ANALYSIS OF THE COMPLEXITY OF THE FORMALIZED CIRCUITS OF RAYCHEV

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Abstract - In this study is carried out an analysis of the classical and quantum complexity of the defined by the author formalized circuits and is shown, that the circuits require several classic computations. The formalized circuits of Raychev have almost the same quantum complexity as the non-general circuits. Since the represented circuit models are independent of the techniques for matrix decomposition and the processes for global optimization, used to find the quantum circuits for a given operator, on quantum computers can be made simulations with a high accuracy for the unitary propagators of molecular Hamiltonians. As an instance, we show how to be constructed a circuit model for a hydrogen molecule.

Key words: Quantum computing, circuit, operators, gates

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1. INTRODUCTION

In classic formalized schemes three factors determine the parameters of the implementation: the quality of the tools for computer design, which are used for mapping of the formalized circuits, the quality of the architecture, and the design on electrical/transistor level. Similarly, the three most important factors, which determine the parameters of the implementation of the quantum logic are summarized in: the tools for computer design, the programmable architecture and the implementation of the quantum operators. The quantum logic synthesis has shown that each unitary transformation can be realized by a set of single qubit operators plus CNOT. It should be noted that the arrays of quantum operators [22,23] usually are based on matrix decompositions. The goal of this study is to optimize the number of the used operators. However, these methods are suitable for execution according to the needs of the target logic, and not in a fixed architecture. The proposed formalized quantum scheme is suitable for simulation of each operator, by determining the values of the angle in the circuit; Thus, it can provide a certain target scheme through controlled operators. Considering the current limits of the quantum mechanics, on the basis of that formalized logic it may not be possible to realize a large quantum circuit. In this article, we use a method, based on several decompositions that can decompose an arbitrary n-qubit operator into a circuit, containing m-qubit operators and several diagonal operators. Mathematically, this means that each n-bit quantum operator can be expressed through the product of several m-qubit operators and several diagonal matrices.

2. THE CIRCUITS

In the classical and quantum complexities cases of the circuits, explained in [33], it is easy to be seen that they depend mainly on the values of the constantly controlled networks, such as the one in Fig. 5. Such a network, controlled by k qubits may be decomposed as 2^k CNOT gates and 2^k single rotational gates [12]. For example, the circuit, as illustrated for $k = 2$ in Fig. 5a, may be decomposed as in Fig. 5b. The values of the angles in the decomposed circuit are a solution of the linear equation system $M^k\theta = \phi$:

$$M^k = \begin{pmatrix} \theta_1 \\ \theta_2 \\ \vdots \\ \theta_{2^k} \end{pmatrix} = \begin{pmatrix} \phi_1 \\ \phi_2 \\ \vdots \\ \phi_{2^k} \end{pmatrix} \quad (1),$$

where k is the number of the control qubits in the network, and the entered values of M are defined as:

$$M_{ij} = (-1)^{b_i - 1 \cdot q_j - 1} \ (2),$$

in which the power is found by taking the scalar product of the standard binary code of the $i - 1$, b_{i-1} index, and the binary representation of $j - 1$ integer of the code of Gray g_{j-1}. Since M^k is a version of the matrix of Hadamard with reordered columns, we see that M is unitary. Thus $(M^k)^{-1} = 2^{-k}(M^k)^T$, the new values of the angles in the decomposed circuit are the result of a clean matrix vector multiplication [12]:

$$\theta = 2^{-k}(M^k)^T\phi \quad (3).$$

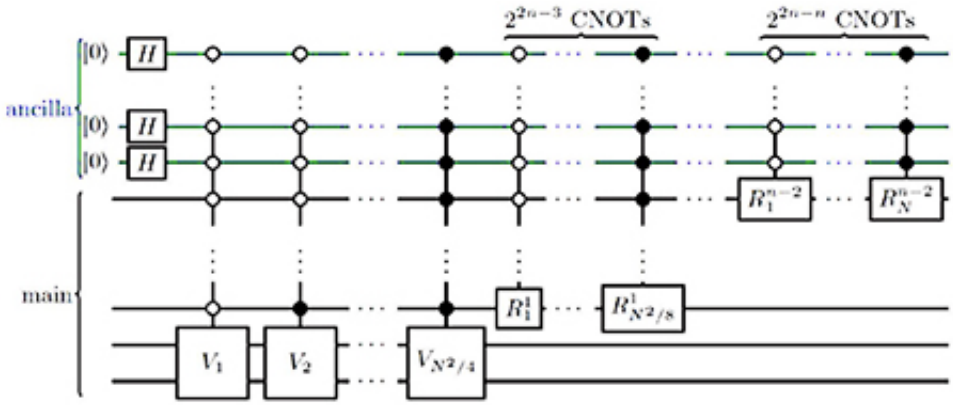


Fig. 1: The second circuit with initial blocks 4 by 4: The quantum gates in the networks controlled in a various way, after the V_i blocks, combine small blocks and construct the N by N blocks at the end. The initial Hadamards are for modification of the input data. The V_i blocks are for the step of formation.

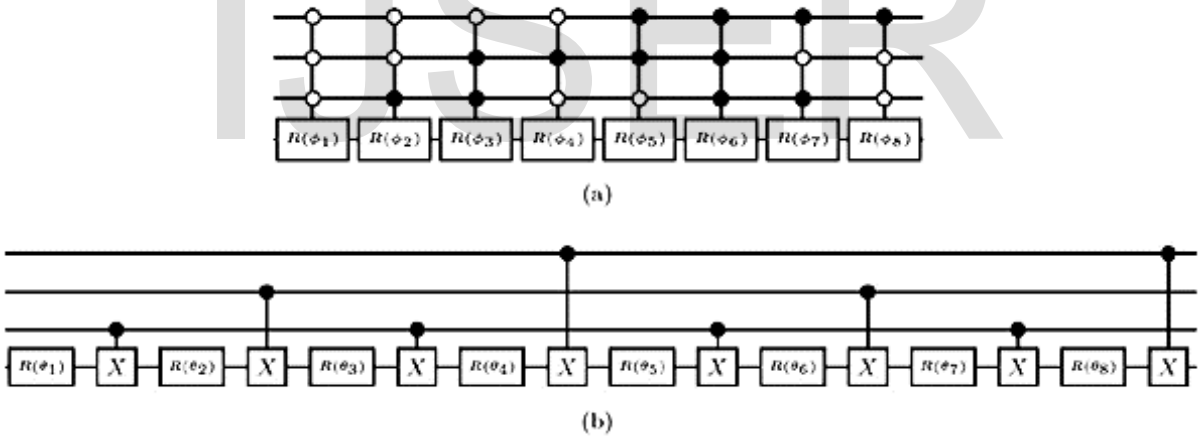


Fig. 2: (a) Multi-controlled network with a code of Gray. (b) The decomposition of the network with a code of Gray in (a) into CNOT and into single quantum gates.

A. The complexity of the first circuit model

1. The classical complexity

In the first diagram of a circuit (see Fig. 3), because there is only one such network, we must multiply the $2^{2n} \times 2^{2n}$ matrix by the vector of dimension 2^{2n}, designed by taking the arc-cosines of each element of U. From here the classical complexity for each first circuit is $O(2^{4n})$. Since M is a reordered version of the matrix of Hadamard, through the use of a fast Hadamard transform [21], that requires $O(NlogN)$ computations for vector transformation through a matrix of Hadamard, this can be achieved in:

$$O(2^{2n}\log(2^{2n})) = O(2n2^{2n}) \quad (4).$$

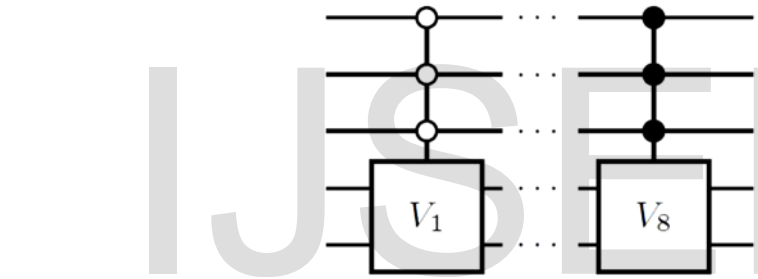
2. The quantum complexity

The quantum complexity of the circuit is the number of the gates needed to decompose the network, the combination of the blocks and their input modifications: 2^{2n} CNOT, 2^{2n} single rotation, $2n$ Hadamard, and n SWAP gates.

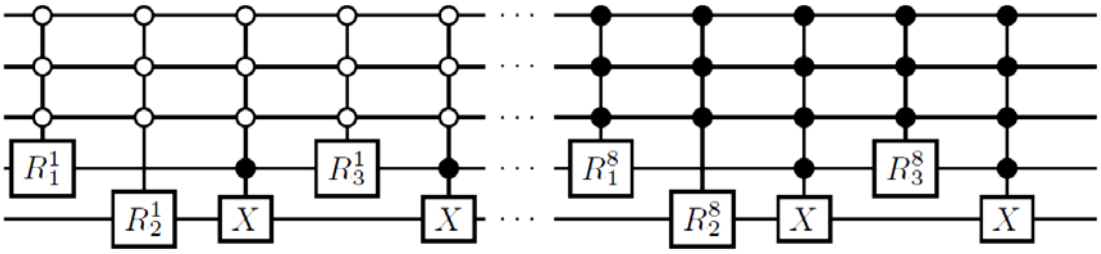
B. The complexity of the second circuit

The classical and quantum complexity for the second circuit are defined by the number of networks, which are formed by placing the quantum gates in blocks, controlled together, as shown in Fig. 6 and from the steps for combination. Since the quantum gates in the different blocks with the same angles operate for all cases of the control qubits, their placement together does not produce networks. Instead, they must be applied only once such as the control X gates, shown in Fig. 6c. From here, if the initial blocks of 2^c by 2^c (operating on c qubits) include m various quantum gates (the type of the gates is the same, but each ones requires various angles in various blocks such as R^1_1 and R^8_1 in Fig. 6), these blocks together produce m networks with code of Gray, controlled by 2^{2n-c} qubits.

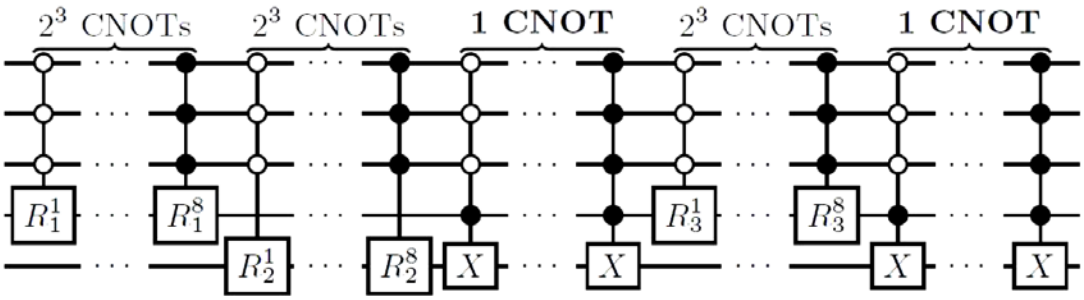
Additionally, in the step for combination we use binary coded networks on each one of the main qubits with the exception of the last c qubits for producing N by N blocks. Thus, we also have $n - c$ networks with code of Gray for the step for combination, for which the number of the control qubits decrease by one from one step of combination to another (or from one network with code of Gray to another). The classical and quantum complexity will be determined mainly by the decompositions of these $m + (n - c)$ networks.



(a)



(b)



(c)

Fig. 3: The circuit in (a) with initial blocks 4 by 4 can be represented as in (b) through the use of the circuit, given in Fig. (7). Without altering the order of the gates, that have the same control state, the gates can be relocated in order to form permanently controlled networks, such as in (c): If a gate have the same value of the angle for all control states such as the control X gates in the circuit, they are equivalent to a single gate (in the case of a X gate in the circuit is necessary only one CNOT).

1. Classical complexity

As we said in [33], in the step of forming, the combination of decomposed block circuits together form m networks with code of Gray for m different gate as represented for two-qubit blocks in Fig. 6. From here in order to find the decompositions of these networks, as in Fig. 5b through the formula given in equation (15), are necessary m number of matrix-vector multiplications: The dimensions of the matrices are $2^{2n-c}\times 2^{2n-c}$, and the dimensions of the vectors are 2^{2n-c}. Using a fast Hadamard transform, the complexity of this part will be $O_f = O\ (m(2n-c)(2^{2n-c}))$ instead of $O\ (m(2^{2n-c})^2)$ by a simple matrix-vector multiplication.

In addition, the step for combination is summation of the computations made to find the angles of the $(n\text{-}c)$ networks with code of Gray (remember, that the number of the control qubits reduces by one from one network to another). This is equal to $O\ ((2^{2n-c-1})2)+O\ ((2^{2n-c-2})^2)+\cdots+O\ ((2^{2n-c-n+c})^2) = O\ (2^{4n-2c}-2^{2n})$ through a simple matrix-vector multiplication. Through a fast Hadamard transform, the complexity of the step for combination is as follows:

$$O_c = O\big((2n-c-1)(2^{2n-c-1})\big) + O\big((2n-c-2)(2^{2n-c-2})\big) + \cdots + O(n2^n)$$
$$= O\Big(2\times(1-(2n-c)2^{2n-c-1} + (2n-c-1)2^{2n-c}) - O\big(2\times(1-n2^{2n-1} + (n-1)2^n)\big)\Big)$$
$$= O\big((2n-c-2)2^{n-c} - (n-2)2^n\big) \qquad (5).$$

Thus, while the total complexity through the elementary multiplication is

$$= O(2^{4n-2c} - 2^{2n}) + O(m(2^{2n-c})^2)$$
$$= O\big((m+1)2^{4n-2c} - 2^{2n}\big) \qquad (6),$$

through a fast Hadamard transform, it is:

$$O_f + O_c = O\big((m+1)(2n-c)2^{2n-c} - 2^{2n-c+1} - (n-2)2^n\big) \qquad (7).$$

2. The quantum complexity

In regard to the quantum complexity the analysis follows the same structure: as was mentioned before, the m different gates in the blocks on c qubits create m networks, that are controlled by $2n-c$ qubits. The decomposition of these networks requires $m2^{2n-c}$ CNOT and the same number of single gates.
Since the $n-c$ combinations ($n-c$ *network*) are needed, the complexity of the step for combination is the sum of the $n-c$ periods: $2^{2n-c-1} + 2^{2n-c-2} + \cdots + 2^{2n-c-n+c} = 2^{2n-c} - 2n$.

After this the total CNOT complexity shall be read as:

$$2^{2n-c} - 2^n + m2^{2n-c} + \Phi = (m+1)2^{2n-c} - 2^n + \Phi \quad (8),$$

where Φ represents the gates in each block, which must be run only once.

For example: As an example the complexity of a basic block circuit with size of 4 by 4 can be found as follows: Through the use of a decomposition of Schmidt[4] each 1 by 4 single vector $\mathbf{u_x}$ may be decomposed as: $\boldsymbol{u_x} = \sum^2{}_{i=1}\ a_i \boldsymbol{v^1}_i \otimes \boldsymbol{v^2}_i$. Since V_1 and V_2, composed of vectors $v^1{}_i$ and $v^2{}_i$, are 2 by 2 unitary matrices, these matrices (with the elements (cos_1 and sin_1 for V_1 and cos_2 and sin_2 for V_2) and the coefficients satisfying $|a_1|^2 + |a_2|^2 = 1$, can be accepted for rotational gates. For the coefficients, a_1 and a_2 are values of cosine and sine of a rotational gate ($a_1 = cos_a$ *and* $a_2 = sin_a$). The obtained decomposition becomes equal to the following:

$$U_x^T = \begin{pmatrix} a_1 cos_1 cos_2 + a_2 sin_1 sin_2 \\ -a_1 cos_1 sin_2 + a_2 sin_1 cos_2 \\ -a_1 sin_1 cos_2 + a_2 cos_1 sin_2 \\ a_1 sin_1 sin_2 + a_2 cos_1 cos_2 \end{pmatrix} \quad (9),$$

which generally requires three rotational gates. The circuit, given in Fig. 7, form each $\mathbf{u_x}$ as a leading row of its 4 by 4 matrix.

Therefore, this circuit for realization of the blocks in Fig. 4 gives $c = \Phi = 2$ and $m = 3$; thus the CNOT complexity of the entire circuit in Fig. 4 is reported as $2^{2n} - 2n + 2$. Please also pay attention that if the blocks in the circuit, shown in Fig. 4, were of a size 2 by 2, then the complexity would be $2^{2n} - 2^n$.

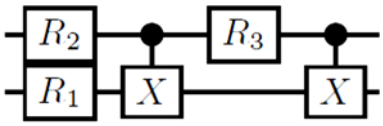


Fig. 4: The quantum circuit, which is found by following the decomposition of Schmidt and can generate any vector of a size 4 as the first row of its matrix presentation.

C. Comparison with the non-formalized circuit models

The reported non-general circuit models possess CNOT complexities, varying from $O(n^3 2^{2n})$ to the most effective one $\frac{3}{4}\, 2^{2n} - \frac{3}{2}\, 2^n$. The proven lower limit for the CNOT complexity is $(2^{2n-2} - 3n/4 - 1/4)$ without the use of ancilla qubits[20]. Although the circuit models given in this report, are main and fixed dimensions for each operator, their complexity is greater approximately by a factor of 2, in comparison with the non-general circuits. Additionally, if we can make m less than or equal to 2^{c-2}, then we can also go below the lower limit. This is likely to become, since the usual quantum gates in the blocks (as two CNOT in 4 by 4 blocks) do not have influence on the upper limit of the complexity. From here, by taking advantage of this property, the upper limit of the complexity can be decreased by using higher Hilbert spaces.

D. Simulation of Molecular Hamiltonians

The exponential growth of computational complexity in terms of the number of atoms is a huge challenge for the accuracy of the quantum chemical computations. Even for a simple molecule such as the methanol, the use only of 6-31G** basis for valence electrons, exist 50 orbitals. The 18 valence electrons may be distributed in these orbitals in a manner that satisfies the principle of exclusion of Pauli. This leads to around 10^{17} possible configurations, which makes the computation of the full configuration interaction (FCI) almost impossible on the classical computers[6]. It is known, however, that the quantum computer can be used for effective evaluation of the energies in the ground and exited state of the molecules[6,23–32]. For simulation of the quantum systems it is necessary to be found an equivalent quantum circuit to the unitary propagator of the Hamiltonian that represents this system. The molecular electronic Hamiltonian, in the approximation of Born-Oppenheimer, has been described in the second quantization form as [6,16,27]:

$$H = \sum_{pq} h_{pq} a_p^\dagger a_q + \frac{1}{2} \sum_{pqrs} h_{pqrs} a_p^\dagger a_q^\dagger a_s a_r \quad (10),$$

where the matrix elements h_{pq} and h_{pqrs} are a set of one- and two-electron integrals, and a_j and $a^\dagger_j$ spinless fermionic operators of annihilation and creation. Lets suppose that the set of single-particle spatial functions compose the molecular orbitals $\{\varphi(\mathbf{r})\}^M_{k=1}$ and the set of spin orbitals$\{\chi(\mathbf{x})\}^{2M}_{p=1}$ is defined by $\chi_p = \varphi_i \sigma_i$, and the set of the spatial-spin coordinates x = (r, ω), where σ_i is a spin-function. The single-electron integral is defined as

$$h_{pq} = \int dx \chi_p^*(x) \left(-\frac{1}{2}\nabla^2 - \sum_\alpha \frac{Z_\alpha}{r_{\alpha x}} \right) \chi_q(x) = \langle \varphi_p | H^1 | \varphi_q \rangle \delta_{\sigma_p \sigma_q} \quad (11),$$

and the two-electron integral is:

$$h_{pqrs} = \int dx_1 dx_2 \frac{\chi_p^*(x_1) \chi_q^*(x_2) \chi_s(x_1) \chi_r(x_2)}{r_{12}} = \langle \varphi_p | \langle \varphi_q | H^2 | \varphi_r \rangle | \varphi_s \rangle \delta_{\sigma_p \sigma_q} \delta_{\sigma_r \sigma_s} \quad (12),$$

where r_{ax} is the distance between the a^{th} nucleus and the electron, r_{12} is the distance between the electrons, ∇^2 is the Laplacian of electron-spatial coordinates, and $\chi_p(x)$ is a selected single-particles basis: $\chi_p = \varphi_p\sigma_p$, $\chi_q = \varphi_q\sigma_q$,$\chi_r = \varphi_r\sigma_r$, и $\chi_s = \varphi_s\sigma_s$.

In order to describe the hydrogen molecule in a minimal basis, which is the minimum number of spatial functions required to describe the system, one spatial function is necessary per one atom, marked as φ_{H1} and φ_{H2}. The molecular spatial orbitals are defined by symmetry: φg = φH1 + φH2 and φu = φH1 − φH2; which corresponds to four spin-orbitals: $|\chi 1\rangle = |\varphi g\rangle|a\rangle$, $|\chi 2\rangle = |\varphi g\rangle|\beta\rangle$, $|\chi 3\rangle = |\varphi u\rangle|a\rangle$, and $|\chi 4\rangle = |\varphi u\rangle|\beta\rangle$. The basis STO-3G is used in order to calculate the dimensional integrals of the Hamiltonian which is defined as $H = H^{(1)} + H^{(2)}$, where since $h_{pqrs} = h_{pqsr}$, $H^{(1)}$ *and* $H^{(2)}$ are simplified as[6,16,27]:

$$H^1 = h_{11}a_1^\dagger a_1 + h_{22}a_2^\dagger a_2 + h_{33}a_3^\dagger a_3 + h_{44}a_4^\dagger a_4 \quad (13)$$

and

$$H^2 = h_{1221}a_1^\dagger a_2^\dagger a_1 a_2 + h_{3443}a_3^\dagger a_4^\dagger a_3 a_4 + h_{1441}a_1^\dagger a_4^\dagger a_1 a_4 + h_{2332}a_3^\dagger a_2^\dagger a_3 a_2 + (h_{1331} - h_{1313})a_1^\dagger a_3^\dagger a_1 a_3 + (h_{2442} - h_{2424})a_2^\dagger a_4^\dagger a_4 a_2 + h_{1423}\left(a_1^\dagger a_4^\dagger a_2 a_3 + a_3^\dagger a_2^\dagger a_4 a_1\right) + +h_{1243}(a_1^\dagger a_2^\dagger a_4 a_3 + a_3^\dagger a_4^\dagger a_2 a_1) \quad (14).$$

The values of the spatial integral, calculated for the atomic distance 1.401a.u., the Hamiltonian matrix, found as 16 by 16 matrix[6], such that 4 qubits are necessary for realizing an unitary propagator of this Hamiltonian, which is found by e^{-iHt} by adjusting t = 1. [33].

The accuracy of the circuit model for the unitary propagator also defines the simulation accuracy. The quantum circuits generation through the use of techniques for matrix decomposition or methods of global optimization [34] requires the search of a huge complex space and simulation of the quantum systems unitary matrices on classical computers. For large matrices, this affects the efficiency, and consequently, the circuits's accuracy. Since the angles of the rotational gates in our circuits are defined directly by the matrix elements (e.g. in the first circuit, Fig. 3), we only take the values arcosine, and the generation of these angles requires only a few calculations; the circuits always have high accuracy and efficiency. This helps to be obtained very accurate circuit models for the simulation of the quantum circuit. For example, for the 16 by 16 unitary propagator of hydrogen molecules, given in reference 6, are required nine qubits in the circuit scheme in Fig. 3. Since the unitary propagator is extremely disperse and has only 19 non-null elements, the most of the constantly controlled gates in the circuit will be identity, except for 19 of them. From here in Annex B, we show how to reduce the number of the qubits to 6 qubits, Fig. 8. We give the rotational values for the gates in Table I. Therefore, since our circuit models have a fixed model, the use of different basic sets or parameters for computation of the Hamiltonian will not change the circuit model, and its accuracy.

Briefly, we represent general formalized quantum circuits, which can simulate any given 2^n by 2^n real matrix. Due to the structure of the circuits, they may be used for production of specific or multi-functional quantum chips and processors. Since the circuit models depend exclusively from the matrix elements, for the application of specific circuits, aiming to realize a certain type of systems, each level of rarity in the system can reduce the number of the gates significantly. Additionally, we show that, the generation of circuits with complexity less than the lower limit is possible, by making $m \leq 2^{c-2}$ and increasing Φ in the given complexity.

3. CONCLUSION

It is important to note that, in this work, although we have in mind real matrices, it is not difficult to realize each complex case both through consideration of each rotational gate as capable to produce each complex element of an unitary matrix in the first model of a circuit. This may require more than one conventional rotational gate, but should not increase the upper limit of the quantum complexity. The modification of the second circuit, however, may not be so simple, as in the first one: it may require additional gates during the steps for combination and formation.

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