duration. In the case of selective rotation gate, the minimal time found by optimization depends on the quadrupole interaction constant  $q$  and the angle of rotation  $\theta$ . This time coincide with the minimal duration of composite pulse  $T_\infty$  [7] for a spin  $I = 1$ . In the case of spin  $I = 3/2$ , the numerical calculations leads to the less values of duration in comparison with the composite pulse. Therefore, the pulse sequences with less total duration can exist. In addition, we show in example of  $QFT$  gate that the straightforward optimization for complex gate (without decomposition on selective rotations) allows to reduce the time of operation.

The estimation of minimum time obtained in this work is useful to the further calculations of optimal control field parameters for implementing quantum computation by means of NMR techniques on quadrupole nuclei in real experimental conditions.

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## References

- [1] K. A. Valiev and A. A. Kokin, Quantum Computers:Hopes and Reality (Research Center “Regular and Chaotic Dynamics”, Izhevsk, 2001) [in Russian].
- [2] L. M. K. Vandersypen, M. Steffen, G. Breyta *et al.*, Phys. Rev. Lett. **85**, 5452 (2000).
- [3] L. M. K. Vandersypen, M. Steffen, G. Breyta, *et al.*, Nature. **414**, 883 (2001).
- [4] J. Daboul, X. Wang, B. C. Sanders, J. Phys. A. **36**, 7063 (2003).
- [5] Ch. Slichter, Principles of Magnetic Resonance (Springer, Heidelberg, 1978; Mir, Moscow, 1981).
- [6] P. Rebentrost, F. K. Wilhelm. Phys. Rev. B **79**, 060507 (2009).
- [7] V. E. Zobov and V. P. Shauro, Zh. Eksp. Teor. Fiz. **135**, 10 (2009).
- [8] M. D. Bowdrey, J. A. Jones, Phys. Rev. A. **74**, 052324 (2006).
- [9] A. M. Frydryszak, V. M. Tkachuk. Phys. Rev. A. **77**, 014103 (2008).
- [10] N. Khaneja, R. Brockett, S. J. Glaser. Phys. Rev. A. **63**, 032308 (2001).
- [11] E. M. Fortunato, M. A. Pravia, N. Boulant, G. Teklemariam, T. F. Havel, and D. G. Cory, J. Chem. Phys. **116**, 7599 (2002).
- [12] N. Khaneja, T. Reiss, C. Kehlet *et al.*, J. Magn. Reson. **172**, p. 296 (2005).
- [13] C. A. Ryan, C. Negrevergne, M. Laforest *et al.*, Phys. Rev. A. **78**, 012328 (2008).
- [14] S. G. Schirmer, P. J. Pemberton-Ross, X. Wang. ArXiv: 0801.0746v1 [quant-ph] 2008.
- [15] A. S. Ermilov and V. E. Zobov, Opt. Spektrosk. **103**, 994 (2007).
- [16] V. E. Zobov, V. P. Shauro, A. S. Ermilov, Pis'ma Zh. Éksp. Teor. Fiz. **87**, 385 (2008).