

Analytic Constructions of General n -Qubit Controlled Gates

Yang Liu¹, Gui Lu Long^{1*}, † and Yang Sun²

¹Key Laboratory of Atomic and Molecular NanoSciences and Department of Physics,
Tsinghua University, Beijing 100084, P. R. China

² Department of Physics and Astronomy, University of Notre Dame, Indiana 46556, USA
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In this Letter, we present two analytic expressions that most generally simulate n -qubit controlled- U gates with standard one-qubit gates and CNOT gates using exponential and polynomial complexity respectively. Explicit circuits and general expressions of decomposition are derived. The exact numbers of basic operations in these two schemes are given using gate counting technique.

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I. Introduction— The study of quantum computers has been developing very rapidly over the past years. It provides exponential speedup in factoring [1], or square-root speedup in unsorted database search [2]. In the circuit model of universal quantum computer [3], the unitary operation that completes a computation task is a series of gates on a fixed number of qubits. Any unitary gate can be constructed from a set of universal gates [3, 4]. Using the smallest number of basic gates to construct an arbitrary unitary transformation is very important, not only for using less executing time, but also for resulting less errors.

Complexity of circuit is measured in terms of the number of basic gates, namely the one-bit gate and the two-bit CNOT gate. For a general $2^n \times 2^n$ unitary matrix U with 4^n degrees of freedom, $O(4^n n^2)$ elementary operations are needed in principle [5]. Later on, efficient schemes implementing arbitrary quantum gates have reduced the circuit complexity to $O(4^n)$ [6, 7, 8]. They are achieved by using the QR decomposition [6], or the cos-sin decomposition [7]. General scheme for decomposing an arbitrary gate is given in Ref. [8] using numerical method. For some quantum information task, such as initialization, a more efficient scheme with complexity $O(2^n n^2)$ was proposed [9].

$C^n(U)$ gates are typical n -qubit fully controlled- U gates that apply a unitary U to the target qubit if and only if all the first $n - 1$ control qubits are 1. Circuits for $C^2(U)$, $C^3(U)$ and $C^4(U)$ gates have been constructed [10, 11, 12, 13]. But for the general case with $n \geq 5$, the explicit construction is absent. In this Letter, we present two different construction schemes for an arbitrary $C^n(U)$ gate, one uses an exponential and the other uses polynomial number of CNOT and one-qubit gates. The polynomial complexity scheme is good for large scale quantum computing. The exponential complexity scheme prevails for a circuit with a small qubit number. In particular, they are analytic. These results

are very appealing in designing quantum computer programming language, because it not only saves computing time for its construction, but also avoids errors in numerical construction because of error accumulation.

II. Exponential Construction Scheme— First we introduce some notation. For a generic n -qubit circuit, its qubits are numbered from the top from 1 to n . $\wedge^k(V)$ stands for a controlled- V gate with k control qubits and one target qubit, so $C^n(U)$ gate is equally represented by $\wedge^{n-1}(U)$ whose $n - 1$ control qubits positioned at the top and the target qubit at the bottom. Order of operations in an expression as well as in circuits are performed from left to right.

Previous investigations gave explicit networks of $C^n(U)$ gates for $n = 2, 3, 4$. In this Letter, we present a general analytic scheme implementing $C^n(U)$ gates for arbitrary values of n and any unitary operator U . Firstly, we define two kinds of quantum gate-array blocks, the A -block and the B -block as shown in Fig.1.

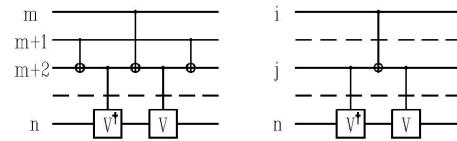


FIG. 1: A and B blocks in repair section. The left part is a A -block, the right one is a B -block.

The A -block is indicated as A^m , where $m = 1, \dots, n - 3$. Its qubit nodes involve qubits $m, m + 1, m + 2$ and n . The B -block is labeled as B_j^i , where $1 \leq i < j < n$. Its qubit nodes involve qubits i, j and n . First we suppose the explicit gate-array components of $C^{n-1}(U)$ network has been known, then we give a general analytic expression. Our strategy for $C^n(U)$ network is a two-step procedure: basic section constructing in the left part and repair section constructing in the right part of the circuit. Basic section is obtained by combining $C^{n-1}(U)$ network with a control input that is the $(n - 1)$ -th line without any performance. The basic section of $C^n(U)$ network is indicated as $\widetilde{C^{n-1}}$. $\widetilde{C^{n-1}}$ contains $2^{n-2} - 2$ CNOT gates, $(2^{n-2} - 1)$ number of $\wedge^1(V)$ and $\wedge^1(V^\dagger)$ gates,

*Corresponding author

where $V^{2^{n-2}} = U$. Repair section is yielded by placing A^m and B_j^i gate-array blocks in an alternating sequence with respective number of 2^{n-4} .

A β -bit Gray code [14] strings $\{g_\alpha\}$, where $\alpha = 1, \dots, 2^\beta$ is a palindromelike ordering with special property that the adjacent bit strings differ only by a single bit. We define a function $\gamma(\alpha, \beta)$ to represent the numerical value of the position where g_α and $g_{\alpha+1}$ differ. In the repair section of $C^n(U)$, the index m of A^m block is definite as $n - 3$, the index j of B_j^i blocks is definite as $n - 1$, whereas index i varies complying with a $(n-4)$ -bit binary

Gray code strings sequence. Denote \widetilde{C}^k as a network obtained from $C^k(U)$ gate combined with $n - k$ extra qubits positioned between its last two qubits. Carrying out the recursion, the following results are obtained:

$$\begin{aligned} C^5(U) &= \widetilde{C}^4 A^2 B_4^1 A^2 B_4^1, \\ C^6(U) &= \widetilde{C}^5 A^3 B_5^2 A^3 B_5^1 A^3 B_5^2 A^3 B_5^1, \\ C^7(U) &= \widetilde{C}^6 A^4 B_6^3 A^4 B_6^2 A^4 B_6^3 A^4 B_6^1 A^4 B_6^3 A^4 B_6^2 A^4 B_6^3 A^4 B_6^1, \\ &\vdots \\ C^n(U) &= \widetilde{C}^{n-1} A^{n-3} B_{n-1}^{n-4} A^{n-3} B_{n-1}^{n-3} \dots A^{n-3} B_{n-1}^1. \end{aligned} \quad (1)$$

So a generic $C^n(U)$ circuit where $n \geq 5$ can be expressed:

$$C^n(U) = \widetilde{C}^4 \prod_{\beta=1}^{n-4} \prod_{\alpha=1}^{2^\beta} A^{\beta+1} B_{\beta+3}^{\gamma(\alpha, \beta)}. \quad (2)$$

Given a unitary operator V , there must exist one-qubit unitary operations D , E , F and real number a such that $DEF = I$ and $e^{ia} D \sigma_x E \sigma_x F = V$. σ_x and G are unitary one-qubit operations corresponding to matrices

$\sigma_x = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$ and $G = \begin{bmatrix} 1 & 0 \\ 0 & e^{ia} \end{bmatrix}$. Let $C_{k'}^k(U)$ denote a $\wedge^1(U)$ gate where qubit k controls the qubit k' . We rewrite Eq. (2) in terms of CNOT and one-qubit gates after certain gate counting:

$$\begin{aligned} C^n(U) &= \widetilde{C}^4 \prod_{\beta=1}^{n-4} \prod_{\alpha=1}^{2^\beta} F_n^\dagger C_{\beta+3}^{\beta+2}(\sigma_x) C_n^{\beta+3}(\sigma_x) G_{\beta+3}^\dagger E_n^\dagger C_{\beta+3}^{\beta+1}(\sigma_x) \\ &\quad C_n^{\beta+1}(\sigma_x) G_{\beta+3} E_n C_{\beta+3}^{\beta+2}(\sigma_x) C_n^{\beta+2}(\sigma_x) G_{\beta+3}^\dagger E_n^\dagger \\ &\quad C_{\beta+3}^{\gamma(\alpha, \beta)}(\sigma_x) C_n^{\gamma(\alpha, \beta)}(\sigma_x) G_{\beta+3} E_n C_n^{\beta+3}(\sigma_x) F_n, \end{aligned} \quad (3)$$

where

$$\begin{aligned} \widetilde{C}^4 &= D_n C_n^1(\sigma_x) E_n C_n^2(\sigma_x) C_2^1(\sigma_x) G_2^\dagger E_n^\dagger C_n^2(\sigma_x) C_2^1(\sigma_x) E_n \\ &\quad C_n^3(\sigma_x) C_3^2(\sigma_x) E_n^\dagger G_2^\dagger C_3^1(\sigma_x) C_4^1(\sigma_x) G_3 E_n C_3^2(\sigma_x) \\ &\quad C_n^2(\sigma_x) G_3^\dagger E_n^\dagger C_3^1(\sigma_x) C_n^1(\sigma_x) E_n C_n^3(\sigma_x) G_1 G_2 G_3 F_n. \end{aligned} \quad (4)$$

In Eqs. (3,4), $C_{k'}^k(\sigma_x)$ are CNOT gates and the D , E , F , G and their hermitian conjugate are the one-qubit gates and their subscripts represent the positions. The β -bit binary Gray code strings reflected in a sequence of $B_{\beta+3}^{\gamma(\alpha, \beta)}$ can be chosen freely in an arbitrary cyclic β -qubit Gray code sequence and the $C^n(U)$ circuit for ($n \geq 3$) are self-inverse.

We can prove this exponential simulation fulfills the action of $C^n(U)$ faithfully. After a carefully accounting of merges of CNOT gates and single-qubit, we find this exponential simulation scheme for a $C^n(U)$ gate finally utilizes $2^n - 2$ CNOT gates and 2^n one-qubit gates.

III. Polynomial Construction Scheme – The above scheme is advantageous for small values of n , but it becomes inefficient for a large value of n , for instance $n > 8$ because of its exponential complexity. Here we propose a $C^n(U)$ circuit using $O(n^2)$ basic CNOT and one-qubit gates.

We know for $n \geq 3$, $C^n(U)$ can be simulated by a network with its own inverse, where $V^2 = U$ in Fig. 2.

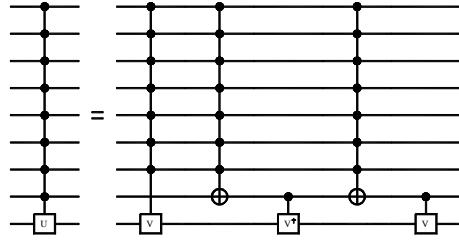


FIG. 2: A quantum circuit for implementing $C^n(U)$ gates with unitary V meeting $V^2 = U$.

Given the explicit construction of arbitrary $C^{n-1}(U)$ gate is known, the key procedure is to simulate two $\wedge^{n-2}(\sigma_x)$ gates. For $n \geq 4$ and $m_1 \in 1, \dots, n-2$, a $\wedge^{n-2}(\sigma_x)$ gate can be partitioned into two $\wedge^{m_1}(\sigma_x)$ gates and two $\wedge^{m_2}(\sigma_x)$ gates, where $m_1 + m_2 = n - 1$ as shown in Fig. 3.

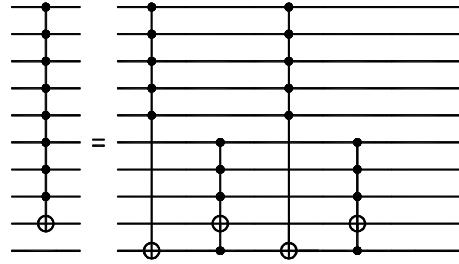


FIG. 3: A quantum circuit for implementing a $\wedge^{n-2}(\sigma_x)$ gate with $\wedge^{m_1}(\sigma_x)$ and $\wedge^{m_2}(\sigma_x)$ gates where $m_1 + m_2 = n - 1$.

So the problem is reduced to how to construct $\wedge^{m_1}(\sigma_x)$ and $\wedge^{m_2}(\sigma_x)$ gates. If we assign $m_1 = [n/2]$, $m_2 = n - [n/2] - 1$, $\wedge^{m_1}(\sigma_x)$ and $\wedge^{m_2}(\sigma_x)$ can be decomposed into several Toffoli gates. It is worthy noting that these decompositions are only applicable to $\wedge^{m_1}(\sigma_x)$ for $n \geq 6$ and to $\wedge^{m_2}(\sigma_x)$ for $n \geq 7$. So for $n \geq 6$, we investigate the most regular arrangement of Toffoli gates implementing $\wedge^{m_1}(\sigma_x)$ in Fig. 4. Let T_c^a denote a Toffoli gate with control qubits a and b , the target qubit c . Consider the characteristic features of such network: $\wedge^{m_1}(\sigma_x)$ network consists of $4[n/2] - 8$ Toffoli gates and the indices of Toffoli gates is symmetric around $i_0 = [n/2] - 1$ and periodic

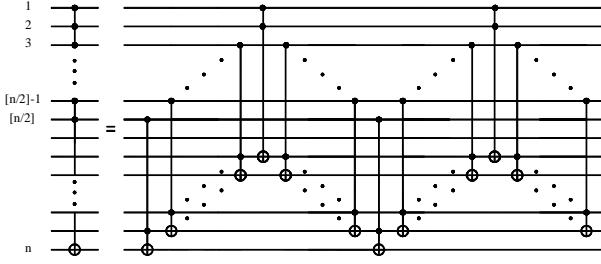


FIG. 4: A quantum circuit for a $\wedge^{m_1}(\sigma_x)$ gate consisting of Toffoli gates arranged most regularly.

with period $d = 2[n/2] - 4$, then use a formula to describe the regulation of Toffoli gates

$$\wedge^{m_1}(\sigma_x) = \prod_{i=1}^{4[n/2]-8} T_{n-[n/2]+2+f(n)}^{1+(1-\delta_{i,i_0})(1-\delta_{i,i_0+d})(n-[n/2]+f(n))}, \quad (5)$$

where $f(n) = |\frac{d}{2} + \frac{d}{\pi} \arctan(\tan(\frac{\pi}{d}i - \frac{\pi}{2})) - [\frac{n}{2}] + 1|$. It denotes the deviation of i to $\frac{n}{2} - 1$ when $1 \leq i \leq d$ or to $\frac{n}{2} - 1 + d$ when $d + 1 \leq i \leq 2d$. The absolute value function expresses symmetric property, the arctan function fixes periodic regulations, and the δ functions correspond to certain singular points at $i = [n/2] - 1$ and $3[n/2] - 5$ referred in above formalism.

Similarly, for $n \geq 7$, $\wedge^{m_2}(\sigma_x)$ gates can be simulated

by the network in Fig. 5. We find that there are $4n -$

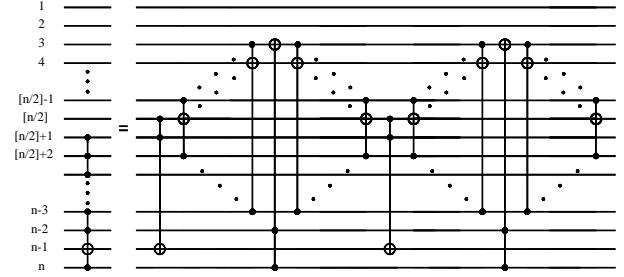


FIG. 5: A quantum circuit for a $\wedge^{m_2}(\sigma_x)$ gate consisting of Toffoli gates arranged most regularly.

$4[n/2] - 12$ Toffoli gates in $\wedge^{m_2}(\sigma_x)$ network. Inspecting the mathematic property of indices, it is periodic with period $d' = 2n - 2[n/2] - 6$, symmetric around $j_0 = n - [n/2] - 2$ and $j_0 + d' = 3n - 3[n/2] - 8$, we obtain the following formula

$$\wedge^{m_2}(\sigma_x) = \prod_{j=1}^{4n-4[n/2]-12} T_{n-1+(1-\delta_{j,1})(1-\delta_{j,2n-2[n/2]-5})}^{n+(1-\delta_{j,j_0})(1-\delta_{j,j_0+d'})(2[n/2]-2n+3+g(n))}, \quad (6)$$

where $g(n) = |\frac{d'}{2} + \frac{d'}{\pi} \arctan(\tan(\frac{\pi}{d'}j - \frac{\pi}{2})) - n + [\frac{n}{2}] + 2|$. Then we propose a cascade decomposition of $C^n(U)$ ($n \geq 7$) gate by a recursive method shown in Fig. 6, where unitary V_i is defined by $V_i^{2^i} = U$.

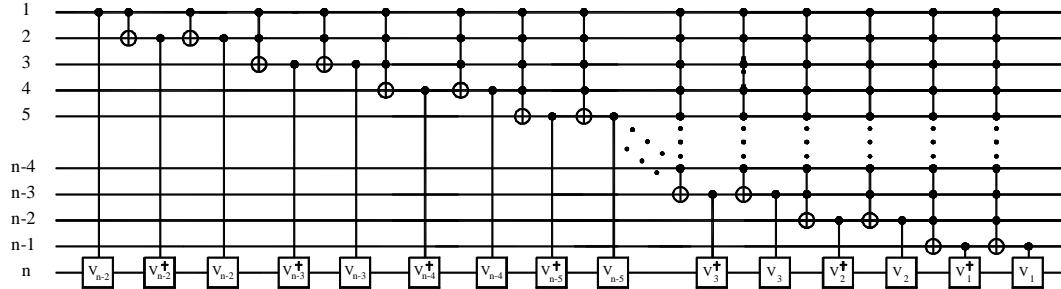


FIG. 6: Cascade structure of $C^n(U)$ gates where unitary V_i satisfies $V_i^{2^i} = U$.

Suppose $T_k^{\{1,2,\dots,k-1\}}$ is a $\wedge^{k-1}(\sigma_x)$ whose first $k - 1$ qubits control the last one qubit. Then above decomposition can be described in formula

$$\begin{aligned} C^n(U) &= \widetilde{C^{n-1}(V_1)} T_{n-1}^{\{1,2,\dots,n-2\}} C_n^{n-1}(V_1^\dagger) T_{n-1}^{\{1,2,\dots,n-2\}} C_n^{n-1}(V_1) \\ &= \widetilde{C^6(V_{n-6})} \prod_{k=7}^n T_{k-1}^{\{1,2,\dots,k-2\}} C_n^{k-1}(V_{n-k+1}^\dagger) T_{k-1}^{\{1,2,\dots,k-2\}} C_n^{k-1}(V_{n-k+1}), \end{aligned} \quad (7)$$

where $T_{k-1}^{\{1,2,\dots,k-2\}} = \wedge^{m_1}(\sigma_x) \wedge^{m_2}(\sigma_x) \wedge^{m_1}(\sigma_x) \wedge^{m_2}(\sigma_x)$. After tedious calculation, we find out a $C^n(U)$ gate totally requires 2 CNOT gates, $8n^2 - 72n + 174$

Toffoli gates and $2n - 3$ two-qubit controlled gates. Then the problem is reduced to simulating Toffoli gate with basic CNOT and one-qubit gates. Using well-known congruent modulo phase shift (CMPS) methods [15] for Toffoli gates, it can be expressed as $T_c^b = R_c C_c^b(\sigma_x) R_c C_c^a(\sigma_x) R_c^\dagger C_c^b(\sigma_x) R_c^\dagger$, where $R = R_y(\pi/4)$. The CMPS scheme only requires 7 basic operations which is much less than 14 basic operations in the usual simulation scheme. $\widetilde{C^6(V_{n-6})}$ part is congruent to the circuit

for $C^6(U)$ and we have proven that the Toffoli gates labeled as 4, 6, 8, 10, 15, 20, 25, 30 as shown in Fig. 7 for $\widetilde{C^6(V_{n-6})}$ part, and all the Toffoli gates other than $C^6(V_{n-6})$ in Eq. (7) can be replaced by the modulo phase shift of Tollofi gates.

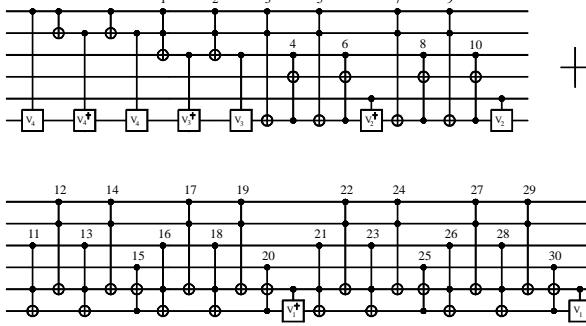


FIG. 7: The explicit structure of $C^6(U)$ (congruent to $\widetilde{C^6(V_{n-6})}$) in terms of Toffoli and two-qubit controlled gates.

Given a unitary operator V_{n-k+1} , L , P , R and S are one-qubit unitary gates such that $e^{ib}L\sigma_xP\sigma_xQ = V_{n-k+1}$, $LPQ = I$ and $S = \begin{bmatrix} 1 & 0 \\ 0 & e^{ib} \end{bmatrix}$, their subscripts represent which qubit they are performed on. Now we obtain the $C^n(U)$ in terms of CNOT and one-qubit gates:

$$\begin{aligned} C^n(U) = & \widetilde{C^6(V_{n-6})} \prod_{k=7}^n W_{k-1} W_{k-1} S_{k-1}^\dagger Q_n^\dagger C_n^{k-1}(\sigma) P_n^\dagger C_n^{k-1}(\sigma) L_1^\dagger \\ & W_{k-1} W_{k-1} L_n C_n^{k-1}(\sigma) P_n C_n^{k-1}(\sigma) S_{k-1} Q_n, \end{aligned} \quad (8)$$

where

$$\begin{aligned} W_{k-1} = & \left\{ \prod_{i=1}^{4[k/2]-8} R_{k-[k/2]+2+f(k)} \right. \\ & C_{k-[k/2]+2+f(k)}^{1+(1-\delta_{i,i_0})(1-\delta_{i,i_0+d})(k-[k/2]+f(k))}(\sigma_x) \\ & R_{k-[k/2]+2+f(k)} C_{k-[k/2]+2+f(k)}^{2+f(k)}(\sigma_x) R_{k-[k/2]+2+f(k)}^\dagger \\ & C_{k-[k/2]+2+f(k)}^{1+(1-\delta_{i,i_0})(1-\delta_{i,i_0+d})(k-[k/2]+f(k))}(\sigma_x) \\ & \left. R_{k-[k/2]+2+f(k)}^\dagger \right\} \\ & \left\{ \prod_{j=1}^{4k-4[k/2]-12} R_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))} \right. \\ & C_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))}^{k-2-g(k)}(\sigma_x) \\ & R_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))} \\ & C_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+3+g(k))}^{k+(1-\delta_{j,j_0})(1-\delta_{j,j_0+d'})(2[k/2]-2k+3+g(k))}(\sigma_x) \\ & R_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))}^\dagger \\ & C_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))}^{k-2-g(k)}(\sigma_x) \\ & \left. R_{k-1+(1-\delta_{j,1})(1-\delta_{j,1+d'})(2[k/2]-2k+5+g(k))}^\dagger \right\}. \end{aligned}$$

Taking account of the merges of CNOT gates and one-qubit gates, we obtain the total number of basic operations in $C^n(U)$ construction are $24n^2 - 212n + 540$ CNOT gates and $32n^2 - 288n + 739$ one bit gates ultimately.

IV. Conclusions— In conclusion, we have given two analytic schemes for constructing a $C^n(U)$ gate for arbitrary value of n and any unitary U operator, one with exponential complexity and the other with polynomial complexity. General expression for decomposition of $C^n(U)$ gats with basic one-qubit gates and CNOT gates has been derived explicitly. We have compared the exact numbers of basic operations required in these two methods for $n = 1 - 20$. It shows that the exponential construction is advantageous for the value of $n = 1 - 8$, whereas the polynomial simulation is efficient for larger values of $n > 8$.

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[†] Electronic address: gllong@mail.tsinghua.edu.cn

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