# REALIZATIONS OF STANDARD QUANTUM COMPUTATIONAL CIRCUITS BY ADIABATIC EVOLUTION 

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#### Abstract

We study the adiabatic equivalent of the standard quantum circuit of elementary logic operators. We propose a scheme for constructing time variations of the Hamiltonian. This scheme can be implemented sufficiently simply, for example, on nuclear spins controlled by radio-frequency pulses. As an illustration, we numerically simulate an adiabatic quantum algorithm for finding the permutation order for a system of five spins (qubits).


Keywords: quantum algorithm, adiabatic evolution, nuclear magnetic resonance

## 1. Introduction

In standard quantum computation, the algorithms are implemented as sequences of discrete unitary transformations (elementary quantum logical operators or gates that form a circuit) [1], [2]. This representation is convenient for comparing the work of quantum computers with that of classical computers. Quantum computation can also be performed differently, for example, using adiabatic evolution [3]. An adiabatic algorithm is implemented by a time-dependent Hamiltonian. This Hamiltonian varies continuously from the initial Hamiltonian $H(0)$, whose ground state $|0\rangle$ is easy to construct, to the final Hamiltonian $H(1)$, whose ground state $|\Psi\rangle$ encodes the solution of the problem under study. If the Hamiltonian varies sufficiently slowly, then the quantum adiabatic theorem guarantees that the quantum computer is in the ground state with a high probability. The noise tolerance of the ground state gives reason to hope [4] that the probability of errors in adiabatic quantum computation decreases.

It was recently proved [5], [6] that not only the search algorithm [3] but any standard quantum circuit can be realized using adiabatic evolution. In [5], the Hamiltonian varies with time according to a linear law. In [6], a more complicated unitary transformation of the Hamiltonian was proposed that guarantees that a given value of the gap between the ground and the nearest excited energy level remains the same during the evolution process. This parameter plays an important role because its value determines the admissible rate of variation of the Hamiltonian, i.e., the accuracy and the running time of the experiment.

In this paper, we study the version of the adiabatic algorithm proposed in [6] from the standpoint of its realization on nuclear spins controlled by radio-frequency ( RF ) pulses. This type of quantum system is chosen because simulation of many standard quantum algorithms, including the adiabatic algorithm for seeking the maximal cut [7] as the Hamiltonian varies linearly with time, have now been simulated by nuclear magnetic resonance (NMR) methods. The obtained results can be easily generalized to other quantum systems used in quantum computation [2]. We show how the version proposed in [6] should be modified to simplify the experiment. As an example, we consider an algorithm for finding the permutation order; the quantum circuit for this algorithm in standard form was realized on five spins (qubits) in [8]. We simulate an adiabatic algorithm for this circuit for different versions of the Hamiltonian variation with time on a computer and study how the result depends on the parameters.
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## 2. Quantum computational circuit for finding the permutation order

The standard circuit for a quantum algorithm can be implemented by a sequence of some $n$ unitary operators (one- or two-qubit gates)

$$
\begin{equation*}
|\psi\rangle=U|0\rangle=U_{n} U_{n-1} \cdots U_{1}|0\rangle \tag{1}
\end{equation*}
$$

As an example, we consider the quantum algorithm for finding the permutation order $r$ [8]. We present sequence (1) for this algorithm omitting the details, which can be found in [8]. For the permutation order $r=4$, we have

$$
\begin{equation*}
U=H_{3} B_{23}\left(\frac{\pi}{2}\right) B_{13}\left(\frac{\pi}{4}\right) H_{2} B_{12}\left(\frac{\pi}{2}\right) H_{1} \mathrm{CNOT}_{24} \mathrm{CNOT}_{35} H_{3} H_{2} H_{1} \tag{2}
\end{equation*}
$$

For the permutation order $r=2$, the product does not contain $\mathrm{CNOT}_{24}$. Formula (2) contains the following operators:
the Hadamard operator $H_{i}$ acting on spin (qubit) $i$,
the operator $B_{i j}(\theta)$ of controlled phase shift by the angle $\theta=\pi / 2^{i-j}$, and
the "not" operator $\mathrm{CNOT}_{i j}$ acting on the spin $j$ and controlled by the spin $i$, which can be expressed in terms of $B_{i j}$ according to the formula [9] $\mathrm{CNOT}_{i j}=H_{j} B_{i j}(\pi) H_{j}, i, j=1, \ldots, 5$.

These operators can be represented by matrices in the standard computational basis of eigenvalues of the projection operator of each spin on the direction of the constant magnetic field:

$$
H=\frac{1}{\sqrt{2}}\left(\begin{array}{rr}
1 & 1  \tag{3}\\
1 & -1
\end{array}\right), \quad B_{i j}(\theta)=\left(\begin{array}{cccc}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i \theta}
\end{array}\right)
$$

The matrices of the operators in (2) are $32 \times 32$ matrices and can be obtained from matrices (3) by straightforward (tensor) multiplication by the unit $2 \times 2$ matrices $E$ for the qubits that do not belong to this gate. For example, $H_{3}=E \otimes E \otimes H \otimes E \otimes E$.

We briefly explain the purpose of the operators in (2). First, the Hadamard operators use the ground state to prepare a superposition state for the first three spins. Then the operators CNOT expose them to transformations corresponding to a permutation chosen by the oracle. Finally, the quantum Fourier transformation over the spins 1,2 , and 3 permits finding the period of the obtained state, which coincides with the desired permutation order.

The experiment described in [10] was performed on five-spin molecules with the Hamiltonian

$$
\begin{equation*}
H=-\sum_{i} \omega_{i} I_{i}^{z}+\sum_{i<j} 2 \pi J_{i j} I_{i}^{z} I_{j}^{z} \tag{4}
\end{equation*}
$$

where $\omega_{i}$ is the frequency of the Larmor precession in a constant magnetic field $B_{0}$ with the chemical shift taken into account, the second term describes the indirect spin-spin interaction, and $I_{i}^{z}$ is the $z$ component of the vector operator of spin $i, i=1, \ldots, 5$. Hereafter, the energy is measured in frequency units. The gates are realized by a sequence of RF-field pulses applied to the system [2], [8]-[10]

$$
\begin{equation*}
H_{\mathrm{rf}}=-2 \sum_{i} \omega_{1 i}(t) I_{i}^{x} \cos \left(\omega_{\mathrm{rf} i} t+\varphi_{i}(t)\right) \tag{5}
\end{equation*}
$$

where $\omega_{\text {rfi }}$ is the frequency of the RF field. The amplitude $\omega_{1 i}(t)$ and the phase $\varphi_{i}(t)$ vary with time according to (2), i.e., the RF field with such characteristics is switched on at the instants when it is required to ensure the result of work of the corresponding gate. In the rotating (with the frequency $\omega_{\mathrm{rf} i}$ ) coordinate system (RCS) [11], the coefficient $\omega_{i}$ in the first term in Hamiltonian (4) is replaced with $\omega_{i}-\omega_{\mathrm{rf} i}$ and becomes zero at resonance.

The Hadamard gate $H_{i}$ is realized by successive rotations using the RF field first through the angle $\pi / 2$ about the $y$ axis and then through the angle $\pi$ about the $x$ axis of the RCS. For the first rotation, the RF field with the phase $\varphi_{i}=\pi / 2$ is switched on for the time interval $\tau_{i}$ satisfying the condition $\tau_{i} \omega_{1 i}=\pi / 2$. For the second rotation, the RF field with the phase $\varphi_{i}=0$ is switched on for the time interval $\tau_{i} \omega_{1 i}=\pi$. According to [9], [10], the operator $B_{i j}(\theta)$ can be obtained if we maintain (set) the time interval $\tau_{i}$ between the pulses such that the condition $\pi \tau_{i} J_{i j}=\theta / 2$ is satisfied and then additionally shift the phase by applying the operator $\exp \left(-i \theta\left(I_{i}^{z}+I_{j}^{z}\right) / 2\right)$.

On the free evolution interval, the system evolves under the action of the evolution operator $\exp (i t H)$ with Hamiltonian (4). To ensure the required sign of the phase, we add one operator of the RF pulse, which rotates the spin $i$ about the $x$ axis through the angle $\pi$ both before and after the free evolution operator.

The product of the corresponding matrices

$$
\left(\begin{array}{cccc}
e^{i \pi \tau J_{i j} / 2} & 0 & 0 & 0 \\
0 & e^{-i \pi \tau J_{i j} / 2} & 0 & 0 \\
0 & 0 & e^{-i \pi \tau J_{i j} / 2} & 0 \\
0 & 0 & 0 & e^{i \pi \tau J_{i j} / 2}
\end{array}\right)\left(\begin{array}{cccc}
e^{-i \theta / 2} & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i \theta / 2}
\end{array}\right)=e^{-i \theta / 4} B_{i j}(\theta)
$$

gives the desired operator $B_{i j}(\theta)$. An additional phase shift can be obtained, for example, by shifting the phases of the preceding pulses or by using three RF pulses. On the free evolution interval, the interactions of the other spins that are not required in this gate are eliminated by RF pulses rotating these spins through the angle $\pi$ [2], [8]-[10].

The authors of [8] used the RF field to control the dynamics of the system of five spins and thus realized the standard circuit of the quantum algorithm for finding the permutation order. We note that under the conditions of the NMR experiment, the operator $U$ acts on the system density matrix determining the state of the system at high temperatures [2], [9].

## 3. Adiabatic quantum algorithm

We now consider the adiabatic equivalent of standard quantum circuit (1) consisting of elementary logic operators. Following [6], we introduce the operators

$$
\begin{equation*}
K=-i \log U, \quad U(s)=e^{i s K} \tag{6}
\end{equation*}
$$

where $s=t / T$ is the dimensionless time, $T$ is the evolution time, $U(0)=1$, and $U(1)=U$. Then the adiabatic realization of quantum algorithm (1)

$$
\begin{equation*}
|\Psi(T)\rangle=U_{T}|0\rangle \tag{7}
\end{equation*}
$$

is determined by the evolution operator

$$
\begin{equation*}
U_{T}=\widehat{P} \exp \left(-i T \int_{0}^{1} H(s) d s\right) \tag{8}
\end{equation*}
$$

where $\widehat{P}$ is the time-ordering operator [12] and

$$
\begin{equation*}
H(s)=U(s) H(0) U^{\dagger}(s) \tag{9}
\end{equation*}
$$

We perform the identity transformations described in the appendix to rewrite Eq. (8) as

$$
\begin{equation*}
U_{T}=U \exp \left\{-i T\left(H(0)+\frac{K}{T}\right)\right\} \tag{10}
\end{equation*}
$$

The condition that this equation is adiabatic means that the difference between the energy levels of $H(0)$ must be larger than the corresponding elements of the matrix $K / T$ :

$$
\begin{equation*}
\left.\frac{1}{T}|\langle m| K| n\right\rangle|\ll| E_{n}-E_{m} \mid \tag{11}
\end{equation*}
$$

We note that there is an analogy with the transition to an RCS [11] used to solve the problem of spin motion in a slowly rotating strong magnetic field. The strong field holds the magnetic moment rotating together with the field in this case. The action of adiabatic RF pulses used in the NMR experiments is based on this property (see, e.g., the theoretical results and references in [13]). An effective field perpendicular to the plane of rotation of the real field arises in this case in the Hamiltonian in (10). In the same way, an effective Hamiltonian other than the Hamiltonians controlling the variations in the system under the action of each of the elementary unitary operators in (1) arises if the circuit of gates $U_{n} U_{n-1} \cdots U_{1}$ in (1) is represented in form (10).

The operator $K$ in general form relates all the qubits acting in the problem. It is difficult to find this operator and more difficult to implement it experimentally. Another method for modifying the Hamiltonian with time was therefore proposed in [6]:

$$
\begin{equation*}
H\left(s_{1}, s_{2}, \ldots, s_{n}\right)=U_{n}\left(s_{n}\right) \cdots U_{2}\left(s_{2}\right) U_{1}\left(s_{1}\right) H(0) U_{1}^{\dagger}\left(s_{1}\right) U_{2}^{\dagger}\left(s_{2}\right) \cdots U_{n}^{\dagger}\left(s_{n}\right) \tag{12}
\end{equation*}
$$

where each operator $U_{j}$ in (1) satisfies formulas (6) for its own parameter $s_{j}(j=1, \ldots, n)$ varying from 0 to 1 . In expression (12), all the parameters $s_{j}$ can be set equal to each other ( $s_{j}=s$ ) and can be increased synchronously as time increases in formula (8), where $H(s)$ is replaced with $H(s, s, \ldots, s)$. Along with this case, a stepwise successive variation of Hamiltonian (12) by the operators $U_{j}\left(s_{j}\right), j=1,2, \ldots, n$, i.e., first under the action of $U_{1}\left(s_{1}\right)$, then under the action of $U_{2}\left(s_{2}\right)$, and so on up to $U_{n}\left(s_{n}\right)$, was also studied in [6]:

$$
H(t)= \begin{cases}U_{1}\left(t / T_{1}\right) H(0) U_{1}^{\dagger}\left(t / T_{1}\right) & \text { for } 0<t<T_{1} \\ U_{2}\left(t / T_{2}-T_{1} / T_{2}\right) U_{1}(1) H(0) \times & \\ \quad \times U_{1}^{\dagger}(1) U_{2}^{\dagger}\left(t / T_{2}-T_{1} / T_{2}\right) & \text { for } T_{1}<t<T_{1}+T_{2} \\ \vdots & \\ U_{n}\left(t / T_{n}-\sum_{i=1}^{n-1} T_{i} / T_{n}\right) \times & \\ \quad \times U_{n-1}(1) \cdots U_{1}(1) H(0) U_{1}^{\dagger}(1) \cdots U_{n-1}^{\dagger}(1) \times & \\ \quad \times U_{n}^{\dagger}\left(t / T_{n}-\sum_{i=1}^{n-1} T_{i} / T_{n}\right), & \text { for } \sum_{i=1}^{n-1} T_{i}<t<T\end{cases}
$$

where $T_{j}$ is the length of the time interval on which the operator $U_{j}$ acts and $T=\sum_{j=1}^{n} T_{j}$. In this case, (8)
becomes

$$
\begin{align*}
U_{T}= & \widehat{P} \exp \left(-i T_{n} \int_{0}^{1} H\left(1, \ldots, 1, s_{n}\right) d s_{n}\right) \times \cdots \times \\
& \times \widehat{P} \exp \left(-i T_{j} \int_{0}^{1} H\left(1, \ldots, 1, s_{j}, 0, \ldots, 0\right) d s_{1}\right) \times \cdots \times \\
& \times \widehat{P} \exp \left(-i T_{1} \int_{0}^{1} H\left(s_{1}, 0, \ldots, 0\right) d s_{1}\right) \tag{13}
\end{align*}
$$

The variation of the Hamiltonian in expression (13) is simpler and more understandable than that in general case (8), but the methods for implementing this variation in experiments remain unclear. The point is that this time dependence is inverse to the time dependence following from the Heisenberg representation or from the interaction representation (see, e.g., the appendix). Indeed, we assume that we have the initial Hamiltonian $H(0)$. Then we want it to be time dependent. For this, we can add a controlling Hamiltonian, for example, a Hamiltonian describing the interaction with strong RF pulses, and obtain $H(0)+V(t)$. After passing to the interaction representation in $V(t)$ (see the appendix), we obtain

$$
H(t)=U_{V}^{-1}(t) H(0) U_{V}(t)
$$

(the correspondence between the operators can be easily established by comparing with formula (9)). For $t+\Delta t$, we obtain

$$
H(t+\Delta t)=U_{V}^{-1}(t) U_{V}^{-1}(\Delta t) H(0) U_{V}(\Delta t) U_{V}(t)
$$

i.e., the increasing part of the evolution operators, which form the operators enclosing the time-dependent operator, is still inside. Then, conversely, just as in the case of (13), the increasing part of the evolution operators in the dependence of Hamiltonian (12) on time turns out to be outside. Because the method proposed in [6] is thus unnatural, all the results become more complicated.

We show that the method can be simplified significantly if Hamiltonian (12) is modified stepwise with the operators $U_{j}\left(s_{j}\right)$ applied starting from the last, which is more natural, i.e., the operator $U_{n}\left(s_{n}\right)$ acts first, and the operator $U_{1}\left(s_{1}\right)$ acts at the end:

$$
H(t)= \begin{cases}U_{n}\left(t / T_{n}\right) H(0) U_{n}^{\dagger}\left(t / T_{n}\right) & \text { for } 0<t<T_{n} \\ U_{n}(1) U_{n-1}\left(t / T_{n-1}-T_{n} / T_{n-1}\right) H(0) \times & \\ \times U_{n-1}^{\dagger}\left(t / T_{n-1}-T_{n} / T_{n-1}\right) U_{n}^{\dagger}(1) & \text { for } T_{n}<t<T_{n-1}+T_{n} \\ \vdots & \\ U_{n}(1) \cdots U_{2}(1) U_{1}\left(t / T_{1}-\sum_{i=2}^{n} T_{i} / T_{1}\right) H(0) \times & \\ \times U_{1}^{\dagger}\left(t / T_{1}-\sum_{i=2}^{n} T_{i} / T_{1}\right) U_{2}^{\dagger}(1) \cdots U_{n}^{\dagger}(1) & \text { for } \sum_{i=2}^{n} T_{i}<t<T\end{cases}
$$

In this case, instead of (8), we obtain

$$
\begin{align*}
U_{T}= & \widehat{P} \exp \left(-i T_{1} \int_{0}^{1} H\left(s_{1}, 1, \ldots, 1\right) d s_{1}\right) \times \cdots \times \\
& \times \widehat{P} \exp \left(-i T_{j} \int_{0}^{1} H\left(0, \ldots, 0, s_{j}, 1, \ldots, 1\right) d s_{j}\right) \times \cdots \times \\
& \times \widehat{P} \exp \left(-i T_{n} \int_{0}^{1} H\left(0, \ldots, 0, s_{n}\right) d s_{n}\right) \tag{14}
\end{align*}
$$

Because the increasing part of the evolution operators, which form the operators enclosing the timedependent operator in (12), turns out to be inside in the method proposed here, we can perform the further transformations

$$
\begin{aligned}
\widehat{P} \exp \left(-i T_{j} \int_{0}^{1} H\left(0, \ldots, 0, s_{j}, 1, \ldots, 1\right) d s_{j}\right)= & U_{n}\left(s_{n}\right) \times \cdots \times U_{j+1}\left(s_{j+1}\right) \times \\
& \times \widehat{P} \exp \left(-i T_{j} \int_{0}^{1} H\left(0, \ldots, 0, s_{j}, 0, \ldots, 0\right) d s_{j}\right) \times \\
& \times U_{j+1}^{\dagger}\left(s_{j+1}\right) \ldots U_{n}^{\dagger}\left(s_{n}\right) \\
U_{T}= & U U_{1}^{\dagger} \widehat{P} \exp \left(-i T_{1} \int_{0}^{1} H\left(s_{1}, 0, \ldots, 0\right) d s_{1}\right) \times \cdots \times \\
& \times U_{j}^{\dagger} \widehat{P} \exp \left(-i T_{j} \int_{0}^{1} H\left(0, \ldots, 0, s_{j}, 0, \ldots, 0\right) d s_{j}\right) \times \cdots \times \\
& \times U_{n}^{\dagger} \widehat{P} \exp \left(-i T_{n} \int_{0}^{1} H\left(0, \ldots, 0, s_{n}\right) d s_{n}\right)
\end{aligned}
$$

After the exponentials are transformed (see the appendix), we hence obtain the simple expression

$$
\begin{align*}
U_{T}= & U \exp \left\{-i T_{1}\left(H(0)+\frac{K_{1}}{T_{1}}\right)\right\} \times \\
& \times \exp \left\{-i T_{2}\left(H(0)+\frac{K_{2}}{T_{2}}\right)\right\} \cdots \exp \left\{-i T_{n}\left(H(0)+\frac{K_{n}}{T_{n}}\right)\right\} . \tag{15}
\end{align*}
$$

Condition (11) that Eq. (10) is adiabatic must be satisfied on each interval. We do not restrict our discussion to the case $T_{j}=T / n$, because for a fixed $T$, we can increase the accuracy by choosing a larger $T_{j}$ for a larger $K_{j}$ (for example, choosing a larger $T_{j}$ for a larger angle in the case of the phase shift gates given by (18), which we consider later).

If condition (11) is satisfied, then according to (10) or (15), the state $|0\rangle$ is preserved up to a phase factor at the first stage of evolution (7) and is transformed into the state $|\Psi(T)\rangle$ by the operator $U$ at the second stage. In the adiabatic limit as $T \rightarrow \infty$, we must obtain exact result (1) independently of the method of applying the operators. For a finite $T$, we inevitably obtain an error, whose value may depend on the method of applying the operators. In the next section, we analyze this problem by investigating a specific example. The importance of this analysis is that it is simpler to realize expression (15) than expression (10) because the effective Hamiltonian $K$ must contain interactions of many spins [6], while the Hamiltonians $K_{j}$ in (15) corresponding to the one- and two-qubit gates must contain only one- and two-spin interactions.

Nevertheless, the problem remains because it is necessary to modify the effective Hamiltonian of the system with time in the sequence obtained in formula (15). A method for this variation was proposed in [7] and is based on the Trotter formula for two noncommuting operators

$$
\begin{align*}
\exp \left\{-i T_{j}\left(H(0)+\frac{K_{j}}{T_{j}}\right)\right\} & =\lim _{N_{j} \rightarrow \infty}\left\{\exp \left(-i \Delta t_{j} H(0)\right) \exp \left(-\frac{i \Delta t_{j} K_{j}}{T_{j}}\right)\right\}^{N_{j}}= \\
& =\lim _{N_{j} \rightarrow \infty}\left\{\exp \left(-i \Delta t_{j} H(0)\right) U_{j}^{\dagger}\left(\frac{1}{N_{j}}\right)\right\}^{N_{j}} \tag{16}
\end{align*}
$$

where $\Delta t_{j}=T_{j} / N_{j}$. Under the conditions of a real experiment, the value of $\Delta t_{j}$ is bounded by the device potentialities. As a result, for some finite $\Delta t_{j}=\Delta t=T / N$ (where $N=\sum_{j=1}^{n} N_{j}$ ) with (16) taken into account, we obtain the approximate expression for operator (15)

$$
\begin{align*}
U_{T, \Delta t}= & U\left\{\exp (-i \Delta t H(0)) U_{1}^{\dagger}\left(\frac{1}{N_{1}}\right)\right\}^{N_{1}} \times \\
& \times\left\{\exp (-i \Delta t H(0)) U_{2}^{\dagger}\left(\frac{1}{N_{2}}\right)\right\}^{N_{2}} \times \cdots \times\left\{\exp (-i \Delta t H(0)) U_{n}^{\dagger}\left(\frac{1}{N_{n}}\right)\right\}^{N_{n}} \tag{17}
\end{align*}
$$

which can already be realized experimentally.

## 4. Numerical simulation of the NMR realization of an adiabatic quantum algorithm

In the preceding section, we studied general formulas and did not specify the form of the quantum system and the quantum algorithm. Here, we use the specific example considered in Sec. (2) to study the accuracy of formula (17).

To implement quantum algorithm (2) for finding the permutation order using adiabatic evolution, we vary the Hamiltonian in accordance with formula (12) applying the operators

$$
\begin{align*}
\prod_{j} U_{j}\left(s_{j}\right)= & H_{3} B_{23}\left(\pi \frac{s_{5}}{2}\right) H_{3} H_{3} B_{13}\left(\pi \frac{s_{4}}{4}\right) H_{3} H_{2} B_{12}\left(\pi \frac{s_{3}}{2}\right) H_{2} \times \\
& \times H_{2} H_{4} B_{24}\left(\pi s_{2}\right) H_{4} H_{2} H_{3} H_{5} B_{35}\left(\pi s_{1}\right) H_{5} H_{3} \tag{18}
\end{align*}
$$

We do not introduce the parameters $s$ for the Hadamard operators, because the condition $U_{j}(0)=1$ is satisfied according to the properties $H_{j} H_{j}=1$ and $B_{i j}(0)=1$. By the method described in Sec. 2, we can further elaborate by assigning each gate of the controlled phase shift in (18) the required sequence of RF pulses and the free evolution intervals. Because our goal is to investigate the error arising because $\Delta t$ is finite for different methods for modifying Hamiltonian (12) with time by the operators $U_{j}\left(s_{j}\right)$, we use expressions (3), already obtained for these operators, in (18) in our computation.

We choose the ground state in which all five spins are directed along the $z$ axis as the initial state. This state is assigned the Hamiltonian

$$
\begin{equation*}
H(0)=-\omega \sum_{i=1}^{5} I_{i}^{z} \tag{19}
\end{equation*}
$$

The exponential in (17) containing $\Delta t H(0)$ is a rotation about the $z$ axis or a phase shift. We already discussed the methods for realizing this transformation.

The results of adiabatic quantum computation (7) by three methods for increasing the parameters $s_{j}$ in (18) were obtained using the formula

$$
\begin{equation*}
U_{T, \Delta t}=\prod_{m=1}^{N} \exp \left(-i \Delta t H\left(\frac{m}{N}\right)\right)=\prod_{m=1}^{N} U\left(\frac{m}{N}\right) \exp (-i \Delta t H(0)) U^{\dagger}\left(\frac{m}{N}\right) \tag{20}
\end{equation*}
$$

which follows from general formula (8) if we divide the time interval $T$ into $N$ intervals $\Delta t=T / N$ and neglect the variations of Hamiltonian (12) inside these small intervals. When the $s_{j}$ increase synchronously, this implies that the unit range of each parameter $s_{j}=s$ is divided into $N$ parts. When the $s_{j}$ increase successively, formula (8) transforms into formulas (13)-(15). Based on the ratio of the angles $\theta_{j}$ in the
operators $B_{i j}=B_{i j}\left(\theta_{j}\right)$ in (18), we set $N_{1}=N_{2}=4 N_{4}$ and $N_{3}=N_{5}=2 N_{4}$ to ensure equal increments of the angles, $\Delta s_{j} \theta_{j}=13 \pi /(4 N)$, where $\Delta s_{j}=1 / N_{j}=\Delta t / T_{j}$. We note that if we apply the sequence of operators starting from the last, then formula (20) transforms into formula (17).

The computer calculations were performed using MATLAB for different values of the parameters $\omega \Delta t$ and $N=T / \Delta t$ (we set $\Delta t=$ const guided by the experimental conditions [7]). The degree of agreement between the computed and exact theoretical vectors of state $|\psi\rangle$ given by (1) was estimated using the formula given in [9] as $|\langle\Psi(T) \mid \psi\rangle|$. The obtained error is shown in Fig. 1. The parameter $\omega \Delta t$ determines the value of the gap. Therefore, as this parameter decreases, the accuracy also decreases because condition (11) that Eq. (10) is adiabatic is violated. On the other hand, as $\omega \Delta t$ approaches $\pi$, the error due to replacing the continuous variation with a discrete variation increases. The dependence of the error on $N$ calculated for the optimal value $\omega \Delta t=1.6$ shows that the accuracy of the inverse method proposed here, with the operators applied successively, is not less than the accuracy of the method proposed in [6]. Applying the operators simultaneously (when the $s_{j}$ increase synchronously) gives a smaller error because the angle increment then decreases: $\Delta s_{j} \theta_{j} \leq \pi / N$. An additional contribution to the error in the case where the operators are applied successively occurs because the Hamiltonian in evolution operator (15) varies discretely. The value of the steps can be decreased by dividing the intervals of the operator action into several parts. For example, all the $s_{j}$ can be successively increased to 0.5 in the first stage and from 0.5 to 1 in the second stage.

## 5. Conclusion

The performed computation confirms the admissibility of the algorithm in which we apply operator sequence (12) starting from the last and thus obtain formula (17). Following this formula, we can construct the required sequence of RF pulses. The exponential containing $\Delta t H(0)$ in (17) is rotation about the $z$ axis. According to (18), the operators $U_{j}\left(1 / N_{j}\right)$ are products of the Hadamard operators and the operators of the controlled phase shift by a small angle. The NMR methods for implementing these operators for spin systems were described in Sec. 2. Here, we note that $T$ is the formal time, while the actual running time of the experiment is determined by the time required to realize the operators of the controlled phase shift, i.e., eventually, by the time required to rotate spins by a required angle as a result of the spin-spin interaction. The times of one-qubit operators that rotate spins using the RF-field pulses are usually significantly shorter. It follows from (17) that the time required to simulate adiabatic computation is twice as large as the running time of standard quantum computation (1).

The above transformation of the evolution operator thus permits avoiding difficulties due to constructing a nonlocal multiparticle Hamiltonian $H(s)$ given by (9), which implements adiabatic algorithm (7). The effective Hamiltonian of the required form is now formed automatically as a result of the action on the spin-spin interaction Hamiltonian of RF-pulse sequence (17) chosen according to the algorithm. This transformation, which is identical under the ideal conditions, unfortunately ceases to be identical because of environmental excitations. The point is that the operators enclosing $H(s)$ in formula (12) are reproduced in (17) using the spin-spin interaction taken at different (other) instants of real time. Whether the proposed scheme tolerates noises of different types is left for further investigation.

## Appendix

Based on the well-known properties of exponential operators (see, e.g., Sec. 15 in [12]), we derive several formulas used in the text. The equation of motion for the evolution operator of a quantum system whose Hamiltonian consists of two parts, time-dependent and time-independent, has the form

$$
\begin{equation*}
\frac{d}{d t} U(t)=-i\left\{H_{0}+V(t)\right\} U(t) \tag{A.1}
\end{equation*}
$$



Fig. 1. Errors in the results of quantum adiabatic computation presented (a) as functions of the evolution time $N=T / \Delta t$ for $\omega \Delta t=1.6$ in the three methods for applying the sequence of operators in (12) (the solid line corresponds to applying them simultaneously, the triangles correspond to applying them successively from the beginning to the end of the sequence, and the dots correspond to applying them successively from the end to the beginning of the sequence) and (b) as functions of the value of the locking field $\omega \Delta t / \pi$ for different values of $N$.

If we explicitly distinguish the operator of evolution under the action of the time-dependent part in this operator,

$$
U_{V}(t)=\widehat{P} \exp \left(-i \int_{0}^{t} V\left(t_{1}\right) d t_{1}\right)
$$

then

$$
\begin{equation*}
U(t)=\widehat{P} \exp \left(-i \int_{0}^{t}\left(H_{0}+V\left(t_{1}\right)\right) d t_{1}\right)=U_{V}(t) U_{H}(t) \tag{A.2}
\end{equation*}
$$

For the operator $U_{H}$ in the last formula, Eq. (A.1) implies the equation

$$
\frac{d}{d t} U_{H}(t)=-i\left\{U_{V}^{-1}(t) H_{0} U_{V}(t)\right\} U_{H}(t)
$$

whose solution is given by

$$
\begin{equation*}
U_{H}(t)=\widehat{P} \exp \left(-i \int_{0}^{t} H_{0}\left(t_{1}\right) d t_{1}\right) \tag{A.3}
\end{equation*}
$$

where

$$
\begin{equation*}
H_{0}(t)=U_{V}^{-1}(t) H_{0} U_{V}(t) \tag{A.4}
\end{equation*}
$$

On the other hand, it follows from (A.2) that

$$
\begin{equation*}
U_{H}(t)=U_{V}^{-1}(t) U(t)=U_{V}^{-1}(t) \widehat{P} \exp \left(-i \int_{0}^{t}\left(H_{0}+V\left(t_{1}\right)\right) d t_{1}\right) \tag{A.5}
\end{equation*}
$$

Formulas (A.3)-(A.5) coincide with (8)-(10) if

$$
H_{0}=H(0), \quad V(t)=\frac{K}{T}, \quad U_{V}^{-1}(t)=U
$$

are chosen as the parts of the Hamiltonian.

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