

# Quantum Circuits of AES with a Low-depth Linear Layer and a New Structure

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**Abstract.** In recent years quantum computing has developed rapidly. The security threat posed by quantum computing to cryptography makes it necessary to better evaluate the resource cost of attacking algorithms, some of which require quantum implementations of the attacked cryptographic building blocks. In this paper we manage to optimize quantum circuits of AES in several aspects. Firstly, based on de Brugière *et al.*'s greedy algorithm, we propose an improved depth-oriented algorithm for synthesizing low-depth CNOT circuits with no ancilla qubits. Our algorithm finds a CNOT circuit of AES MixColumns with depth 10, which breaks a recent record of depth 16. In addition, our algorithm gives low-depth CNOT circuits for many MDS matrices and matrices used in block ciphers studied in related work. Secondly, we present a new structure named compressed pipeline structure to synthesize quantum circuits of AES, which can be used for constructing quantum oracles employed in quantum attacks based on Grover and Simon's algorithms. When the number of ancilla qubits required by the round function and its inverse is not very large, our structure will have a better trade-off of  $D$ - $W$  cost. We then give detailed quantum circuits of AES-128 under the guidance of our structure and make some comparisons with other circuits. Finally, our encryption circuit and key schedule circuit have their own application scenarios. The Encryption oracle used in Simon's algorithm built with the former will have smaller depth. For example, we can construct an AES-128 Encryption oracle with  $T$ -depth 33, while the previous best result is 60. A small variant of the latter, along with our method to make an Sbox input-invariant, can avoid the allocation of extra ancilla qubits for storing key words in the shallowed pipeline structure. Based on this, we achieve a quantum circuit of AES-128 with the lowest  $T$  of  $D$ - $W$  cost 130720 to date.

**Keywords:** Quantum circuit · Depth · AES · Encryption oracle

## 1 Introduction

Quantum computers provide a great potential of solving certain important information processing tasks that are intractable for any classical computer. Shor's algorithm [Sho94] showed that a sufficiently large quantum computer allows to factor numbers and compute discrete logarithms in polynomial time, which represents an exponential speed-up compared to classical algorithms and can be devastating to many public-key encryption schemes in use today.

The possible emergence of large-scale quantum computing devices in the near future has brought new security threats and raised concerns about post-quantum security. Not only the public-key cryptosystem, the security of the symmetric-key cryptosystem is also under threat. A trivial application of Grover's algorithm [Gro96] results in a quadratic

speedup of the exhaustive search attack. Simon’s algorithm [Sim97] answers the question of how to find the period of a periodic function with  $n$  input bits in  $O(n)$  quantum queries. As a result, many encryption structures and the most widely used modes of operation for authentication and authenticated encryption were attacked by using Simon’s algorithm [KLLNP16a, LM17]. Both of these two algorithms require the quantum oracle of the symmetric building block to be attacked. Moreover, the National Institute of Standards and Technology (NIST) used the complexity of the quantum circuit for AES with a bound of depth called MAXDEPTH as a baseline to categorize the post-quantum public-key schemes into different security levels in the call for proposals to the standardization of post-quantum cryptography<sup>1</sup>. Both these reasons give rise to the growing appeals for studying the quantum implementations of symmetric-key building blocks as well as how to optimize them. This helps understand the quantum security of current encryption schemes and guides future post-quantum encryption designs.

The synthesis and optimization of quantum circuits have been studied for many years [SBM05, SM13, JST<sup>+</sup>20, AMMR13, AMM14, STY<sup>+</sup>23]. Given an  $n$ -qubit unitary operator and an available gate set  $\mathcal{G}$ , synthesis algorithms find one of its implementations described as a sequence of  $G$  quantum gates in  $\mathcal{G}$  with width (number of qubits)  $W$ , full depth  $FD$  and  $T$ -depth  $TD$ . The optimization of  $G$  and  $W$  is related to the saving of resources and qubits, while the optimization of  $FD, TD$  is also concerned due to the phenomenon of quantum decoherence. In addition, it is worth noting that there is a lot of work on optimizing quantum circuits on some noisy intermediate-scale quantum (NISQ) devices (see [Pre18, WHY<sup>+</sup>19, ZFX22] for an incomplete list). In the process of quantum computation, since it has been difficult to isolate qubits for a long time, qubits would interact unintentionally with external elements, which would distort the results. Assuming that two non-overlapping gates can run in parallel, the running time of the circuit is related to its depth. Therefore, the proper execution of complex algorithms can be significantly facilitated by optimizing the depth of quantum circuits since the decoherence time is very limited. The reduction of  $T$ -depth is more important in fault-tolerant computations where the running time is dominated by  $T$ -depth [Fow12].

Recent research on quantum implementation of symmetric ciphers mainly focuses on AES due to its popularity and importance. The main concerns are the structure, AES MixColumns and AES S-box. At the same time, there is also related work focusing on quantum implementations of other symmetric building blocks [ZLW<sup>+</sup>22]. One research line is to optimize the width. Grassl *et al.* proposed the first quantum circuit of AES under the so-called zig-zag structure with low width [GLRS16]. Zou *et al.* proposed the improved zig-zag structure, and then Huang *et al.* presented the OP-based round-in-place structure with a similar idea. Jaques *et al.* first proposed the straight-line structure of key schedule process with no ancilla states and first adopted the pipeline structure. Furthermore, Jang *et al.* proposed the shallowed pipeline structure to reduce the full depth. Li *et al.* directly designed an in-place quantum circuit of AES S-box with low width and constructed a straight-line circuit of AES with the lowest width to date [LGQW23]. During the research on quantum circuits of AES, many researchers studied low-width quantum circuits of AES S-box.

The other research line is to reduce the circuit depth. In Clifford+ $T$  circuits,  $T$ -depth is the main concern since Clifford gates are much cheaper than the  $T$  gate. The pipeline structure, first mentioned in reversible logic implementations of AES in [DSSR13], is straightforward to provide a low  $T$ -depth circuit of AES in many studies. To synthesize low  $T$ -depth AES S-box, usually a low Toffoli-depth Sbox which computes redundant states is designed. Jaques *et al.* constructed an Sbox with Toffoli-depth 6, and then gave a quantum circuit of AES-128 with  $T$ -depth 120. Li *et al.* [LCS<sup>+</sup>22] proposed an Sbox

<sup>1</sup><https://csrc.nist.gov/CSRC/media/Projects/Post-Quantum-Cryptography/documents/call-for-proposals-final-dec-2016.pdf>

with Toffoli-depth 4. Huang *et al.* also gave an Sbox with Toffoli-depth 4, and further gave one with Toffoli-depth 3, which is the theoretical minimum. Therefore, the  $T$ -depth of quantum circuit of AES-128 is reduced to 60 [HS22]. The width of Sbox was further reduced by Jang *et al.*'s and Liu *et al.*'s techniques [JBK<sup>+</sup>22, LPZW23], while the saving of qubits made the optimized Sbox no longer input-invariant.

Full depth is a forward-looking time-cost measure for quantum circuits, so optimizing the depth of a CNOT circuit can reduce the full depth of the entire circuit. CNOT circuits which consist only of CNOT gates appear as subcircuits of larger circuits, such as quantum oracles of symmetric ciphers, stabilizer circuits [AG04], and CNOT+ $T$  circuits. Patel *et al.* and Jiang *et al.* proposed methods to generate CNOT circuits with asymptotic optimal gate count and space-depth trade-off, respectively [PMH08, JST<sup>+</sup>20]. For specific matrices, Xiang *et al.*'s method [XZL<sup>+</sup>20] is based on some reduction rules for matrix decomposition, can effectively reduce the number of gates of given CNOT circuits and provides CNOT circuits with the smallest CNOT gates to date for many MDS matrices and matrices used in block ciphers. A lot of work on quantum circuits of AES (see [ZWS<sup>+</sup>20, HS22, JBK<sup>+</sup>22, LGQW23] for an incomplete list) adopted the implementation of AES MixColumns with 92 CNOT gates provided by Xiang *et al.*'s method. Its depth estimation given by the Q# resource estimator is 30. However, their method does not take the circuit depth into account. Zhu *et al.* defined the exchange-equivalence of sequences, and proposed a framework of optimizing the depth a given CNOT circuit [ZH22] by exploring the possibility of exchanging CNOT gates. They started the optimization with the results of Xiang *et al.*'s method and gave a better estimation of depth 28 for AES MixColumns. Recently Liu *et al.* proposed a method for computing the depth of given quantum circuits and provided a circuit of AES MixColumns with depth 16 by computing the depth of many search results of Xiang *et al.*'s method. Some CNOT circuits of AES MixColumns with ancilla qubits are synthesized on the basis of optimized low-depth classical circuits, and the state-of-art classical circuit of AES MixColumns with minimum depth 3 requires 99 XOR gates [SFX23]. In addition, de Brugière *et al.* proposed a depth-oriented greedy method and a block algorithm for small and middle scale matrices, respectively [dBBV<sup>+</sup>21b]. However, their methods have not been tested on the linear layers of many cryptographic building blocks.

## 1.1 Our contributions

This paper mainly focuses on optimizing quantum circuits of AES and gives improvements in several aspects.

**Improved greedy algorithm for finding low-depth CNOT circuits with no ancilla qubits.** We first notice that related works of providing CNOT circuits of AES Mixcolumns either adopted non-depth-oriented search methods or determined the depth based on existing circuits. Instead, we use a depth-oriented search method. Since de Brugière *et al.* proposed a depth-oriented cost-minimization greedy algorithm that is suitable for random small scale matrices, we first apply their algorithm to AES Mixcolumns and find a circuit with depth 12, which is much better than a recent record of depth 16 in [LPZW23]. We then propose an improved greedy algorithm based on de Brugière *et al.*'s algorithm and successfully find a circuit with depth 10, which can be used to reduce the full depth of quantum circuits of AES. The improvement of our algorithm is reflected in three aspects. First, in addition to considering the logarithm of each row's Hamming weight, we also consider the *square* of each row's Hamming weight, which gives priority to rows or columns that are "far from being done" and is beneficial to reduce the circuit depth in many cases. Second, we treat two cases of row and column operations differently when evaluating the cost, that is, each column's Hamming weight is considered when column operations are performed. Finally, we give an equivalent condition of determining whether a matrix can be implemented with depth 1 to better handle sparse matrices. As applications, our

improved greedy method provides low-depth CNOT circuits for many MDS matrices and matrices used in block ciphers (see Table 3, 4). Except for some matrices with depth 3, all the results are much better than those in [ZH22]. de Brugière *et al.*'s algorithm is also applied to these matrices for comparison.

**Compressed pipeline structure for quantum circuits of AES.** We observe that the pipeline structure has a low depth but too many intermediate states, while the OP-based round-in-place structure has fewer intermediate states but a greater depth. To combine the advantages of the above two structures, We propose a new structure named compressed pipeline structure, which computes new states and eliminates intermediate states in parallel for qubit reuse. If the round function is taken as a unit, our structure will have lower  $D-W$  cost than the above two structures when the number of ancilla qubits of a round function is small enough. To give detailed quantum circuits of AES-128, we propose iterative round functions for the encryption circuit under the guidance of our structure. Since two consecutive roundkeys are needed in the round functions, we also present a new circuit for the key schedule of AES-128 which provides linear components of consecutive two roundkeys in one round. Both cases of NCT-based circuit and qAND-based circuit are considered. Our circuit only needs such quantum circuits of AES S-box where the output register is  $|0\rangle$  and has lower  $TD-W$  or  $TofD-W$  cost when the number of ancilla qubits of AES S-box is small enough. The cost for the AES Grover oracle can be evaluated by referring to the cost of the encryption circuit.

**The AES-128 Encryption oracle with lower  $T$ -depth.** The encryption circuit in our structure can be used to construct the Encryption oracle employed in Simon's algorithm with simplified cleaning of redundant states. If the round function is taken as a unit, our constructed Encryption oracle will have depth  $r + 1$ , which is almost half of the previous best result  $2r$ . When it comes to AES-128, the AES-128 Encryption oracle can be constructed with smaller  $T$ -depth. Since the redundant states of the encryption circuit can be cleaned by  $|c\rangle$  with one layer of AES S-box, the AES-128 Encryption oracle can be constructed with  $T$ -depth 33, which breaks the previous record of  $T$ -depth 60 in [HS22].

**Key schedule of the shallowed pipeline structure with input-invariant Sbox.** In the key schedule of the shallowed pipeline structure,  $10 \times 32$  qubits need to be allocated for storing the input register of low Toffoli-depth Sbox which cannot keep the input register unchanged. We find that adding some CNOT gates can make such Sbox input-invariant without increasing the Toffoli-depth and ancilla qubits, which ensures that the information of the input register is not lost. Based on this, we propose a new key schedule for the shallowed pipeline structure which is actually a small variant of the key schedule in the compressed pipeline structure. It can avoid the allocation of extra  $10 \times 32$  qubits for storing key words and can be used to synthesize a quantum circuit of AES-128 with the lowest  $TofD-W$  cost 130720 to date.

All the source codes and results of this paper are available at <https://gitee.com/Haotian-Shi/Quantum-circuits-of-aes-with-a-low-depth-linear-layer-and-a-new-structure>.

## 1.2 Organization

In Section 2 we introduce some background knowledge about quantum computation. In Section 3 we introduce some existing methods for optimizing the depth of CNOT circuits. Our new method and its application on some matrices are illustrated in Section 4. In Section 5 we propose our compressed pipeline structure for iterative building blocks. Specific quantum implementations of AES in different scenarios and the resource costs are given in Section 6. We conclude our work in Section 7.

## 2 Preliminaries

### 2.1 Notations

We assume that the reader is familiar with AES, and a brief description of AES is given in Appendix B for completeness. Some notations used throughout the paper are listed as follows:

Table 1: Some notations used throughout the paper.

Notation	Definition
$\mathbb{F}_2$	The finite field with two elements 0 and 1
$\oplus$	The XOR computation
$\text{GL}(2, n)$	The set of all $n \times n$ invertible matrices over $\mathbb{F}_2$
$\text{GF}(n, \mathbb{F}_2)$	The finite field with $2^n$ elements
$I_n$	The $n$ -by- $n$ identity matrix over $\mathbb{F}_2$ .
$E(i + j)$	The resulting matrix by adding the $j$ -th row to the $i$ -th row of $I_n$ (type-3 elementary matrix in $\text{GL}(2, n)$ )
$E(i, j)$	The CNOT gate of adding the $i$ -th qubit to the $j$ -th qubit
$E(i \leftrightarrow j)$	The resulting matrix by exchanging the $i$ -th and $j$ -th row of $I_n$ (type-1 elementary matrix in $\text{GL}(2, n)$ ), or the swapping of the $i$ -th and $j$ -th qubits.
$ u\rangle$	A state vector $u$
$S(x)$	The function of AES S-box.
$\mathcal{O}_{\mathcal{R}}$	The quantum oracle: $ x\rangle  y\rangle \mapsto  x\rangle  y \oplus \mathcal{R}(x)\rangle$
$\mathcal{O}_{\mathcal{R}^{-1}}$	The quantum oracle: $ x\rangle  y\rangle \mapsto  x\rangle  y \oplus \mathcal{R}^{-1}(x)\rangle$
$k_j^k$	The $k$ -th 32-bit word of the $j$ -th roundkey, or $W_{4j+k}$ in the key schedule of AES-128.

### 2.2 Quantum computation

The simplest quantum system is a single qubit state. It can be described as a unit vector  $|u\rangle$  in a Hilbert Space  $\mathcal{H} = \mathbb{C}^2$  and has two computational basis states  $|0\rangle$  and  $|1\rangle$ . Then  $|u\rangle = \alpha |0\rangle + \beta |1\rangle$ , where  $|\alpha|^2 + |\beta|^2 = 1$ . An  $n$ -qubit state  $|u\rangle$  can be described as a unit vector in  $\mathcal{H}^{\otimes n}$ , and a computational basis state can be described as a state of  $n$ -bit 0/1 string:  $|x_1 x_2 \dots x_n\rangle$ .

The evolution of an  $n$ -qubit quantum state can be described as a quantum gate represented by a  $2^n \times 2^n$  unitary matrix  $U$ . It acts on an  $n$ -qubit state  $|u\rangle$  by left matrix multiplication  $U|u\rangle$ . Several typical quantum gates include:

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S = \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}, T = \begin{pmatrix} 1 & 0 \\ 0 & e^{\frac{i}{4\pi}} \end{pmatrix}, \text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$

$$\text{Toffoli} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

In this paper we mainly focus on quantum circuits which compute classical vectorial boolean functions, so the input states we are concerned with are only computational basis states. The X gate, CNOT gate and Toffoli gate all act on computational basis states as shown in Figure 1:

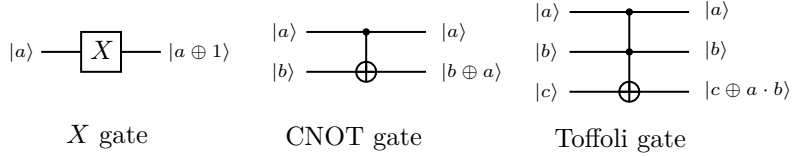


Figure 1: Circuits of X gate, CNOT gate and Toffoli gate. The changed qubit is called the target qubit.

One can see that the roles they play in quantum computation are NOT gate, XOR gate and AND gate in classical computation, respectively. An NCT-based circuit is often designed to compute a vectorial boolean function and is defined as follows:

**Definition 1** (NCT-based circuit). An NCT-based circuit is a quantum circuit consisting only of X gates, CNOT gates and Toffoli gates.

There is another quantum gate called a quantum AND gate (qAND in short) which simulates the functionality of a classical AND gate. It differs from the Toffoli gate in that the target qubit must be  $|0\rangle$ . This gate together with its adjoint is illustrated in Figure 2.

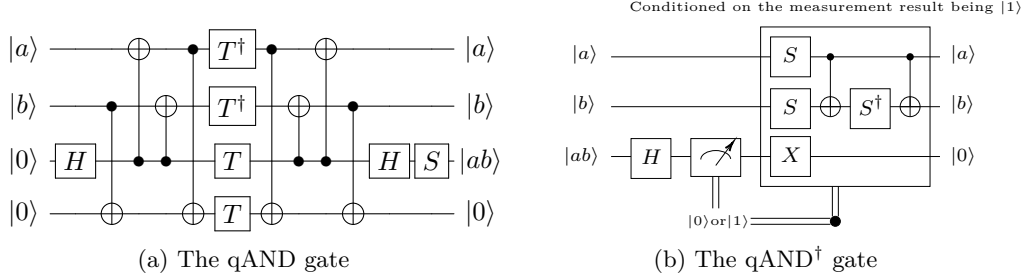


Figure 2: The quantum AND gate together with its adjoint.

### 2.3 Optimization goals

Due to the limited decoherence time and qubit resources, it is crucial to reduce the time cost and storage cost in quantum circuits. In NCT-based circuits, the metrics of width ( $W$ ), Toffoli depth ( $TofD$ ), and  $TofD-W$  cost are crucial for evaluating the cost. In practice, the Toffoli gate can be decomposed with  $T$ -depth  $3/4$  and full depth  $9/8$ , respectively, using 0 ancilla qubit [AMMR13], or decomposed with  $T$ -depth 1 using 4 ancilla qubits [Sel13]. If the target qubit of a Toffoli gate is identically equal to  $|0\rangle$ , the Toffoli gate can be replaced by qAND with  $T$ -depth 1 using 1 ancilla qubit and its adjoint can be replaced by qAND<sup>†</sup> with  $T$ -depth 0 using 0 ancilla qubit. As is shown in [NC00], the Clifford gates are much cheaper than the  $T$ -gate. Therefore,  $T$ -depth ( $TD$ ) is a key parameter to measure the running time of a circuit. At the same time, a forward-looking perspective assumes that each gate has a unit depth and defines the full depth ( $FD$ ) as a time-cost metric.

### 3 State-of-art heuristics for optimizing the depth of CNOT circuits

In this section, we first introduce some background knowledge of CNOT circuits. We then introduce some existing methods for optimizing the depth of CNOT circuits, including methods for handling existing circuits [ZH22, LPZW23] and the depth-oriented greedy algorithm [dBBV<sup>+</sup>21b].

#### 3.1 CNOT circuits

A CNOT circuit is a quantum circuit that contains only CNOT gates. One can see from Figure 1 that a CNOT gate adds one boolean tuple to another, so it can be seen as an invertible linear transformation  $\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}$  in  $\mathbb{F}_2^2$ . Similarly, for an  $n$ -qubit system, the CNOT gate  $E(i, j)$  controlled by the  $i$ -th qubit and targeting on the  $j$ -th qubit can be seen as the type-3 elementary matrix  $E(j + i)$ . Therefore, a CNOT circuit of  $n$ -qubits can be seen as a product of type-3 elementary matrices. Actually the linear layer of a cipher is an  $n$ -bit reversible linear boolean function and can be interpreted as an invertible matrix  $A$  in  $GL(2, n)$ . Therefore, the CNOT circuit of a linear layer  $A$  can be synthesized by referring to a proper form of matrix decomposition of  $A$ . Recall that the general form of matrix decomposition is illustrated below as Theorem 1:

**Theorem 1.** *Any  $A$  in  $GL(2, n)$  can be expressed as a product of type-1 and type-3 elementary matrices.*

Note that the only type-2 matrix in  $GL(2, n)$  is the identity matrix and therefore does not appear in the matrix decomposition. However, this form does not promise a consecutive product of type-3 elementary matrices. In general, it is clear that the matrix multiplication does not satisfy the commutative law, but given two elementary matrices  $E(i + j)$  (type-3) and  $E(k \leftrightarrow l)$  (type-1), we have the following property:

**Property 1.**  $E(i + j)E(k \leftrightarrow l) = E(k \leftrightarrow l)E(f_{k,l}(i) + f_{k,l}(j))$ ,  $E(k \leftrightarrow l)E(i + j) = E(f_{k,l}(i) + f_{k,l}(j))E(k \leftrightarrow l)$ , where

$$f_{k,l}(x) = \begin{cases} k, & \text{if } x = l; \\ l, & \text{if } x = k; \\ x, & \text{else.} \end{cases} \quad (1)$$

As a result, we can have the following form of matrix decomposition which is easy converted to a CNOT circuit:

**Theorem 2.** *Any  $A$  in  $GL(2, n)$  can be expressed as*

$$A = PE(i_1 + j_1)E(i_2 + j_2) \dots E(i_L + j_L), \quad (2)$$

where  $P$  is a permutation matrix.

Since the swapping of two qubits can be realized by rewiring for free, it is easy to convert a decomposition of  $A$  to a CNOT circuit of  $A$  and vice versa. Based on Theorem 2, Xiang *et al.* defined the sequential XOR (s-XOR) metric which describes the minimum gate cost of implementing  $A$  by updating input variables to output variables:

**Definition 2** (s-XOR). [XZL<sup>+</sup>20] Let  $M \in GL(n, \mathbb{F}_2)$  be an invertible matrix. Assume  $(x_1, x_2, \dots, x_n)$  are the  $n$  input bits of  $M$ . It is always possible to perform a sequence of XOR instructions  $x_i = x_i \oplus x_j$  with  $1 \leq i, j \leq n$ , such that the  $n$  input bits are updated to the  $n$  output bits. The s-XOR count of  $M$  is defined as the minimum number of XOR instructions to update the inputs to the outputs.

Xiang *et al.* proposed some reduction rules to reduce the number of type-3 elementary matrices in a matrix decomposition and obtained in-place implementations of the many constructed MDS matrices and matrices used in block ciphers with minimum XOR gates up to date [XZL<sup>+</sup>20]. The specific results of their method can serve as a fairly good starting point for optimizing the quantum depth of the corresponding CNOT circuits.

### 3.2 Computing the depth of given circuits

Zhu *et al.* used a sequence  $SEQ = \{E(c_1, t_1), E(c_2, t_2), \dots, E(c_L, t_L)\}$  to describe a given CNOT circuit [ZH22]. To compute the depth of a sequence  $SEQ$ , the authors divide it into  $D$  subsequences:  $SEQ_1, SEQ_2, \dots, SEQ_D$  such that  $SEQ = \bigcup_{i=1}^D SEQ_i$ .  $\{SEQ_1, SEQ_2, \dots, SEQ_D\}$  is called a parallel partition of  $SEQ$  if any two gates in  $SEQ_i$  can act in parallel for all  $1 \leq i \leq D$ . Then the sequence depth of  $SEQ$  is defined as the minimum  $D$  such that there is a parallel partition of  $SEQ$  with  $D$  subsequences.

It is easy to see that if two adjacent gates  $E(c_i, t_i), E(c_{i+1}, t_{i+1})$  can act in parallel,  $E(c_{i+1}, t_{i+1})$  can move forward and  $E(c_i, t_i)$  can move backward without changing the output of the sequence. The depth of  $SEQ$  evaluated from most quantum resource estimators, such as the Q# resource estimator of Microsoft [Q#], is the sequence depth of one of its move-equivalent sequences. The Q# resource estimator works by moving all  $E(c_i, t_i)$  forward as far as possible. However, the definition of move-equivalence can be extended. Zhu *et al.* noticed this and clarified the equivalent condition of exchanging two CNOT gates:

**Property 2.** Given  $E(c_i, t_i)$  and  $E(c_j, t_j)$ ,  $E(c_i, t_i)E(c_j, t_j) = E(c_j, t_j)E(c_i, t_i)$  if and only if  $t_i \neq c_j$  and  $t_j \neq c_i$ .

They then gave the definition of exchange-equivalent sequences and proposed an algorithm named One-way-opt, which involves iteratively extracts a layer of CNOT gates by exploring gates that can be exchanged forward and can run in parallel with the gates of the current layer. One-way-opt is executed twice in both forward and backward directions to search for low-depth exchange-equivalent sequences. Redecomposition of  $SEQ$ 's subsequences is also considered to explore more possibilities. Recently, Jang *et al.* also adopted the idea of reordering gates to optimize the depth of linear layers [JBK<sup>+</sup>22].

Liu *et al.* proposed an algorithm FINDDEPTH to quickly determine the full depth of a given quantum circuit [LPZW23]. They record the updated qubits (target qubits) and used qubits (control qubits) of previous CNOT gates in each depth layer to determine the minimum depth  $d$  where the current CNOT gate  $E(c, t)$  can be placed. Specifically, the control qubit  $c$  should not be updated in larger depths, and the target qubit  $t$  should not be used in larger depths. At the same time, qubits  $c, t$  should not emerge in depth layer  $d$ . Note that from Zhu *et al.*'s perspective this algorithm actually returns the sequence depth of a exchange-equivalent sequence of the given  $SEQ$ .

### 3.3 Greedy method

de Brugière *et al.* [dBBV<sup>+</sup>21b] proposed a depth-oriented greedy method to find low-depth CNOT circuits of invertible linear layers. It is a cost-minimization algorithm, that is, a cost function needs to be defined to evaluate the cost of reducing the matrix  $A$  to a permutation matrix, and then a strategy for exploring effective elementary transformations is designed according to the cost function.

The authors considered four cost functions to guide the optimization of gate count [dBBV<sup>+</sup>21a]:



$$\begin{aligned}
(1) h_{sum}(A) &= \sum_{i,j} a_{ij}; \\
(2) H_{sum}(A) &= h_{sum}(A) + h_{sum}(A^{-1}); \\
(3) h_{prod}(A) &= \sum_i \log_2(\sum_j a_{ij}); \\
(4) H_{prod}(A) &= h_{prod}(A) + h_{prod}(A^{-1}).
\end{aligned}$$

These four cost functions roughly estimate the cost of decomposition through the sparsity of a matrix  $A$ , and reach their minimum when  $A$  is a permutation matrix. Therefore, they can guide the search in the cost-minimization process.  $h_{sum}$  is a rough estimation since there can be too many operations which lead to the same cost, and the remaining cost functions have two major improvements over  $h_{sum}$ . On the one hand, the inverse of the matrix is taken into account, which was first proposed in [SP14]. Since a row operation on  $A$  is equivalent to a corresponding column operation on  $A^{-1}$ , adding the cost of the inverse matrix can provide a balanced estimation of the distance to a permutation matrix. On the other hand, the logarithm of every row's Hamming weight is taken into account, which was first presented in [dBBV<sup>+</sup>21a].  $h_{prod}$  gives priority to "almost done" rows such that the overall efficiency of elimination is guaranteed. Note that with cost-minimization algorithms one may end up with a sparse matrix but where the rows and columns have few nonzero common entries. This type of matrix represents a local minimum from which it might be difficult to escape. Both these two considerations can help to avoid getting stuck in local minima and can lead to better results.

Once a fairly well cost function is chosen (such as (2) or (4)), the greedy method for optimizing gate count works by memorizing the operations that minimize the cost function and randomly choosing one from them, and some restrictions exist in the case of depth optimization. The author defines two sets  $L_r$  and  $L_c$ , which record the previously applied row and column operations [dBBV<sup>+</sup>21a] that can run in parallel. In each iteration of choosing an operation, the available row or column operations must meet the following two conditions:

- Reduce the cost function.
- Can act in parallel with  $L_r$  or  $L_c$ .

If no available row or column operations exist, one resets  $L_r, L_c$  to empty. Each time a non-empty  $L_r$  or  $L_c$  is reset to empty, the depth count is increased by one. The algorithm ends when the cost function is equal to its minimum, that is, the current matrix is a permutation matrix, or when the depth counter exceeds a certain threshold, that is, the algorithm falls into local minima.

According to their experiments with random matrices, this depth-oriented greedy method behaves well for small  $n$  (roughly  $n < 40$ ). When  $n$  is larger, it performs worse than their block algorithm and often falls into local minima. Their block algorithm [dBBV<sup>+</sup>21b] and Jiang *et al.*'s algorithm [JST<sup>+</sup>20] have asymptotic optimal bounds and can handle larger matrices better.

## 4 Our method and its applications

In this section, we first propose an improved greedy algorithm for finding low-depth CNOT circuits. Then we apply our algorithm to different linear building blocks with sizes of  $16 \times 16$  and  $32 \times 32$  that have been studied in [ZH22]. Since the original greedy method in [dBBV<sup>+</sup>21b] is not applied to these matrices, we also apply their method to these matrices for comparison.

## 4.1 Our method

Our method is based on the framework of the original greedy method [dBBV+21b], and differs from it in three aspects. First, in addition to considering the logarithm of each row's Hamming weight, we also consider the *square* of each row's Hamming weight. Second, we treat two cases of row and column operations differently when evaluating the cost, that is, each column's Hamming weight is considered when column operations are performed. Finally, we add a judgement of whether the current matrix can be implemented with depth 1 to better handle sparse matrices.

We first make an intrinsic observation about the problem of synthesizing low-depth CNOT circuits. Though not strict, the larger Hamming weight of a row  $i$ , the more potential gates need to be done on the row  $i$ . Therefore, prioritizing the rows or columns with larger Hamming weights might be a preferable choice to obtain lower circuit depth. Intuited by this, we propose a new cost function  $h_{sq}$  which is based on the square of every row's Hamming weight:

$$h_{sq}(A) = \sum_i \left( \sum_j a_{ij} \right)^2.$$

We also notice that focusing on the Hamming weight of the rows ignores the effect of the column operations. So we propose two cost functions  $H_{sqr}, H_{sqc}$  which are based on  $h_{sq}$  to evaluate row operations and column operations respectively:

$$\begin{aligned} H_{sqr}(A) &= h_{sq}(A) + h_{sq}((A^{-1})^T); \\ H_{sqc}(A) &= h_{sq}(A^T) + h_{sq}(A^{-1}). \end{aligned}$$

Note that the cost of corresponding transformation of inverse matrix is under consideration. In our method, the cost after row operations is evaluated by  $H_{sqr}(A)$ , and the cost after column operations is evaluated by  $H_{sqc}(A)$ . In addition, the cost of current matrix is defined as the maximum evaluation of  $H_{sqr}$  and  $H_{sqc}$  to explore more possibilities.

According to our experiments, using row and column cost functions based on  $h_{prod}$  will sometimes yield better results than using row and column cost functions based on  $h_{sq}$ , which means that  $h_{sq}$  is not the best choice for all matrices. So in practice, we also use cost functions  $H_{prodr}$  and  $H_{prodc}$  defined as follows:

$$\begin{aligned} H_{prodr}(A) &= h_{prod}(A) + h_{prod}((A^{-1})^T); \\ H_{prodc}(A) &= h_{prod}(A^T) + h_{prod}(A^{-1}). \end{aligned}$$

In our algorithm, we adopt a hybrid strategy of randomly using  $H_{prodr}, H_{prodc}$  or  $H_{sqr}, H_{sqc}$ , since both cases are likely to give the best result.

In addition, we give an equivalent condition to test whether a matrix can have depth 1. This helps determine whether the last searched  $L_r$  and  $L_c$  can be implemented in parallel, since the original algorithm can only find this better case with probability  $\frac{2}{2^t}$ , where  $t$  is the total number of CNOT gates in the last searched  $L_r$  and  $L_c$ .

**Theorem 3.** *Suppose the implementation of a permutation matrix is free. Given an invertible matrix  $A_{n \times n}$  on  $\mathbb{F}_2$ ,  $A$  can be implemented with depth 1 if and only if the following conditions hold:*

- (a) *The Hamming weights of all  $A$ 's rows are less than or equal to 2.*
- (b) *For any two rows  $i, j$  of  $A$  with Hamming weight 2,  $a_{ik}a_{jk} = 0$  for all  $k$ .*

---

**Algorithm 1** Improved greedy algorithm for synthesizing low-depth CNOT circuits.
 

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**Input:** An invertible matrix  $A_{n \times n}$ 
**Output:** A depth  $d$  and a vector of layers  $Layers$  that implement  $A$  with length  $d$ .

 $Layers \leftarrow \emptyset, Layers_r \leftarrow \emptyset, Layers_c \leftarrow \emptyset;$ 
 $L_r \leftarrow \emptyset, L_c \leftarrow \emptyset;$ 
 $List \leftarrow \emptyset;$ 
 $B \leftarrow A;$ 

 Randomly determine  $H_r, H_c \leftarrow H_{sqr}, H_{sqc}$  or  $H_{sqr}, H_{sqc}$ .

 $cost \leftarrow \max\{H_r(B), H_c(B)\};$ 
 $one \leftarrow \text{False};$ 
 $d \leftarrow 0;$ 
**while True do**
 $cost \leftarrow \max\{H_r(B), H_c(B)\};$ 
 $mincost \leftarrow$  minimum resulting cost of all available row operations adding  $i$ -th row to the  $j$ -th row (denoted  $\{i, j, 0\}$ ) to  $B$ , and all available column operations adding  $i$ -th column to the  $j$ -th column (denoted  $\{i, j, 1\}$ ) to  $B$  (if not  $one$ );

 $List \leftarrow \{\text{All operations that lead to the } mincost\};$ 
**if**  $mincost = cost$  **then**
**if** not  $one$  and  $\text{can-depth-one}(A)$  **then**
 $one \leftarrow \text{True};$ 
**end if**
**if**  $L_r.size() > 0$  **then**
 $d \leftarrow d + 1, Layers_r.append(L_r), L_r.clear();$ 
**end if**
**if**  $L_c.size() > 0$  **then**
 $d \leftarrow d + 1, Layers_c.append(L_c), L_c.clear();$ 
**end if**
**if**  $cost = 2n$  **then**
**break;**
**end if**
**if**  $d \geq 100$  **then**
**return**  $d, \emptyset$ .  $\triangleright$  Too large  $d$  means the matrix may fall into a local minima.

**end if**
**else**

 Randomly choose one operation  $\{i, j, op\}$  that minimizes the cost function of the resulting matrix, add  $\{i, j, op\}$  to  $L_r$  if  $op = 0$ , or  $L_c$  if  $op = 1$ ;

 $B \leftarrow E(j+i)^{1-op} B E(i+j)^{op};$ 
**end if**
 $List.clear();$ 
**end while**

 Record a permutation  $P$ , satisfying  $P(i) = j$  if  $B[i][j] = 1$ ;

**for**  $i$  from 0 to  $Layers_c.size() - 1$  **do**
 $l \leftarrow \emptyset;$ 
**for**  $j$  from 0 to  $Layers_c[i].size() - 1$  **do**
 $\{t, c, op\} \leftarrow Layers_c[i][j], l.append(\{c, t\});$ 
**end for**
 $Layers.append(l);$ 
**end for**
**for**  $i$  from  $Layers_r.size() - 1$  down to 0 **do**
 $l \leftarrow \emptyset;$ 
**for**  $j$  from 0 to  $Layers_r[i].size() - 1$  **do**
 $\{c, t, op\} \leftarrow Layers_r[i][j], l.append(\{P[c], P[t]\});$ 
**end for**
**end for**
**return**  $d, Layers;$ 


---

*Proof.* It is easy to see that a set of row operations on a permutation matrix can be interpreted as a set of column operations and vice versa. So we only need to consider the parallelism of row operations to reduce a matrix to a permutation matrix.

*Necessity.* It is easy to see that target rows of type-3 matrices have Hamming weight 2 and other rows have Hamming weight 1. (b) holds since the reduced matrix is a permutation matrix.

*Sufficiency.* Without loss of generality, assume that the  $i$ -th row has Hamming weight 2 for  $0 \leq i < l$ , and other rows have Hamming weight 1. For each  $i$  such that  $a_{i,p_i} = 1, a_{i,q_i} = 1$ , there exist only one corresponding row  $t_i$  with Hamming weight 1 such that either  $a_{t_i,p_i} = 1$  or  $a_{t_i,q_i} = 1$ , since  $A$  is invertible. Applying  $E(t_i, i)$  for  $0 \leq i < l$  gives the implementation with depth 1.  $\square$

Detailed procedures of our improved greedy algorithm is illustrated as Algorithm 1. The running time of this algorithm is dominated by evaluating the cost of all possible row or column operations. Suppose the considered matrix  $A$  is  $n$  by  $n$ . Ignoring the limitation of parallelism, at most  $n^2$  row operations and  $n^2$  column operations need to be evaluated. Since  $A^{-1}$  can be computed first and updated according to the corresponding operations on  $A$ , the cost of the resulting matrix can be computed in  $O(n)$  times based on the cost of  $A$ . Therefore, the complexity of determining of an operation to be done for a current matrix is upper bounded by  $O(n^3)$ . Similar to de Brugière *et al.*'s greedy method, our algorithm behaves well for small scale matrices (roughly  $n < 40$ ), and our often falls into local minima when  $n$  is larger. Our algorithm is repeated tens of thousands of time for a matrix and the best result is recorded.

## 4.2 Application to AES MixColumns

We first focus on CNOT circuits of AES MixColumns. Previous researchers synthesized quantum circuits of AES MixColumns with different methods. Some CNOT circuits with low depth were designed by converting optimized classical circuits (see [LSL<sup>+</sup>19, BFI21, LWF<sup>+</sup>22] for an incomplete list) into quantum style using ancilla qubits. Zhu *et al.* studied the exchange-equivalence sequence of the CNOT circuit provided by Xiang *et al.*'s method [ZH22] and found an implementation that has depth 28. Recently Liu *et al.* proposed a method for computing the depth of quantum circuits and then used it to evaluate many circuits generated by Xiang *et al.*'s method [XZL<sup>+</sup>20]. They obtained a circuit with 98 CNOT gates and depth 16. Jang *et al.* optimized the circuit built upon the work in [LSL<sup>+</sup>19] and obtained an out-of-place circuit with depth 8 [JBK<sup>+</sup>22].

We observe that related works of providing CNOT circuits of AES MixColumns either adopt non-depth-oriented search methods or determine the depth based on existing circuits. Instead, we use depth-oriented search algorithms to generate low-depth CNOT circuits with no ancilla qubits. We first apply the greedy algorithm in [dBBV<sup>+</sup>21b] with cost function  $H_{prod}$  to AES MixColumns and obtain a circuit with depth 12 and 128 gates. Then using our improved greedy algorithm, we can find a circuit with depth 10 and 131 gates. It can be used to reduce the full depth of quantum circuits of AES without increasing the circuit width. The comparison with previous results is shown in Table 2.

## 4.3 Applications to many proposed matrices

Following the work of [ZH22], we apply our method to various matrices in the literature including:

- some matrices which are used in block ciphers [DR02, Bar00, SSA<sup>+</sup>07, JV05, Ava17, SKW<sup>+</sup>98, BNN<sup>+</sup>10, JNP15, BBI<sup>+</sup>15, CMR05, ADK<sup>+</sup>14, BCG<sup>+</sup>12, BJK<sup>+</sup>16].

- some MDS matrices which are independently constructed in [SKOP15, SS16, SS17, JPST17, LS16, LW16, BKL16];

Table 2: Comparison of CNOT circuits of the AES MixColumns matrix.

Source	# CNOT	$W$	$FD$
[BFI21, LWF <sup>+</sup> 22]	206	135	13
[LSL <sup>+</sup> 19]	210	137	11
[JBK <sup>+</sup> 22]	169	96	8
[JNRV20]	277	32	111
[GLRS16, ZWS <sup>+</sup> 20]	277	32	39
[XZL <sup>+</sup> 20]	92	32	30
[ZH22]	92	32	28
[LPZW23]	98	32	16
[dBBV <sup>+</sup> 21b]	128	32	12
<b>This paper</b>	131	32	<b>10</b>

Based on the CNOT circuits of these matrices provided by Xiang *et al.*'s method, Zhu *et al.* evaluated their move-equivalent sequence depth by  $Q\#[Q\#]$ , and investigated their exchange-equivalent sequence depth. Except for a few small-scale matrices, we can find better results with lower depths for these matrices. For the matrices used in block ciphers, we have succeeded in reducing the circuit depth for all of them except for a few matrices that already have CNOT circuits with small depth (see Table 3). For the many constructed MDS matrices, we can optimize the depth of CNOT circuits for all of them (see Table 4). Overall, our improved greedy algorithm gives the best results with the lowest depth for all of the matrices<sup>2</sup>.

<sup>2</sup>Note that for a few matrices, implementations with the same depth but fewer gates can be searched using de Brugière *et al.*'s algorithm. Therefore, their algorithm could be used in combination with our algorithm in order to search for better low depth CNOT circuits.

Table 3: Comparison of the depth/gate count of CNOT circuits for matrices used in block ciphers

Cipher	Size	Q#	[ZH22]	This paper	[dBBV+21b]
AES <sup>a</sup> [DR02]	32	30/92	28/92	<b>10</b> /131	12/128
ANUBIS [Bar00]	32	26/98	20/98	<b>10</b> /119	14/136
CLEFIA M0 [SSA+07]	32	30/98	27/98	<b>10</b> /110	13/126
CLEFIA M1 [SSA+07]	32	21/103	16/103	<b>10</b> /128	13/127
FOX MU4 [JV05]	32	55/136	48/136	<b>21</b> /265	<b>21</b> /200
QARMA128 [Ava17]	32	6/48	5/48	<b>3</b> /48	<b>3</b> /48
TWOFISH [SKW+98]	32	37/111	29/111	<b>15</b> /175	18/187
WHIRLWIND M0 [BNN+10]	32	65/183	51/183	<b>28</b> /331	<b>28</b> /286
WHIRLWIND M1 [BNN+10]	32	69/190	54/190	<b>22</b> /290	25/279
JOLTIK [JNP15]	16	20/44	17/44	<b>7</b> /52	9/48
MIDORI [BBI+15]	16	<b>3</b> /24	<b>3</b> /24	<b>3</b> /24	<b>3</b> /24
SmallScale AES [CMR05]	16	20/43	19/43	<b>10</b> /62	11/59
PRIDE L0 [ADK+14]	16	<b>3</b> /24	<b>3</b> /24	<b>3</b> /24	<b>3</b> /24
PRIDE L1 [ADK+14]	16	5/24	5/24	<b>3</b> /24	<b>3</b> /24
PRIDE L2 [ADK+14]	16	5/24	5/24	<b>3</b> /24	<b>3</b> /24
PRIDE L3 [ADK+14]	16	6/24	6/24	<b>3</b> /24	<b>3</b> /24
PRINCE M0 [BCG+12]	16	6/24	6/24	<b>3</b> /24	<b>3</b> /24
PRINCE M1 [BCG+12]	16	6/24	6/24	<b>3</b> /24	<b>3</b> /24
QARMA64 [Ava17]	16	6/24	5/24	<b>3</b> /24	<b>3</b> /24
SKINNY [BJK+16]	16	<b>3</b> /12	<b>3</b> /12	<b>3</b> /12	<b>3</b> /12

<sup>a</sup> A recent result of 16/98 is given in [LPZW23].

## 5 The compressed pipeline structure for iterative primitives

In this section, we first introduce some structures used for quantum circuits of AES in previous works. Then we propose a new structure named compressed pipeline structure. Finally we make some comparisons in different levels and introduce its application in the Grover oracle and the Encryption oracle.

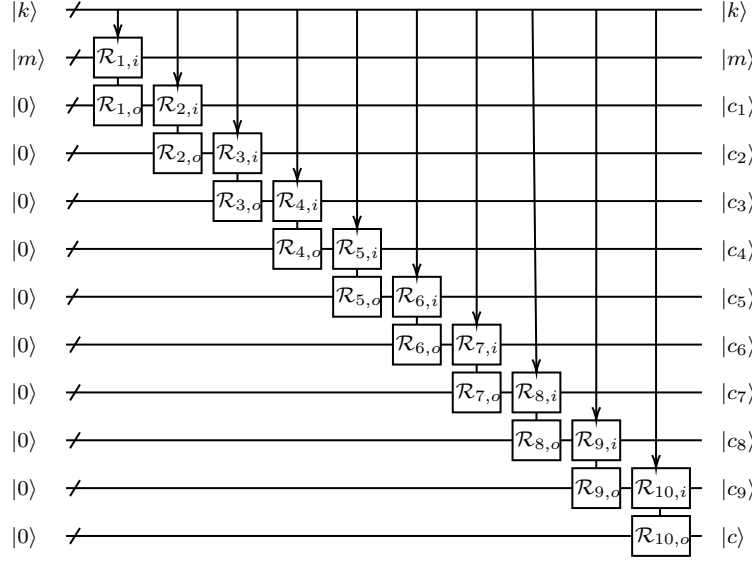
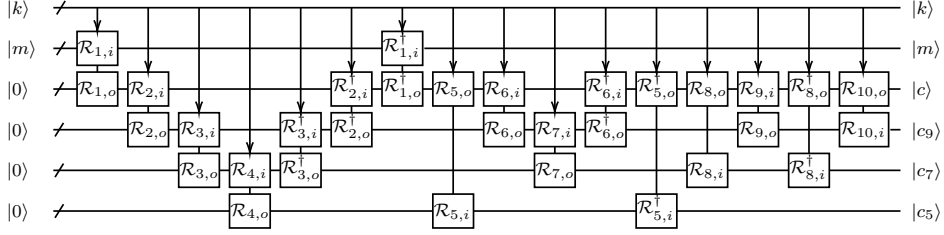
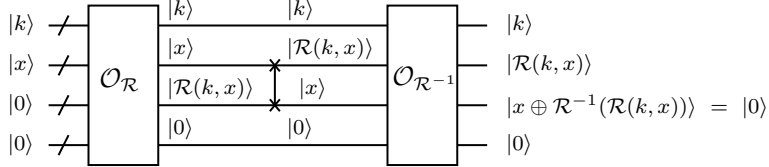
### 5.1 Existing structures

Many structures have been proposed to synthesize quantum circuits of AES. Some of them are based on out-of-place round functions, including the pipeline structure  $\mathcal{S}_p$ , the zig-zag structure  $\mathcal{S}_z$  and the out-of-place based (OP-based in short) round-in-place structure  $\mathcal{S}_i$ . The pipeline structure, which is first mentioned in reversible logic implementations of AES in [DSSR13], was proposed by Jaques *et al.* in [JNRV20]. It has low depth and large width and is used to construct low  $T$ -depth quantum circuits of AES in [JNRV20, HS22, JBK+22, LPZW23]. The zig-zag structure was first put forward by Grassal *et al.* in [GLRS16] to reduce the number of intermediate states. It is used to construct low-width circuits of AES in [GLRS16, ASAM18, LPS20]. To further reduce the number of intermediate states, Zou *et al.* presented the improved zig-zag structure [ZWS+20], and Huang *et al.* proposed the OP-based round-in-place structure to construct in-place circuits on the basis of out-of-place circuits. Denote the  $j$ -th round function  $\mathcal{R}_j$  which satisfies  $\mathcal{R}_j(c_{j-1}) = c_j$ , then the out-of-place oracle  $\mathcal{O}_{\mathcal{R}_j}$  takes  $|x\rangle|y\rangle$  as input and outputs  $|x\rangle|y \oplus \mathcal{R}_j(x)\rangle$ . The input register and output register is distinguished by notation  $\mathcal{R}_{j,i}$  and  $\mathcal{R}_{j,o}$  respectively. For simplicity, the key schedule and the ancilla qubits are omitted.  $\mathcal{S}_p$  and  $\mathcal{S}_z$  compute the desired output  $|c\rangle$  along with some redundant states, as illustrated in Figure 3, 4, respectively. The construction of the in-place function in  $\mathcal{S}_i$  is shown in Figure 5.

Table 4: Comparison of the depth/gate count of CNOT circuits for many constructed MDS matrices

Matrices	Size	Move-eq	[ZH22]	<b>This paper</b>	<b>[dBBV<sup>+</sup>21b]</b>
$4 \times 4$ matrices in $\text{GF}(4, \mathbb{F}_2)$					
[BKL16]	16	23/41	21/41	<b>10/59</b>	12/57
[JPST17]	16	24/41	18/41	<b>9/49</b>	<b>9/48</b>
[LS16]	16	27/41	26/41	<b>11/63</b>	12/65
[SKOP15]	16	25/44	22/44	<b>11/59</b>	<b>11/59</b>
[LW16]	16	29/44	27/44	<b>11/62</b>	12/65
[JPST17](Involutory)	16	15/41	14/41	<b>9/54</b>	13/54
[SKOP15](Involutory)	16	19/44	16/44	<b>7/52</b>	9/48
[LW16](Involutory)	16	27/44	25/44	<b>7/52</b>	9/48
[SS16](Involutory)	16	12/38	11/38	<b>8/46</b>	<b>8/44</b>
$4 \times 4$ matrices in $\text{GF}(8, \mathbb{F}_2)$					
[BKL16]	32	56/144	47/144	<b>18/208</b>	20/188
[JPST17]	32	26/82	22/82	<b>9/100</b>	<b>9/96</b>
[LS16]	32	67/121	54/121	<b>21/235</b>	23/203
[LW16]	32	55/104	42/104	<b>13/164</b>	16/167
[SKOP15]	32	23/90	20/90	<b>10/112</b>	11/118
[SS16]	32	47/114	40/114	<b>20/218</b>	<b>20/190</b>
[JPST17](Involutory)	32	18/83	14/83	<b>9/103</b>	13/108
[SKOP15](Involutory)	32	18/91	16/91	<b>8/101</b>	9/96
[LW16](Involutory)	32	19/87	19/87	<b>8/99</b>	<b>8/98</b>
[SS16](Involutory)	32	19/93	18/93	<b>10/122</b>	12/119
$8 \times 8$ matrices in $\text{GF}(4, \mathbb{F}_2)$					
[SS17]	32	54/183	55/183	<b>29/351</b>	33/302
[SKOP15]	32	59/170	49/170	<b>28/349</b>	29/286
[SKOP15](Involutory)	32	47/185	37/185	<b>29/337</b>	30/300
$8 \times 8$ matrices in $\text{GF}(8, \mathbb{F}_2)$					
[SKOP15](Involutory)	64	50/348	37/348	<b>22/484</b>	25/412

There are also some other structures which do not take the out-of-place round function as a unit. On the one hand, an in-place round function can be directly designed without out-of-place round functions. For example, Li *et al.* proposed an in-place quantum circuit of AES S-box with only 8 ancilla qubits, and then used it to synthesize a quantum circuit of AES under the straight-line structure, which has the lowest width to date [LGQW23]. On the other hand, some out-of-place round functions themselves can be decomposed into computation and uncomputation. The shallowed pipeline structure proposed by Jang *et al.* delays the uncomputation of one round function (if exists) to the next round to reduce the full depth [JBK<sup>+</sup>22]. Liu *et al.* improved this structure by sharing the ancilla qubits of the computation and uncomputation to save qubits [LPZW23].

Figure 3: The pipeline structure  $\mathcal{S}_p$ .Figure 4: The zig-zag structure  $\mathcal{S}_z$ .Figure 5: OP-based round-in-place function in  $\mathcal{S}_i$ .

## 5.2 Compressed pipeline structure

In this section we propose the compressed pipeline structure.

We first make some observations on existing structures. Though the pipeline structure has the lowest depth, too many qubits store the intermediate states. At the same time, the zig-zag structure and its improvements clean some intermediate states to save qubits, but at a cost of almost twice the depth of the pipeline structure. To combine the advantages of the above two structures, we propose a strategy of computing new states and eliminating intermediate states in parallel.

Specifically, when  $c_{j+1}$  ( $j \geq 1$ ) is generated, the register storing  $c_{j-1}$  can be cleaned by  $\mathcal{O}_{\mathcal{R}_{j-1}^{-1}}$  in parallel and then can be reallocated in further use. In fact, our structure can be thought of as adding the clean process to the pipeline structure, hence the name



compressed pipeline structure denoted by  $\mathcal{S}_{cp}$ . Since the input register of both  $\mathcal{O}_{\mathcal{R}_{j-1}^{-1}}$  and  $\mathcal{O}_{\mathcal{R}_j}$  is the same,  $|c_j\rangle$  is copied by CNOT gates so that  $\mathcal{O}_{\mathcal{R}_{j-1}^{-1}}$  and  $\mathcal{O}_{\mathcal{R}_j}$  can act in parallel. Therefore, our structure requires four intermediate message registers, while a round function and its inverse function need to be executed in parallel.  $\mathcal{S}_{cp}$  is illustrated in Figure 6.

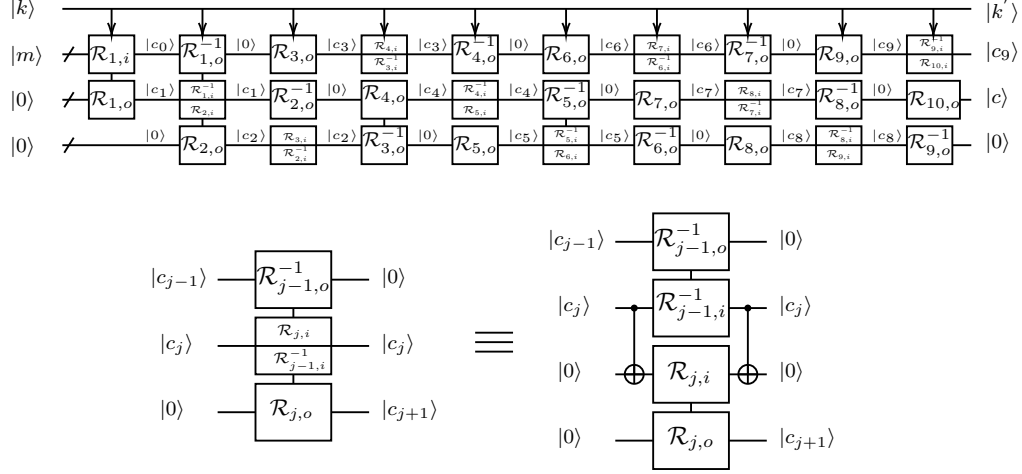


Figure 6: The compressed pipeline structure  $\mathcal{S}_{cp}$ . For convenience, the copy of the  $|c_j\rangle$  state is simplified as "split into two parts".

### 5.3 Comparison of different structures

In this subsection, we will compare the depth and width of different structures that takes round function as a unit and illustrate the use of our  $\mathcal{S}_{cp}$  in two scenarios: the Grover oracle and the Encryption oracle.

We first clarify some parameters for the different structures. Suppose  $\mathcal{O}_{\mathcal{R}_j}$  has a unit depth and needs  $\alpha$  ancilla qubits. Since the components of  $\mathcal{O}_{\mathcal{R}_j}$ ,  $\mathcal{O}_{\mathcal{R}_j^{-1}}$  are almost the same, it is reasonable to regard them as having the same cost. Suppose the round function iterates for  $r$  rounds, and one message register needs  $n$  qubits. The width of the key schedule is set to  $k'$  to show the difference from the other structures, because in our structure, the parallel execution of a round function with its inverse means that two consecutive roundkeys are required.

The comparison with previous structures under the above parameters is outlined in Table 5. Since we treat a round function as a unit, only the comparison between  $\mathcal{S}_p$ ,  $\mathcal{S}_z$ ,  $\mathcal{S}_i$  with our  $\mathcal{S}_{cp}$  are considered.

Table 5: The comparison of different structures, where  $t$  is the minimal number such that  $\sum_{i=1}^t i > r$ .

Structure	Depth	Width
$\mathcal{S}_p$	$r$	$k + (r + 1)n + \alpha$
$\mathcal{S}_z$	$\approx 2r$	$k + tn + \alpha \approx k + \sqrt{2rn} + \alpha$
$\mathcal{S}_i$	$2r$	$k + 2n + \alpha$
<b>This paper</b>	$r$	$k' + 4n + 2\alpha$

Our  $\mathcal{S}_{cp}$  has the same depth  $r$  as  $\mathcal{S}_p$ , and at the same time needs 4 message registers instead of  $r + 1$  message registers in  $\mathcal{S}_p$ . Therefore, our  $\mathcal{S}_{cp}$  will have lower width than  $\mathcal{S}_p$

and lower  $D$ - $W$  cost than  $\mathcal{S}_z, \mathcal{S}_i$  if  $\alpha$  and  $k'$  are small enough.

*Circuits for Grover oracles.* We first consider the Grover oracle:  $|y\rangle |q\rangle \rightarrow |y\rangle |q \oplus f(y)\rangle$ , where  $f(y)$  is a boolean function which outputs one bit 1 or 0. An exhaustive key search Grover oracle has input state  $|k\rangle$ , and the correctness of the key is verified by some plaintext-ciphertext pairs. For simplicity we consider the case of one pair  $(m_0, c_0)$ . Denote an encryption circuit as  $C_*$ , the Grover oracle works as follows:

- $C_*$  computes  $|c\rangle$  with  $|m_0\rangle$  and  $|k\rangle$ .
- A comparison process compares  $|c\rangle$  with  $|c_0\rangle$  to decide whether to flip  $|q\rangle$ .
- Do the uncomputation with  $C_*^\dagger$ .

It can be seen that the cost of the Grover oracle is almost twice that of the encryption circuit. Therefore, the cost of Grover oracles with different structures can be evaluated directly by referring to the cost of different encryption circuits in Table 5.

Since uncomputation of recovering  $m$  is necessary in the Grover oracle, the depth of the Grover oracle is dominated by that of  $C_*$ . Thus,  $\mathcal{S}_p$  is used to construct low-depth circuits of the Grover oracle in related research. Our circuit  $\mathcal{S}_{cp}$  greatly reduces the use of message registers to store intermediate states and will have lower width than  $\mathcal{S}_p$  if the number of ancilla qubits required in round functions is small enough.

*Circuits for Encryption oracles.* We then consider the Encryption oracle defined in [KLLNP16b]:  $|m\rangle |0\rangle \rightarrow |m\rangle |E(m)\rangle$ , where  $m$  is the plaintext and  $E(m)$  is the encryption of  $m$ . Encryption oracles allows the input register to be in a superposition  $\sum_m |m\rangle$ , and then the output will be a superposition  $\sum_m |m\rangle |E(m)\rangle$ . Note that the key register is not needed in the Encryption oracle since the roundkeys can be precomputed classically and the AddRoundKey can be realized by applying  $X$  gates on specified qubits. The construction of Encryption oracles using  $\mathcal{S}_p, \mathcal{S}_z$  or  $\mathcal{S}_i$  is shown in Figure 7.

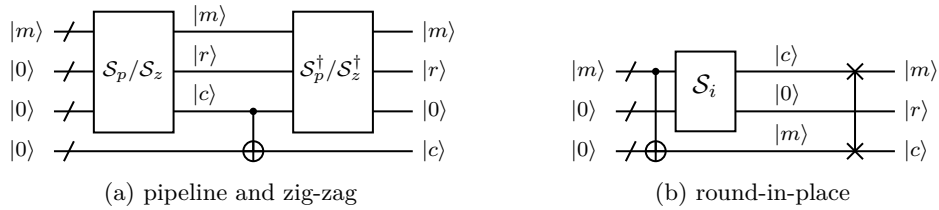


Figure 7: The Encryption oracle based on different structures

We show that our structure  $\mathcal{S}_{cp}$  can be used to construct an Encryption oracle that has a smaller depth. The depth of an Encryption oracle using  $\mathcal{S}_i$  is  $2r$  since there is no redundant intermediate states, and the depth of an Encryption oracle using  $\mathcal{S}_p/\mathcal{S}_z$  is twice the depth of  $\mathcal{S}_p/\mathcal{S}_z$  since uncomputation is needed to clean redundant states. However, the advantage of our structure is that  $\mathcal{S}_{cp}$  can greatly reduce the cost for cleaning redundant states. Since  $|c_{j-1}\rangle$  is cleaned by  $|c_j\rangle$ , the remaining redundant states contains only  $|c_{r-1}\rangle$ , which can be cleaned by  $|c\rangle$  using  $\mathcal{R}_r^{-1}$ . Thus, the depth of an Encryption oracle using  $\mathcal{S}_{cp}$  and  $\mathcal{R}_r^{-1}$  is only  $r + 1$ , almost half the previous record. The comparison with previous results is outlined in Table 6.

Table 6: The depth and width of Encryption oracles with different structures

	$\mathcal{S}_p$	$\mathcal{S}_z$	$\mathcal{S}_i$	<b>This paper</b>
depth	$2r$	$\approx 4r$	$2r$	<b><math>r + 1</math></b>
width	$(r + 1)n + \alpha$	$\approx \sqrt{2rn} + \alpha$	$(1 + 2)n + \alpha$	$(1 + 4)n + 2\alpha$

## 6 Quantum circuits of AES

In this section we give detailed quantum circuits of AES under the guidance of our structure. Quantum circuits for the encryption circuit and the key schedule of AES-128<sup>3</sup> are specified, and the cost is compared with other circuits in different cases. The encryption circuit can be used to synthesize an Encryption oracle with the lowest  $T$ -depth to date, and a small variant of the key schedule with our design of input-invariant Sbox can be used in the shallowed pipeline structure to save qubits for key registers.

### 6.1 Quantum circuits of AES S-box

We first introduce some knowledge on quantum circuits of AES S-box. The  $C_2$  circuit of AES S-box defined by  $C_2 : |x\rangle |y\rangle \mapsto |x\rangle |y \oplus S(x)\rangle$  is the main concern for out-of-place implementations, since  $C_1$  circuits defined by  $C_1 : |x\rangle |0\rangle \mapsto |x\rangle |S(x)\rangle$  are special cases of  $C_2$  circuits and are easier to design. The  $C_3$  circuit defined by  $C_3 : |S(x)\rangle |x\rangle \mapsto |S(x)\rangle |0\rangle$  can be efficiently constructed on a  $C_1$  circuit with a few more CNOT gates by the method in [HS22]. Moreover, some  $C_2$  circuits of AES S-box can be decomposed into Sbox and SubS<sup>†</sup>. The Sbox circuit is defined by Sbox:  $|x\rangle |0\rangle |y\rangle \mapsto |x'\rangle |r\rangle |y \oplus S(x)\rangle$ , where  $|r\rangle$  is the redundant state. Sbox can be decomposed into two parts denoted by SubS and SubC. SubS takes  $|x\rangle |0\rangle$  as input and outputs  $|x'\rangle |r\rangle$ , where  $|r\rangle$  contains linear components of  $S(x)$ . Then SubC adds them to  $|y\rangle$  to get  $|y \oplus S(x)\rangle$ .

Related works have studied some low Toffoli-depth Sboxes illustrated in Table 7. In these related works, the target qubit of each Toffoli gate in SubS is always a new qubit  $|0\rangle$ , so the Toffoli gates can be replaced by qAND gates with  $T$ -depth 1, and SubS<sup>†</sup> can be realized with  $T$ -depth 0 using qAND<sup>†</sup>. Therefore, these related works can be used to synthesize low  $T$ -depth qAND-based  $C_2$  circuits of AES S-box.

Note that the input register of some Sboxes can remain unchanged while others cannot. An Sbox is defined to be input-invariant if it can keep the input register unchanged, which means the information of the input register  $|x\rangle$  is not lost before SubS<sup>†</sup> or Sbox<sup>†</sup> is done. We observe that, the reason why some Sboxes are not input-invariant is that the input register is updated by some ancilla qubits with CNOT gates to save qubits, and these ancilla qubits themselves are also updated. It is worthy to note that the updating of  $|x\rangle$  can be uncomputed with only CNOT gates, as the target qubit of all Toffoli gates is always a new qubit  $|0\rangle$  in related works of low Toffoli-depth Sboxes. Therefore, adding some CNOT gates can make this kind of Sbox input-invariant without increasing the number of ancilla qubits and the Toffoli-depth (see Table 7 for our results). The full depth is also not increased when the Toffoli gates are decomposed.

<sup>3</sup>We omit the quantum circuit analysis of AES-192 and AES-256 because their analysis is similar to AES-128, but the key schedules are a little different but easier to design, and the added comparison is somewhat cumbersome.

Table 7: Some low *TofD* Sboxes

Source	#CNOT	#1qClifford	#Toffoli	<i>TofD</i>	Ancilla qubits	Input-invariant
[JNRV20]	186	4	34	6	120	✓
[HS22]	214	4	34	4	120	✓
[HS22]	356	4	78	3	182	✓
[LPZW23]	168	4	34	4	74	✗
<b>This paper</b>	179	4	34	4	74	✓
[LPZW23]	196	4	34	4	60	✗
<b>This paper</b>	207	4	34	4	60	✓
[JBK <sup>+</sup> 22]	313	4	78	3	136	✗ <sup>b</sup>
[JBK <sup>+</sup> 22]	162	4	34	4	68 <sup>a</sup>	✗ <sup>b</sup>

<sup>a</sup> The full depth of this circuit is smaller when the Toffoli gates are decomposed.

<sup>b</sup> Since the authors does not give specific implementations, we cannot give detailed costs for their input-invariant versions.

The process of finding a sequence of CNOT gates added to a given low Toffoli-depth Sbox to make it input-invariant can be integrated into an algorithm. It involves recording the qubits whose updatings should be memorized. All the input qubits are recorded at the beginning, and each qubit used to update a recorded qubit is recorded. Finally, a sequence of uncomputing the memorized updatings is returned. The detailed process is illustrated in Algorithm 2. Note that in order not to increase the Toffoli-depth, this algorithm is only suitable for such low Toffoli-depth Sboxes where the updating of input qubits is related with only CNOT gates.

Some  $C_1$  circuits for low-width Toffoli-based circuits are also studied, see Table 8 for some recent works. If these  $C_1$  circuits are used for AES S-box, our quantum circuit of AES-128 in Subsection 6.3 will have the lowest *TofD-W/TD-W* cost.

Table 8: Some Toffoli-based  $C_1$  circuits of AES S-box

Source	#CNOT	#1qClifford	#Toffoli	Toffoli-depth	Ancilla qubits
[LXX <sup>+</sup> 23]	193	4	57	24	5
[LXX <sup>+</sup> 23]	195	4	57	22	6
[LGQW23]	197	4	44	32	4

## 6.2 Round function and key schedule

In this subsection we give the detailed circuits of the iterative functions that we define for the encryption circuit and key schedule of AES-128.

For the encryption circuit, we define the beginning function  $B$  and the  $j$ -round function  $F_j$  which are shown in Figure 8. For simplicity, the result of applying multiple AES S-boxes on a qubit register  $|x\rangle$  is denoted by  $|S(x)\rangle$  throughout the rest of the paper.  $B$  and  $F_j$  acts as follows:

$$\begin{aligned}
 B &: |m\rangle |0\rangle |0\rangle |0\rangle \mapsto |c_0\rangle |S(c_0)\rangle |c_1\rangle |0\rangle, \\
 F_j &: |c_{j-1}\rangle |S(c_{j-1})\rangle |c_j\rangle |0\rangle \mapsto |c_j\rangle |S(c_j)\rangle |c_{j+1}\rangle |0\rangle.
 \end{aligned} \tag{3}$$

As a result, our circuit  $C_{cp}$  is synthesized by connecting  $B, F_1, F_2, \dots, F_9$ . Note that  $C_{cp}$  does not strictly adhere to the structure  $\mathcal{S}_{cp}$  in Figure 6. One can see that outputs of AES S-box are copied for cleaning the inputs in the next round, which saves the cost of the inverse of linear layers, and that our circuit  $C_{cp}$  is more compact, has clear linear and nonlinear layers, and has fewer linear layer components of AES than the circuit which adhere strictly to  $\mathcal{S}_{cp}$ . In a nonlinear layer, 16  $C_1$  circuits and 16  $C_3$  circuits are executed in parallel for the encryption circuit.

---

**Algorithm 2** Make an Sbox input-invariant.
 

---

**Input:** An NCT-based circuit  $\mathcal{C} = \{g_0 g_1 \dots g_{t-1}\}$  of an Sbox with input qubits  $|x_0 x_1 \dots x_7\rangle$ , ancilla qubits  $|r_0 r_1 \dots r_{m-1}\rangle$  and output qubits  $|y_0 y_1 \dots y_7\rangle$ . The updating of input qubits in the input Sbox should be related with only CNOT gates.

**Output:** A sequence of CNOT gates which is added to the Sbox to make it input-invariant.

```

seq ← [];
for i from 0 to m − 1 do
  updated[i] ← 0;
end for
for i from 0 to t − 1 do
  if  $g_i$  is not a CNOT gate then
    Continue;
  end if
  Let  $a$  be the control qubit and  $b$  be the target qubit of  $g_i$ .
  if  $b$  is some  $|x_i\rangle$  or some  $|r_j\rangle$  with  $updated[j] = 1$  then
    seq.append( $g_i$ );
    if  $a$  is some  $|r_j\rangle$  then
      updated[j] ← 1;
    end if
  end if
end for
seq.reverse();
return seq;

```

---

We then present a new key schedule circuit which is suitable with our new encryption circuit, since in  $F_j$ , two consecutive roundkeys  $|k_j\rangle, |k_{j+1}\rangle$  should be able to be computed simultaneously by CNOT gates. Instead of storing  $|k_j\rangle, |k_{j+1}\rangle$  in eight 32-qubit registers, we store linear components of two consecutive roundkeys registers to save qubits<sup>4</sup>. The linear components of two consecutive roundkeys  $|k_j\rangle, |k_{j+1}\rangle$  include  $|k_j^0\rangle |k_j^1\rangle |k_j^2\rangle |k_j^3\rangle |S(k_j^3)\rangle$ , and the computation of  $|k_j\rangle, |k_{j+1}\rangle$  with CNOT gates is based on the dependence of

<sup>4</sup>It is relatively easy for AES-192 and AES-256 to provide two consecutive roundkeys with eight 32-qubit key registers.

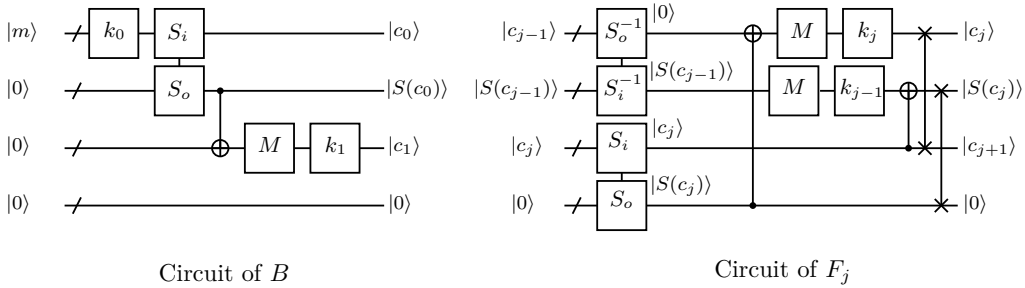


Figure 8: Circuits of  $B$  and  $F_j$ .  $S_i, S_o$  and  $S_i^{-1}, S_o^{-1}$  stand for the input and output registers of  $C_1$  circuits and  $C_3$  circuits, respectively. MixColumns no longer acts on the first message register in  $F_9$ . ShiftRows are omitted for simplicity throughout the rest of the paper.

consecutive roundkeys illustrated below:

$$\begin{cases} k_{j+1}^0 = Const_{j+1} \oplus S(k_3^j) \oplus k_j^0 \\ k_{j+1}^1 = Const_{j+1} \oplus S(k_3^j) \oplus k_j^0 \oplus k_j^1 \\ k_{j+1}^2 = Const_{j+1} \oplus S(k_3^j) \oplus k_j^0 \oplus k_j^1 \oplus k_j^2 \\ k_{j+1}^3 = Const_{j+1} \oplus S(k_3^j) \oplus k_j^0 \oplus k_j^1 \oplus k_j^2 \oplus k_j^3 \end{cases}, \quad (4)$$

where  $Const_{j+1}$  is the  $(j+1)$ -th round constant.

By the dependence of consecutive roundkeys, we construct a circuit of key schedule which can compute linear components of two consecutive roundkey states with six 32-qubit registers. The beginning iteration  $K_0$  and the  $j$ -th iteration  $K_j$  act as follows:

$$\begin{aligned} K_0 : |k_0^0\rangle |k_0^1\rangle |k_0^2\rangle |k_0^3\rangle |0\rangle |0\rangle &\mapsto |k_0^0\rangle |k_0^1\rangle |k_0^2\rangle |k_0^3\rangle |S(k_0^3)\rangle |0\rangle \\ K_j : |k_{j-1}^0\rangle |k_{j-1}^1\rangle |k_{j-1}^2\rangle |k_{j-1}^3\rangle |S(k_{j-1}^3)\rangle |0\rangle &\mapsto |k_j^0\rangle |k_j^1\rangle |k_j^2\rangle |k_j^3\rangle |S(k_j^3)\rangle |0\rangle. \end{aligned} \quad (5)$$

The circuit of  $K_j$  is illustrated in Figure 9, and the circuit of  $K_0$  is omitted due to its simplicity. In the nonlinear layer of  $K_j$ , 4  $C_1$  circuits and 4 reversed  $C_1$  circuits are executed in parallel. Therefore,  $F_j$  and  $K_j$  can be synchronized. It is easy to see that  $|k_j\rangle |k_{j+1}\rangle$  can be computed by the linear components with depth 5, thus a small increase in the depth of AddRoundKey trades for key register savings.

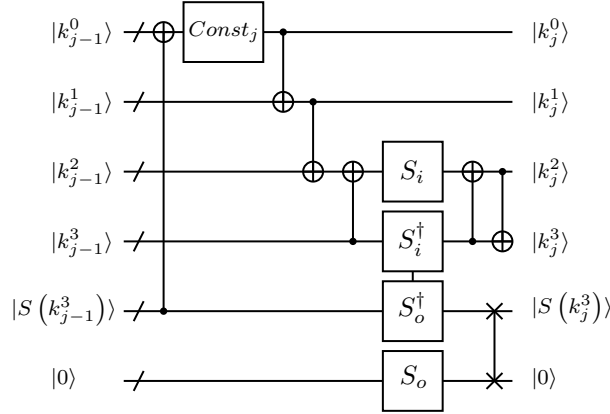


Figure 9: The  $j$ -th iteration  $K_j$  of the key schedule.

Moreover, only five 32-qubit registers are enough if one uses the qAND-based Sbox, since  $Sbox^\dagger$  can clear the redundant states without increasing the  $T$ -depth. The beginning iteration  $K'_0$  and the  $j$ -th iteration  $K'_j$  acts as follows:

$$\begin{aligned} K'_0 : |k_0^0\rangle |k_0^1\rangle |k_0^2\rangle |k_0^3\rangle |0\rangle |0\rangle &\mapsto |k_0^0\rangle |k_0^1\rangle |k_0^2\rangle |k_0^3\rangle |r_0\rangle |0\rangle \\ K_j : |k_{j-1}^0\rangle |k_{j-1}^1\rangle |k_{j-1}^2\rangle |k_{j-1}^3\rangle |r_{j-1}\rangle |0\rangle &\mapsto |k_j^0\rangle |k_j^1\rangle |k_j^2\rangle |k_j^3\rangle |r_j\rangle |0\rangle \end{aligned} \quad (6)$$

The corresponding circuit  $K'_j$  is shown in Figure 10.  $|r_{j-1}\rangle$  and  $|r_j\rangle$  are the redundant states within the computations of  $|S(k_{j-1})\rangle$  and  $|S(k_j)\rangle$ , respectively. Similarly,  $K_0$ 's corresponding circuit  $K'_0$  needs 4 Sboxes. It is worthy to note that the *Sbox* is actually input-invariant, which is easy to achieve based on our analysis in Subsection 6.1.

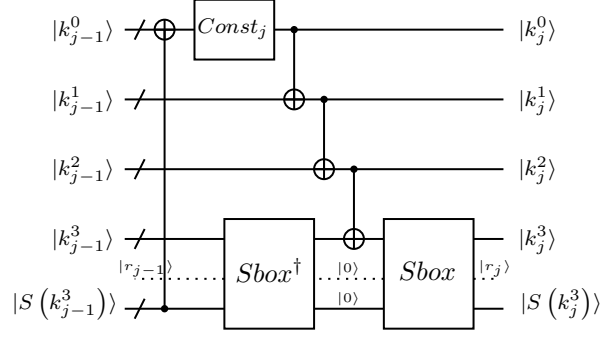


Figure 10:  $K'_j$  with Sbox and Sbox $^\dagger$ . The dashed line represents the ancilla qubits of qAND-based Sbox.

### 6.3 Quantum circuits of AES-128

AES-128 can be constructed with iterative circuits  $F_j, B, K_j, K'_j$  defined by us.  $F_j$  runs in parallel with  $B_j$ , where  $k_j, k_{j-1}$  are to add specific 32-qubit registers to the message registers by CNOT gates. See Figure 11 for the hierarchy of our quantum circuit of AES-128.

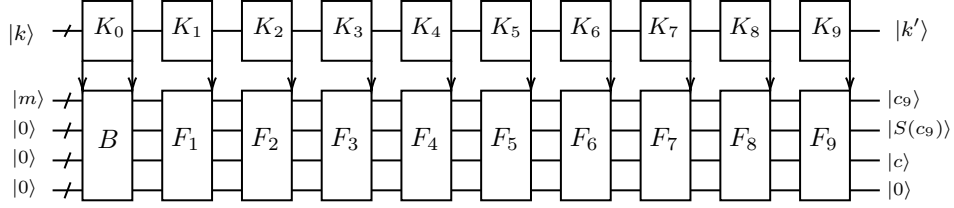


Figure 11: Our quantum circuit of AES-128. The arrows indicate the AddRoundKey process at the beginning or end of  $K_j$ .

We then compare the cost of our  $C_{cp}$  with that of  $\mathcal{S}_p$  and  $\mathcal{S}_i$  in both Toffoli-based and qAND-based AES S-box scenarios. For different circuits, the number of qubits required for key registers and message registers, parallel  $C_1, C_2$  circuits<sup>5</sup> and layers of AES S-box are shown in Table 9. One can see that our circuit  $C_{cp}$  do not need  $C_2$  circuits.

Table 9: Costs of different structures for AES-128

Circuits	$C_p$	$C_i$	$C_{cp}$ with $K_j$	$C_{cp}$ with $K'_j$
Qubits of key registers	128	128	192	160
Qubits of message registers	$128 \times 11$	$128 \times 2$	$128 \times 4$	$128 \times 4$
$C_1$ circuits in parallel	16	16	40	36
$C_2$ circuits in parallel	4	2	0	0
Layers of AES S-box	10	20	10	10

The cost of different structures can be computed when the number of ancilla qubits and the Toffoli/ $T$ -depth of AES S-box are determined. For simplicity of comparison, assume that both  $C_1$  and  $C_2$  circuits require  $m$  ancilla qubits. In case of using Toffoli-based AES S-box, our circuit needs fewer ancilla qubits than  $C_p$  when  $m < 42$ , and has lower  $TofD-W$  cost than  $C_i$  when  $m < 16$ . So our circuit will have lower  $TofD-W$ -cost with state-of-art

<sup>5</sup>Since a  $C_3$  circuit can be constructed by a  $C_1$  circuit with a few more CNOT gates using the method in [HS22], we regard them as the same type of  $C_1$  circuits.

low-width AES S-box. In case of using qAND-based Sbox, our circuit needs fewer ancilla qubits than  $C_p$  when  $m < 54$ , and has lower  $TD-W$  cost than  $C_i$  for all  $m > 0$ .

Since a Grover oracle is composed of  $AES$ ,  $AES^\dagger$  and a small comparison process, the choice of parameters to make the  $TD-W$  cost of Grover search lower is basically consistent with the above analysis.

## 6.4 AES Encryption oracle with lower $T$ -depth

As introduced in Subsection 5.3, previous research synthesized the AES Encryption oracle which cannot break the limit of  $2 \times 10$  layers of AES S-box. Since the roundkeys can be precomputed in the AES Encryption oracle, the redundant states of our circuit  $C_{cp}$  only include  $|c_9\rangle |S(c_9)\rangle$ , which can be cleaned with only one layer of AES S-box. The clear function  $C$  shown in Figure 12 takes  $|c_9\rangle |S(c_9)\rangle |c\rangle |0\rangle$  as input and outputs  $|0\rangle |0\rangle |c\rangle |0\rangle$ . Therefore, the AES Encryption oracle can be constructed with  $(10 + 1)$  layers of AES S-box.

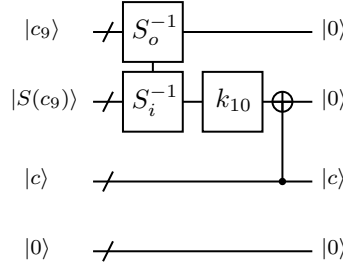


Figure 12: The clear function  $C$ .

Using the qAND-based  $C_1$  circuits and  $C_3$  circuits with  $T$ -depth 3, we construct an AES-128 Encryption oracle with  $T$ -depth 33, which breaks the previous record of  $T$ -depth 60 in [HS22].

Since in AES-like Hasing the roundkeys are actually constants, our circuit can also be used to construct quantum oracles of AES-like Hasing with lower  $T$ -depth.

## 6.5 Key schedule of the shallowed pipeline structure with lower width

Jang *et al.* proposed the shallowed pipeline structure using AES S-box that can be decomposed into Sbox and  $\text{SubS}^\dagger$ , where the cleaning of redundant states  $\text{SubS}^\dagger$  is delayed to the next round [JBK<sup>+</sup>22]. Then, Liu *et al.* improved the structure by sharing the ancilla qubits in Sbox and  $\text{SubS}^\dagger$  [LPZW23]. They both adopted the straight line structure for the key schedule, where  $|k_{j-1}\rangle$  will be updated by  $|k_j\rangle$  in the  $j$ -th round. As introduced in Subsection 6.1, the Sbox given in [HS22] with unoptimized width is input-invariant, but the Sbox given in [LPZW23] with optimized width is no longer input-invariant, which leads to the loss of information in the input register. Since Sbox and  $\text{SubS}^\dagger$  need  $|k_j^3\rangle$  and  $|k_{j-1}^3\rangle$  for each  $j$ , respectively, Jang *et al.* allocated extra 32 qubits for storing  $|k_{j-1}^3\rangle$  when using input-invariant Sbox. Since the Sbox used by Liu *et al.* has smaller width but is no longer input-invariant,  $10 \times 32$  qubits are allocated for storing all  $|k_{j-1}^3\rangle$  with  $1 \leq j \leq 10$ . We show that extra allocation of qubits for storing keywords is not necessary.

On the one hand, we have succeeded to make a low Toffoli-depth Sbox input-invariant with a few more CNOT gates. On the other hand, by the dependence of consecutive roundkeys in Equation 4 used in  $K_j$ 's, we have  $k_{j-1}^3 = k_j^2 \oplus k_j^3$ . Therefore, unchanged  $|k_j^3\rangle$  and the feasibility of computing  $|k_{j-1}^3\rangle$  with  $|k_j^2\rangle, |k_j^3\rangle$  means that the allocation of extra qubits for key schedule in [JBK<sup>+</sup>22, LPZW23] is unnecessary. Our  $K_j''$ 's for the shallowed



pipeline structure which are similar to  $K_j$ 's only need 128 qubits for key registers and work as follows:

$$\begin{aligned} K''_0 &: |k_0^0\rangle |k_0^1\rangle |k_0^2\rangle |k_0^3\rangle |0\rangle \mapsto |k_1^0\rangle |k_1^1\rangle |k_1^2\rangle |k_1^3\rangle |r_0, 0\rangle. \\ K''_j &: |k_j^0\rangle |k_j^1\rangle |k_j^2\rangle |k_j^3\rangle |r_{j-1}, 0\rangle \mapsto |k_{j+1}^0\rangle |k_{j+1}^1\rangle |k_{j+1}^2\rangle |k_{j+1}^3\rangle |r_j, 0\rangle. \end{aligned} \quad (7)$$

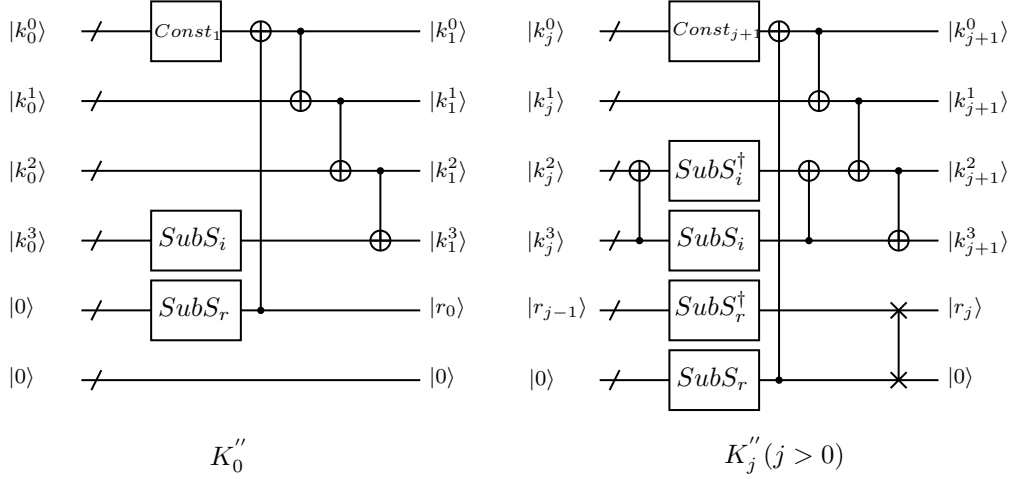


Figure 13:  $K''_j$  for the shallowed pipeline structure.  $SubS_i$  represents the input register of  $SubS$ , and  $SubS_r$  represents the register that will store the redundant state.

Using our  $K''_j$  and our input-invariant Sbox, we achieve a quantum circuit of AES-128 under the shallowed pipeline structure with the lowest  $TofD-W$  cost 130720 to date<sup>6</sup>.

## 7 Conclusion

In this work, quantum circuits of AES are studied and optimized. We first propose an improved greedy algorithm based on it. When applied to many MDS matrices and matrices used in block ciphers, our improved greedy algorithm gives the best results with the lowest depth for all of them. For example, our improved method finds an in-place CNOT circuit of AES MixColumns with depth 10, which breaks the recent record of depth 16 and helps to reduce the full depth of AES. To further optimize quantum circuits of AES, we propose a new compressed pipeline structure for iterative building blocks. If the round function is taken as a unit, our structure will have lower  $D-W$  cost when the number of ancilla qubits of a round function is small enough. Detailed quantum circuit of AES-128 under the guidance of our structure is given and compared with previous circuits. Moreover, the encryption circuit can be used to synthesis an AES-128 Encryption oracle with  $T$ -depth 33, and a small variant of the key schedule along with our input-invariant Sbox can avoid the allocation of  $10 \times 32$  qubits for storing key words in the shallowed pipeline structure where the Sbox is not input-invariant. Further optimization of low Toffoli-depth Sbox is left as a future work. Our methods in this paper can be used to optimize quantum circuits of other iterative building blocks.

<sup>6</sup>We contacted the author of [JBK<sup>+</sup>22] and learned that their not-yet-public circuit of Sbox with 68 ancilla qubits makes the combined Sbox and  $SubS^\dagger$  require 93 ancilla qubits. Our circuit uses the input-invariant version of Sbox and has a maximum width of 3268 which is internally optimized via ProjectQ [SHT18].

## References

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## A The depth 10 implementation of AES MixColumns.

Table 10: The implementation of AES MixColumns with quantum depth 10. The outputs  $|y_0\rangle, |y_1\rangle, \dots, |y_{31}\rangle$  are represented by 0, 17, 18, 27, 28, 21, 22, 15, 16, 25, 26, 3, 20, 29, 30, 7, 24, 1, 10, 19, 12, 5, 6, 31, 8, 9, 2, 11, 4, 13, 14, 23, respectively.

Operation	Operation	Operation
Depth 1	CNOT   (24, 16)	CNOT   (7, 17)
CNOT   (12, 28)	CNOT   (22, 23)	CNOT   (1, 18)
CNOT   (20, 4)	Depth 4	CNOT   (9, 26)
CNOT   (19, 3)	CNOT   (20, 27)	CNOT   (14, 23)
CNOT   (27, 11)	CNOT   (22, 31)	CNOT   (31, 8)
CNOT   (21, 5)	CNOT   (16, 17)	CNOT   (29, 13)
CNOT   (13, 29)	CNOT   (10, 18)	CNOT   (28, 12)
CNOT   (6, 22)	CNOT   (4, 21)	CNOT   (11, 4)
CNOT   (30, 14)	CNOT   (25, 9)	CNOT   (6, 15)
CNOT   (23, 31)	CNOT   (7, 0)	CNOT   (20, 27)
CNOT   (15, 7)	CNOT   (29, 6)	CNOT   (16, 25)
CNOT   (18, 2)	CNOT   (2, 26)	CNOT   (0, 24)
CNOT   (26, 10)	CNOT   (11, 19)	CNOT   (10, 3)
CNOT   (24, 1)	CNOT   (3, 23)	Depth 9
CNOT   (0, 8)	CNOT   (8, 24)	CNOT   (31, 7)
CNOT   (9, 25)	Depth 5	CNOT   (29, 5)
CNOT   (16, 17)	CNOT   (18, 26)	CNOT   (2, 10)
Depth 2	CNOT   (27, 12)	CNOT   (22, 14)
CNOT   (31, 7)	CNOT   (17, 9)	CNOT   (15, 23)
CNOT   (19, 27)	CNOT   (7, 3)	CNOT   (4, 28)
CNOT   (12, 20)	CNOT   (31, 15)	CNOT   (3, 11)
CNOT   (13, 21)	CNOT   (22, 8)	CNOT   (25, 1)
CNOT   (4, 28)	CNOT   (23, 20)	CNOT   (30, 6)
CNOT   (30, 6)	CNOT   (24, 16)	CNOT   (0, 16)
CNOT   (16, 0)	Depth 6	CNOT   (13, 21)
CNOT   (24, 8)	CNOT   (3, 23)	CNOT   (12, 20)
CNOT   (26, 18)	CNOT   (8, 24)	CNOT   (24, 9)
CNOT   (15, 23)	CNOT   (17, 1)	CNOT   (19, 27)
CNOT   (2, 10)	CNOT   (31, 19)	CNOT   (8, 17)
CNOT   (29, 5)	CNOT   (22, 30)	CNOT   (26, 18)
CNOT   (3, 11)	CNOT   (7, 4)	Depth 10
CNOT   (25, 17)	CNOT   (2, 12)	CNOT   (21, 5)
CNOT   (1, 9)	CNOT   (25, 18)	CNOT   (13, 29)
CNOT   (22, 14)	CNOT   (5, 21)	CNOT   (30, 14)
Depth 3	Depth 7	CNOT   (6, 22)
CNOT   (17, 26)	CNOT   (23, 24)	CNOT   (15, 7)
CNOT   (18, 19)	CNOT   (7, 18)	CNOT   (23, 31)
CNOT   (20, 13)	CNOT   (1, 2)	CNOT   (27, 3)
CNOT   (31, 12)	CNOT   (16, 9)	CNOT   (20, 4)
CNOT   (11, 3)	CNOT   (22, 19)	CNOT   (19, 11)
CNOT   (8, 9)	CNOT   (31, 20)	CNOT   (12, 28)
CNOT   (21, 30)	CNOT   (10, 27)	CNOT   (9, 25)
CNOT   (28, 4)	CNOT   (5, 13)	CNOT   (26, 2)
CNOT   (2, 27)	CNOT   (28, 29)	CNOT   (18, 10)
CNOT   (7, 25)	CNOT   (25, 26)	CNOT   (24, 16)
CNOT   (14, 6)	Depth 8	CNOT   (8, 0)
CNOT   (29, 15)	CNOT   (5, 22)	CNOT   (17, 1)



## B Brief description of the AES family.

The AES family [DR02] contains three instances, denoted as AES-128, AES-192 and AES-256 respectively according to the length of the key.

The round function of the AES family consists of four transformations, i.e., SubBytes, ShiftRows, MixColumns and AddRoundKey. The total number of rounds equals 10, 12 and 14 for AES-128, AES-192 and AES-256, respectively. 16 bytes are arranged in a  $4 \times 4$  matrix state. The SubBytes replaces each byte in the state by another one according to the AES S-box. The ShiftRows changes the position of the bytes by cyclically rotating the bytes in the  $i$ -th row to the left by  $i$  bytes, where  $i = 0, 1, 2, 3$ . The MixColumns is a right circulant matrix  $(0x02, 0x03, 0x01, 0x01)$  over  $\text{GF}(8, \mathbb{F}_2)$  and acts on each column of the state by matrix multiplication. Note that the MixColumns is absent in the last round. The AddRoundKey adds the roundkey to the state by bitwise XOR.

The key schedule of AES-128 is based on 32-bit words. Denote the master key by  $W_0, W_1, \dots, W_{s-1}$ , where  $s = 4$  for AES-128. Except the given words (i.e., the words in the master key), 40 words are required by AES-128. For AES-128, the word  $W_i$  can be calculated by the following equation:

$$W_i = \begin{cases} W_{i-4} \oplus \text{SubWord}(\text{RotWord}(W_{i-1})) \oplus \text{Const}(i/4), & \text{if } i \equiv 0 \pmod{4}, \\ W_{i-4} \oplus W_{i-1}, & \text{otherwise,} \end{cases}$$

where  $i = 4, 5, \dots, 43$ .  $k_j^i$  equals  $W_{4j+i}$  is the  $i$ -th 32-bit word of the  $j$ -th roundkey.

The SubWord applies four AES S-boxes to the bytes in one word. The RotWord cyclically rotates the bytes in the word to the left by one byte. The Rcon adds the round constant to the word by bitwise XOR.