Russian Physics Journal, Vol. 50, No. 6, 2007

QUANTUM ELECTRONICS

A COMPARATIVE ANALYSIS OF TWO METHODS OF REALIZING ELEMENTARY LOGIC OPERATORS FOR A QUANTUM COMPUTER ON QUTRITS

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UDC 530.145, 539.143.43

In the present work, elementary logic operators (including selective rotation, Fourier transform, controlled phase shift, and controlled NOT operators) for a quantum computer on tristable systems (qutrits) are examined. Computer modeling of realization of these operators based on a system of two nuclear spins I = 1 is carried out by the methods of nuclear magnetic resonance. Two different methods of realizing the controlled NOT operator are presented: with the help of weak pulses of radio-frequency magnetic field selective in spin-spin interaction and with the help of strong pulses selective in quadrupole interaction. A dependence of realization errors on the interaction parameters, variable field amplitude, and pulse duration is calculated. Advantages and disadvantages of each method in the process of realization are indicated.

1. INTRODUCTION

Interest has been increased recently in the control over the dynamics of quantum systems with the purpose of realization of quantum algorithms [1]. Operation of the first quantum computers on the basis of bistable quantum systems – qubits – was investigated both theoretically and experimentally [1]. However, multistable quantum systems are much more often encountered in nature. The tristable systems having three basic states – qutrits [2] – are considered to be the most perspective. Mathematically, it has been proved that any quantum algorithm can be realized with the help of one or two elementary logic qutrit operators (gates). An example of the single-qutrit gate is the Fourier transform operator [2]

$$F|j\rangle = \frac{1}{\sqrt{3}}\sum_{k=0}^{2} e^{2i\pi k j/3}|k\rangle . \tag{1.1}$$

The controlled NOT operator (controlled-NOT or XOR gate) [2]:

$$CNOT_{12}|i\rangle_1|j\rangle_2 = |i\rangle_1|i+j\,(\mathrm{mod}\,3)\rangle_2 , \tag{1.2}$$

serves as an example of two-qutrit gate, where $|i\rangle_1$ is the state of the control qutrit, and $|j\rangle_2$ is the state of the operating qutrit. By the present time, the problem of realization of these gates is insufficiently studied theoretically. In [2], a method of their realization with the help of strong laser pulses nonselective in interaction between ions was suggested.

In the present work, computer modeling is performed of *CNOT* gate realization based on two quadrupole nuclei with spin $I = 1$ in a radio-frequency magnetic field. The matter is that the most significant results of quantum calculations are currently obtained by the methods of nuclear magnetic resonance (NMR) [1]. Moreover, the simplest single-qutrit gates

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1064-8887/07/5006-0566

on quadrupole deuterium nucleus with spin $I = 1$ have already been realized [3]. Alongside with the method suggested in [2], the method based on weak radio-frequency pulses selective in dipole-dipole interaction between nuclei is examined here. This method has already been used for milticubit systems [1, 4]. The purpose of numerical modeling is to study a dependence of the error on the magnitudes of internal interactions and radio-frequency-field parameters and, finally, to establish optimal conditions for experimental realization.

2. A TWO-QUTRIT SYSTEM

Let us consider two nuclei with spin $I = 1$, different gyromagnetic ratios γ_1 and γ_2, and different quadrupole interaction constants q_1 and q_2 in a constant magnetic field B_0 directed along the Z axis. The Hamiltonian of this system has the form [5]

$$H_0 = -\omega_1 I_1^z - \omega_2 I_2^z + q_1\left(I_1^{z\,2} - \frac{2}{3}\right) + q_2\left(I_2^{z\,2} - \frac{2}{3}\right) - d\left(2I_1^z I_2^z - \frac{1}{2}I_1^+ I_2^- - \frac{1}{2}I_1^- I_2^+\right), \tag{2.1}$$

where $\omega_i = B_0\gamma_i$ is the Larmor precession frequency in the magnetic field, d is the dipole-dipole interaction constant, I_i^z is the operator of spin projection onto the Z axis for the ith nucleus, $I_i^{\pm} = I_i^x \pm iI_i^y$ are raising and lowering operators. We will measure energy in frequency units and set $\hbar = 1$. Interaction with the magnetic radio-frequency field B_1 is written in the form

$$V = -\tfrac{1}{2}\Omega_1(e^{-i(\omega t+\varphi)}I_1^- + e^{i(\omega t+\varphi)}I_1^+) - \tfrac{1}{2}\Omega_2(e^{-i(\omega t+\varphi)}I_2^- + e^{i(\omega t+\varphi)}I_2^+)\,. \tag{2.2}$$

Here $\Omega_i = B_1\gamma_i$ is the radio-frequency field amplitude, ω is the field frequency, and φ is the phase.

It should be noted that in actual systems, as a rule, $d \ll q, \omega$. Nitrogen $^{14}\mathrm{N}$ and deuterium $^{2}\mathrm{H}$, for which typical experimental values of the ratio $2d/q$ are of the order of $\sim 10^{-4}$ and $\sim 10^{-2}$, respectively, can be considered as examples of nuclei with spin $I = 1$. These ratios of the dipole to quadrupole interaction are used below.

Each nucleus can be considered as a separate qutrit with different spin projections on the selected axis:

$$\left|I^z = 1\right\rangle = |0\rangle, \quad \left|I^z = 0\right\rangle = |1\rangle, \quad \left|I^z = -1\right\rangle = |2\rangle. \tag{2.3}$$

taken as a basis. According to rules of quantum calculations, we must have an opportunity to apply a radio-frequency field to the required transitions between the energy levels of each qutrit. Therefore, we will choose ω_i and q_i so that to avoid the coincidence of transition frequencies for different qutrits. In this case, the shift of energy levels and the admixture of other states to the computer basis states owing to the transverse dipole-dipole interaction component will be insignificant. We now number the states corresponding to nine non-equidistant levels ε_n of the two-qutrit system as follows:

$$|1\rangle = |0\rangle|0\rangle,\ |2\rangle = |0\rangle|1\rangle,\ |3\rangle = |0\rangle|2\rangle,\ |4\rangle = |1\rangle|0\rangle,\ \ldots,\ |8\rangle = |2\rangle|1\rangle,\ |9\rangle = |2\rangle|2\rangle\,. \tag{2.4}$$

For a quantum-mechanical description of the system dynamics, we must solve the Schrödinger equation:

$$i\frac{d\Psi}{dt} = (H_0 + V)\Psi\,. \tag{2.5}$$

To solve it, we take advantage of a rotating system of coordinates [5] using the following substitution:

$$\Psi = e^{i\omega t(I_1^z + I_2^z)}\Psi^* .$$

As a result, we obtain Schrödinger equation (2.5) with the effective Hamiltonian:

$$\begin{aligned} H &= H_0 + \omega(I_1^z + I_2^z) + e^{-i\omega t(I_1^z + I_2^z)}\, V\, e^{i\omega t(I_1^z + I_2^z)} \\ &= H_0 + \omega(I_1^z + I_2^z) - \tfrac{1}{2}\Omega_1(e^{-i\varphi} I_1^- + e^{i\varphi} I_1^+) - \tfrac{1}{2}\Omega_2(e^{-i\varphi} I_2^- + e^{i\varphi} I_2^+). \end{aligned} \tag{2.6}$$

In this case, the time dependence of the Hamiltonian disappears upon exposure to the radio-frequency field, and only the dependence on the amplitude and phase of this field remains. The phase specifies the direction of the radio-frequency field in the rotating system of coordinates. At $\varphi = 0$, the field is directed along the X axis, and at $\varphi = \pi/2$, it is directed along the Y axis. Because the Hamiltonian is independent of time, we obtain a solution to the Schrödinger equation in the rotating system of coordinates in the following form:

$$\Psi^*(t) = e^{-iHt}\Psi^*(0) .$$

Thus, the system evolution operator is determined by Hamiltonian (2.6):

$$U(t) = e^{-iHt} . \tag{2.7}$$

We can control the system evolution applying the radio-frequency field in a pulsed regime, that is, during a finite time period $t_\mathrm{p} >> 1/\omega$. In this case, if we choose the frequency of the variable field equal to the frequency of transitions between energy levels $\omega = \omega^{m-n} = \varepsilon_n - \varepsilon_m$, the states corresponding to these energy levels will change first of all. These transitions are called selective rotations. Let us designate rotation through the angle θ as follows:

$$\{\theta\}_\alpha^{m-n} , \tag{2.8}$$

where α denotes the rotation axis, and m and n are serial numbers of the energy levels between which the transition occurs.

Since for the *CNOT* operator we must change states of the second qutrit, the pulse duration will be determined by the amplitude Ω_2 :

$$t_\mathrm{p} = \theta/(\sqrt{2}\Omega_2) . \tag{2.9}$$

3. REALIZATION OF THE *CNOT* GATE WITH THE HELP OF WEAK PULSES

In basis (2.4), two-qutrit *CNOT* gate (1.2) is a 9×9 block matrix:

$$CNOT_{12} = \begin{bmatrix} E & 0 & 0 \\ 0 & A & 0 \\ 0 & 0 & A' \end{bmatrix}, \quad \text{where } A = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \tag{3.1}$$

A' is the transposed matrix, and E is the unit matrix.

The most obvious method of obtaining the *CNOT* operator is realization of transitions between the qutrit states related by nonzero matrix elements in matrix (3.1) upon exposure to the radio-frequency-field, that is, between the following states:

$$\begin{bmatrix} |1\rangle|0\rangle \to |1\rangle|1\rangle & (\varepsilon_4 \to \varepsilon_5) \\ |1\rangle|1\rangle \to |1\rangle|2\rangle & (\varepsilon_5 \to \varepsilon_6) \\ |1\rangle|2\rangle \to |1\rangle|0\rangle & (\varepsilon_6 \to \varepsilon_4) \end{bmatrix}, \quad \begin{bmatrix} |2\rangle|0\rangle \to |2\rangle|2\rangle & (\varepsilon_7 \to \varepsilon_9) \\ |2\rangle|1\rangle \to |2\rangle|0\rangle & (\varepsilon_8 \to \varepsilon_7) \\ |2\rangle|2\rangle \to |2\rangle|1\rangle & (\varepsilon_9 \to \varepsilon_8) \end{bmatrix}.$$

Transitions (indicated in the parentheses) are realized with the help of selective rotations (2.8) through the angle π at the corresponding resonant frequency.

The pulse train used to realize the gate is [3]

$$\{\pi\}_X^{7-8} \to \{\pi\}_X^{8-9} \to \{\pi\}_X^{5-6} \to \{\pi\}_X^{4-5}. \tag{3.2}$$

The arrows here indicate the sequence of pulses in time. This pulse train provides rotations not only at the allowed transitions, but also at the 7–9 and 4–6 forbidden transitions. The resonant frequencies of radio-frequency pulses in Eq. (3.2) are close to the following values:

$$\begin{aligned} &\omega^{7-8} = \omega_2 - q_2 - 2d, \quad \omega^{8-9} = \omega_2 + q_2 - 2d, \\ &\omega^{5-6} = \omega_2 + q_2, \qquad\quad \omega^{4-5} = \omega_2 - q_2. \end{aligned} \tag{3.3}$$

The transverse component of the dipole-dipole interaction introduces a small correction to resonant frequencies (3.3), which can be calculated in the context of perturbation theory and makes $\sim d^2/(\omega_1 - \omega_2)$. Because close frequencies in (3.3) differ by $2d$ ($d << q$), the condition of selective action on the states of the second qutrit is the smallness of the radio-frequency field amplitude in comparison with the dipole-dipole interaction constant ($\Omega_2 << d$).

The duration of each pulse is specified by Eq. (2.9) with $\theta = \pi$.

4. GATE REALIZATION WITH THE HELP OF STRONG PULSES

Let us consider another method of obtaining *CNOT* operator (3.1) [2]. This gate can be obtained with the help of two others: the single-qutrit Fourier transform operator F acting on the second spin and the two-qutrit operator of controlled phase shift P_{12}:

$$CNOT_{12} = (E \otimes F)^{-1} P_{12} (E \otimes F). \tag{4.1}$$

The single-qutrit Fourier transform operator in the matrix form is expressed as follows:

$$F = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 & 1 \\ 1 & \frac{-1 - i\sqrt{3}}{2} & \frac{-1 + i\sqrt{3}}{2} \\ 1 & \frac{-1 + i\sqrt{3}}{2} & \frac{-1 - i\sqrt{3}}{2} \end{bmatrix}. \tag{4.2}$$

It is transformed into a 9×9 block-diagonal matrix by taking the direct (tensor) product of matrices $E \otimes F$.

To realize operator (4.2), we used the pulsed train obtained by A. S. Ermilov [6]:

$$\left\{\frac{1}{2}\pi\right\}_Y^{2-3.5-6.8-9} \to \left\{2\cdot\arctan\left(\sqrt{2}\right)\right\}_Y^{1-2.4-5.7-8} \to \{\pi\}_Z^{1-2.4-5.7-8} \to \left\{\frac{7}{2}\pi\right\}_Y^{2-3.5-6.8-9} . \tag{4.3}$$

Here each pulse should act simultaneously on three transitions of the second qutrit whose resonant frequencies differ by $\pm 2d$. Therefore, the radio-frequency pulses should be taken with the amplitudes satisfying the condition $d \ll \Omega_2 \ll q_2$ and with frequencies

$$\omega^{1-2,4-5,7-8} = \omega_2 - q_2, \quad \omega^{2-3,5-6,8-9} = \omega_2 + q_2 . \tag{4.4}$$

The qutrits are coupled by the controlled phase shift operator [7]

$$P_{12} = \exp\left(i\frac{2\pi}{3}N_1 N_2\right). \tag{4.5}$$

The action of the operator involves the shift of the state phase through the angle depending on the qutrit states N_1 and N_2 which can take values 0, 1, or 2.

The diagonal operator P_{12} given by Eq. (4.5) can be expressed through operators I_1^z and I_2^z based on the relation

$$\frac{2\pi}{3}N_1 N_2 = \frac{2\pi}{3}\left(1 - I_1^z\right)\left(1 - I_2^z\right) = \frac{2\pi}{3}\left(I_1^z I_2^z - I_1^z - I_2^z + 1\right). \tag{4.6}$$

After substitution of Eq. (4.6), P_{12} is transformed into the product of three operators:

$$P_{12} = \exp\left(i\frac{2\pi}{3}I_1^z I_2^z\right)\exp\left(-i\frac{2\pi}{3}I_2^z\right)\exp\left(-i\frac{2\pi}{3}\left(I_1^z - 1\right)\right). \tag{4.7}$$

First of them is obtained by free evolution of the system with the spin-spin interaction Hamiltonian $H_d = -2dI_1^z I_2^z$ during time period

$$t_d = \pi/(3d) . \tag{4.8}$$

To eliminate the phase shift caused by the quadrupole interactions, the time period is chosen multiple to the period $2\pi/q_2$ [8]. The second operator is reduced to the action of two additional *Z*-pulses on the second spin:

$$\left\{\frac{4}{3}\pi\right\}_Z^{2-3,5-6,8-9} \to \left\{\frac{4}{3}\pi\right\}_Z^{1-2,4-5,7-8} . \tag{4.9}$$

The third operator is the phase multiplier that has no effect on the result; therefore, it can be rejected.

In practice (and in our calculations), the pulses in schemes (4.3) and (4.9) with rotation about the *Z* axis are realized with the help of the compound *Z*-pulse [1, 5, 8]:

$$\{\theta\}_Z^{m-n} \equiv \left\{-\frac{1}{2}\pi\right\}_X^{m-n} \to \{\theta\}_Y^{m-n} \to \left\{\frac{1}{2}\pi\right\}_X^{m-n} .$$

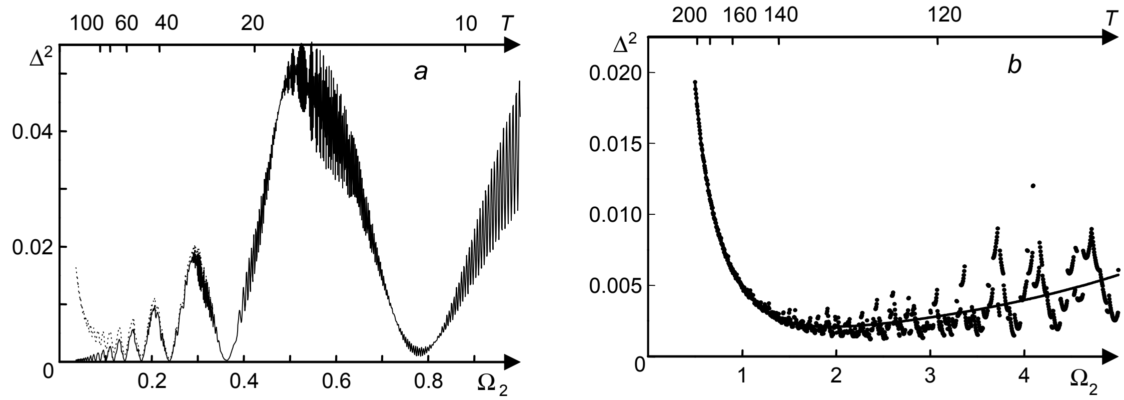

Fig. 1. Dependence of the resultant error of the *CNOT* gate realization on the radio-frequency-field amplitude and/or the total time of experiment (the upper scale) for the first method with $d = 1$ (*a*) and for the second method with $d = 0.01$ (*b*). The solid curve (*b*) shows the average curve obtained by approximation of the calculated dependence by the sum of three exponents.

5. CALCULATIONS OF THE SYSTEM EVOLUTION AND DISCUSSION OF RESULTS

To model the quantum gate realization by the method of nuclear magnetic resonance, we took advantage of the software package MATLAB version 7.1. The action of separate pulses on the system was calculated from Eq. (2.7) with substitution of the corresponding pulse duration and Hamiltonian. Multiplication of the evolution matrices of each pulse gives the resultant pulse train. After modeling of the pulse action on the system for both cases, the error of the result obtained can be found from the formula

$$\Delta^2 = \frac{1}{3}\sum_{i=1}^{3}\Delta_i^2, \quad \text{where} \quad \Delta_i^2 = \frac{1}{9}\sum_{m,n=1}^{3}\left(|A_{mn}| - A_{mn}^0\right)^2 . \tag{5.1}$$

Here A_{mn} are elements of the corresponding block of the calculated *CNOT* operator matrix given by Eq. (3.1) or (4.1), A_{mn}^0 are elements of the corresponding block of the theoretical operator matrix, and the sum over i yields the total error for the three blocks.

Relative values were taken for the parameters, and one hundredth of the quadrupole interaction constant q_2 was chosen as a measurement unit:

$$\omega_1 = 500, \quad \omega_2 = 300, \quad q_1 = 200, \quad q_2 = 100. \tag{5.2}$$

Figure 1 shows plots of dependences of the resultant error on the radio-frequency field amplitude for both cases and the corresponding total time of experiment which equals to the sum of durations (2.9) of all pulses plus the free evolution period given by Eq. (4.8) for the second method.

From the plots it can be seen that the resultant error, on average, increases with the radio-frequency field amplitude for both realizations. This is explained by the action of pulses with high field amplitudes not only on the necessary transitions but also on all others transitions in different degrees.

In the first realization variant described by Eq. (3.2), vividly expressed oscillations of the error are observed, which decreases to $\sim 10^{-3}$ in the first minimum (to the right of Fig. 1*a*). This result is caused by the special feature of application of the radio-frequency field to nonresonant transitions of the second (operating) spin, given that other states of the control spin differ by $2d$ from resonant state (3.3) due to spin-spin interaction. In the process of rotation of resonant transitions of

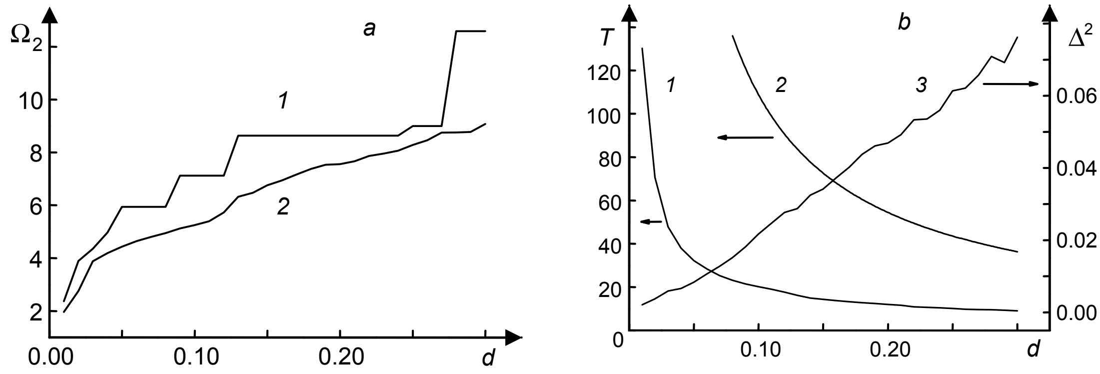

Fig. 2. Dependence of the radio-frequency field amplitude (*a*), total experiment time (*b*, curve *1*), and error (*b*, curve *3*) in the minimum on the magnitude of dipole-dipole interaction for the second method. Curve *1* (*a*) shows the calculated dependence, whereas curves *2* (*a*), *1* (*b*), and *3* (*b*) show the approximated results. For a comparison, curve *2* (*b*) shows time period (5.3).

the second spin with frequency Ω_2, these nonresonant states will rotate with frequency $\sqrt{\Omega_2^2/2+d^2}$, thereby introducing an error. However, if the amplitude is such that the resonant rotation of the spin through the angle π will be accompanied by the rotation of nonresonant states through angles multiple of 2π, the calculation error will be minimal [4], as can be seen from the plot. A small error remains from parasitic transitions in the first block of the *CNOT* operator matrix given by Eq. (3.1) with frequencies that differ by 4*d* from resonant frequencies given by Eq. (3.3). Using relation $\Omega_2 = \sqrt{2/3}d$ for the first minimum, we obtain the following dependence of the experiment time on *d*:

$$T = 2\sqrt{3}\pi/d\,. \tag{5.3}$$

When the radio-frequency field amplitude decreases, the error tends to zero (see the solid curve in Fig. 1*a*) for exact frequency tuning considering the correction for the dipole-dipole interaction. If weak pulses are tuned to frequencies (3.3) without corrections, they cease to perform necessary rotations because of violation of the resonance conditions; as a result, the error increases (see the dashed curve in Fig. 1*a*).

In the second realization variant described by Eq. (4.1), the error increases for large field amplitudes because of violation of pulse selectivity in the quadrupole interaction. On the contrary, the radio-frequency-field of small amplitude does not rotate completely two energy levels (3.3) (whose resonant frequencies differ by ±2*d* from the resonant frequency of the radio-frequency pulse) necessary to take the Fourier transform. This also introduces a resultant error. For the joint action of the given mechanisms, the minimum is observed in which their influence on the error becomes comparable. The dependence of the characteristics of this minimum on *d* is shown in Fig. 2. A sharp increase in the experiment time for small *d* is caused by the increased free evolution time of the system given by Eq. (4.8) which becomes dominant for such *d* values. Nevertheless, this time period is by a factor of several tens shorter than the time period of *CNOT* realization by the first method given by Eq. (5.3).

CONCLUSIONS

The main purpose of modeling was a comparison of the experiment time for different methods of *CNOT* gate realization, since for a successful realization of the experiment on an actual experimental setup, the entire pulse train should be transmitted during time period shorter than the relaxation (decoherence) time of the system. The method based on the application of weak pulses selective in spin-spin interaction is simpler; however, because small radio-frequency field amplitudes are used, the total experiment time given by Eq. (5.3) increases. In the second method based on strong pulses selective in quadrupole interactions, the pulse train is much more complicated, and the free evolution time of the system is added; however, the requirement of pulse selectivity in quadrupole interaction allows pulse amplitudes to be increased by a factor of several tens in comparison with the first realization. The experiment time is then decreased several folds. However, our analysis has demonstrated that the given method is inefficient for large d values because of the increased error value.

Thus, based on consideration of pulse train duration, we can conclude that realization with the help of strong pulses selective in quadrupole interaction is preferable for systems with weak dipole-dipole interaction ($d/q \sim 10^{-3} - 10^{-4}$). For systems with strong dipole-dipole interaction ($d/q \sim 10^{-1} - 10^{-2}$), on the contrary, the realization method with the help of weak pulses selective in dipole-dipole interaction is preferable.

The results obtained can be used to choose optimal conditions for experimental *CNOT* gate realization (1.2) and implementation of algorithms based on it as well as algorithms based on quantum Fourier transform (1.1) that are of great independent importance.

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