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Effect of a Phase Factor on the Minimum Time of a Quantum Gate

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Abstract—A relationship between the phase factor of a quantum gate, the layout of energy levels of its effective Hamiltonian, and the implementation time of the gate is demonstrated. By an example of the direct and inverse quantum Fourier transforms (QFT) gates for a qutrit represented by a quadrupole nucleus with spin $I = 1$, as well as for a system of two qubits ($I = 1/2$), effective Hamiltonians and minimum implementation times corresponding to different global phases are obtained. Implementation schemes are proposed for these Hamiltonians by the nuclear magnetic resonance (NMR) technique with the use of sequences of radio-frequency (RF) pulses separated by intervals of free evolution. Analytic results for the minimum times of gates are in agreement with the results obtained by numerical optimization methods. The phase considered is divided into dynamic and geometric parts.

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1. INTRODUCTION

For the processing of quantum information, one should be able to implement a sequence of basic quantum logical operations (gates) on a given physical system [1, 2]. Quantum computing can be performed both on two-level quantum systems (qubits) and on multilevel quantum systems—qudits [3–5] (when there are d levels). The latter systems have a number of advantages; for example, the same size of computational basis can be guaranteed by a smaller number of qudits. When considering the implementation of quantum algorithms, one should take into account, in addition to the operational complexity (the number of gates to perform an algorithm [2]), the time complexity (time taken to perform an algorithm) [6–11]. The reduction of this time minimizes losses due to interaction with the environment. The time complexity of quantum logical operations is determined by the quantum system and the method of its control. In the general case, the presence of a certain minimum time $T_{\min}$ within which a quantum gate can be implemented with an acceptable error is a fundamental limitation on the speed of quantum operations.

Finding efficient methods of control of quantum systems to implement gates with the maximum accuracy and in the minimum time is one of the most important problems in the development of a full-scale quantum computer. Among the physical systems used for this purpose, systems of nuclear spins are distinguished by their relative simplicity. Therefore, many experimental studies have been carried out on such systems, that demonstrate the implementation of quantum algorithms by the nuclear magnetic resonance (NMR) technique [12]. In some simple cases, the minimum time of the gate and the corresponding effective Hamiltonian for its implementation by a radio-frequency (RF) magnetic field can be found analytically (see, for example, [8–10, 13, 14]). In more complex systems, numerical methods have been used for this purpose [7, 11, 15–20].

The quantum Fourier transform (QFT) [1, 2, 12] plays a key role in many quantum algorithms. Computations of QFT on spin-1/2 systems have shown that the minimum time $T_{\min}$ strongly depends on the phase factor in the definition of a gate [7, 11]. The point is that the evolution operator $U(T)$ of a spin system during time T with a traceless Hamiltonian belongs to a special unitary group $SU(N)$ (N is the dimension of the Hilbert space of the system). Hence, the equality $\det\{U(T)\} = 1$ holds. At the same time, the quantum gates U_G are defined in the group of unitary operators $U(N)$ such that the moduli of determinants satisfy the equality $\left|\det\{U_G\}\right| = 1$. Therefore, we can implement gates only up to a phase factor:

$$U_G = \exp(-i\phi_p)U(T). \quad (1)$$

The global phase in (1) can be chosen from a certain set of values [7],

$$\phi_p = \phi_0 + 2\pi p/N, \quad p = 0, 1, \ldots, N-1, \quad (2)$$

where $N = 2^n$ for a system of n spins 1/2 and ϕ_0 is the minimum value of the angle $\phi_0 \in [0, \pi]$ such that $\det\{\exp(i\phi_0)U_G\} = 1$. Numerical calculation [7] for a QFT gate on three spins 1/2 has shown that the minimum time $T_{\min}$ depends on the value (2) of the global phase. In [11], a similar result was obtained for gates of QFT and the rearrangement of states (SWAP) on two spins 1/2. In [20], numerical simulation of the implementation of QFT on qudits with the numbers of states $d = 3$ and $d = 4$ represented by quadrupole nuclei with

spins $I = 1$ and $I = 3/2$, respectively, has also demonstrated that the minimum time of a gate strongly depends on the value of the global phase.

Today, there are a lot of publications devoted to the analysis of various manifestations of the quantum phase (see the reviews [21–23]). Most often, one considers the Berry phase [24] under adiabatic evolution and the Aharonov–Anandan phase [25] under nonadiabatic evolution. In the general case, the total phase is a sum of dynamic and geometric parts. In the field of quantum computations, the main focus is placed on the implementation of quantum gates by means of a geometric phase (see [12, 23, 26–28] and references therein). In [29], the authors analyze the phase and the Hamiltonian of a gate by examples of qubit rotation gate and SWAP gate between the ends of a spin chain. The above-mentioned relationship between the phase factor of the gate and the minimum time of its implementation has not been explained, as far as we know; in the present study, we consider this relationship by an example of QFT.

Earlier [7, 11, 20], it has been established by numerical methods that one can find such time dependence of RF field that allows one to implement a gate with one of possible values of the global phase (2) each of which corresponds to its own minimum implementation time. It is clear that the phase factor in itself cannot affect the duration of a pulse. Hence, there should be another reason for such a relationship. However, it is very difficult to understand the mechanism of this relationship by the computed complex time dependence of the RF field. Therefore, in the present study, we apply analytic methods to the investigation of effective Hamiltonians that implement a gate and consider simple methods for its approximate construction. In Section 2, we obtain general formulas that describe the relation between the phase factor of a quantum gate and the effective Hamiltonian that implements this gate. In Section 3, we consider an example of QFT for a qutrit represented by a quadrupole nucleus with spin $I = 1$. In Section 4, we obtain an effective Hamiltonian of QFT for a system of two qubits. In Section 5, we accomplish the division of the phase into dynamic and geometric parts.

2. RELATIONSHIP BETWEEN THE PHASE FACTOR AND THE EFFECTIVE HAMILTONIAN OF A GATE

Suppose that a unitary operator of some gate in a computational basis is represented by a matrix U_G, which is expressed in exponential form as

$$U_G = e^{iK}. \tag{3}$$

Using transformation P, we reduce the matrices U_G and K to a diagonal form:

$$P^\dagger K P = D = \sum_{f=1}^{N} \Lambda_f |f\rangle\langle f|, \tag{4}$$

$$P^\dagger U_G P = \exp(iD) = \sum_{f=1}^{N} \exp(i\Lambda_f)|f\rangle\langle f|, \tag{5}$$

where $|f\rangle\langle f|$ is the projector onto the eigenstate $|f\rangle$. Now, if we add the number $2\pi m_k$ to the eigenvalues Λ_k, where m_k is an integer, then the value of the exponential function in (5) remains unchanged, but the matrix D is changed; hence, the matrix K is transformed into a new matrix

$$\begin{aligned} K_m &= P(D + 2\pi m_k |k\rangle\langle k|)P^\dagger \\ &= K + 2\pi m_k P|k\rangle\langle k|P^\dagger. \end{aligned} \tag{6}$$

In this case, the trace of the matrix is changed:

$$\mathrm{Tr}K_m = \mathrm{Tr}K + 2\pi m_k \equiv N\Phi_m. \tag{7}$$

Suppose that we want to implement the gate U_G on a given physical system by the effective Hamiltonian H_{eff}. Since its trace is zero, we should take a matrix

$$TH_{\text{eff}}^m = -K_m + \Phi_m E, \tag{8}$$

to implement this gate, where E is the unit matrix. Let us explain transformations (6) and (8) in physical terms. When one chooses different sets of numbers m_k in (6), the effective Hamiltonian (8) is changed so that one or several of its energy levels are shifted by $2\pi m_k/T$. The associated variation of the mean energy is eliminated by a scale shift such that this mean value is taken as the origin. As a result, we obtain the operator

$$U_m(T) = \exp(-iTH_{\text{eff}}^m) = U_G \exp(-i\Phi_m). \tag{9}$$

Note that transformation (7) has allowed us to change the trace of the matrix K and pass from one value of the global phase to another, whereas unitary transformations (for example, rotations caused by the external field) preserve the trace of the matrix.

Comparing operators (9) and (11), we obtain

$$\phi_p = -\Phi_m \mod (2\pi).$$

Thus, we have obtained an operator U_G (1) up to a global phase each of whose values from the set (2) corresponds to its own effective Hamiltonian. Such an implementation of a gate allows one to choose, from among the effective Hamiltonians H_{eff}^m, the one that has advantages, for example, that can be implemented in less time.

Consider a QFT gate with a matrix:

$$U_G = \mathrm{QFT}_N = \frac{1}{\sqrt{N}} \times \begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & \sigma & \sigma^2 & \dots & \sigma^{N-1} \\ 1 & \sigma^2 & \sigma^4 & \dots & \sigma^{2(N-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \sigma^{N-1} & \sigma^{2(N-1)} & \dots & \sigma^{(N-1)^2} \end{pmatrix}, \quad (10)$$

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

Let us analyze the above-described transformations by an example of a qutrit. Then, in expressions (3)–(5) for the matrix $U_G = \mathrm{QFT}_3$(10), we have

$$K = \frac{\pi}{2}\begin{pmatrix} 2g_1 & -g_2 & -g_2 \\ -g_2 & 1+g_2/2 & g_2/2 \\ -g_2 & g_2/2 & 1+g_2/2 \end{pmatrix}, \quad (11)$$

$$D = \pi\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1/2 \end{pmatrix},$$

where $g_1 = \sin^2(\theta/2)$, $g_2 = \cos\theta = 1/\sqrt{3}$, and $\theta = \arctan\sqrt{2}$. The matrix

$$P = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{2} & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & -1 \end{pmatrix} \times \begin{pmatrix} \sin(\theta/2) & \cos(\theta/2) & 0 \\ -\cos(\theta/2) & \sin(\theta/2) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (12)$$

transforms matrices K and D to diagonal form. The matrices

$$2\pi m_1 P|1\rangle\langle 1|P^\dagger = \pi m_1\begin{pmatrix} 2g_1 & -g_2 & -g_2 \\ -g_2 & 1-g_1 & 1-g_1 \\ -g_2 & 1-g_1 & 1-g_1 \end{pmatrix},$$

$$2\pi m_2 P|2\rangle\langle 2|P^\dagger = \pi m_2\begin{pmatrix} 2(1-g_1) & g_2 & g_2 \\ g_2 & g_1 & g_1 \\ g_2 & g_1 & g_1 \end{pmatrix}, \quad (13)$$

$$2\pi m_3 P|3\rangle\langle 3|P^\dagger = \pi m_3\begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \end{pmatrix}$$

define variations of the effective Hamiltonian.

Returning to the general case, notice that the QFT gate (10) can be obtained by a series of rotations selective with respect to transitions between levels [30, 31]. In this case, the variation of the phase factor (1) affects the numerical values of the exponents in the diagonal part of the QFT expansion but does not affect the sequence of selective rotation operators themselves. This method of obtaining a QFT gate is not time optimal, as demonstrated by numerical calculations in [16]. For the optimal implementation of a gate, one should act on all the transitions simultaneously, as this is done in a QFT gate implemented by an optimized RF pulse or by the effective Hamiltonian (8).

3. CONSTRUCTION OF AN EFFECTIVE HAMILTONIAN OF QFT ON A QUTRIT

Consider a qudrupole nucleus with spin $I = 1$ placed in a strong static magnetic field and a control RF magnetic field. In the reference frame rotating about the direction of the static field (z axis) with the frequency ω_{rf} of the RF field [32], the Hamiltonian takes the form

$$H(t) = -(\omega_0 - \omega_{\mathrm{rf}})I_z + u_x(t)I_x + u_y(t)I_y + H_q, \quad H_q = q(I_z^2 - 2/3). \quad (14)$$

Here ω_0 is the Larmor frequency, I_α is the spin projection operator onto axis α ($\alpha = x, y, z$), q is the constant of quadrupole interaction of the nucleus with the gradient of the axially symmetric crystal field, and the amplitude $u_\alpha(t)$ is the projection of the control RF field onto the axis α. Assume that $\hbar = 1$; then the energy is measured in the units of frequency. Let us pass to dimensionless time and dimensionless frequencies expressed in the units of $1/q$ and q, respectively. As qutrits, we can take, following, for example, [33], deuterium nuclei ($I = 1$) in a liquid crystal. The NMR spectrum consists of two narrow lines with splitting of 200 Hz, which allows one to control all the transitions between three levels by an optimized RF pulse [20] with practically attainable amplitude.

Table 1. The values of parameters for obtaining H_{eff}^{m} for QFT_3

Φ_m	m_1, m_2, m_3	φ	ψ	ξ	δ	t_1	t_2	T
$3\pi/6$	0, 0, 0	0	1.083	0.3206	0.6802	1.08	2.32	3.40
$7\pi/6$	0, 1, 0	$\pi/2$	1.326	−1.431	−1.466	2.41	0.63	3.04
$-\pi/6$	−1, 0, 0	$\pi/2$	−0.6657	0.7901	0.1052	3.44	4.27	7.71

To implement a gate for quantum computations, one should find a control field $u_\alpha(t)$ (14) such that the evolution operator

$$U(T) = \hat{T}\exp\left(-i\int_0^T H(t)dt\right) \tag{15}$$

performs, in time T, the necessary logical unitary operation of the qutrit state up to the phase factor (1). Here $\hat{T}$ is the time ordering operator. A variant of numerical solution of this problem is given in [20]. In the present section, we analytically construct an effective Hamiltonian that implements a QFT gate.

In the absence of the RF field, system (14) has three nonequidistant energy levels for states with different values of I_z:

$$|I_z = 1\rangle = |1\rangle, \quad |I_z = 0\rangle = |2\rangle, \quad |I_z = -1\rangle = |3\rangle. \tag{16}$$

We take these states as a computational basis of a qutrit. Earlier [13], we found an effective Hamiltonian for rotations selective with respect to transitions between the levels of this qutrit. To obtain a QFT on qutrit, we should construct an effective Hamiltonian in the form of the matrix H_{eff}^{m} (8) with the substitution of (11) and (13). Moreover, this Hamiltonian should be constructed from operators that describe actions on the system that are admissible in our model. Introduce the notations

$$A = \exp(-i\varphi I_x)(H_q t_1)\exp(i\varphi I_x),$$
$$B = \exp(-i\psi I_y)(H_q t_2)\exp(i\psi I_y), \tag{17}$$
$$C = \xi I_x + \delta I_z,$$

where the first two operators can be obtained from the free evolution operators and the operators of nonselective rotations through angles φ and ψ due to the following property of exponential operators:

$$\exp(-i\varphi I_x)\exp(iHt)\exp(i\varphi I_x) = \exp[\exp(-i\varphi I_x)iHt\exp(i\varphi I_x)].$$

The operator C in (17) is obtained by an RF field (in contrast to the case of selective rotations [13], we take a z-field instead of a y-field). Equating the sum of matrices of the operators (17) to (8), we obtain a system of equation

$$-K_m + \Phi_m E = \begin{pmatrix} \frac{1}{6}[(3\cos^2\varphi - 1)t_1 + (3\cos^2\psi - 1)t_2] + \delta & \frac{1}{\sqrt{2}}(-it_1\sin\varphi\cos\varphi + t_2\sin\psi\cos\psi + \xi) & -\frac{1}{2}(t_1\sin^2\varphi - t_2\sin^2\psi) \\ \frac{1}{\sqrt{2}}(it_1\sin\varphi\cos\varphi + t_2\sin\psi\cos\psi + \xi) & -\frac{1}{3}[(3\cos^2\varphi - 1)t_1 + (3\cos^2\psi - 1)t_2] & \frac{1}{\sqrt{2}}(it_1\sin\varphi\cos\varphi - t_2\sin\psi\cos\psi + \xi) \\ -\frac{1}{2}(t_1\sin^2\varphi - t_2\sin^2\psi) & \frac{1}{\sqrt{2}}(-it_1\sin\varphi\cos\varphi - t_2\sin\psi\cos\psi + \xi) & \frac{1}{6}[(3\cos^2\varphi - 1)t_1 + (3\cos^2\psi - 1)t_2] - \delta \end{pmatrix}. \tag{18}$$

The joint solution of these equations yields the sought values of the parameters, which are given in Table 1. For every value of the phase, solutions with positive evolution times are chosen that lead to the minimum value of the sum $T = t_1 + t_2$.

Thus, for the parameters given in Table 1, we obtain the matrix $-K_m + \Phi_m E$ for QFT in the form of the sum

$$TH_{\text{eff}}^{m} = A + B + C. \tag{19}$$

Since the operators in this expression do not commute with each other, to obtain a pulse sequence that implements the given Hamiltonian, we apply the Trotter–Suzuki formula [34] for exponential operators:

$$(e^{-iA/2r}e^{-iB/2r}e^{-iC/r}e^{-iB/2r}e^{-iA/2r})^r = e^{-i(A+B+C)} + O(r^{-3}). \tag{20}$$

In view of expression (19), this product converges, as $r \longrightarrow \infty$, to the ideal QFT gate (10): $\text{QFT}_3\exp\{-i\Phi_m\}$.

The r-times repeated product of operators in parentheses on the left-hand side of (20) can be obtained by the operators of nonselective rotations $\{\theta\}_\alpha = \exp(-i\theta I_\alpha)$, separated by intervals of free evolution, that are shown by arrows $\xrightarrow{t} \equiv \exp(-itH_q)$:

$$\{\varphi\}_x \xrightarrow{t_1/2r} \{\varphi\}_{-x}\{\psi\}_y \xrightarrow{t_2/2r} \{\psi\}_{-y}\{\Omega/r\}_\Omega \times \{\psi\}_y \xrightarrow{t_2/2r} \{\psi\}_{-y}\{\varphi\}_x \xrightarrow{t_1/2r} \{\varphi\}_{-x}, \quad (21)$$

where the central position in the sequence is occupied by the rotation through angle $\Omega/r = \sqrt{\xi^2 + \delta^2}/r$ about the axis with the direction cosines ξ/Ω and δ/Ω along the axes x and z. A nonselective rotation can be obtained by a simple or composite pulse of RF field of large amplitude [14].

In quantum algorithms, in addition to the direct QFT, one uses the inverse QFT: $U_G^\dagger = \mathrm{QFT}_3^{-1}$. Since we cannot change the sign of time in formulas (9) and (19), we should change the sign of the effective Hamiltonian under invariant original quadrupole interaction (14). The parameters obtained after solving Eqs. (18) for this case are presented in Table 2.

Above, we used a standard relation (16) between the physical basis of the system (states with different projections of spin) and the logical basis of a qutrit. However, we can change this relation to another,

$$|I_z = 0\rangle = |1\rangle, \quad |I_z = 1\rangle = |2\rangle, \quad |I_z = -1\rangle = |3\rangle, \quad (22)$$

which better correlates with the layout of the energy levels of the Hamiltonian in the rotating reference frame. As an example, we point out paper [35], in which the authors demonstrated the enhancement of the efficiency of an adder on a quadrupole nucleus ^{133}Cs ($I = 7/2$) after renaming the computational basis. The change of the basis (16) to (22) leads to a simple permutation of the matrix elements of the effective Hamiltonian on the right-hand side of Eq. (18):

$$\Pi T H_{\mathrm{eff}}^m \Pi = \Pi(A + B + C)\Pi, \quad \Pi = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

By solving the new systems of equations, we find the values of the parameters given in Tables 3 and 4.

In the new basis, the solution of system (18) has a simpler form than in the old basis. This is associated with the fact that the matrix of the effective Hamiltonian (18) in the new basis has the same symmetry as the matrix of the operator K (11) for a QFT. According to Table 3, for given permutation, the minimum time $T = 2.72$ is implemented for the phase $\Phi_m = 3\pi/6$ and is less than that in the case of the standard logical basis (16).

Effective Hamiltonians corresponding to all the cases considered above and the sequences of nonselective RF pulses separated by intervals of free evolution that are necessary for implementing these Hamiltonians can be obtained by formulas (20) and (21). The same gates can be implemented by optimized RF pulses the time dependence of whose amplitudes ($u_\alpha(t)$ in expression (14)) are determined numerically as described in [20]. As a result of calculations, we have found that the minimum durations $T_{\min}$ of such pulses

Table 2. The values of parameters for obtaining H_{eff}^m for QFT_3^{-1}

Φ_m	m_1, m_2, m_3	φ	ψ	ξ	δ	t_1	t_2	T
$-3\pi/6$	0, −1, 1	0	−0.6532	3.653	3.036	0.85	4.91	5.76
$-7\pi/6$	0, −1, 0	0	−1.489	1.431	1.466	2.36	1.83	4.19
$\pi/6$	1, 0, 0	$\pi/2$	0.9051	−0.7901	−0.1052	0.83	4.27	5.09

Table 3. The values of parameters for obtaining $\Pi H_{\mathrm{eff}}^m \Pi$ for QFT_3

Φ_m	m_1, m_2, m_3	φ	ψ	ξ	δ	t_1	t_2	T
$3\pi/6$	0, 0, 0	$\pi/2$	$\pi/2$	1.283	0	1.81	0.907	2.72
$7\pi/6$	−1, 0, 0	$\pi/2$	0	3.848	0	5.86	0.421	6.28
$-\pi/6$	1, 0, 0	0	$\pi/2$	−1.283	0	1.81	4.05	5.86

Table 4. The values of parameters for obtaining $\Pi H_{\mathrm{eff}}^m \Pi$ for QFT_3^{-1}

Φ_m	m_1, m_2, m_3	φ	ψ	ξ	δ	t_1	t_2	T
$-3\pi/6$	0, 0, 0	0	$\pi/2$	−1.283	0	1.81	0.907	2.72
$-7\pi/6$	0, 1, 0	$\pi/2$	$\pi/2$	1.283	0	1.81	4.05	5.86
$\pi/6$	−1, 0, 0	$\pi/2$	0	1.283	0	4.05	2.23	6.28

Table 5. The values of phases Φ_m when implementing variants of QFTs by means of optimized RF pulses

$T_{\min}$	QFT_3	QFT_3^{-1}	$\Pi QFT_3 \Pi$	$\Pi QFT_3^{-1} \Pi$
1.86	$7\pi/6$	$-7\pi/6$	$3\pi/6$	$-3\pi/6$
3.15	$3\pi/6$	$\pi/6$	$-\pi/6$	$-7\pi/6$
4.51	$-\pi/6$	$-3\pi/6$	$7\pi/6$	$\pi/6$

take one of three values, depending on the value of the phase factor. For all the variants of a QFT on qutrit considered above, these three durations coincide to within the accuracy of computation, but the corresponding phase factors change places, as is shown in Table 5. Note that the time dependence of the amplitudes of optimized RF pulses calculated for different variants of QFT strongly differs in these cases.

We find that the relationship between the durations $T_{\min}$ of QFT implementations for different values of the global phase taken from the tables for the effective Hamiltonians qualitatively agrees with the relationship between the results of a numerical experiment that are shown in Table 5. The quantitative values of $T_{\min}$ after numerical optimization turn out to be less, which suggests that the Hamiltonian H_{eff} should be complicated or made explicitly time-dependent to achieve optimality in the analytic approach. Nevertheless, the value $T = 2.72$ obtained is about half the calculated minimum duration $T = 5.36$ of a QFT gate implemented as a sequence of optimal selective rotations [16].

4. CONSTRUCTION OF AN EFFECTIVE HAMILTONIAN OF QFT OF TWO QUBITS

As the second example, we consider a system of two spins 1/2 with a Hamiltonian

$$H = 4J_z I_{1z} I_{2z} + 4J_x (I_{1x} I_{2x} + I_{1y} I_{2y}) + 2b(I_{1z} + I_{2z}) \tag{23}$$

with the matrix

$$H = \begin{pmatrix} J_z + 2b & 0 & 0 & 0 \\ 0 & -J_z & 2J_x & 0 \\ 0 & 2J_x & -J_z & 0 \\ 0 & 0 & 0 & J_z - 2b \end{pmatrix}$$

in a standard computational basis $|1\rangle = |00\rangle$, $|2\rangle = |01\rangle$, $|3\rangle = |10\rangle$, and $|4\rangle = |11\rangle$, where 0 and 1 are the values of the projections $I_z = 1/2$ and $I_z = -1/2$, respectively.

In [9], the authors showed that if one takes the values of constants $J_x = 4J_z$ and $b = J_z$, then as a result of evolution of the system, within time $T = \pi/8J_z$, we obtain an operator $U_{\text{“QFT”}}(T) = \exp(-iHT)$, which can easily be transformed into a QTF gate (10) under the action of the Hadamard operator W on the first qubit:

$$QFT_4 = W U_{\text{“QFT”}}(T) W, \quad W = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes E.$$

This solution corresponds to the global phase $\Phi_m = 3\pi/8$. Let us find effective Hamiltonians and durations for other values of phases (2) by the method proposed in Section 2 above. First, we reduce the matrices H and $U_{\text{“QFT”}}(T)$ to a diagonal form by the transformation

$$P = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{pmatrix}. \tag{24}$$

After that, according to (8), we obtain the following system of four equations to calculate the parameters of the effective Hamiltonian:

$$\begin{aligned} 2\pi m_1 - \Phi_m &= -(J_z + 2b)T, \\ 2\pi m_2 - \Phi_m &= -(2J_x - J_z)T, \\ \pi + 2\pi m_3 - \Phi_m &= (2J_x + J_z)T, \\ \pi/2 + 2\pi m_4 - \Phi_m &= -(J_z - 2b)T, \end{aligned} \tag{25}$$

where $\Phi_m = \pi(m_1 + m_2 + m_3 + m_4)/2 + 3\pi/8$. Let us find a solution to the system:

$$\begin{aligned} -J_z T &= \pi(m_1 + m_4 - m_2 - m_3)/2 - \pi/8, \\ -J_x T &= \pi(m_2 - m_3)/2 - \pi/4, \\ bT &= \pi(m_4 - m_1)/2 + \pi/8. \end{aligned} \tag{26}$$

The global phase Φ_m is defined up to 2π and can take four different values for different values of $\sum_i m_i$:

$$\Phi_m = \begin{cases} 3\pi/8, & m_1 + m_2 + m_3 + m_4 = 0, \\ 7\pi/8, & m_1 + m_2 + m_3 + m_4 = 1, \\ -\pi/8, & m_1 + m_2 + m_3 + m_4 = -1, \\ 11\pi/8, & m_1 + m_2 + m_3 + m_4 = 2. \end{cases} \tag{27}$$

One can express time T in terms of this phase:

$$T = \frac{1}{J_z} \left\{ \frac{\pi}{2} - \Phi_m + \pi(m_2 + m_3) \right\}. \tag{28}$$

For each possible value of the phase, by varying the number m, one can find the minimum time T of the QFT and the corresponding values of the parameters J_x and b.

In real experiments, one usually assumes that the spin–spin interaction constant is invariant (defined by nature). For example, in [11], the authors took an isotropic original Hamiltonian (23) with the constants

$$J_x^0 = J_y^0 = J_x^0 = J/4. \tag{29}$$

Table 6. The values of parameters for obtaining QFT_4

Φ_m	T	t_0	t_x	t_y	t_z	m_1, m_2, m_3, m_4	bT
$3\pi/8$	$3\pi/2J$	$2T/3$	$T/6$	$T/6$	0	0, 0, 0, 0	$\pi/8$
$11\pi/8$	$3\pi/2J$	0	$T/6$	$T/6$	$2T/3$	1, 1, 0, 0	$-3\pi/8$
						0, 1, 0, 1	$5\pi/8$
$-\pi/8$	$5\pi/2J$	$5T/8$	0	0	$3T/8$	0, 0, 0, -1	$-3\pi/8$
						-1, 0, 0, 0	$5\pi/8$
$7\pi/8$	$5\pi/2J$	$3T/8$	0	0	$5T/8$	0, 1, 0, 0	$\pi/8$

Table 7. The values of parameters for obtaining QFT_4^{-1}

Φ_m	T	t_0	t_x	t_y	t_z	m_1, m_2, m_3, m_4	bT
$-3\pi/8$	$5\pi/2J$	0	$3T/10$	$3T/10$	$2T/5$	0, 0, 0, 0	$-\pi/8$
$-11\pi/8$	$5\pi/2J$	$2T/5$	$3T/10$	$3T/10$	0	$-1, -1$, 0, 0	$3\pi/8$
						0, -1, 0, -1	$-5\pi/8$
$\pi/8$	$3\pi/2J$	$5T/8$	0	0	$3T/8$	0, 0, 1, 0	$-\pi/8$
$-7\pi/8$	$3\pi/2J$	$3T/8$	0	0	$5T/8$	-1, 0, 0, 0	$3\pi/8$
						0, 0, 0, -1	$-5\pi/8$

Let us describe how an effective QFT Hamiltonian is derived from this Hamiltonian. We turn one of the spins through an angle of 180° about one of the axes x, y, or z by an RF pulse. Then the interaction between the spin projections onto this axis remains unchanged, whereas the interaction between the other two projections changes its sign. Denote these changes as follows:

$$H_x = (+--), \quad H_y = (-+-), \quad H_z = (--+),$$

where the indices x, y, and z denote the rotation axis and $\pm$ are the new signs of interactions (in the original interaction, $H = H_0 = (+++)$. The effective Hamiltonian with the necessary values of the interaction constants (26) is obtained by summing four Hamiltonians:

$$TH_{\text{eff}} = t_0H_0 + t_xH_x + t_yH_y + t_zH_z. \tag{30}$$

The parameters for solving this problem with minimum time for each value of the phase are shown in Table 6. Table 7 presents the parameters for obtaining the inverse Fourier transform. Note that identical durations of the direct and inverse QFTs are obtained for different phases.

In [11], the authors found the minimum durations of the QFTs of two qubits for different phases and values of J by a numerical optimization method. In particular, for $J = 0.8$, we obtain two values for the minimum duration from Table 6: $3\pi/2J = 5.89$ and $5\pi/2J = 9.82$, which well agree with the results of the numerical experiment of [11] for appropriate phases $\phi_m = (\Phi_m + 5\pi/8) \bmod (2\pi)$. The forms of the dependence of the QFT duration on J for small values of J also coincide.

To obtain experimentally the effective Hamiltonian with the parameters given in Tables 6 and 7 with the use of the procedure described in the previous section, we can construct a sequence of RF pulses separated by intervals of free evolution.

For a different form of the original spin–spin interaction, the necessary Hamiltonian can also be constructed by the above-described method with some variations. For example, if, in the original Hamiltonian, only the interaction between z components of spins is nonzero, as in [7], then the interactions between the x and y components can be obtained by rotations through an angle of 90° about the axes y and x, respectively.

5. ANALYSIS OF THE PHASE

We refer the phase considered in this work to the Aharon–Anandan phases [25] because there occurs a nonadiabatic cyclic evolution. Indeed, let us successively apply first the direct QFT and then the inverse QFT to an arbitrary state $|\Psi\rangle$. Denote the variables of the inverse QFT by an upper bar:

$$|\Psi(T + \overline{T})\rangle = \overline{U}(\overline{T})U(T)|\Psi\rangle = \exp\{-i\overline{\Phi}_m\}U_G^{-1}U_G \times \exp\{-i\Phi_m\}|\Psi\rangle = \exp\{-i\Delta\Phi\}|\Psi\rangle. \tag{31}$$

Depending on the parameters, the phase difference takes different values $\Delta\Phi = \overline{\Phi} + \Phi_m = -2\pi(p + \bar{p})/N$

according to (2). Following [25], we divide the phase obtained into the dynamic

$$\beta = \int_0^{\bar{T}} \langle\Psi|\bar{H}(\bar{t})|\Psi\rangle d\bar{t} + \int_0^T \langle\Psi|H(t)|\Psi\rangle dt \qquad (32)$$

and the geometric $\gamma = \Delta\Phi - \beta$ parts. For different states $|\Psi\rangle$ and different Hamiltonians, the relation between β and γ takes different values.

The study of the phases of optimized pulses with complex time dependence of the control field in expressions (14) and (15) for $H(t)$ requires separate consideration. Now we return to the case of time-independent Hamiltonians H_{eff} and $\bar{H}_{\text{eff}}$ for the direct and inverse QFTs, respectively. The eigenfunctions of these Hamiltonians coincide (by construction) with the eigenfunctions of the gate (5). In this basis,

$$|\Psi\rangle = \sum_{f=1}^{N} c_f|f\rangle, \quad \sum_{f=1}^{N} |c_f|^2 = 1. \qquad (33)$$

According to (8) and (9), Eq. (31) for a particular state of the basis yields

$$\bar{T}\langle f|\bar{H}_{\text{eff}}|f\rangle + T\langle f|H_{\text{eff}}|f\rangle = \Delta\Phi - 2\pi(\bar{m}_f + m_f). \quad (34)$$

Summing up these equations over f and taking into account that the traces of the Hamiltonians H_{eff} and $\bar{H}_{\text{eff}}$ are zero, we obtain

$$\Delta\Phi = 2\pi\sum_{f=1}^{N} \frac{\bar{m}_f + m_f}{N}. \qquad (35)$$

Substituting expressions (33)–(35) into (32), we obtain the following expressions for the dynamic and geometric phases:

$$\beta = -2\pi\sum_{f=1}^{N} (\bar{m}_f + m_f)\left(|c_f|^2 - \frac{1}{N}\right),$$
$$\gamma = 2\pi\sum_{f=1}^{N} (\bar{m}_f + m_f)|c_f|^2. \qquad (36)$$

For every set $\bar{m}_f$, m_f, by varying c_f, we can change the relation between the two phases (36), for example, we can get rid of the dynamic phase.

Note that the value of the phase (31) can be measured experimentally by an auxiliary spin, for example, by the NMR interferometer scheme from [36]

6. CONCLUSIONS

One and the same logical operator (gate) can be represented mathematically as an exponential function with different matrices in the exponent, whose eigenvalues may differ by values divisible by 2π. Each such matrix can be implemented on a physical system by an appropriate effective Hamiltonian. When an eigenvalues is changed by 2π, we pass to a new solution with the global phase changed by $2\pi/N$. First, the corresponding energy level of the effective Hamiltonian is shifted by $-2\pi/T$, and, second, all the levels experience a compensatory shift by $2\pi/NT$. As a result of such shifts, the implementation time T of a gate by the given Hamiltonian is changed. The construction rules for effective Hamiltonians and the values of implementation times depend on a chosen physical system. Above, we have considered the implementation of a QFT gate on a qutrit represented by a quadrupole nucleus with spin $I = 1$, as well as on a system of two qubits ($I = 1/2$). We have found effective Hamiltonians and minimum implementation times corresponding to different global phases. We have proposed schemes for their implementation by the NMR method by means of a sequence of RF pulses separated by intervals of free evolution. The conclusions made above have been confirmed by the agreement between analytic results for the minimum times of gates and the results obtained by numerical optimization methods.

Thus, we have explained how the phase factor affects the minimum implementation time of a gate. The general relations obtained on this way for the variation of the phase factor under the variation of the effective Hamiltonian of the gate will be useful both for systems of qubits and for systems of qudits. The phase factors considered should be controlled when constructing complex quantum circuits. Otherwise, they may spoil the interference pattern necessary for implementing a quantum algorithm [12]. Specific results obtained for the QFT are practically important for implementing quantum algorithms on nuclei with spin $I = 1$ with weak quadrupole interaction in a liquid-crystal matrix [33], as well as on heteronuclear systems of two spins with $I = 1/2$. In addition, they may find application in other multilevel physical systems, for example, for the QFT on atoms controlled by laser pulses, which were considered in [4, 30, 37].

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