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ATOMS, MOLECULES, OPTICS

# Implementation of a Quantum Adiabatic Algorithm for Factorization on Two Qudits

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**Abstract**—Implementation of an adiabatic quantum algorithm for factorization on two qudits with the number of levels $d_1$ and $d_2$ is considered. A method is proposed for obtaining a time-dependent effective Hamiltonian by means of a sequence of rotation operators that are selective with respect to the transitions between neighboring levels of a qudit. A sequence of RF magnetic field pulses is obtained, and a factorization of the numbers 35, 21, and 15 is numerically simulated on two quadrupole nuclei with spins 3/2 ($d_1 = 4$) and 1 ($d_2 = 3$).

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## 1. INTRODUCTION

To implement the main ideas and advantages of quantum computing, it suffices to consider operations on two-level quantum systems—qubits [1]. In nature, one more frequently encounters multilevel quantum systems. The redundant levels can just be ignored; however, they cause interference if they are closely spaced on the energy scale, and one has to remove such interference [2, 3]. It is more preferable to use additional states corresponding to these levels directly during computation. For example, in [4], the authors proposed using a third level for implementing the Toffoli gate on qubits. The efficiency of such an approach was demonstrated on photonic [5] and superconducting [6] systems. The implementation of quantum algorithms directly on multilevel systems (on qudits, in the presence of $d$ levels) seems to be even more promising [7, 8]. The conception of virtual qubits allows one to perform quantum computations even on the level of a single qudit: a quadrupole nucleus [9–14], a molecular magnetics [15], or a Rydberg atom [16]. However, to implement all the advantages of quantum computations over classical ones, one should apply multiqudit systems and multilevel logic [7, 8, 17–22].

One of advantages of multiqudit systems over multiqubit ones is that they can provide the same size of the computational basis by a smaller number of physical elements. A decrease in the number of elements should facilitate their control; however, the methods of control of qudits have not yet been sufficiently developed. For quadrupole nuclei ($d = 2I + 1$, where $I$ is the spin of a nucleus), on which a large number of experiments have been carried out (see, for example, [10–14, 23, 24]), a survey of control methods is given in [25]. In [26], we considered the implementation of a quantum order-finding algorithm on two qudits with $d_1 = 8$ and $d_2 = 4$, instead of five qubits, which were used in [27] for the experimental implementation of such an algorithm for the permutation of four elements by an NMR method.

Quantum computing can be implemented not only by circuits of gates [1], but also by an adiabatic variation of a Hamiltonian [28–31] from the initial Hamiltonian $H(0) = H_c$, whose ground state $|\Psi(0)\rangle$ can be easily prepared, to the final Hamiltonian $H(T) = H_p$, whose ground state $|\Psi(T)\rangle$ encodes the solution of the problem posed. When implementing quantum adiabatic algorithms [28–31] or quantum annealing [30, 32], the system is in the ground state; this allows one to hope that the system has high noise immunity. In this way one can solve, for example, the ground state problem in the Ising model [32] or complex combinatorial problems [28–31]. Recently, an adiabatic quantum algorithm for factorization (decomposition of a number $N = pq$ into its prime factors) has been proposed [31] and implemented by an NMR method on three qubits given by spins $I = 1/2$ [33]. The algorithm is based on searching for the ground state of a system that minimizes the weight function $W = (N - pq)^2$. Note that, in the case of a classical computer, the problem of factoring a large number belongs to the class of exponentially complex problems; however, when solving this problem on a quantum computer by Shor's well-known algorithm, its complexity is changed to polynomial complexity. The question of whether exponential speedup can be achieved in adiabatic computation remains disputable [34].

Methods for implementing the above-mentioned adiabatic factorization algorithm on qudits have not been considered and are the subject of the present study. We consider the implementation of this algo-

rithm on two qudits $d_1$ and $d_2$. Since there is at least one pair of factors ($N = 2p$) for any even number, we will consider only odd numbers. Thus, the maximum size of a number to be factored is $N = (2d_1 - 1)(2d_2 - 1)$. It turned out that three spins used in the experiment in [33] were sufficient for the adiabatic factorization of the number 21. In our case, $d_1 = 4$ and $d_2 = 2$ suffice for factoring the number 21, whereas $d_1 = 4$ and $d_2 = 3$ allow one to factor the number 35. The implementation on qubits would require four spins $I = 1/2$, and one would need a four-spin effective interaction (in addition to the three-spin interaction, which was needed to factor number 21 in [33]) to control these qubits. For two spins, one does not need multiparticle interaction. However, the control of qudits requires operators that are selective with respect to the transitions between levels instead of operators selective with respect to the spins, which are used to control qubits. In Section 2, we propose a method for constructing a time-dependent effective Hamiltonian for multilevel systems by means of rotation operators that are selective with respect to the transitions between levels. As an example, in Section 3 we take two quadrupole nuclei with spins $I_1 = 3/2$ ($d_1 = 4$) and $I_2 = 1$ ($d_2 = 3$). $I = 3/2$ is, for example, the spin of the nucleus of $^{23}$Na on which quantum algorithms were implemented experimentally by the NMR method in [10–12]. $I = 1$ is the spin of the nucleus of deuterium $^2$H; an NMR control of the state of this nucleus was implemented in [23]. To control such systems, one applies RF magnetic field pulses that are selective with respect to the transitions between neighboring levels [10, 11, 13, 23]. Quantum algorithms on the system of two quadrupole nuclei coupled by spin–spin interaction have not yet been implemented. We will find appropriate sequences of RF pulses and carry out a computer simulation of a quantum adiabatic algorithm for factorization.

## 2. DERIVATION OF AN EFFECTIVE HAMILTONIAN BY ROTATION OPERATORS THAT ARE SELECTIVE WITH RESPECT TO TRANSITIONS

The Hamiltonian of two nuclei placed in an axially symmetric crystal filed and a strong static magnetic field can be represented as [35]

$$H_0 = -\omega_1 I_1^z - \omega_2 I_2^z + q_1\left[(I_1^z)^2 - \frac{1}{3}I_1(I_1+1)\right] + q_2\left[(I_2^z)^2 - \frac{1}{3}I_2(I_2+1)\right] - JI_1^zI_2^z, \quad (1)$$

where $\omega_j = B_0\gamma_j$ is the Larmor frequency of spin $j$, $q_1$ and $q_2$ are the corresponding quadrupole constants, $J$ is the spin–spin interaction constant, and $I_j^z$ is the operator of projection of the spin of appropriate nucleus onto the direction of the static magnetic field (the $z$ axis). The energy is measured in the units of frequency; i.e., we set $\hbar = 1$. As a computational basis, we take the eigenfunctions $|m_1, m_2\rangle$ of the operators $I_1^z$ and $I_2^z$ with projections $m_1$ and $m_2$, respectively. Let us enumerate the functions by natural numbers starting from the ground state level; for example, $n = I_j - m_j + 1$ for one spin.

The adiabatic algorithm is implemented by means of a time-dependent Hamiltonian that continuously varies, for example, by the linear law

$$H(t) = \left(1 - \frac{t}{T}\right)H_c + \left(\frac{t}{T}\right)H_p, \quad 0 \le t \le T. \quad (2)$$

If the Hamiltonian varies sufficiently slowly, then the quantum adiabatic theorem guarantees that the quantum computer will be in the ground state with high probability [28–34].

The weight function $W = (N - pq)^2$ corresponds to the Hamiltonian

$$H_p = Q[N - (d_1 - 2I_1^z)(d_2 - 2I_2^z)]^2, \quad (3)$$

where $d_j = 2I_j + 1$ and $Q$ is a scaling factor that is necessary to ensure commensurability with the Hamiltonian (1). If $N = pq$, then the ground state of the Hamiltonian $H_p$ with zero energy is attained for $p = d_1 - 2I_1^z$ and $q = d_2 - 2I_2^z$, i.e., for

$$I_1^z = \frac{d_1 - p}{2}, \quad I_2^z = \frac{d_2 - q}{2}.$$

To obtain the answer, one should measure the projections of the spins.

As the initial state, take the equal superposition state

$$|\Psi(0)\rangle = |S\rangle = \left(\frac{1}{d_1}\sum_{n=1}^{n=d_1}|n\rangle\right) \otimes \left(\frac{1}{d_2}\sum_{k=1}^{k=d_2}|k\rangle\right) = \frac{1}{\sqrt{d_1 d_2}}\sum_{m_1=-I_1}^{m_1=I_1}\sum_{m_2=-I_2}^{m_2=I_2}|m_1, m_2\rangle.$$

For a system of spins $I = 1/2$, such a state is obtained by Hadamard gates; as the initial Hamiltonian, one usually takes $H_c = w\sum_j I_j^x$. In the case of qudits ($I > 1/2$), the state $|S\rangle$ is not an eigenstate of such a Hamiltonian. The state $|S\rangle$ can be obtained from the ground state of Hamiltonian (1) with maximum projections $|I_1, I_2\rangle$ of the two spins on the $z$ axis by the quantum Fourier transform (QFT) operator:

$$|S\rangle = F|I_1, I_2\rangle,$$

where $F = F_1 \otimes F_2$, $F_j = \mathrm{QFT}_{d_j}$ ($j = 1, 2$),

$$\mathrm{QFT}_d = \frac{1}{\sqrt{d}}\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \sigma & \sigma^2 & \dots & \sigma^{d-1} \\ 1 & \sigma^2 & \sigma^4 & \dots & \sigma^{2(d-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \sigma^{d-1} & \sigma^{2(d-1)} & \dots & \sigma^{(d-1)^2} \end{pmatrix},$$

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

Since $|S\rangle$ should be the ground state of the Hamiltonian $H_c$, we take, as $H_c$, the operator

$$H_c = (F_1 \otimes F_2)H_0(F_1 \otimes F_2)^{-1}. \quad (4)$$

Following [33], we represent the operator of adiabatic evolution during time $T = \Delta tM$ with linear Hamiltonian (2) as a product of evolution operators on the sequence of $M$ small time intervals $\Delta t$:

$$U_T = \hat{P}\exp\left(-i\int_0^T H(t)dt\right) = \prod_{m=0}^{M} U_m, \quad (5)$$

where $\hat{P}$ is the time-ordering operator. On each such interval, we neglect the variation of Hamiltonian (2) and approximately represent the evolution operator as a product of three noncommuting operators:

$$U_m = \exp\left[-i\left(1-\frac{m}{M}\right)\frac{\Delta tH_c}{2}\right] \times \exp\left(-i\Delta tH_p\frac{m}{M}\right)\exp\left[-i\left(1-\frac{m}{M}\right)\frac{\Delta tH_c}{2}\right], \quad (6)$$

where $m$ is discrete time ($0 \le m \le M$).

We well derive operators needed in (6) with the use of rotation operators $\{\theta\}_{\alpha,j}^{k\leftrightarrow n}$ selective with respect to the transitions between the levels of the spin $j$, where $\theta$ is the angle of rotation about the axis $\alpha$ ($\alpha = x, y, z$) and $k$ and $n$ are the numbers of levels that vary from unity to $d_j$. In the matrix form,

$$\{\theta\}_{y,j}^{k\leftrightarrow n} = \begin{bmatrix} E_{k-1} & 0 & 0 & 0 & 0 \\ 0 & \cos\frac{\theta}{2} & 0 & -\sin\frac{\theta}{2} & 0 \\ 0 & 0 & E_{n-k-1} & 0 & 0 \\ 0 & \sin\frac{\theta}{2} & 0 & \cos\frac{\theta}{2} & 0 \\ 0 & 0 & 0 & 0 & E_{d_j-n} \end{bmatrix},$$

$$\{\theta\}_{z,j}^{k\leftrightarrow n} = \begin{bmatrix} E_{k-1} & 0 & 0 & 0 & 0 \\ 0 & \exp\left(-i\frac{\theta}{2}\right) & 0 & 0 & 0 \\ 0 & 0 & E_{n-k-1} & 0 & 0 \\ 0 & 0 & 0 & \exp\left(i\frac{\theta}{2}\right) & 0 \\ 0 & 0 & 0 & 0 & E_{d_j-n} \end{bmatrix}. \quad (7)$$

Here $E_k$ is a unit matrix of dimension $k$. The matrix of $x$ rotation differs from the matrix of $y$ rotation by coefficients equal to $-i$ in front of both sine functions.

To accomplish a selective rotation, we will switch on a magnetic RF field of amplitude $B_{\mathrm{rf}}$ and frequency $\omega$ for a finite period of time $t_p$ ($t_p \gg 1/\omega$). In a reference frame rotating with frequency $\omega$ [35], the time-variation of the evolution operator is given by

$$U_p(t) = e^{-iHt}$$

with the time-independent Hamiltonian $H$:

$$H = H_0 + \omega(I_1^z + I_2^z) - \Omega_1(I_1^x\cos\varphi + I_1^y\sin\varphi) - \Omega_2(I_2^x\cos\varphi + I_2^y\sin\varphi).$$

Here $\Omega_j = \gamma_j B_{\mathrm{rf}}$. The phase $\varphi$ of the RF field determines the direction of the field in the rotating frame. When $\varphi = 0$, the rotation is about $x$ axis ($\alpha = x$, $x$ rotation), whereas, $\varphi = \pi/2$, the rotation is about $y$ axis ($\alpha = y$, $y$ rotation). If we choose the frequency of the RF field to be equal to the transition frequency between the energy levels, $\omega = \varepsilon_n - \varepsilon_k$, then the states corresponding to these levels will change first, and we obtain a

selective rotation $\{\theta\}_{\alpha,j}^{k\leftrightarrow n}$ through an angle $\theta = t_p\Omega_j I_{jkn}$, where $I_{jkn}$ is the modulus of a matrix element of the operator $I_j^x$. The amplitude of the RF pulse should satisfy the selectivity condition: $J \ll \Omega_j \ll q_j$. For rotations about the $z$ axis, we will apply a composite RF pulse:

$$\{\theta\}_{z,j}^{k\leftrightarrow n} = \{-\pi/2\}_{y,j}^{k\leftrightarrow n}\{\theta\}_{x,j}^{k\leftrightarrow n}\{\pi/2\}_{y,j}^{k\leftrightarrow n}. \quad (8)$$

Let us construct an evolution operator in (6) with $H_p$:

$$\begin{aligned} H_p/Q = {} & C(N) + A(N)I_1^z + B(N)I_2^z + 4d_2^2(I_1^2)^2 \\ & + 4d_1^2(I_2^z)^2 + D(N)I_1^zI_2^z - 8d_1(I_2^z)^2I_1^z \\ & - 8d_2(I_1^z)^2I_2^z + 16(I_1^z)^2(I_2^z)^2, \end{aligned} \quad (9)$$

where

$$C(N) = (N-d_1d_2)^2, \quad A(N) = 4d_2(N-d_1d_2),$$
$$B(N) = 4d_1(N-d_1d_2), \quad D(N) = -8(N-2d_1d_2).$$

The evolution operator with Hamiltonian (9) can be expressed as a product of exponential operators corresponding to the terms in (9). The constant $C(N)$ appearing in the Hamiltonian, even though depends on $N$, gives only a common phase factor; therefore, it can be omitted.

The operators with one-particle interactions can be implemented by a sequence of operators of selective $z$ rotations in the following way:

$$\exp(-i\theta I^z) = W_+^1(I)W_-^1(I) \quad (10)$$

for integer spins $I$, where

$$W_+^1(K) = \prod_{m=1}^{K}\left\{2\theta\left[mI - \frac{m}{2}(m-1)\right]\right\}_z^{m\leftrightarrow m+1},$$

$$W_-^1(K) = \prod_{m=1}^{K}\left\{2\theta\left(mI - \frac{m}{2}(m-1)\right)\right\}_z^{d-m\leftrightarrow d-m+1},$$

and

$$\begin{aligned} \exp(-i\theta I^z) = {} & W_+^1\left(I-\frac{1}{2}\right)W_-^1\left(I-\frac{1}{2}\right) \\ & \times\left\{2\theta\left[I\left(I+\frac{1}{2}\right) - \left(I-\frac{1}{2}\right)\right]\right\}_z^{I+1/2\leftrightarrow I+3/2}. \end{aligned} \quad (11)$$

for half-integer spins $I$. For the squares of one-particle operators for integer spins $I$, we obtain

$$\exp\{-i\varphi[(I^z)^2 + E_dA]\} = W_+^2(I)W_-^2(I), \quad (12)$$

where

$$W_+^2(K) = \prod_{m=1}^{K}\left\{2\varphi\left[\sum_{n=0}^{n=m-1}(I-n)^2 + mA\right]\right\}_z^{m\leftrightarrow m+1},$$

$$W_-^2(K) = \prod_{m=1}^{K}\left\{-2\varphi\left[\sum_{n=0}^{n=m-1}(I-n)^2 + mA\right]\right\}_z^{d-m\leftrightarrow d-m+1}, \quad (13)$$

for half-integer spins $I$, we have

$$\begin{aligned} & \exp\{-i\varphi[(I^z)^2 + E_dA]\} \\ & = W_+^2\left(I-\frac{1}{2}\right)W_-^2\left(I-\frac{1}{2}\right), \end{aligned} \quad (14)$$

$$A = -\frac{I(I+1)}{3} = -\frac{d^2-1}{12}.$$

Operators with two-particle interactions,

$$U(\lambda, p_1, p_2) = \exp[-i\lambda(I_2^z)^{p_2}(I_1^z)^{p_1}], \quad p_1, p_2 = 1, 2, \quad (15)$$

are constructed by combining several intervals of free evolution under Hamiltonian (1), whose lengths are multiples of periods $2\pi/q_1$, $2\pi/q_2$, $2\pi/\omega_1$, and $2\pi/\omega_2$, and the sets of operators of 180-degree $y$ rotations. For such lengths, only the contribution of the spin–spin interaction remains in the evolution operator:

$$\begin{aligned} U(t) = \exp(itH_0) &= U(tJ, 1, 1) \\ &= \exp(-itJI_2^zI_1^z). \end{aligned} \quad (16)$$

Both operators (15) and (16) are represented by diagonal matrices with matrix elements in the form of exponential functions $\exp(-i\Phi_m)$, $m = 1, 2, \ldots, d_1d_2$, with different phases. We will permute these phase factors by selective operators of rotation through 180°. For example, in the operator $\{-\pi\}_y^{n\leftrightarrow k}U(t)\{\pi\}_y^{n\leftrightarrow k}$, the functions $\exp(-i\Phi_n)$ and $\exp(-i\Phi_k)$ change places.

Note that if we interchange the matrix elements of the operator $I_z$ that are symmetric with respect to the middle of the matrix, then the sign of the operator is reversed:

$$\Pi_d^{\mp}I_z\Pi_d = -I_z, \quad (17)$$

where

$$\Pi_d = \{\pi\}_y^{1\leftrightarrow d}\{\pi\}_y^{2\leftrightarrow d-1}\ldots\{\pi\}_y^{(d-1)/2\leftrightarrow(d+3)/2},$$

for integer spins and

$$\Pi_d = \{\pi\}_y^{1\leftrightarrow d}\{\pi\}_y^{2\leftrightarrow d-1}\ldots\{\pi\}_y^{d/2\leftrightarrow d/2+1},$$

for half-integer spins and $\Pi_d^{\mp}$ is the Hermitian conjugate operator. Note that operators for forbidden tran-

sitions can be obtained through a chain of transitions between adjacent levels:

$$\{\pi\}_y^{k\leftrightarrow d+1-k} = \{\pi\}_y^{k\leftrightarrow k+1}\{\pi\}_y^{k+1\leftrightarrow k+2}\ldots\{\pi\}_y^{d-k\leftrightarrow d-k+1} \times \{\pi\}_y^{d-k-1\leftrightarrow d-k}\ldots\{\pi\}_y^{k\leftrightarrow k+1}.$$

Using (17), we obtain

$$U(t)\Pi_{d_1}^{\mp}U(t)\Pi_{d_1} = U(t)\Pi_{d_2}^{\mp}U(t)\Pi_{d_2} = E_1\otimes E_2. \quad (18)$$

Here and below, $E_j$ is a unit matrix of dimension $d_j$.

If we act on the second operator $U(t)$ in (18) by the operators of selective rotation between the levels $n$ and $n+1$ of the first spin, we obtain a matrix that formally coincides with the matrix of selective rotation $\{\theta_2\}_{z,1}^{n\leftrightarrow n+1}\otimes E_2$, but the angle of rotation depends on the state of the second spin (with these reservations, we keep the sign of the direct product):

$$U(t)\{-\pi\}_{y,1}^{n\leftrightarrow n+1}\Pi_{d_1}^{\mp}U(t)\Pi_{d_1}\{\pi\}_{y,1}^{n\leftrightarrow n+1} = \{2tJI_2^z\}_{z,1}^{n\leftrightarrow n+1}\otimes E_2. \quad (19)$$

To obtain a rotation with opposite sign, $\{-\theta\}_{z,1}^{n\leftrightarrow n+1}$, we should act by the same selective rotations on the first operator $U(t)$ in (19). Thus, if we make up two products of the form (13) from the transformed pairs of evolution operators (19) with lengths varying from factor to factor,

$$2t_mJI_2^z = 2\varphi_2\left[\sum_{n=0}^{n=m-1}(I_1-n)^2+mA_1\right],$$

where

$$\varphi_2 = \tau JI_2^z, \quad \frac{t_m}{\tau} = \left[\sum_{n=0}^{n=m-1}(I_1-n)^2+mA_1\right], \quad (20)$$

then we obtain the operator

$$\exp\{-i\varphi_2[(I_1^z)^2+E_1A_1]\} = \exp\{-i\tau I_2^z[(I_1^z)^2+E_1A_1]\}. \quad (21)$$

Acting analogously on the states of the second spin, we can obtain the operator

$$\exp\{-i\tau I_1^z[(I_2^z)^2+E_2A_2]\}, \quad (22)$$

if we first act on one spin and then on the other, we obtain

$$\exp\{-i\tau[(I_1^z)^2+E_1A_1][(I_2^z)^2+E_2A_2]\}. \quad (23)$$

Following these rules, we determine the final product of operators, which yields the evolution operator $\exp(-i\Delta tH_pm/M)$. Multiplying, according to (6) and (4), this product by the operators

$$\exp(-itH_c) = F\exp(-itH_0)F^{-1} \quad (24)$$

and substituting the result into (5), we obtain the sought evolution operator, in the form of a product, which corresponds to such a time variation of effective Hamiltonian (2) that is needed to implement an algorithm.

## 3. IMPLEMENTATION OF ALGORITHM ON THE SYSTEM OF TWO QUADRUPOLE NUCLEI

Let us simulate the operation of the algorithm. As an example, we take two quadrupole nuclei with spins $I_1 = 3/2$ ($d_1 = 4$) and $I_2 = 1$ ($d_2 = 3$). In this specific case, we can simplify the general formulas of the previous section, using the property

$$(I_1^z)^2 = 2\left|I_1^z\right| - 3E_1/4, \quad (I_2^z)^2 = \left|I_2^z\right|, \quad (25)$$

where $\left|I_i^z\right|$ is the matrix of the moduli of spin projections on the diagonals. Hamiltonian (3) is reduced to the form

$$H_p/Q = C(N) + A(N)I_1^z + B(N)I_2^z + 72\left|I_1^z\right| + 52\left|I_2^z\right| + D(N)I_1^zI_2^z - 64I_1^z\left|I_2^z\right| - 96\left|I_1^z\right|I_2^z + 32\left|I_1^z\right|\left|I_2^z\right|, \quad (26)$$

where

$$A(N) = 12(N-12), \quad B(N) = 4(4N-39), \quad D(N) = -8(N-24).$$

For every $N$, the ground state of $H_p$ gives the sought factors:

(1) $N = 35$: $|\Psi(T)\rangle = |-3/2, -1\rangle$ with $I_1^z = -3/2$ ($p = 7$) and $I_2^z = -1$ ($q = 5$);

(2) $N = 21$: $|\Psi(T)\rangle = |-3/2, 0\rangle$ with $I_1^z = -3/2$ ($p = 7$) and $I_2^z = 0$ ($q = 3$);

(3) $N = 15$: the twofold degenerate state $|\Psi(T)\rangle = |-1/2, 0\rangle/\sqrt{2} + |1/2, -1\rangle/\sqrt{2}$ with $I_1^z = -1/2$ ($p = 5$) and $I_2^z = 0$ ($q = 3$) and $I_1^z = 1/2$ ($p = 3$) and $I_2^z = -1$ ($q = 5$).

Operators with one-particle interactions can be implemented by means of a sequence of operators of selective $z$ rotations as follows:

$$\exp(-i\theta I_1^z) = \{3\theta\}_{z,1}^{1\leftrightarrow 2}\{4\theta\}_{z,1}^{2\leftrightarrow 3}\{3\theta\}_{z,1}^{3\leftrightarrow 4},$$
$$\exp(-i\theta I_2^z) = \{2\theta\}_{z,2}^{1\leftrightarrow 2}\{2\theta\}_{z,2}^{2\leftrightarrow 3},$$
$$\exp(-i3\varphi\left|I_2^z\right|) = \{2\varphi\}_{z,2}^{1\leftrightarrow 2}\{-2\varphi\}_{z,2}^{2\leftrightarrow 3}\exp(-i2\varphi E_2), \quad (27)$$
$$\exp(-i\varphi\left|I_1^z\right|) = \{\varphi\}_{z,1}^{1\leftrightarrow 2}\{-\varphi\}_{z,1}^{3\leftrightarrow 4}\exp(-i\varphi E_1).$$

To obtain operators with two-particle interactions, we include the intervals of free evolution and the operators of 180-degree $y$ rotations:

$$\begin{aligned}
&\exp(-it4JI_2^z|I_1^z|) \\
&= \exp(-itJI_2^z 4E_1)\{-\pi\}_{y,1}^{3\leftrightarrow 4} \\
&\times \{-\pi\}_{y,1}^{2\leftrightarrow 3}\{-\pi\}_{y,1}^{3\leftrightarrow 4}\exp(-itJI_2^z I_1^z) \\
&\times \{\pi\}_{y,1}^{3\leftrightarrow 4}\{-\pi\}_{y,1}^{1\leftrightarrow 2}\exp(-itJI_2^z I_1^z)\{\pi\}_{y,1}^{1\leftrightarrow 2} \\
&\times \{\pi\}_{y,1}^{2\leftrightarrow 3}\{\pi\}_{y,1}^{3\leftrightarrow 4}, \qquad (28)\\
&\exp(-it3JI_1^z|I_2^z|) = \exp(-itJI_1^z 2E_2) \\
&\times \{-\pi\}_{y,2}^{2\leftrightarrow 3}\exp(-itJI_2^z I_1^z) \\
&\times \{-\pi\}_{y,2}^{1\leftrightarrow 2}\exp(-itJI_2^z I_1^z) \\
&\times \{\pi\}_{y,2}^{1\leftrightarrow 2}\{\pi\}_{y,2}^{2\leftrightarrow 3}.
\end{aligned}$$

The final product of operators determined by these rules, which yields the evolution operator $\exp(\Delta itH_p m/M)$, is given in the Appendix. According to (6), we should multiply this product by the operators $\exp(-itH_c)$. It turned out that, when deriving $H_c$ (4), we could apply a simpler transformation, omitting phase shifts and a part of operators of $y$ rotations in the decompositions for the operators of QFT [26, 36]:

$$\begin{aligned}
U_F &= \left\{\frac{\pi}{2}\right\}_{y,1}^{3\leftrightarrow 4}\left\{2\arccos\left(\frac{1}{\sqrt{3}}\right)\right\}_{y,1}^{2\leftrightarrow 3} \\
&\times \left\{\frac{2\pi}{3}\right\}_{y,1}^{1\leftrightarrow 2}\left\{\frac{\pi}{2}\right\}_{y,2}^{2\leftrightarrow 3}\left\{2\arccos\left(\frac{1}{\sqrt{3}}\right)\right\}_{y,2}^{1\leftrightarrow 2}, \qquad (29)\\
\exp(-itH_c) &= U_F\exp(-itH_0)U_F^{-1}.
\end{aligned}$$

Substituting the products obtained into (5), we find an evolution operator that implements the factorization algorithm. In the computations, we will use the following property of neighboring factors in (5):

$$\begin{aligned}
&U_F\exp\{-i[1-(m+1)/M]\Delta tH_0\}U_F^{-1}U_F \\
&\times \exp\{-i[1-m/M]\Delta tH_0\}U_F^{-1} \\
&= U_F\exp(i\Delta tH_0/M)U_F^{-1}.
\end{aligned}$$

## 4. COMPUTATION AND DISCUSSION

In the previous section, we obtained a sequence of selective RF pulses separated by intervals of free evolution. In order to prevent phase distortions, we should make the lengths of RF pulses to be multiples of $2\pi/q_1$. Therefore, for a given amplitude $\Omega_2$ of the RF field, we defined the length of pulses up to the integer part of the period $2\pi/q_1$. Using the operator sequences obtained, we simulated the implementation of a factorization algorithm for the numbers $N = 15$, 21, and 35 for different values of parameters. We compared the final states $|\Psi\rangle = U_T|\Psi(0)\rangle$ of the system with theoretically expected values $|\Psi\rangle_{\text{theor}} = |\Psi(T)\rangle$. The implementation error is determined by the formula

$$\Delta = 1 - |\langle\Psi|\Psi_{\text{theor}}\rangle|. \qquad (30)$$

The results of simulation are depicted as diagrams versus $\Omega_2$ ($\Omega_1 = \Omega_2\gamma_1/\gamma_2 = 0.6\Omega_2$) and $M$. The values of other parameters, $\Delta t$ and $Q$, which also strongly affect the results, were chosen so that to minimize the error.

The error as a function of the RF pulse amplitude, plotted by broken lines in Fig. 1, shows strong oscillations due to phase distortions. To eliminate these distortions, we make changes in the computation of the amplitudes of RF pulses. First, we take the amplitude $\Omega_2 = q_1/2k\sqrt{2}$ of the RF field to implement a $\pi/2$ pulse on spin 2 in time $t_p = 2\pi k/q_1$. For this amplitude, we determine the lengths of other pulses to within the integer part of the period $2\pi/q_1$. After that, we slightly change, if necessary, the amplitude of the RF field of each pulse to obtain the precise value of the required angle of rotation. The computed dependence is shown by symbols in Fig. 1. The remaining error is associated with two main sources. First, in addition to the selective rotation on the chosen transition, an RF pulse acts on other nonresonant transitions. This error grows as the RF pulse amplitude increases. Second, the spin–spin interaction changes the state of the system during the RF pulse action. This error grows as the RF pulse amplitude decreases. As a result of the joint effect of these two sources, we obtain functions with minima at which the error increases with $J$ (monotonically for $N = 35$ and $N = 15$ and nonmonotonically for $N = 21$).

The implementation error as a function of the duration $T = \Delta tM$ of adiabatic evolution is shown in Fig. 2. As $M$ and, hence, $T$ increases, the error decreases, which indicates that the sequence of selective RF pulses is correct and that the adiabaticity condition is satisfied. In the case of $N = 21$, one needs larger value of $T$ to achieve the same accuracy as for other $N$. This is associated with the fact that the gap $\Delta_N$ between the ground and the first excited states of Hamiltonian (3) depends on $N$:

$$\Delta_{21} = 16Q, \quad \Delta_{15} = 36Q, \quad \Delta_{35} = 100Q,$$

and for $N = 21$ this gap is minimal.

The error can be reduced by decreasing the total number of RF pulses. To this end, one should perform selective rotations about $z$ axis using another known method—by shifting the phases of subsequent selective RF pulses acting on this transition—rather than using a composite RF pulse (8). Next, to reduce the error, one can apply Gaussian selective RF pulses [10, 11, 13, 23] instead of simple rectangular RF pulses. The angle of rotation is determined by the area of such a Gaussian pulse. The error due to the deviation of this quantity from the required one has been considered above by an example of rectangular pulses. The deviation of the time dependence of the pulse amplitude

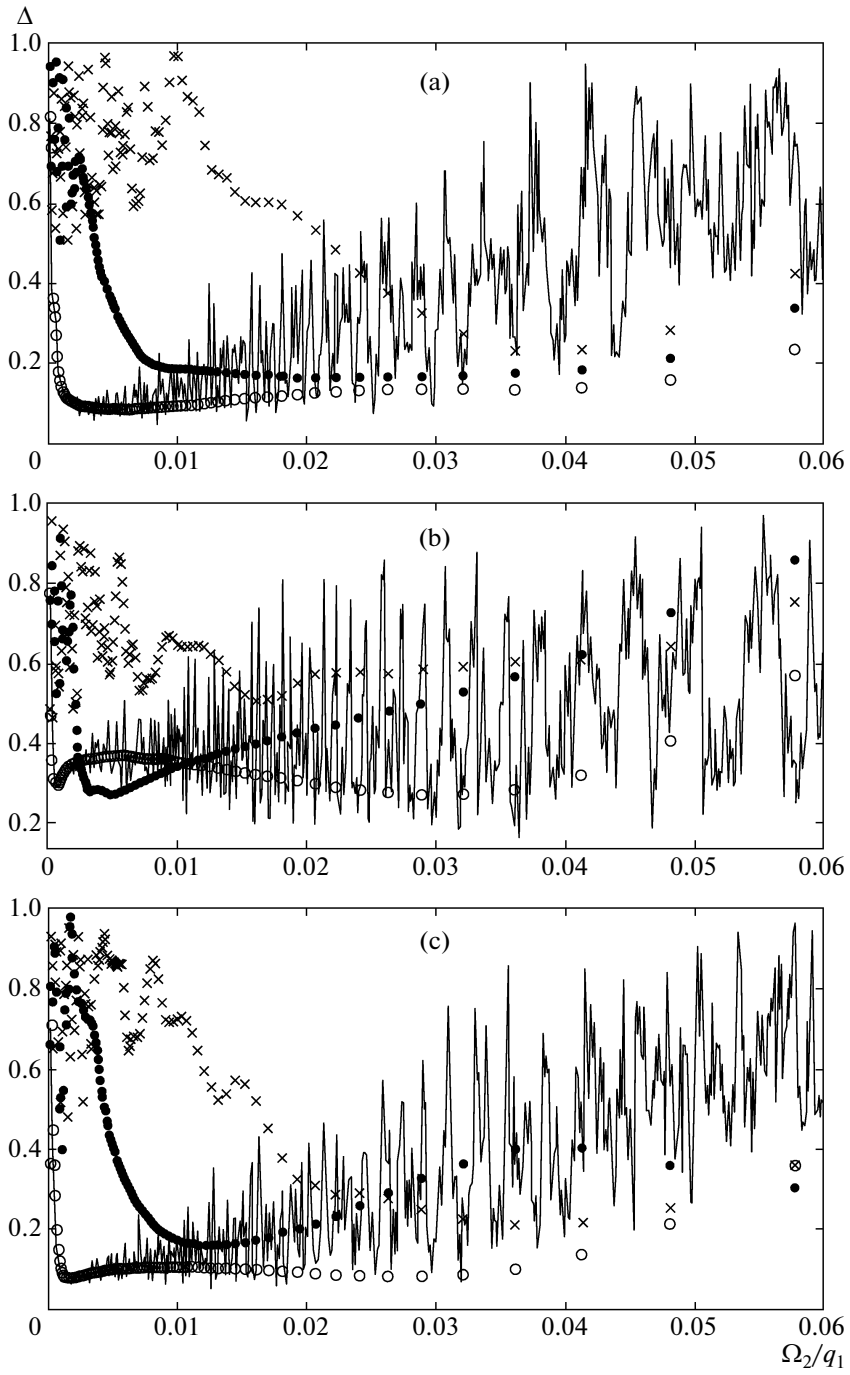


**Fig. 1.** Implementation error $\Delta = 1 - \left|\langle\Psi|\Psi_{\text{theor}}\rangle\right|$ of an adiabatic algorithm for factoring three numbers; (a) $N = 35$ with $Q = q_1/8.08$, (b) $N = 21$ with $Q = q_1/3.6$, and (c) $N = 15$ with $Q = q_1/2.8$, as a function of the amplitude $\Omega_2/q_1$ of the RF field for three values of spin–spin interaction: $J/q_1 = 10^{-6}$ (open circles and broken line), $J/q_1 = 10^{-5}$ (closed circles), and $J/q_1 = 5 \times 10^{-5}$ (crosses). The values of the other parameters are as follows: $M = 20$, $\omega_1 = 30q_1$, $\omega_2 = 50q_1$, $q_2 = 2q_1$, and $\Delta t q_1 = \pi/100$.

from a simple functional form (a constant or a Gaussian function) does not necessarily increase the error. Conversely, one can substantially reduce the error by passing to RF pulses whose shape is determined by optimization methods [37]. For example, in [12], the authors found such a pulse shape for the QFT of a four-level quadrupole nucleus of Na, while, in [38], a complex optimized RF pulse was applied to implement an evolution operator on a small time interval for a system of three nuclear spins 1/2. This evolution

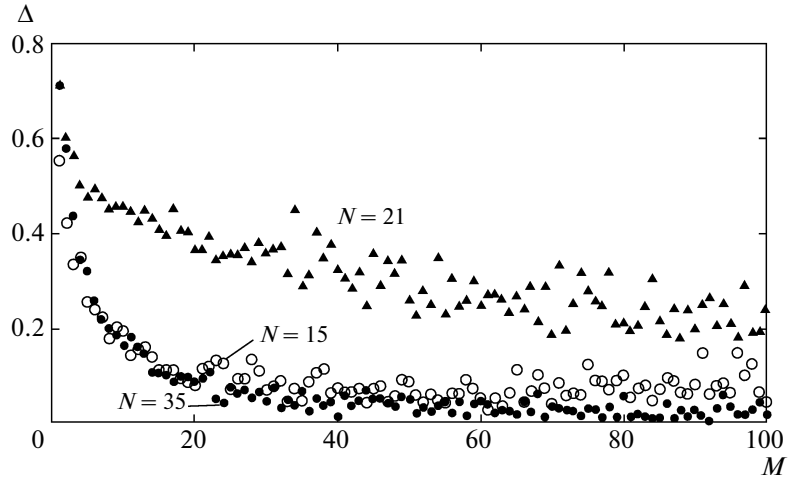


**Fig. 2.** Implementation error $\Delta = 1 - \left|\langle\Psi|\Psi_{\text{theor}}\rangle\right|$ of an adiabatic algorithm for factoring three numbers as a function of the evolution time $M = T/\Delta t$ for $\omega_1 = 30q_1$, $\omega_2 = 50q_1$, $q_2 = 2q_1$, $J/q_1 = 10^{-6}$, $\Delta t q_1 = \pi/100$, and the following values of parameters dependent on $N$: $\Omega/q_1 = 0.005$ and $Q = q_1/8.08$ for $N = 35$, $\Omega_2/q_1 = 0.005$ and $Q = q_1/3.6$ for $N = 21$, and $\Omega/q_1 = 0.0016$ and $Q = q_1/2.8$ for $N = 15$.

operator plays the same role as our operator $U_m$ (6). A generalization of the optimization procedure to a system of quadrupole nuclei was considered in [25].

Thus, we have obtained a sequence of RF pulses that has allowed us to simulate an implementation of a quantum factorization algorithm by an NMR method. The length of the pulse sequence in real time is several times greater than the initial time $T$, because the evolution operator (6) on the time interval $\Delta t = T/M$ is obtained from operators of free evolution (Table 1) with large duration. It is important that we have demonstrated the controllability of the system, and the implementation time can be significantly reduced by the methods described in the previous paragraph.

Finally, note that the demonstration of the operation of quantum algorithms by NMR methods gives rise to a signal from a large ensemble of quantum systems; therefore, the quantum yield probabilities are observed as the intensity of lines in the NMR spectrum in case of spectral detection, or as the elements of the density matrix in case of tomographic detection:

$$\rho_f = \left\{\frac{1-\beta}{d_1 d_2} E_1 \otimes E_2 + \beta|\Psi\rangle\langle\Psi|\right\},$$

where β is the amplitude of a pseudopure state, proportional to inverse temperature. The obtaining of a pseudopure state of the system of two quadrupole nuclei was discussed in [26].

## 5. CONCLUSIONS

We have shown that an adiabatic algorithm for factorization can be implemented on two qudits instead of a large number of qubits. In this case, one does not need three- and four-spin interactions. We have demonstrated that a time-dependent effective Hamiltonian can be obtained by means of a sequence of operators that are selective with respect to transitions. For a system of quadrupole nuclei chosen as qudits, the initial superposition state and the time-dependent effective Hamiltonian can be obtained by a sequence of RF pulses that are selective with respect to transitions. However, since the spin of the most common nuclei is limited by the number 9/2, to factor large numbers, one should extend the theoretical results obtained to other multilevel systems, for example, to molecular magnets, whose spin can be as large as 10 and even more [15, 39]. The method proposed here will also be useful for the control of multilevel states of superconducting systems [6, 8, 40] or atoms [16, 17, 19] by selective microwave or laser pulses, respectively.

## *APPENDIX*

Tables 1–6 show the values of parameters in the rotation operators $\{\theta\}_{\alpha,j}^{k\leftrightarrow n}$ (7) whose product, combined with the operators of free evolution (which are also presented Table 1 as $\exp(-is_r D_r H_0)$, $r = 1, 2, 3,$ and 4), forms the evolution operator $\exp(-i\Delta t H_p m/M)$ with Hamiltonian (26). The operators $V_r$ are added to eliminate one-spin contributions for arbitrary lengths of free evolution intervals, which are not necessarily multiples of the period $2\pi/q_1$. Evolution with negative time in the operators $V_4\exp(-is_4 D_4 H_0)$, as well as in the operators $V_1\exp(-is_1 D_1 H_0)$ for $N = 21$ and $N = 15$, is obtained in two steps. We implement positive-time evolution, taking positive values of the constants $-D_4$

**Table 1.** Operator $\exp(-i\Delta t H_p m/M)$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 1 | 3–4 | $y$ | π |
| 1 | 2–3 | $y$ | π |
| 1 | 1–2 | $y$ | π |
| 2 | 2–3 | $y$ | π |
| 2 | 1–2 | $y$ | π |
| | $\exp(-isD_4H_0/2)$ | | |
| | $V_4$ | | |
| 2 | 1–2 | $y$ | $-\pi$ |
| | $\exp(-isD_4H_0/2)$ | | |
| | $V_4$ | | |
| 1 | 3–4 | $y$ | π |
| 1 | 1–2 | $y$ | $-\pi$ |
| 2 | 1–2 | $y$ | π |
| | $\exp(-isD_4H_0/2)$ | | |
| | $V_4$ | | |
| 2 | 1–2 | $y$ | $-\pi$ |
| | $\exp(-isD_4H_0/2)$ | | |
| | $V_4$ | | |
| 2 | 2–3 | $y$ | $-\pi$ |
| 1 | 1–2 | $y$ | π |
| 1 | 3–4 | $y$ | $-\pi$ |
| | $\exp(-3isD_3H_0/2)$ | | |
| | $V_3$ | | |
| 1 | 3–4 | $y$ | π |
| 1 | 1–2 | $y$ | $-\pi$ |
| | $\exp(-3isD_3H_0/2)$ | | |
| | $V_3$ | | |
| 1 | 3–4 | $y$ | $-\pi$ |
| 1 | 2–3 | $y$ | $-\pi$ |
| 1 | 3–4 | $y$ | $-\pi$ |
| 2 | 2–3 | $y$ | π |
| 2 | 1–2 | $y$ | π |
| | $\exp(-2isD_2H_0)$ | | |
| | $V_2$ | | |
| 2 | 1–2 | $y$ | $-\pi$ |
| | $\exp(-2isD_2H_0)$ | | |
| | $V_2$ | | |
| 2 | 2–3 | $y$ | $-\pi$ |
| | $\exp(-6isD_1H_0)$ | | |
| | $V_1V_J$ | | |

**Table 2.** Product of operators $V_4$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 2 | 1–2 | $z$ | $sD_4(\omega_2 - q_2/3)$ |
| 2 | 2–3 | $z$ | $sD_4(\omega_2 + q_2/3)$ |
| 1 | 1–2 | $z$ | $sD_4(3\omega_1/2 - q_1)$ |
| 1 | 2–3 | $z$ | $2sD_4\omega_1$ |
| 1 | 3–4 | $z$ | $sD_4(3\omega_1/2 + q_1)$ |

**Table 3.** Product of operators $V_3$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 2 | 1–2 | $z$ | $sD_3(3\omega_2 - q_2)$ |
| 2 | 2–3 | $z$ | $sD_3(3\omega_2 + q_2)$ |
| 1 | 1–2 | $z$ | $sD_3(9\omega_1/2 - 3q_1)$ |
| 1 | 2–3 | $z$ | $6sD_3\omega_1$ |
| 1 | 3–4 | $z$ | $sD_3(9\omega_1/2 + 3q_1)$ |

**Table 4.** Product of operators $V_2$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 2 | 1–2 | $z$ | $sD_2(4\omega_2 - 4q_2/3)$ |
| 2 | 2–3 | $z$ | $sD_2(4\omega_2 + 4q_2/3)$ |
| 1 | 1–2 | $z$ | $sD_2(6\omega_1 - 4q_1)$ |
| 1 | 2–3 | $z$ | $8sD_2\omega_1$ |
| 1 | 3–4 | $z$ | $sD_2(6\omega_1 + 4q_1)$ |

**Table 5.** Product of operators $V_1$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 2 | 1–2 | $z$ | $4sD_1(3\omega_2 - q_2)$ |
| 2 | 2–3 | $z$ | $4sD_1(3\omega_2 + q_2)$ |
| 1 | 1–2 | $z$ | $6sD_1(3\omega_1 - 2q_1)$ |
| 1 | 2–3 | $z$ | $24sD_1\omega_1$ |
| 1 | 3–4 | $z$ | $6sD_1(3\omega_1 + 2q_1)$ |

**Table 6.** Product of operators $V_J$

| $j$ | $k$–$n$ | α | θ |
|---|---|---|---|
| 2 | 1–2 | $z$ | $4sJ(b - 3D_3 - D_4 + 52)$ |
| 2 | 2–3 | $z$ | $4sJ(b - 3D_3 + D_4 - 52)$ |
| 1 | 1–2 | $z$ | $2sJ(3a - 6D_2 - 2D_4 + 3a + 216)$ |
| 1 | 2–3 | $z$ | $8sJ(a - 2D_2)$ |
| 1 | 3–4 | $z$ | $2sJ(3a - 6D_2 + 2D_4 + 3a - 216)$ |

and $-D_1$ in these operators, and apply rule (17) to change the sign.

For short, we introduce the following notation:

$$s = \frac{m}{M}\frac{Q}{6J}\Delta t, \quad a = 3A(N), \quad b = 3B(N),$$

$$D_1 = -D(N), \quad D_2 = 64, \quad D_3 = 96, \quad D_4 = -32.$$

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