Advancing Quantum State Preparation using LimTDD

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Abstract-Quantum state preparation (QSP) is a fundamental task in quantum computing and quantum information processing. It is critical to the execution of many quantum algorithms, including those in quantum machine learning. In this paper, we propose a family of efficient QSP algorithms tailored to different numbers of available ancilla qubits ranging from no ancilla qubits, to a single ancilla qubit, to a sufficiently large number of ancilla qubits. Our algorithms are based on a novel decision diagram that is fundamentally different from the approaches used in previous QSP algorithms. Specifically, our approach exploits the power of Local Invertible Map Tensor Decision Diagrams (LimTDDs) — a highly compact representation of quantum states that combines tensor networks and decision diagrams to reduce quantum circuit complexity. Extensive experiments demonstrate that our methods significantly outperform existing approaches and exhibit better scalability for large-scale quantum states, both in terms of runtime and gate complexity. Furthermore, our method shows exponential improvement in best-case scenarios. This paper is an extended version of [1], with three more algorithms proposed.

Index Terms—quantum state preparation, decision diagrams, quantum circuits

I. INTRODUCTION

Quantum computing represents a transformative leap in computation capabilities, by leveraging the principles of quantum mechanics to achieve exponential speedups in specific computational tasks. This technology harnesses the unique properties of quantum bits (qubits), such as superposition and entanglement, to tackle complex problems more efficiently than classical computers. For instance, quantum algorithms like Shor's algorithm factor large integers exponentially faster than existing classical algorithms, thereby posing a significant challenge to traditional cryptographic methods [2]. In the realm of material science and drug development, quantum computing also enables faster simulations of molecular behaviours and chemical reactions, accelerating the discovery of new materials and pharmaceuticals [3], [4]. Moreover, quantum computing holds vast potential for applications in optimisation problems and artificial intelligence [5], [6] as well.

One of the fundamental challenges in quantum computing and quantum information processing is the efficient preparation of quantum states, known as Quantum State Preparation (QSP). The success of many quantum algorithms, for example, quantum machine learning [7] and HHL [8], requires encoding classical data into quantum states efficiently. However, as the number of qubits in a quantum system increases, the complexity of representing and manipulating quantum states also grows exponentially, making efficient preparation of quantum states a highly challenging problem, particularly for large-scale quantum systems.

Work partially supported by Innovation Program for Quantum Science and Technology under Grant No. 2024ZD0300502, Beijing Nova Program Grant No. 20220484128 and 20240484652, and the National Natural Science Foundation of China Grant No. 12471437.

Significant progress has been made in recent years in developing efficient algorithms for QSP. Various methods have been proposed to prepare states of special types, such as sparse quantum states [9], [10], [11]. Techniques based on gate decomposition [12], [13], [14] and uniformly controlled rotations [15] have been developed for the preparation of general quantum states. Some works focus on minimising the number of ancilla qubits [16], while others aim to minimise the circuit depth [17]. Theoretical bounds for QSP have also been established [18]. However, most existing methods rely on explicit representations of quantum states, such as vector representations, which grow exponentially as the number of qubits increases, limiting the scale of quantum states that can be efficiently prepared.

Decision diagrams have emerged as a powerful tool for representing and manipulating quantum states efficiently due to their compactness. These compact data structures were first used in classical computation, and have found wide application in classical circuit synthesis [19] and verification [20]. Recently, researchers have explored the application of decision diagrams in quantum computing. By adapting classical decision diagrams to support quantum operations or designing new decision diagrams, significant progress has been made in the efficient simulation and verification of quantum circuits [21], [22]. Moreover, decision diagrams have also been applied to QSP [23], [24], [25]. With the compactness of decision diagrams, these algorithms demonstrate high efficiency and the ability to prepare relatively large-scale quantum states, circumventing the issue that the quantum states require exponential memory space. For example, Mozafari et al. proposed an efficient algorithm for preparing uniform quantum states [23]. Other works have attempted to further optimise the preparation process using one or multiple ancilla qubits to [24], [25]. In such methods, the compression efficiency of the decision diagrams used is the key factor that influences the effectiveness of the final state preparation.

A recent advancement in this field is the proposal of the Local Invertible Map Tensor Decision Diagram (LimTDD) [26]. LimTDD combines the strengths of tensor networks and decision diagrams, offering a highly compact representation of quantum states. It can identify isomorphic structures between tensors, achieving exponential improvement in compression efficiency compared to other decision diagrams like TDD and LIMDD.

This paper explores the use of LimTDD for quantum state preparation, leveraging its high compression efficiency to develop more efficient algorithms. We first investigate the fundamental properties of LimTDD and propose a QSP algorithm that does not require any ancilla qubits. We then extend this approach to algorithms that use one or multiple ancilla qubits, inspired by previous works [24], [25]. The time and gate complexity of both algorithms correspond to the number of paths and of nodes of the underlying decision

diagram, respectively. Since LimTDD normally has fewer paths and fewer nodes, our algorithms demonstrate significant improvements in efficiency and circuit complexity, particularly in the best-case scenario. Finally, we propose a flexible algorithm that can adapt to different numbers of available ancilla qubits to maximise resource usage.

Our experiments show that the proposed algorithms can handle large-scale quantum states more efficiently, reducing the number of quantum gates and circuit depth. This work highlights the potential of LimTDD in QSP and provides a robust foundation for the future development of quantum computing technologies. We have developed an interface that converts state vectors into LimTDDs and synthesises these representations into executable state preparation circuits. This tool streamlines the workflow for quantum physicists and experimentalists, enabling them to efficiently generate the quantum states required for their research. Future work will focus on integrating our algorithms into widely used quantum computing frameworks, such as Qiskit, to further accelerate and standardise the QSP process.

The structure of this paper is as follows. In section II, we provide basic concepts of quantum computing, QSP, and LimTDD. In section III, we introduce the basic constructions for QSP using LimTDD. From section VI to IV, we give algorithms for QSP using LimTDD with no ancilla qubits, one ancilla qubit, sufficient number of ancilla qubits, and a given number of ancilla qubits. Then, we conduct experiments to carefully analyse the performance of our algorithm in section VIII. Finally, in section IX, we give a brief conclusion on our paper.

II. BACKGROUND

In this section, we give basic background on quantum computing, quantum state preparation, and LimTDD.

A. Quantum Computing

1) Quantum States: Quantum computing harnesses the principles of quantum mechanics to perform computations using quantum bits (qubits), which can exist in superpositions of states, unlike classical bits that are either 0 or 1. A qubit is described by a two-dimensional complex vector space with orthonormal basis states $|0\rangle$ and $|1\rangle$, satisfying:

$$\langle 0|0\rangle = \langle 1|1\rangle = 1$$
 and $\langle 0|1\rangle = \langle 1|0\rangle = 0$.

A general qubit state can be in a linear combination $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, where α and β are complex numbers with $|\alpha|^2 + |\beta|^2 = 1$. This superposition allows qubits to represent multiple states simultaneously and parallelly, offering an advantage over classical bits.

For multi-qubit systems, the state space grows exponentially with the number of qubits. An n-qubit system is described by a 2^n -dimensional complex vector, with basis states $|k\rangle$ (binary strings of length n). For example, $|000\rangle$ represents all three qubits in the $|0\rangle$ state $|000\rangle = |0\rangle \otimes |0\rangle \otimes |0\rangle$.

Example 1: Consider the 3-qubit state $\frac{1}{\sqrt{6}}(|000\rangle + |001\rangle + \frac{1}{\sqrt{2}}|010\rangle - \frac{1}{\sqrt{2}}|011\rangle - |100\rangle - \frac{1}{\sqrt{2}}|101\rangle + \frac{1}{\sqrt{2}}|110\rangle + |111\rangle$, represented as an 8-dimensional vector: $\frac{1}{\sqrt{6}}[1,1,\frac{1}{\sqrt{2}},-\frac{1}{\sqrt{2}},-1,-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1]^T$.

2) Quantum Gates: Quantum gates, which are unitary transformation.

- 2) Quantum Gates: Quantum gates, which are unitary transformations on qubits, perform quantum computations. Common gates include:
 - Hadamard gate (H gate): Creates superposition states:

$$H|0\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \quad H|1\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle).$$

• Pauli-Z gate (Z gate): Introduces a phase flip to $|1\rangle$:

$$Z|0\rangle = |0\rangle, \quad Z|1\rangle = -|1\rangle.$$

 Controlled-X gate (CX gate): Flips the target qubit if the control qubit is |1>:

$$CX(|0\rangle \otimes |\psi\rangle) = |0\rangle \otimes |\psi\rangle, \quad CX(|1\rangle \otimes |\psi\rangle) = |1\rangle \otimes X |\psi\rangle.$$

3) Quantum Circuits: Quantum circuits implement quantum algorithms by sequencing these gates. Gates are applied to qubits, and their order determines the overall transformation. Outputs are typically measured in the computational basis. Circuits can be graphically represented, with qubits as lines and gates as symbols.

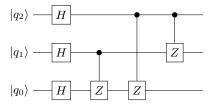


Fig. 1. Example of a quantum circuit with Hadamard and CZ gates.

Fig. 1 shows a quantum circuit with Hadamard and CZ gates, creating superposition and entanglement among three qubits.

B. Quantum State Preparation

The task of preparing a specific quantum state is a cornerstone in quantum computing and quantum information processing. This procedure is vital for executing various quantum algorithms, many of which demand particular quantum states as inputs to harness their computational benefits.

- 1) Formal Definition: Starting with a given initial state, commonly $|0\rangle^{\otimes n}$, the goal of quantum state preparation is to reach a target quantum state $|\psi_v\rangle = \sum_{k=0}^{2^n-1} v_k \, |k\rangle$. Here, $v = (v_0, v_1, \dots, v_{2^n-1})^T \in \mathbb{C}^{2^n}$ is a normalized vector $(\|v\|_2 = 1)$ that encapsulates the amplitudes of the target state in the computational basis. The mission of QSP is to devise a quantum circuit capable of converting the initial state into the target state $|\psi_v\rangle$.
- 2) Key Challenges and Significance: In the general case, the complexity of representing and manipulating quantum states escalates exponentially with the number of qubits n. To fully characterise a general n-qubit state, 2^n complex amplitudes are necessary, rendering the explicit representation and preparation of arbitrary quantum states computationally prohibitive in most scenarios. This makes efficient QSP an exceedingly challenging problem, particularly for large-scale quantum systems. Nevertheless, it is indispensable for practical quantum computing applications, as the efficiency of QSP directly affects the viability and performance of numerous quantum algorithms.

C. LimTDD

LimTDD, or Local Invertible Map Tensor Decision Diagram, is an advanced decision diagram designed to efficiently represent and manipulate tensors and tensor networks. In this work, we employ the LimTDD data structure to depict quantum states, leveraging its remarkable compression ratio to facilitate the preparation of largescale quantum states with high efficiency.

The compact representation of LimTDD is established on the concept of quantum state isomorphism.

Definition 1 (LIM, Quantum State Isomorphism): An n-qubit Local Invertible Map (LIM) is an operator O of the form

$$O = \lambda O_n \otimes \dots \otimes O_1, \tag{1}$$

where $\lambda \in \mathbb{C}$ is a complex number and each O_i is an invertible 2×2 matrix. The set of all such maps is denoted as $\mathcal{M}(n)$, and the set of all LIMs is defined as

$$\mathcal{M} = \bigcup_{n \in N} \mathcal{M}(n). \tag{2}$$

Two n-qubit quantum states $|\Psi\rangle$ and $|\Phi\rangle$ are said to be isomorphic if $|\Phi\rangle = O |\Psi\rangle$ for some $O \in \mathcal{M}(n)$.

Definition 2 (LimTDD): Let \mathcal{G} be a subgroup of \mathcal{M} . A \mathcal{G} -LimTDD \mathcal{F} over a set of indices S is a rooted, weighted, and directed acyclic graph $\mathcal{F} = (V, E, idx, low, high, wt)$ defined as follows:

- V is a finite set of nodes which consists of non-terminal nodes V_{NT} and a terminal node v_T labelled with integer 1. Denote by $r_{\mathcal{F}}$ the unique root node of \mathcal{F} ;
- $idx: V_{NT} \to S$ assigns each non-terminal node an index in S. We call $idx(r_F)$ the top index of F, if r_F is not the terminal node;
- both low and high are mappings in $V_{NT} \to V$, which map each non-terminal node to its 0- and 1-successors, respectively;
- $E = \{(v, low(v)), (v, high(v)) : v \in V_{NT}\}$ is the set of edges, where (v, low(v)) and (v, high(v)) are called the lowand high-edges of v, respectively. For simplicity, we also assume the root node $r_{\mathcal{F}}$ has a unique incoming edge, denoted e_r , which has no source node;
- wt : $E \to \mathcal{G}$ assigns each edge a weight in \mathcal{G} . wt (e_r) is called the weight of \mathcal{F} , and denoted $w_{\mathcal{F}}$. In this paper, if $wt(e) = \lambda \cdot O$, for some complex number λ and invertible map O, we call λ the complex weight and O the (pure) operator.

Although LimTDD can be used to represent all tensors, we only consider cases where it represents quantum states. When used to represent a quantum state, the semantics of the terminal node is defined to be $|v_T\rangle = 1$, the semantics of an edge e, directing to a node v, is defined as

$$|e\rangle = \operatorname{wt}(e) \cdot |v\rangle$$

and the semantics of a non-terminal node v is defined to be

$$|v\rangle = |0\rangle \otimes |(v, low(v))\rangle + |1\rangle \otimes |(v, high(v))\rangle.$$

In this paper, each index corresponds to a qubit, and we will use q_v to represent the qubit corresponding to a node v. For convenience, we assume that the top index represents the most significant qubit $(q_{n-1}$ for an n-qubit state), and the bottom non-terminal node's index represents the least significant qubit (q_0) , with other qubits arranged sequentially. Occasionally, we use notations like $|0\rangle_{n-1}$ and $|0\rangle_0$ to identify specific qubits, and we will use notation $|0\rangle_n$ to represent a $|0\rangle$ state on the qubit corresponding to the node v. In addition, we use will $|*\rangle_n$ to represent all possible computational bases of n qubits, and we will omit n if no ambiguity. The subgroup $\mathcal G$ is set to XP-Operators in [26], but our algorithm applies to any subgroup of \mathcal{M} .

Example 2: Fig. 2 illustrates an example of a LimTDD representing the quantum state from Example 1. In this diagram, low edges are depicted with dotted red lines and high edges with solid blue lines. The qubit corresponds to node v_{20} is q_2 , the qubit corresponds to node v_{10} and v_{11} is q_1 , and the qubit corresponds to node v_{00} and v_{01} is q_0 . Ignoring normalisation coefficients:

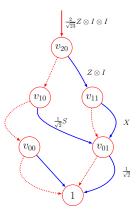


Fig. 2. An example of LimTDD representing the quantum state $|\mathcal{F}\rangle=\frac{2}{\sqrt{23}}[1,1,\frac{1}{\sqrt{2}},\frac{i}{2},-1,-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1]^T.$ We omit the weight 1 and $1\cdot I^{\otimes k}$ in the figure.

- The v_{00} node represents $|v_{00}\rangle=|0\rangle+|1\rangle$, and the v_{01} node represents $|v_{01}\rangle=|0\rangle+\frac{1}{\sqrt{2}}|1\rangle$.
 The v_{10} node represents $|v_{10}\rangle=|0\rangle\,|v_{00}\rangle+\frac{1}{\sqrt{2}}\,|1\rangle\,(S\,|v_{01}\rangle)=|00\rangle+|01\rangle+\frac{1}{\sqrt{2}}\,|10\rangle+\frac{i}{2}\,|11\rangle$, and the v_{11} node represents $|v_{11}\rangle=|0\rangle\,|v_{01}\rangle+|1\rangle\,(X\,|v_{01}\rangle)=|00\rangle+\frac{1}{\sqrt{2}}\,|01\rangle+\frac{1}{\sqrt{2}}\,|10\rangle+|11\rangle$
- The v_{20} node represents $|v_{20}\rangle=|0\rangle\,|v_{10}\rangle+|1\rangle\,(Z\otimes I\,|v_{11}\rangle)=|000\rangle\,+\,|001\rangle\,+\,\frac{1}{\sqrt{2}}\,|010\rangle\,+\,\frac{i}{2}\,|011\rangle\,+\,|100\rangle\,+\,\frac{1}{\sqrt{2}}\,|101\rangle\,-\,\frac{1}{\sqrt{2}}\,|110\rangle\,-\,|111\rangle.$ The entire LimTDD represents the quantum state $\frac{2}{\sqrt{23}}Z\otimes I\otimes I\,|v_{20}\rangle=\frac{2}{\sqrt{23}}(|000\rangle\,+\,|001\rangle\,+\,\frac{1}{\sqrt{2}}\,|010\rangle\,+\,\frac{i}{2}\,|011\rangle\,-\,|100\rangle\,-\,\frac{1}{\sqrt{2}}\,|101\rangle\,+\,\frac{1}{\sqrt{2}}\,|110\rangle\,+\,|111\rangle).$ For convience, we denote the quantum state as $|F\rangle$

We will also use the following graphical notation to describe LimTDDs. Each node within a LimTDD is uniquely characterised by three key elements: its index, the two nodes it points to (successors), and the weights assigned to the edges leading to these successors. This relationship can be visually represented as:

$$(v_0) \stackrel{w_0}{\longleftarrow} (v) \xrightarrow{w_1} (v_1)$$

Moreover, the entire LimTDD structure is uniquely defined by its root node and the weight associated with the edge entering this root node. This can be expressed as:

$$\left(w_{\mathcal{F}}, \ v_0\right) \stackrel{w_0}{\longleftarrow} \left(v\right) \xrightarrow{w_1} \left(v_1\right),$$

or more compactly as:

$$\xrightarrow{w_{\mathcal{F}}} (v)$$

Note that, for a LimTDD representing a quantum state, when normalisation has been applied, every non-terminal node will have the following form:

$$(v_0) \leftarrow V_1 - (v) \xrightarrow{\lambda \cdot O} (v_1).$$

For any unnormalised quantum state $|\psi\rangle$, there exists a unitary operator U such that $U|\psi\rangle = w|0\rangle$, where $w = \sqrt{\langle \psi | \psi \rangle}$ represents the 2-norm of $|\psi\rangle$. When a node $(v_0) \stackrel{\lambda_0 \cdot O}{\longleftarrow} (v) \stackrel{\lambda_1 \cdot O'}{\longleftarrow} (v_1)$ represents the quantum state $|\psi\rangle$, where λ_0 and λ_1 are two complex numbers, the 2-norm of v, denoted as ||v||, is defined to be $\sqrt{\langle \psi | \psi \rangle}$, which can

be computed based on the norms of its two successors. Specifically,

$$||v|| = \sqrt{|\lambda_0|^2 \cdot ||v_0||^2 + |\lambda_1|^2 \cdot ||v_1||^2},$$

with the norm of the terminal node $||v_T||$ set to 1.

In this paper, we use bit-strings $b_{n-1} \cdots b_0$ (where each $b_i \in \{0,1\}$) to represent paths in a LimTDD. The prefix path leading to a node v along a path $b_{n-1} \cdots b_0$ is defined as the prefix $b_{n-1} \cdots b_{k+1}$, if the qubit corresponding to v is q_k . The product of all the weights along a (prefix) path is called an accumulated weight.

Example 3: In Fig. 2, the left-most path (red-red-red) is 000. The prefix path leading to the node v_{10} along this path is 0, and the prefix path leading to the node v_{00} is 00, where the accumulated weights along both paths are $\frac{1}{\sqrt{23}}Z \otimes I \otimes I$.

III. BASIC CONSTRUCTIONS

The methods for QSP using LimTDD are mainly based on the following basic construction components.

A. Basic Construction Components

Basic Construction 1 (Incoming Edge Operator Elimination): Let $\mathcal{F} = \stackrel{\lambda O_n \otimes \cdots \otimes O_1}{\longrightarrow} \stackrel{\smile}{(v)}$ be a LimTDD representing the quantum state $|\psi\rangle$. Then, we have

$$|\psi\rangle = \lambda(O_n \otimes \cdots \otimes O_1) |v\rangle.$$

Applying the operator $(O_n \otimes \cdots \otimes O_1)^{\dagger}$ to $|\psi\rangle$ reduces it to $\lambda |v\rangle$, which can be represented by a LimTDD with the root node v and incoming edge weight λ , that is,

$$\xrightarrow{\lambda} (v)$$

In other words, applying $(O_n \otimes \cdots \otimes O_1)^{\dagger}$ to the LimTDD (i.e., contracting each index x_i (corresponding to q_i) with an operator O_i) eliminates the operator on the incoming edge of the LimTDD.

Basic Construction 2 (High-Edge operator Elimination): Let

$$(v_0) \leftarrow \stackrel{I}{-} (v) \xrightarrow{\lambda O_n \otimes \cdots \otimes O_1} (v_1)$$

be a non-terminal node of a LimTDD \mathcal{F} . Let p be the prefix path leading to v, and assume the accumulated weight along p is a complex number w. Then, the quantum state represented by \mathcal{F} can be expressed as $|\psi\rangle = w \cdot |p\rangle \, |v\rangle + |\mathrm{Res}\rangle = w \cdot |p\rangle \, |0\rangle \, |v_0\rangle + w \cdot \lambda \cdot |p\rangle \, |1\rangle \, (O_n \otimes \cdots \otimes O_1 \, |v_1\rangle) + |\mathrm{Res}\rangle$, where $|\mathrm{Res}\rangle$ is orthogonal to $|p\rangle \, |*\rangle$. By applying the controlled operator $(O_n \otimes \cdots \otimes O_1)^{\dagger}$ with the control condition $|p\rangle \, |1\rangle$, the state is transformed into

$$w \cdot |p\rangle |0\rangle |v_0\rangle + w \cdot \lambda \cdot |p\rangle |1\rangle |v_1\rangle + |\text{Res}\rangle.$$

Consequently, the node is updated to $v_0 \leftarrow v_0 \leftarrow v_0 \leftarrow v_0$ indicating that the operator on the high-edge of the node has been successfully eliminated.

Basic Construction 3 (Outgoing Weight Reduction): Consider a non-terminal node of a LimTDD \mathcal{F} :

$$(v_0) \stackrel{w_0}{\longleftarrow} (v) \xrightarrow{w_1} (v_0),$$

where w_0 and w_1 are complex numbers with $w_0 \neq 0$. Let p denote the prefix path leading to v, and assume the accumulated weight along p is a complex number w. The quantum state represented by \mathcal{F} can then be written as $|\psi\rangle = w \cdot |p\rangle |v\rangle + |\mathrm{Res}\rangle = w \cdot |p\rangle (w_0 |0\rangle + w_1 |1\rangle) |v_0\rangle + |\mathrm{Res}\rangle$, where $|\mathrm{Res}\rangle$ is orthogonal to $|p\rangle |*\rangle$. Define $c = w_1/w_0$. Applying the controlled unitary operator

$$\frac{1}{\sqrt{1+|c|^2}} \begin{bmatrix} 1 & c^{\dagger} \\ -c & 1 \end{bmatrix}$$

to $|\psi\rangle$ with the control condition $|p\rangle$ transforms the state into $w\cdot\sqrt{|w_0|^2+|w_1|^2}\cdot|0\rangle\,|v_0\rangle+|\mathrm{Res}\rangle$. Consequently, the node is updated to $v_0 \leftarrow v_0 \leftarrow v_0 \leftarrow v_0$. This indicates that the complex weights on the two outgoing edges of v_0 have been successfully reduced to $v_0 \leftarrow v_0$, corresponding to $v_0 \leftarrow v_0$.

It is important to note that the accumulated weight leading to the node must be a complex number, in both Constructions 2 and 3. Additionally, in Construction 3, both successor nodes must be identical. This implies that whenever we process a node, we must first eliminate all operators on the paths leading to it. When dealing with the outgoing complex weights of a node, we must first ensure that its two successors are transformed into the same state. Therefore, in the four proposed algorithms, we will first traverse the LimTDD from top to bottom to sequentially eliminate the operators. After reaching the bottom, we will then address the complex weights in reverse order. By the time we handle the outgoing weights of a node, both of its successors will have been converted to represent $|0\rangle^{\otimes k}$ for some k.

B. Branch Condition

Note that in Basic Constructions 2 and 3, we utilise the values of all qubits along a prefix path leading to the node v as the control condition. Typically, this can be simplified to using the values of all branch nodes (branch condition).

For instance, consider a quantum state

$$|\psi\rangle = |0\rangle_3 |+\rangle_2 |1\rangle_1 |v\rangle + |\text{Res}\rangle,$$

where $|{\rm Res}\rangle$ is some state orthogonal to $|0\rangle_3 |0\rangle_2 |1\rangle_1 |*\rangle$ and $|0\rangle_3 |1\rangle_2 |1\rangle_1 |*\rangle$. In this case, the operator on the high-edge of v can be eliminated using the control condition $|0\rangle_3 |1\rangle_1 |1\rangle_v$, and the weights on the two outgoing edges of v can be reduced using the control condition $|0\rangle_3 |1\rangle_1$.

Definition 3 (Branch Condition): A non-terminal node is termed a branch node if its 0-successor and 1-successor are distinct. The branch condition for a node along a path is defined by the values of all branch nodes preceding it on that path.

Consider the LimTDD given in Fig. 2. The nodes v_{20} and v_{10} are branch nodes. The branch condition for the v_{10} node along the path 000 is $|0\rangle_2$, while for the v_{00} node, it is $|0\rangle_2 |0\rangle_1$.

Through this operation, we effectively handle multiple paths simultaneously, which we collectively refer to as a reduced path.

Definition 4 (Reduced paths): Let \mathcal{F} be a decision diagram. The reduced diagram of \mathcal{F} is obtained by merging the edges between any two nodes in \mathcal{F} . We also call paths within this reduced diagram reduced paths of \mathcal{F} .

In the provided example, the node v_{11} has identical 0-successor and 1-successor nodes, meaning its two outgoing edges are merged when determining the reduced paths. The same applies to the nodes v_{00} and v_{01} . Consequently, the LimTDD features only 3 reduced paths. The number of reduced paths is a primary indicator of complexity for some of the algorithms proposed below.

C. Open/Closed Node

It is important to note that while the branch condition is introduced to reduce the number of control qubits, it may still involve a significant number of qubits, thereby increasing the complexity of the resulting circuit. To mitigate this, ancilla qubits can be introduced to further reduce the number of control qubits.

For instance, consider the quantum state $|\psi\rangle = w \cdot |p\rangle |v\rangle + |\text{Res}\rangle = w \cdot |p\rangle |0\rangle |v_0\rangle + w \cdot \lambda \cdot |p\rangle |1\rangle (O_n \otimes \cdots \otimes O_1 |v_1\rangle) + |\text{Res}\rangle$. By introducing an ancilla qubit q_a , we can adjust the quantum state to $w \cdot |1\rangle_a |p\rangle |v\rangle + |0\rangle_a |\text{Res}\rangle = w \cdot |1\rangle_a |p\rangle |0\rangle_v |v_0\rangle + w \cdot \lambda \cdot$

 $|1\rangle_a |p\rangle |1\rangle_v (O_n \otimes \cdots \otimes O_1 |v_1\rangle) + |0\rangle_a |\mathrm{Res}\rangle$. Then, the operator $O_n \otimes \cdots \otimes O_1$ can be eliminated using the control condition $|1\rangle_a |1\rangle_v$. In this case, we say that the node v is marked open by the ancilla qubit q_a . More specifically:

Definition 5 (Open/Closed Node): Let \mathcal{F} be a LimTDD representing the quantum state $|\psi\rangle = \sum_{k=0}^{2^n-1} \lambda_k \, |k\rangle$. By introducing an ancilla qubit q_a and marking each computational basis state $|k\rangle$ with $|b_k\rangle_a$, we obtain the state $\sum_{k=0}^{2^n-1} \lambda_k \, |b_k\rangle_a \, |k\rangle$, where $b_k \in \{0,1\}$. A path p, corresponding to the state $|p\rangle$, is called open (closed, respectively) by q_a if $b_p = 1$ (0, respectively). A node v with prefix path p is called open (closed, respectively) by q_a if all states $|p\rangle \, |*\rangle$ are marked open (closed). A LimTDD is called open (closed) if its root node is open (closed).

In the following sections, we will introduce various strategies to control the opening and closing of nodes so that they can be processed without affecting other parts of the state (decision diagram).

IV. LIMTDD BASED QSP WITH NO ANCILLA QUBIT

Having explored the fundamental concepts, we now turn to the algorithms for efficient quantum state preparation (QSP).

A. Algorithm

We first consider the scenario where no ancilla qubit is available. In this case, all high-edge operators and outgoing weights must be eliminated or reduced using the branch condition. The procedure is detailed in Alg. 1.

Before initiating the procedure, we apply Basic Construction 1 to eliminate the operator on the incoming edge of the LimTDD \mathcal{F} , then execute the algorithm with the input $r_{\mathcal{F}}$.

In this procedure, for each node v represented as

$$(v_0) \leftarrow V \longrightarrow (v_1),$$

where $|v\rangle=|0\rangle\,|v_0\rangle+\lambda\,|1\rangle\,(O\,|v_1\rangle)$, we first address the operator O on the high-edge of v using Basic Construction 2. The state is transformed to

$$|v\rangle = |0\rangle |v_0\rangle + \lambda |1\rangle |v_1\rangle.$$

We then recursively process its successors v_0 and v_1 . If v is a branch node, the circuits cir_0 and cir_1 obtained from processing v_0 and v_1 are appended to the main circuit with control conditions $|0\rangle_v$ and $|1\rangle_v$, respectively. Otherwise, if $v_0 = v_1$ and $cir_0 = cir_1$, we simply add this circuit to the preparation circuit without any additional control conditions. Suppose cir_0 and cir_1 transform $|v_0\rangle$ and $|v_1\rangle$ to $||v_0|||0\rangle^{\otimes k}$ and $||v_1|||0\rangle^{\otimes k}$ for some k. Appending these circuits transforms the original state to $(||v_0|||0\rangle + \lambda ||v_1|||1\rangle)|0\rangle^{\otimes k}$. Subsequently, applying the operator

$$\frac{1}{\sqrt{1+|c|^2}} \begin{bmatrix} 1 & c^{\dagger} \\ -c & 1 \end{bmatrix}$$

with $c=\lambda\cdot||v_1||/||v_0||$ reduces the weight $[||v_0||,\lambda\cdot||v_1||]$ to $\sqrt{||v_0||^2+|\lambda|^2\cdot||v_1||^2}\cdot[1,0]$, where $\sqrt{||v_0||^2+|\lambda|^2\cdot||v_1||^2}=||v||$. Consequently, the node v is transformed to $||v||\,|0\rangle^{\otimes k+1}$ by the resulting circuit.

B. An Example

We now provide a concrete example to illustrate the procedure of our algorithm, with the quantum state to be prepared being $\frac{2}{\sqrt{23}}(|000\rangle+|001\rangle+\frac{1}{\sqrt{2}}|010\rangle+\frac{i}{2}|011\rangle-|100\rangle-\frac{1}{\sqrt{2}}|101\rangle+\frac{1}{\sqrt{2}}|110\rangle+|111\rangle).$ A step-by-step demonstration of our algorithm on the LimTDD is given in Fig. 2. The resulting quantum circuit for preparing the desired quantum state is shown in Fig. 3.

Algorithm 1 STATEPRE1(v)

Input: A node v of an LimTDD representing an n-qubit quantum state $|\psi\rangle$, suppose the qubit corresponding to v is q_v .

Output: A quantum circuit C, corresponding to an unitary matrix U, such that $U|\psi\rangle = |0\rangle^{\otimes n}$.

- cir ← QuantumCircuit(n) ▷ An empty quantum circuit with n qubits
- 2: **if** v is the terminal node **then**
- 3: return cir
- 4: end if
- 5: Suppose wt $((v, high(v))) = \lambda \cdot O$
- 6: Append cir with a controlled O[†] gate, with the control condition set to be |1⟩_n
 ▷ Reduce the operator on the high-edge of v
- 7: **if** low(v) = high(v) **then**
- 8: $cir_0 \leftarrow \text{STATEPRE1}(\text{low}(v))$
- 9: Append cir with cir_0
- 10: else
- 11: $cir_0 \leftarrow StatePrel(low(v))$
- 12: Add a control qubit with control condition $|0\rangle_v$ for every gate in cir_0 and append the circuit to cir
- 13: $cir_1 \leftarrow STATEPRE1(high(v))$
- 14: Add a control qubit with control condition $|1\rangle_v$ for every gate in cir_1 and append the circuit to cir
- 15: end if
- 16: $w_0 \leftarrow || \text{low}(v) ||$
- 17: $w_1 \leftarrow \lambda \cdot || \text{high}(v) ||$
- 18: $c \leftarrow w_1/w_0$
- 19: Append a gate $\frac{1}{\sqrt{1+|c|^2}}\left[\begin{array}{cc} 1 & c^\dagger \\ -c & 1 \end{array}\right]$ to qubit q_v in cir
- 20: $||v|| \leftarrow \sqrt{|w_0|^2 + |w_1|^2}$
- 21: return cir

At first, the quantum state represented by the LimTDD is $\frac{2}{\sqrt{23}}Z\otimes I\otimes I |v_{20}\rangle$ where:

$$\begin{aligned} |v_{20}\rangle &=& |0\rangle \, |v_{10}\rangle + |1\rangle \, (Z\otimes I \, |v_{11}\rangle) \\ |v_{10}\rangle &=& |0\rangle \, |v_{00}\rangle + \frac{1}{\sqrt{2}} \, |1\rangle \, (S \, |v_{01}\rangle) \\ |v_{11}\rangle &=& |0\rangle \, |v_{01}\rangle + |1\rangle \, (X \, |v_{01}\rangle) \\ |v_{00}\rangle &=& |0\rangle + |1\rangle \\ |v_{01}\rangle &=& |0\rangle + \frac{1}{\sqrt{2}} \, |1\rangle \, . \end{aligned}$$

We then explain the procedure of the algorithm step-by-step:

- 1) Cancel the Operator on the Incoming Edge:
 - Apply a Z gate on qubit q_2 to cancel the $Z \otimes I \otimes I$ operator on the incoming edge of the LimTDD. The state becomes: $|v_{20}\rangle$.
- 2) Process the v_{20} Node:
 - a) Process the High-Edge Operator of v_{20} Node:
 - Apply a CZ gate with q_2 as controls and q_1 as the target to cancel the $Z \otimes I$ operator on the high-edge of the v_{20} node. The state becomes: $|0\rangle |v_{00}\rangle + |1\rangle |v_{11}\rangle$.
 - b) Process the v_{10} Node:
 - Process the High-Edge Operator of v_{10} Node:
 - Apply a controlled-controlled- S^{\dagger} gate with control condition $|0\rangle_2 |1\rangle_1$ and target qubit q_0 to cancel the S operator on the high-edge of the y_1 node. The state becomes: $|0\rangle (|0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) + |1\rangle |v_{11}\rangle$.

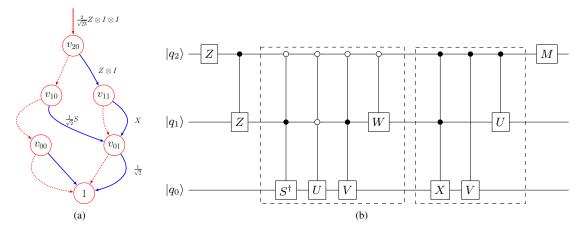


Fig. 3. The quantum circuit that transforms the quantum state $|\mathcal{F}\rangle$ represented by the LimTDD into $|000\rangle$. The two dotted boxes correspond to the processing of the y_1 and y_1' nodes, respectively. In this circuit $U=\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\-1&1\end{bmatrix}$, $V=\frac{1}{\sqrt{3}}\begin{bmatrix}\sqrt{2}&1\\-1&\sqrt{2}\end{bmatrix}$, $W=\frac{1}{\sqrt{11}}\begin{bmatrix}2\sqrt{2}&\sqrt{3}\\-\sqrt{3}&2\sqrt{2}\end{bmatrix}$, $M=\frac{1}{\sqrt{23}}\begin{bmatrix}\sqrt{11}&\sqrt{12}\\-\sqrt{12}&\sqrt{11}\end{bmatrix}$.

- Process the outgoing weights of v_{00} and v_{01} Nodes with prefix path 00 and 01:
 - Since $|v_{00}\rangle = |0\rangle + |1\rangle$, apply a controlled-U gate with control condition $|0\rangle_2 |0\rangle_1$ transform the state to: $|0\rangle (\sqrt{2} |0\rangle |0\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) + |1\rangle |v_{11}\rangle$ where $U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$.
 Since $|v_{01}\rangle = |0\rangle + \frac{1}{\sqrt{2}} |1\rangle$, apply a controlled-V gate with control condition $|0\rangle_2 |1\rangle_1$ transform the
 - Since $|v_{01}\rangle = |0\rangle + \frac{1}{\sqrt{2}}|1\rangle$, apply a controlled-V gate with control condition $|0\rangle_2|1\rangle_1$ transform the state to: $|0\rangle \left(\sqrt{2}|0\rangle + \frac{\sqrt{3}}{2}|1\rangle\right)|0\rangle + |1\rangle |v_{11}\rangle$ where $V = \frac{\sqrt{2}}{\sqrt{3}} \begin{bmatrix} 1 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 1 \end{bmatrix}.$
- Adjust the Weights on Outgoing Edges of the v_{10} Node:
 - Apply a controlled-W gate with control condition $|0\rangle_2$ to adjust the weights on the outgoing edges of the v_{10} node and change the state to: $\frac{\sqrt{11}}{2} |0\rangle |0\rangle |0\rangle + |1\rangle |v_{11}\rangle$ where $W = \frac{1}{\sqrt{11}} \begin{bmatrix} 2\sqrt{2} & \sqrt{3} \\ -\sqrt{3} & 2\sqrt{2} \end{bmatrix}$.
- c) Process the v_{11} Node:
 - Process the High-Edge Operator of v_{11} Node:
 - Apply a CCX gate with control condition $|1\rangle_2 |1\rangle_1$ to cancel the operator on the high-edge of the v_{11} node. The state becomes: $\frac{\sqrt{11}}{2} |0\rangle |0\rangle |0\rangle + \sqrt{3} |1\rangle (|0\rangle + |1\rangle) |v_{01}\rangle$.
 - Process the outgoing weights of v_{01} Node with prefix path 11:
 - Apply a controlled-V gate with $|1\rangle_2$, the state will be changed to $\frac{\sqrt{11}}{2}|0\rangle|0\rangle|0\rangle + |1\rangle\left(\frac{\sqrt{3}}{\sqrt{2}}|0\rangle + \frac{\sqrt{3}}{\sqrt{2}}|1\rangle\right)|0\rangle$.
 - Adjust the Weights on Outgoing Edges of the v_{11} Node:
 - Apply a further gate U controlled by $|1\rangle_2$ and change the state to $\frac{\sqrt{11}}{2}|0\rangle|0\rangle|0\rangle + \sqrt{3}|1\rangle|0\rangle|0\rangle$.
- d) Adjust the Weights on Outgoing Edges of the y_2 Node:
 - Use a $M=\frac{1}{\sqrt{23}}\begin{bmatrix} \frac{\sqrt{11}}{\sqrt{12}} \frac{\sqrt{12}}{\sqrt{11}} \end{bmatrix}$ gate to adjust the weights on the outgoing edges of the v_{20} node, the

state becomes: $\frac{\sqrt{23}}{2} |0\rangle |0\rangle$. Note that the coefficient $\frac{\sqrt{23}}{2}$ is cancelled with the ignored coefficient $\frac{2}{\sqrt{23}}$.

C. Complexity

In this subsection, we consider the time complexity and gate complexity of the algorithm. Here, the time complexity is determined by the number of recursive calls to the function STATEPRE1, and the gate complexity is determined by the number of gates in the returned circuit.

1) Time Complexity: During the process, we traverse the decision graph in a depth-first manner, so each reduced path is visited exactly once. Given there are p reduced paths in the LimTDD, and each path contains n non-terminal nodes (where n is the number of qubits), the time complexity is $\mathcal{O}(np)$.

To optimise this, we can introduce a table to cache the results of previously computed nodes. This allows us to reuse these results if a node is encountered multiple times, thereby reducing the time complexity to $\mathcal{O}(m)$, where m is the total number of nodes in the LimTDD.

2) Gate Complexity: The gate complexity is predominantly influenced by the step of cancelling all high-edge operators and outgoing weights using multi-qubit controlled quantum gates. For a node at level $k \in \{2,\ldots,n\}$ (with the terminal node defined as level 0), the high-edge operator has the form $O_{k-1} \otimes \cdots \otimes O_1$, which includes at most k-1 non-trivial (i.e., non-identity) single-qubit operators. This requires n+2-k qubit-controlled gates for elimination. Additionally, the outgoing weights of a node at level $k \in \{1,\ldots,n\}$ need to be reduced using n+1-k qubit-controlled gates. On any given path, there can be at most n non-trivial outgoing weights (i.e., weights not of the form [w,0] for some complex number $w \neq 0$) that need to be reduced. Moreover, up to n single-qubit gates are required to eliminate the operator on the incoming edge of the LimTDD.

Consequently, the upper bound on the gate complexity is:

- $\bullet \ \ p(n+2-s) \ \ s\text{-qubit gates for} \ \ s\in\{2,\dots,n\},$
- n+1 single-qubit gates.

It is worth noting that the s-qubit gates may involve fewer qubits, as they do not always need to be controlled by all the states corresponding to their prefix path.

3) Special Case: In the special case where the decision diagram is in tower form (i.e., the 0- and 1-successors of each non-terminal node are identical), there is only one reduced path. In this scenario, the upper bound on the gate complexity reduces to 2n single-qubit gates and $\frac{n(n-1)}{2}$ two-qubit gates. In such cases, this algorithm is optimal compared to the other algorithms proposed below.

D. Further optimisation

In this subsection, we explore strategies to reduce the number of multi-qubit control gates by introducing an ancilla qubit q_a .

Consider the scenario where we need to eliminate an operator $O_j \otimes \cdots \otimes O_1$ on the high edge of a node v. The step typically involves using a multi-qubit gate to eliminate all operators O_i for $i \in \{1,\ldots,j\}$ with the same control qubits. Suppose the control condition is $|k\rangle$, which is an $s \geq 2$ qubit state, this would normally require j s+1-qubit gates. However, with an ancilla qubit q_a available, we can proceed as follows:

- Apply an MCX gate with control condition $|k\rangle$ and target q_a to mark the state $|k\rangle$ as open, resulting in the state $|1\rangle_{a'}$ $|k\rangle$ $|v\rangle$ + $|0\rangle_a$ $|\text{Res}\rangle$.
- Use $|1\rangle_a$ as the control condition to eliminate $O_j \otimes \cdots \otimes O_1$.
- Apply another MCX gate with control condition |k⟩ and target q_a to recover q_a.

This approach reduces the number of s + 1-qubit gates from j to 2, while introducing j 2-qubit gates.

Note that this strategy is applicable to all four algorithms proposed in this paper, and has no relations with the Alg. 2 introduced below.

V. LIMTDD BASED OSP WITH ONE ANCILLA QUBITS

In this section, we present a quantum state preparation algorithm leveraging a single ancilla qubit. Our method is conceptually inspired by the algorithm by Mozafari et al. [24], which introduced an efficient algorithm for QSP using decision diagrams. Their method begins with the $|0\rangle$ state and incrementally constructs the target quantum state by traversing the decision diagram path by path. A key feature of their algorithm is the use of an ancilla qubit to mark paths that have already been processed. By leveraging this ancilla qubit as a control qubit, subsequent preparation steps do not interfere with previously prepared paths. Consequently, both the time complexity and the gate complexity of the resulting quantum circuit scale with the number of reduced paths in the decision diagram.

However, the decision diagram employed in [24] - the multi-terminal Algebraic Decision Diagram (ADD)- is less compact compared to the LimTDD used in this paper. As an example, Fig. 4 illustrates the ADD representation of the quantum state presented in Example 1. While the ADD comprises 7 reduced paths, the corresponding LimTDD representation contains only 3, demonstrating a substantial reduction in path counts. Motivated by the observations above, we propose a LimTDD-based QSP algorithm that utilises a single ancilla qubit.

Although our algorithm draws inspiration from [24], their implementation details differ substantially, owing to the fundamental structural distinctions between ADDs and LimTDDs. Specifically, our algorithm eliminates the need to compute the accumulated probability along different branches, thereby streamlining the process. Instead of marking paths, we repurpose the ancilla qubit to indicate the open or closed status of a node. Additionally, we design a circuit that transforms the quantum state represented by the LimTDD into $|0\rangle$, which is the opposite of the reverse transformation presented in [24].

In the following subsections, we provide a detailed exposition of our proposed algorithm.

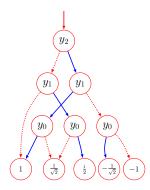


Fig. 4. An example of Multiple-terminal ADD [24] representing the quantum state $\frac{2}{\sqrt{23}}[1,1,\frac{1}{\sqrt{2}},\frac{i}{2},-1,-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1]^T$. The coefficient $\frac{2}{\sqrt{23}}$ was omitted here

A. Algorithm

The core of this algorithm involves introducing an ancilla qubit to control the opening and closing of nodes within the LimTDD. By ensuring that the current node (and its associated subtrees) is the only open node at any moment, we can process it without affecting other nodes. This approach repurposes the ancilla qubit as a control condition, thereby reducing the number of control qubits required in Alg. 1.

Our algorithm, detailed in Alg. 2, begins by eliminating the operator on the incoming edge of the root node. It then proceeds recursively: for each node, we first cancel the operator on its high-edge, process its 0-successor, followed by its 1-successor, and finally adjust the weights on the outgoing edges of the current node.

Throughout this procedure, an ancilla qubit is used to mark the current node v being processed, effectively indicating the open part of the decision diagram. Initially, the entire LimTDD (the root node) is open, marked by $|1\rangle_a$. When a branch node is encountered, we first use a multi-controlled-X (MCX) gate to close its 1-successor, with the control condition set to the branch condition of $\mathtt{high}(v)$. We then proceed to process the 0-successor.

Subsequently, we toggle the open/close condition of the two successors using the branch condition of v, and process the 1-successor. Finally, we reopen the 0-successor using the branch condition of low(v), ensuring the original node remains open. This process is applied recursively; upon completion, the root node is left open, thus the ancilla qubit has been successfully returned to the $|1\rangle_a$ state.

To illustrate, consider a node v with the form

$$(v_0) \leftarrow \stackrel{I}{\longleftarrow} (v) \xrightarrow{\lambda O} (v_1)$$

marked open by q_a with branch condition $|p\rangle$. The state can be represented as $|1\rangle_a |p\rangle |v\rangle + |0\rangle_a |\mathrm{Res}\rangle = |1\rangle_a |p\rangle |0\rangle_v |v_0\rangle + \lambda |1\rangle_a |p\rangle |1\rangle_v (O|v_1\rangle) + |0\rangle_a |\mathrm{Res}\rangle$, where $|\mathrm{Res}\rangle$ is orthogonal to $|p\rangle |*\rangle$. The operator O can be eliminated using a controlled O^\dagger operator with control condition $|1\rangle_a |1\rangle_v$, transforming the state to

$$\left|1\right\rangle_{a}\left|p\right\rangle\left|0\right\rangle_{v}\left|v_{0}\right\rangle+\lambda\left|1\right\rangle_{a}\left|p\right\rangle\left|1\right\rangle_{v}\left|v_{1}\right\rangle+\left|0\right\rangle_{a}\left|\mathrm{Res}\right\rangle.$$

A MCX gate with control condition $|p\rangle\,|1\rangle_v$ is then applied to close the v_1 node, resulting in the state

$$\left|1\right\rangle_{a}\left|p\right\rangle\left|0\right\rangle_{v}\left|v_{0}\right\rangle+\lambda\left|0\right\rangle_{a}\left|p\right\rangle\left|1\right\rangle_{v}\left|v_{1}\right\rangle+\left|0\right\rangle_{a}\left|\mathrm{Res}\right\rangle.$$

Using $|1\rangle_a$ as the control qubit, we process the v_0 node, obtaining a circuit cir_0 that transforms $|1\rangle_a |v_0\rangle$ to $||v_0|| |1\rangle_a |0\rangle^{\otimes k}$ for some

k, while leaving other parts unchanged. Applying this circuit, the original state becomes

$$||v_0|| |1\rangle_a |p\rangle |0\rangle_v |0\rangle^{\otimes k} + \lambda |0\rangle_a |p\rangle |1\rangle_v |v_1\rangle + |0\rangle_a |\text{Res}\rangle.$$

A MCX gate with control condition $|p\rangle$ is then applied to q_a , changing the state to

$$||v_0|| |0\rangle_a |p\rangle |0\rangle_v |0\rangle^{\otimes k} + \lambda |1\rangle_a |p\rangle |1\rangle_v |v_1\rangle + |0\rangle_a |\text{Res}\rangle.$$

We then process the v_1 node with control condition $\left|1\right\rangle_a$, transforming the state to

$$||v_0|| |0\rangle_a |p\rangle |0\rangle_v |0\rangle^{\otimes k} + \lambda ||v_1|| |1\rangle_a |p\rangle |1\rangle_v |0\rangle^{\otimes k} + |0\rangle_a |\text{Res}\rangle.$$

Finally, a MCX gate with control condition $|p\rangle\,|0\rangle_v$ reopens the v_0 part, resulting in the state

$$|1\rangle_a |p\rangle (||v_0|| |0\rangle_v + \lambda ||v_1|| |1\rangle_v) |0\rangle^{\otimes k} + |0\rangle_a |\text{Res}\rangle.$$

An operator

$$\frac{1}{\sqrt{1+|c|^2}} \begin{bmatrix} 1 & c^{\dagger} \\ -c & 1 \end{bmatrix}$$

with $c=\lambda\cdot||v_1||/||v_0||$ and control condition $|1\rangle_a$ is then applied, transforming the state to

$$||v|| |1\rangle_a |p\rangle |0\rangle^{\otimes k+1} + |0\rangle_a |\text{Res}\rangle$$

completing the process of the v node.

B. An Example

In this subsection, we will also use the LimTDD given in Fig. 2 as an example to provide a step-by-step illustration of the algorithm.

We start by adding an ancilla qubit q_a and the initial state becomes $\frac{2}{\sqrt{23}}\ket{1}_a(Z\otimes I\otimes I\ket{v_{20}})$.

Then we explain the procedure of the algorithm step-by-step.

1) Cancel the Operator on the Incoming Edge:

• Apply a Z gate on qubit q_2 to cancel the $Z \otimes I \otimes I$ operator on the incoming edge of the LimTDD. The state becomes: $|1\rangle_a |v_{20}\rangle$.

2) Process the v_{20} Node:

a) Process the High-Edge Operator of v_{20} Node:

• Apply a CCZ gate with q_a and q_2 as controls and q_1 as the target to cancel the $Z \otimes I$ operator on the high-edge of the v_{20} node. The state becomes: $|1\rangle_a (|0\rangle |v_{10}\rangle + |1\rangle |v_{11}\rangle$).

b) Process the v_{10} Node:

• Process the High-Edge Operator of v_{10} Node:

- Use a CX gate with q_2 as the control qubit and q_a as the target qubit to close the v_{11} node. The state becomes: $|1\rangle_a |0\rangle |v_{10}\rangle + |0\rangle_a |1\rangle |v_{11}\rangle$.
- Apply a Controlled-Controlled- S^{\dagger} gate with q_a and q_1 as controls and q_0 as the target to cancel the Z operator on the high-edge of the v_{10} node. The state becomes: $|1\rangle_a |0\rangle (|0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) + |0\rangle_a |1\rangle |v_{11}\rangle$.

• Process the outgoing weights of v_{00} and v_{01} Nodes with prefix path 00 and 01:

– Use a CCX gate with control condition $|0\rangle_2 |1\rangle_1$ to close the v_{01} node, and the state becomes: $|1\rangle_a |0\rangle |0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |0\rangle_a |0\rangle |1\rangle |v_{01}\rangle + |0\rangle_a |1\rangle |v_{11}\rangle.$

Algorithm 2 STATEPRE2 (v, q_a)

Input: A node v of an LimTDD representing an n-qubit quantum state $|\psi\rangle$, and an ancilla qubit q_a .

Output: A quantum circuit C, corresponding to an unitary matrix U, such that $U\ket{1}_a\ket{\psi}=\ket{1}_a\ket{0}^{\otimes n}$.

- 1: $cir \leftarrow \text{QuantumCircuit}(n+1) \quad \triangleright \text{ An empty quantum circuit}$ with n+1 qubits
- 2: **if** v is the terminal node **then**
- 3: return cir
- 4: end if
- 5: Suppose wt $((v, high(v))) = \lambda \cdot O$
- 6: Append cir with a controlled O^{\dagger} gate, with the control condition set to be $|1\rangle_a$ \triangleright Reduce the operator on the high-edge of v
- 7: **if** low(v) = high(v) **then**
- 8: $cir_0 \leftarrow \text{STATEPRE2}(\text{low}(v), q_a)$
- 9: Append cir with cir_0
- 10: else
- 11: Use the branch condition of high(v) to close the high-branch of the node
- 12: $cir_0 \leftarrow \text{StatePre2}(\text{low}(v), q_a)$
- 13: Append cir with cir_0
- 14: Use the branch condition of v to close the low-branch and open the high-branch
- 15: $cir_1 \leftarrow \text{STATEPRE2}(\text{high}(v), q_a)$
- 16: Append cir with cir_1
- 17: Use the branch condition of low(v) to open the low-branch
- 18: end if
- 19: $w_0 \leftarrow || \mathsf{low}(v) ||$
- 20: $w_1 \leftarrow \lambda \cdot || \text{high}(v) ||$
- 21: $c \leftarrow w_1/w_0$
- 22: Append a controlled $\frac{1}{\sqrt{1+|c|^2}}\begin{bmatrix} 1 & c^\dagger \\ -c & 1 \end{bmatrix}$, with the control condition $|1\rangle_a$ and target q_v
- 23: $||v|| \leftarrow \sqrt{|w_0|^2 + |w_1|^2}$.
- 24: return cir
 - Apply a controlled-U gate with q_a as the control qubit to transform the state to: $\sqrt{2} \ket{1}_a \ket{0} \ket{0} \ket{0} + \frac{1}{\sqrt{2}} \ket{0}_a \ket{0} \ket{1} \ket{v_{01}} + \ket{0}_a \ket{1} \ket{v_{11}}$.

 Apply a CX gate with control condition $\ket{0}_2$ and
 - Åpply a CX gate with control condition $|0\rangle_2$ and target qubit q_a to close the v_{00} node and open the v_{01} node and change the state to: $\sqrt{2} |0\rangle_a |0\rangle |0\rangle |0\rangle + \frac{1}{\sqrt{2}} |1\rangle_a |0\rangle |1\rangle |v_{01}\rangle + |0\rangle_a |1\rangle |v_{11}\rangle$.
 - $\begin{array}{l} \frac{1}{\sqrt{2}}\left|1\right\rangle_{a}\left|0\right\rangle\left|1\right\rangle\left|v_{01}\right\rangle + \left|0\right\rangle_{a}\left|1\right\rangle\left|v_{11}\right\rangle.\\ \text{ Apply a controlled-V gate with } q_{a} \text{ as the control qubit to transform the state to: } \sqrt{2}\left|0\right\rangle_{a}\left|0\right\rangle\left|0\right\rangle\left|0\right\rangle + \\ \frac{\sqrt{3}}{2}\left|1\right\rangle_{a}\left|0\right\rangle\left|1\right\rangle\left|0\right\rangle + \left|0\right\rangle_{a}\left|1\right\rangle\left|v_{11}\right\rangle. \end{array}$
 - Apply a CCX gate with control condition $|0\rangle_2 |0\rangle_1$ to reopen the v_{00} node and change the state to: $|1\rangle_a |0\rangle (\sqrt{2} |0\rangle + \frac{\sqrt{3}}{2} |1\rangle) |0\rangle + |0\rangle_a |1\rangle |v_{11}\rangle.$
 - Adjust the Weights on Outgoing Edges of the v_{10}
 - Apply a controlled-W gate with q_a as the control qubit to adjust the weights on the outgoing edges of the v_{10} node and change the state to: $\frac{\sqrt{11}}{2} |1\rangle_a |0\rangle |0\rangle |0\rangle + |0\rangle_a |1\rangle |v_{11}\rangle.$

c) Process the v_{11} Node:

• Process the High-Edge Operator of v_{11} Node:

- Use an X gate on q_a to switch the branches and open the v_{11} node. The state becomes:

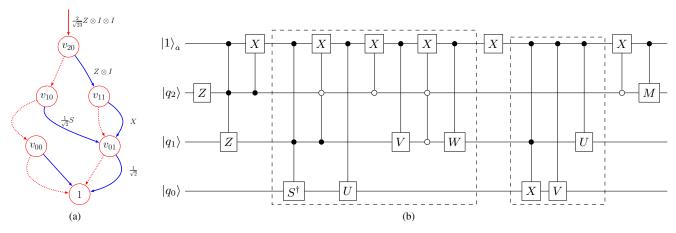


Fig. 5. The quantum circuit that transforms the quantum state $|1\rangle$ $|\mathcal{F}\rangle$ into $|1\rangle$ $|000\rangle$. The two dotted boxes correspond to the processing of the y_1 and y_1' nodes, respectively. In this circuit $U=\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\-1&1\end{bmatrix}, V=\frac{\sqrt{2}}{\sqrt{3}}\begin{bmatrix}1&\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}&1\end{bmatrix}, W=\frac{1}{\sqrt{11}}\begin{bmatrix}2\sqrt{2}&\sqrt{3}\\-\sqrt{3}&2\sqrt{2}\end{bmatrix}, M=\frac{1}{\sqrt{23}}\begin{bmatrix}\sqrt{11}&\sqrt{12}\\-\sqrt{12}&\sqrt{11}\end{bmatrix}$

- $\begin{array}{l} \frac{\sqrt{11}}{2}\left|0\right\rangle_a\left|0\right\rangle\left|0\right\rangle + \left|1\right\rangle_a\left|1\right\rangle\left|v_{11}\right\rangle. \\ \text{ Apply a CCX gate controlled by } q_a \text{ and } q_1 \text{ to} \end{array}$ cancel the operator on the high-edge of the v_{11} node. The state becomes: $\frac{\sqrt{11}}{2}\ket{0}_a\ket{0}\ket{0}\ket{0}$ + $\sqrt{3} |1\rangle_a |1\rangle (|0\rangle + |1\rangle) |v_{01}\rangle.$
- Process the outgoing weights of v_{01} Node with prefix path 11:
- Apply a controlled-V gate with q_a as the control qubit, the state will be changed to $\frac{\sqrt{11}}{2} |0\rangle_a |0\rangle |0\rangle + |1\rangle_a |1\rangle \left(\frac{\sqrt{3}}{\sqrt{2}} |0\rangle + \frac{\sqrt{3}}{\sqrt{2}} |1\rangle\right) |0\rangle$. Adjust the Weights on Outgoing Edges of the v_{11}
- - Apply a further gate U controlled by $|1\rangle_a$ and change the state to $\frac{\sqrt{11}}{2}\ket{0}_a\ket{0}\ket{0}\ket{0}+\sqrt{3}\ket{1}_a\ket{1}\ket{0}\ket{0}$. Apply a CX gate with the control qubit q_2 set to be
 - $|0\rangle$ and target qubit q_a , to reopen the v_{10} node, thus making the all branches of v_{20} node open, and the state becomes: $|1\rangle_a \left(\frac{\sqrt{11}}{2}|0\rangle + \sqrt{3}|1\rangle\right)|0\rangle|0\rangle$.

d) Adjust the Weights on Outgoing Edges of the y_2 Node:

• Use a controlled-M gate with q_a as the control qubit to adjust the weights on the outgoing edges of the v_{20} node, the state becomes: $\frac{\sqrt{23}}{2} |1\rangle_a |0\rangle |0\rangle$. Also, the coefficient $\frac{\sqrt{23}}{2}$ cancels with complex weight $\frac{2}{\sqrt{23}}$ on the incoming edge.

The resulted quantum circuit for preparing the desired quantum state is shown in Fig. 5.

C. Complexity

- 1) Time Complexity: In this algorithm, we traverse the decision graph in a depth-first manner, ensuring that each reduced path is visited exactly once. Given that there are p reduced paths, the time complexity of this algorithm is $\mathcal{O}(np)$, where n is the number of qubits.
- 2) Gate Complexity: The gate complexity is determined by the number of operations required to eliminate high-edge operators and to adjust outgoing weights. Specifically, high-edge operators are eliminated using 3-qubit controlled gates, and outgoing weights are adjusted using 2-qubit controlled gates. Additionally, the operator on

the incoming edge is handled using no more than n single-qubit gates. For each branch node at level $k \in \{1, \dots, n\}$, the algorithm requires one controlled gate to close its 1-branch, one controlled gate to flip the open/close status of both branches, and one controlled gate to reopen the 0-branch. Given n-k nodes preceding the current node on the path, this necessitates two controlled gates with at most n-k+2qubits and one controlled gate with at most n - k + 1 qubits.

In summary, the upper bounds are:

- 2p n + 1-qubit gates,
- 3p s-qubit gates for $s \in \{4, \cdots n\}$, $\frac{n(n-1)}{2}p + 3p$ 3-qubit gates, np + 3p 2-qubit gates,

- n+1 single-qubit gates.
- 3) Special Case: For decision diagrams in the tower form, the upper bound reduces to n single-qubit gates, n two-qubit gates, and $\frac{n(n-1)}{2}$ three-qubit gates. In this scenario, the circuit generated by Alg. 2 is similar to that of Alg. 1, with the exception that all gates are controlled by $|1\rangle_a$, except those used to eliminate the operator on the incoming edge of the LimTDD.

VI. LIMTDD BASED QSP WITH SUFFICIENT NUMBER OF ANCILLA QUBITS

In this section, we address the problem of quantum state preparation with access to a sufficient number of ancilla qubits. Our approach is inspired by the work of Tanaka et al. [25], which introduced an efficient algorithm for quantum state preparation (QSP) using decision diagrams. Their algorithm begins with the $|0\rangle$ state and prepares the target quantum state by traversing the decision diagram in a breadth-first manner. For each non-terminal node, an ancilla qubit is employed to mark the node as open or closed, and the algorithm processes the node accordingly. Consequently, both the time complexity and the gate complexity of the resulting quantum circuit scale with the number of nodes in the decision diagram, and $size(\mathcal{F})$ ancilla qubits are required, where $size(\mathcal{F})$ denotes the number of non-terminal nodes in the decision diagram \mathcal{F} .

However, the decision diagram used in [25] is a weighted free binary decision diagram (WFBDD), which is also less compact compared to the LimTDD representation. For instance, the WFBDD shown in Fig. 6 has 7 nodes, whereas the LimTDD representation has

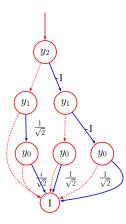


Fig. 6. An example of FBDD [25] representing the quantum state $\frac{2}{\sqrt{23}}[1,1,\frac{1}{\sqrt{2}},\frac{i}{2},-1,-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}},1]^T$. The coefficient $\frac{2}{\sqrt{23}}$ was omitted here.

only 6 nodes. To bridge this gap, we have designed a LimTDD-based QSP algorithm that also utilises $\operatorname{size}(\mathcal{F})$ ancilla qubits.

A. Algorithm

Our algorithm, described in Alg. 3, begins by eliminating the operator on the incoming edge of the root node. For any non-terminal node v, an ancilla qubit q_{av} is assigned to it. Initially, the ancilla qubit corresponding to the root node is set to $|1\rangle$, marking the root node as open, while the ancilla qubits corresponding to other non-terminal nodes are set to $|0\rangle$.

Consider a non-terminal node v with the form

$$(v_0) \stackrel{I}{\leftarrow} - (v) \xrightarrow{\lambda O} (v_1).$$

Whenever a predecessor node v' marked open by $q_{a_{v'}}$ is reached, and v is the b-successor of v', where $b \in \{0,1\}$, v can be marked open with the control condition $|1\rangle_{a_{v'}}|b\rangle_{v'}$ along the path. After all predecessors have been processed, the node v will be marked open by q_{a_v} , and any of its brother nodes will be marked closed. This can be represented as

$$|1\rangle_{a_n}|p\rangle|v\rangle + |0\rangle_{a_n}|\text{Res}\rangle$$
,

where $|{\rm Res}\rangle$ is orthogonal to $|p\rangle\,|*\rangle$, and $|p\rangle$ represents all possible prefix paths leading to v.

We first address the operator O on the high-edge of v. This can be eliminated using a Controlled-Controlled- O^{\dagger} gate with the control condition $|1\rangle_{a}$, $|1\rangle_{v}$, transforming the state to

$$|1\rangle_{a_v}|p\rangle\left(|0\rangle_v|v_0\rangle + \lambda|1\rangle_v|v_1\rangle\right) + |0\rangle_{a_v}|\text{Res}\rangle.$$

At this point, the ancilla qubits $q_{a_{v_0}}$ and $q_{a_{v_1}}$ for v_0 and v_1 are in the state $|0\rangle$ along the path p. We then apply two CCX gates with control conditions $|1\rangle_{a_v} |0\rangle_v$ and $|1\rangle_{a_v} |1\rangle_v$ and target qubits $q_{a_{v_0}}$ and $q_{a_{v_1}}$ to mark v_0 and v_1 open along the path. The state can be simplified to

$$\left|1\right\rangle_{a_{v}}\left|p\right\rangle \left(\left|0\right\rangle_{v}\left|1\right\rangle_{a_{v_{0}}}\left|v_{0}\right\rangle +\lambda\left|1\right\rangle_{v}\left|1\right\rangle_{a_{v_{1}}}\left|v_{1}\right\rangle \right)+\left|0\right\rangle_{a_{v}}\left|\mathrm{Res}\right\rangle .$$

After marking all prefix paths leading to v_0 or v_1 , we process v_0 and v_1 by first eliminating the operators on their high-edges, then processing their successor nodes, and finally adjusting the outgoing weights. Ultimately, both successor nodes are transformed into $|0\rangle^{\otimes k}$ for some k. The state then becomes

$$\left|1\right\rangle_{a_{v}}\left|p\right\rangle \left(\left|\left|v_{0}\right|\right|\left|0\right\rangle_{v}\left|1\right\rangle_{a_{v_{0}}}+\lambda\left|\left|v_{1}\right|\right|\left|1\right\rangle_{v}\left|1\right\rangle_{a_{v_{1}}}\right)\left|0\right\rangle^{\otimes k}+\left|0\right\rangle_{a_{v}}\left|\mathrm{Res'}\right\rangle.$$

We then apply two additional CCX gates with control conditions $|1\rangle_{a_v}\,|0\rangle_v$ and $|1\rangle_{a_v}\,|1\rangle_v$ and target qubits $q_{a_{v_0}}$ and $q_{a_{v_1}}$ to unmark v_0 and v_1 along the path, transforming the state to

$$|1\rangle_{a...}|p\rangle\left(||v_0|||0\rangle_v + \lambda||v_1|||1\rangle_v\right)|0\rangle^{\otimes k} + |0\rangle_{a...}|Res'\rangle$$
.

Finally, we apply an operator

$$\frac{1}{\sqrt{1+|c|^2}} \begin{bmatrix} 1 & c^{\dagger} \\ -c & 1 \end{bmatrix}$$

with $c=\lambda\cdot||v_1||/||v_0||$ and control condition $|1\rangle_{a_v}$ to transform the state to

$$||v|| |1\rangle_{a_n} |p\rangle |0\rangle^{\otimes k+1} + |0\rangle_{a_n} |\text{Res}'\rangle.$$

Note that the state $|\text{Res}\rangle$ has changed to $|\text{Res}'\rangle$, as there could be components connecting to nodes in the sub-tree of v. But it remains orthogonal to $|p\rangle |*\rangle$.

B. An Example

The circuit for preparing the quantum state corresponding to the quantum state shown in Fig. 2 was given in Fig. 7. In the following part, we introduce the procedure step-by-step. The initial state is in $\frac{2}{\sqrt{23}}\ket{0}^{\otimes 4}\ket{1}(Z\otimes I\otimes I\ket{v_{20}})$. We will omit the state of the ancilla qubits if it is in $\ket{0}$ for convenience. Also, we will omit the state $\ket{1}_{\alpha_{20}}$, since it is always in $\ket{1}$.

1) Cancel the Operator on the Incoming Edge:

Apply a Z gate on qubit q₂ to cancel the Z⊗I⊗I operator
on the incoming edge of the LimTDD. The state becomes:
|v₂₀⟩.

2) Ordered traversal to cope with the Operators:

- a) Process the v_{20} Node:
 - Apply a CCZ gate with $q_{a_{20}}$ and q_2 as controls and q_1 as the target to cancel the $Z \otimes I$ operator on the highedge of the v_{20} node. The state becomes: $|0\rangle |v_{10}\rangle + |1\rangle |v_{11}\rangle$.
 - Apply two CCX gates to mark the two nodes v_{10} and v_{11} as open with $q_{a_{10}}$ and $q_{a_{11}}$. The state becomes: $|0\rangle |1\rangle_{a_{10}} |v_{10}\rangle + |1\rangle |1\rangle_{a_{11}} |v_{11}\rangle$.

b) Process the v_{10} Node:

- Apply a CC- S^{\dagger} gate to cancel the S operator on the high-edge of the v_{10} node. The state becomes: $|0\rangle\,|1\rangle_{a_{10}}\,(|0\rangle\,|v_{00}\rangle\,+\,\frac{1}{\sqrt{2}}\,|1\rangle\,|v_{11}\rangle)\,+\,|1\rangle\,|1\rangle_{a_{11}}\,|v_{11}\rangle.$ Apply two CCX gates to mark the two nodes
- Apply two CCX gates to mark the two nodes v_{00} and v_{01} along the prefix path 00 and 01 as open with $q_{a_{00}}$ and $q_{a_{01}}$. The state becomes: $|0\rangle\,|1\rangle_{a_{10}}\,(|0\rangle\,|1\rangle_{a_{00}}\,|v_{00}\rangle\,+\,\frac{1}{\sqrt{2}}\,|1\rangle\,|1\rangle_{a_{01}}\,|v_{01}\rangle)\,+\,|1\rangle\,|1\rangle_{a_{11}}\,|v_{11}\rangle.$

c) Process the v_{11} Node:

- Apply a CCX gate to cancel the X operator on the high-edge of the v_{11} node. The state becomes: $|0\rangle\,|1\rangle_{a_{10}}\,(|0\rangle\,|1\rangle_{a_{00}}\,|v_{00}\rangle\,\,+\,\,\frac{1}{\sqrt{2}}\,|1\rangle\,|1\rangle_{a_{01}}\,|v_{01}\rangle)\,\,+\,|1\rangle\,|1\rangle_{a_{11}}\,(|0\rangle\,+\,|1\rangle)\,|v_{01}\rangle.$
- Apply two CCX gates to mark the node v_{01} along the prefix path 10 and 11 as open. The state becomes: $|0\rangle\,|1\rangle_{a_{10}}\,(|0\rangle\,|1\rangle_{a_{00}}\,|v_{00}\rangle\,+\,\,\frac{1}{\sqrt{2}}\,|1\rangle\,|1\rangle_{a_{01}}\,|v_{01}\rangle)\,\,+\,|1\rangle\,|1\rangle_{a_{11}}\,(|0\rangle\,+\,|1\rangle)\,|1\rangle_{a_{01}}\,|v_{01}\rangle.$

3) Reverse order traversal to cope with the Weights:

- a) Process the v_{01} and v_{00} Node:
 - Apply CV gate to change the state $|v_{01}\rangle$ to $\frac{\sqrt{3}}{\sqrt{2}}|0\rangle$, and apply CU gate to change the state $|v_{00}\rangle$ to

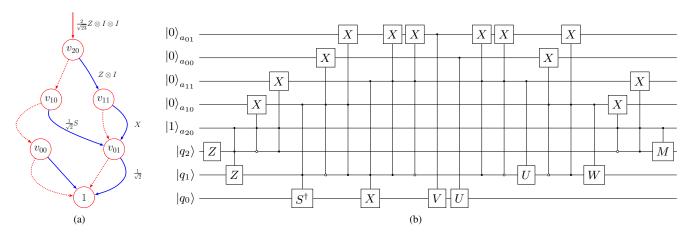


Fig. 7. The quantum circuit that transforms the quantum state $|0\rangle^{\otimes 5} |1\rangle |\mathcal{F}\rangle$ into $|0\rangle^{\otimes 5} |1\rangle |000\rangle$. In this circuit $U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$, $V = \frac{\sqrt{2}}{\sqrt{3}} \begin{bmatrix} 1 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 1 \end{bmatrix}$, $W = \frac{1}{\sqrt{11}} \left[\begin{smallmatrix} 2\sqrt{2} & \sqrt{3} \\ -\sqrt{3} & 2\sqrt{2} \end{smallmatrix} \right]\!,\, M = \frac{1}{\sqrt{23}} \left[\begin{smallmatrix} \sqrt{11} & \sqrt{12} \\ -\sqrt{12} & \sqrt{11} \end{smallmatrix} \right]$

 $\begin{array}{c} \sqrt{2}\left|0\right\rangle, \text{ the state becomes: }\left|0\right\rangle\left|1\right\rangle_{a_{10}}\left(\sqrt{2}\left|0\right\rangle\left|1\right\rangle_{a_{00}}+\\ \frac{\sqrt{3}}{2}\left|1\right\rangle\left|1\right\rangle_{a_{01}}\right)\left|0\right\rangle+\frac{\sqrt{3}}{\sqrt{2}}\left|1\right\rangle\left|1\right\rangle_{a_{11}}\left(\left|0\right\rangle+\left|1\right\rangle\right)\left|1\right\rangle_{a_{01}}\left|0\right\rangle. \\ \text{b) Process the } v_{11} \text{ Node:} \end{array}$

- Apply two CCX gates to unmark the v_{01} along prefix path 10 and 11, and change the state to: $|0\rangle\,|1\rangle_{a_{10}}\,(\sqrt{2}\,|0\rangle\,|1\rangle_{a_{00}}\,+\,\frac{\sqrt{3}}{2}\,|1\rangle\,|1\rangle_{a_{01}})\,|0\rangle\,+\,\frac{\sqrt{3}}{\sqrt{2}}\,|1\rangle\,|1\rangle_{a_{11}}\,(|0\rangle\,+\,|1\rangle)\,|0\rangle.$ • Apply a CU gate reduce the weight on the
- outgoing edges of v_{11} and change the state to: $|0\rangle |1\rangle_{a_{10}} \left(\sqrt{2} |0\rangle |1\rangle_{a_{00}} + \frac{\sqrt{3}}{2} |1\rangle |1\rangle_{a_{01}}\right) |0\rangle + \sqrt{3} |1\rangle |1\rangle_{a_{11}} |0\rangle |0\rangle.$

c) Process the v_{10} Node:

- ullet Apply two CCX gates to unmark v_{00} and v_{01} along prefix paths 00 and 01, and the state becomes:
- outgoing edges of the v_{10} node, the state becomes: $\frac{\sqrt{11}}{2}\ket{0}\ket{1}_{a_{10}}\ket{0}\ket{0} + \sqrt{3}\ket{1}\ket{1}_{a_{11}}\ket{0}\ket{0}$.

d) Process the v_{20} Node:

- Apply two CCX gates to unmark v_{10} and v_{11} , and the state becomes: $\frac{\sqrt{11}}{2} |0\rangle |0\rangle |0\rangle + \sqrt{3} |1\rangle |0\rangle |0\rangle$.
- Apply a CM gate to reduce the weight on the outgoing edges of the v_{20} node, the state becomes: $\frac{\sqrt{23}}{2} |0\rangle |0\rangle |0\rangle.$

C. Complexity

- 1) Time Complexity: In this algorithm, we traverse the decision graph in a breadth-first manner, ensuring that each non-terminal node is visited exactly twice. Given that there are m non-terminal nodes, the time complexity of this algorithm is $\mathcal{O}(m)$.
- 2) Gate Complexity: The gate complexity is determined by the operations required to eliminate high-edge operators and adjust outgoing weights. Specifically, high-edge operators are eliminated using 3-qubit controlled gates, outgoing weights are adjusted using 2-qubit controlled gates, and the operator on the incoming edge is handled using no more than n single-qubit gates. For each nonterminal node, 4 CCX gates are required to open or close its two successors.

In summary, the upper bound on the gate complexity is:

- (3n+4)m 3-qubit gates,
- m 2-qubit gates,
- n single-qubit gates.
- 3) Special Case: For decision diagrams in the tower form, the upper bound reduces to n single-qubit gates, n two-qubit gates, and $\frac{(\hat{n}-1)}{2} + 2n$ three-qubit gates.

D. Further Optimisation

It is important to note that although an ancilla qubit is assigned to every non-terminal node, only branch nodes require ancilla qubits to maintain the described complexity in practice. The trade-off is that when processing non-branch nodes, each gate must incorporate an additional control qubit. For instance, consider a branch node v with a 0-successor v_0 that is not a branch node. When processing node v, we can use the control condition $|1\rangle_{a_n}$. However, when processing node v_0 , we need to use the control condition $|1\rangle_{a_n}|0\rangle_v$.

Furthermore, the minimum number of ancilla qubits required to maintain this complexity can be reduced to $\lceil \log(m) \rceil + 1$, where m is the number of branch nodes. In this scenario, each branch node is encoded with a $\lceil \log(m) \rceil$ -qubit state. For example, suppose a node v is encoded with $|001\rangle$, and its 0-successor and 1-successor are encoded with $|010\rangle$ and $|011\rangle$, respectively. Also, suppose v has been marked open as $|001\rangle |v\rangle = |001\rangle (|0\rangle_{v_1} |v_0\rangle + \lambda O |1\rangle_{v_1} |v_1\rangle)$. Then, we can introduce another ancilla qubit q_a and adjust the entire state to $|1\rangle_a |001\rangle (|0\rangle_v |v_0\rangle + \lambda O |1\rangle_v |v_1\rangle) + |0\rangle_a |\text{Res}\rangle$. Subsequently, we can use the control conditions $|1\rangle_a |0\rangle_v$ and $|1\rangle_a |1\rangle_v$ to adjust the quantum state to $|1\rangle_a (|0\rangle_v |010\rangle |v_0\rangle + \lambda O |1\rangle_v |011\rangle |v_1\rangle) +$ $|0\rangle_a |\text{Res}\rangle$. Finally, we recover q_a using the control conditions $|010\rangle$ and $|011\rangle$, resulting in the state $|0\rangle_a (|0\rangle_v |010\rangle |v_0\rangle +$ $\lambda O \ket{1}_v \ket{011} \ket{v_1} + \ket{0}_a \ket{\text{Res}}$. We then use $\ket{010}$ and $\ket{011}$ as control conditions to process v_0 and v_1 , respectively. However, the cost is that each gate, which originally required one control qubit (q_{a_n}) , now requires $\lceil \log(m) \rceil$ control qubits. This strategy is also applicable to Alg. 4 introduced below.

Algorithm 3 STATEPRE3(v)

37: end while

38: return cir

Input: The root node v of an LimTDD $\mathcal F$ representing an n-qubit quantum state $|\psi\rangle$, suppose there are m non-terminal nodes in $\mathcal F$, and the qubit and ancilla qubit corresponding to v are denoted as q_v and q_{a_v} , respectively.

Output: A quantum circuit C, corresponding to an unitary matrix U, such that $U|0\rangle^{\otimes m-1}|1\rangle|\psi\rangle = |0\rangle^{\otimes m-1}|1\rangle|0\rangle^{\otimes n}$.

```
1: Q \leftarrow \{v\}
                     > An queue (First-In-First-Out) initialled with the
    \mathsf{node}\ v
 2: S \leftarrow []
                                     3: E \leftarrow the set of all edges in \mathcal{F}
 4: cir \leftarrow QuantumCircuit(n+m)
 5: while Q is not empty do
         Remove a node v from Q
 6:
         Push v to the stack S
 7:
         Suppose wt ((v, high(v))) = \lambda \cdot O
 8:
         Append cir with a controlled O^{\dagger} gate with the control
 9:
    condition |1\rangle_v |1\rangle_{a_v}
10:
         for b = 0 to 1 do
             u \leftarrow b-successor of v
11:
12:
             Remove edge (v, u) from E
13:
             if u is the terminal node then
                                                  ⊳ Nothing need to be done
14:
                  pass
15:
             else
                  if u has no incoming edge then
16:
                      Add u to Q
17:
18:
                  Append cir with a CCX gate with control condition
19:
     |b\rangle_v |1\rangle_{a_v}, and target qubit q_{a_u}
20:
              end if
         end for
21:
22: end while
23:
    while S is not empty do
24:
         Remove a node v from S
25:
         for b = 0 to 1 do
26:
             u \leftarrow b-successor of v
27:
             if u is not the terminal node then
28:
                  Append cir with a CCX gate with control condition
     |b\rangle_v |1\rangle_{a_v}, and target qubit q_{a_u}
29:
             end if
30:
         Suppose wt((v, high(v))) = \lambda \cdot O
31:
32:
         w_0 \leftarrow ||\text{low}(v)||
         w_1 \leftarrow \lambda \cdot || \text{high}(v) ||
33:
         c \leftarrow w_1/w_0
34:
    Append a controlled \frac{1}{\sqrt{1+|c|^2}}\begin{bmatrix} 1 & c^\dagger \\ -c & 1 \end{bmatrix}, with the control condition |1\rangle_{a_v} and target q_v
35:
         ||v|| \leftarrow \sqrt{|w_0|^2 + |w_1|^2}.
36:
```

VII. LIMTDD BASED QSP WITH OPTIONAL NUMBER OF ANCILLA QUBITS

In this section, we introduce an algorithm that can flexibly utilise up to m ancilla qubits. This algorithm serves as a bridge between Alg. 2 and Alg. 3, leveraging the available ancilla resources as much as possible to reduce computational complexity.

A. Algorithm

This algorithm combines the procedure of Alg. 2 and Alg. 3. We begin by reserving one ancilla qubit for the procedure outlined in Alg. 2. If additional ancilla qubits are available, we proceed with the steps described in Alg. 3; otherwise, we revert to the procedure in Algorithm 2. Essentially, when the number of available ancilla qubits exceeds $\operatorname{size}(\mathcal{F})$, the algorithm defaults to Alg. 3. Conversely, when only one ancilla qubit is available, the algorithm reduces to Alg. 2.

Consider a non-terminal node v with the form

$$v_0 \leftarrow V_1 \longrightarrow V_1$$

which has been marked open by q_{a_v} , represented as $|1\rangle_{a_v}|v\rangle+|0\rangle_{a_v}|{\rm Res}\rangle$. The operator O can be eliminated using the control condition $|1\rangle_{a_v}$. Suppose neither v_0 nor v_1 has been assigned an ancilla qubit. The circuit generated by using Alg. 2 can transform $|1\rangle_a|v_0\rangle$ and $|1\rangle_a|v_1\rangle$ into $||v_0||\,|1\rangle_a\,|0\rangle^{\otimes k}$ and $||v_1||\,|1\rangle_a\,|0\rangle^{\otimes k}$, respectively. Applying these circuits with control conditions $|1\rangle_{a_v}\,|0\rangle_v$ and $|1\rangle_{a_v}\,|1\rangle_v$ changes the original state to

$$\left|1\right\rangle_{a_{v}}\left(\left|\left|v_{0}\right|\right|\left|0\right\rangle_{v}+\lambda\left|\left|v_{1}\right|\right|\left|1\right\rangle_{v}\right)\left|0\right\rangle^{\otimes k}+\left|0\right\rangle_{a_{v}}\left|\mathrm{Res}\right\rangle.$$

Subsequently, applying an operator

$$\frac{1}{\sqrt{1+|c|^2}} \begin{bmatrix} 1 & c^{\dagger} \\ -c & 1 \end{bmatrix}$$

with $c = \lambda \cdot ||v_1||/||v_0||$ and control condition $|1\rangle_{a_v}$ transforms the state to

$$||v|| |1\rangle_{a_n} |0\rangle^{\otimes k+1} + |0\rangle_{a_n} |\text{Res}\rangle.$$

If either successor node has been assigned an ancilla qubit, we follow the procedure in Algorithm 3 to process the node, which involves adding further gates to transform it into $|0\rangle^{\otimes k}$. We then unmark the node and proceed to adjust the outgoing edge weights of v.

B. An Example

The circuit for preparing the quantum state corresponding to the quantum state shown in Fig. 2 is given in Fig. 7. In the remainder of this subsection, we describe the preparation procedure step-by-step. For clarity, we will also omit the state $|1\rangle_{a_{20}}$ and the state of other ancilla qubits if it is in $|0\rangle$.

1) Cancel the Operator on the Incoming Edge:

Apply a Z gate on qubit q₂ to cancel the Z⊗I⊗I operator
on the incoming edge of the LimTDD. The state becomes:
|v₂₀⟩.

2) Ordered traversal to cope with the Operators:

- a) Process the v_{20} Node:
 - Apply a CCZ gate with q_{a20} and q₂ as controls and q₁ as the target to cancel the Z ⊗ I operator on the highedge of the v₂₀ node. The state becomes: |0⟩ |v₁₀⟩ + |1⟩ |v₁₁⟩.
 - Apply two CCX gates to mark the two nodes v_{10} and v_{11} as open with $q_{a_{10}}$ and $q_{a_{11}}$. The state becomes: $|0\rangle |1\rangle_{a_{10}} |v_{10}\rangle + |1\rangle |1\rangle_{a_{11}} |v_{11}\rangle$.
- b) Process the v_{10} Node:

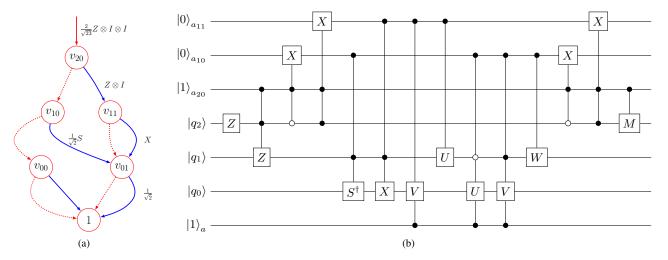


Fig. 8. The quantum circuit that transforms the quantum state $|0\rangle^{\otimes 2}|1\rangle|\mathcal{F}\rangle$ into $|0\rangle^{\otimes 2}|1\rangle|000\rangle$. In this circuit $U=\frac{1}{\sqrt{2}}\begin{bmatrix}1&1\\-1&1\end{bmatrix}$, $V=\frac{\sqrt{2}}{\sqrt{3}}\begin{bmatrix}1&\frac{1}{\sqrt{2}}\\-\frac{1}{\sqrt{2}}&1\end{bmatrix}$, $W = \frac{1}{\sqrt{11}} \begin{bmatrix} 2\sqrt{2} & \sqrt{3} \\ -\sqrt{3} & 2\sqrt{2} \end{bmatrix}, M = \frac{1}{\sqrt{23}} \begin{bmatrix} \sqrt{11} & \sqrt{12} \\ -\sqrt{12} & \sqrt{11} \end{bmatrix}$

• Apply a CC- S^{\dagger} gate to cancel the S operator on the high-edge of the v_{10} node. The state becomes: $\left|0\right\rangle \left|1\right\rangle _{a_{10}}\left(\left|0\right\rangle \left|v_{00}\right\rangle +\frac{_{1}}{\sqrt{2}}\left|1\right\rangle \left|v_{11}\right\rangle \right)+\left|1\right\rangle \left|1\right\rangle _{a_{11}}\left|v_{11}\right\rangle .$

c) Process the v_{11} Node:

ullet Apply a CCX gate to cancel the X operator on the high-edge of the v_{11} node. The state becomes: $|0\rangle |1\rangle_{a_{10}} (|0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) + |1\rangle |1\rangle_{a_{11}} (|0\rangle + |1\rangle_{a_{11}} (|$

3) Reverse order traversal to cope with the Weights:

a) Process the v_{11} Node:

- Use Alg. 2 to cope with the v_{01} node, a CV gate will be returned which can change the state $|v_{01}\rangle$ to $\frac{\sqrt{3}}{2}|0\rangle$, add it to the circuit with control condition $|\tilde{1}\rangle_{a_{11}},$ and the state will becomes: $|0\rangle |1\rangle_{a_{10}} (|0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) + \frac{2}{\sqrt{2}} |1\rangle |1\rangle_{a_{11}} (|0\rangle + |1\rangle) |0\rangle.$ • Apply a CU gate reduce the weight on the outgoing edges of v_{11} and change the
- state to: $|0\rangle |1\rangle_{a_{10}} (|0\rangle |v_{00}\rangle + \frac{1}{\sqrt{2}} |1\rangle |v_{01}\rangle) +$ $\sqrt{3} |1\rangle |1\rangle_{a_{11}} |0\rangle |0\rangle.$

b) Process the v_{10} Node:

- Use Alg. 2 to cope with the v_{00} node and v_{01} node respectively, two gates CU and CV will be returned, which can change state $|v_{00}\rangle$ and $|v_{01}\rangle$ to $\sqrt{2}|0\rangle$ and $\frac{\sqrt{3}}{2}|0\rangle$, respectively. Adding them to the circuit with control condition $|1\rangle_{a_{10}}\,|0\rangle_{1}$ and $|1\rangle_{a_{10}}\,|1\rangle_{1},$ and the state becomes: $|0\rangle\,|1\rangle_{a_{10}}\,(\sqrt{2}\,|0\rangle\,+\,\frac{\sqrt{3}}{2}\,|1\rangle)\,|0\rangle\,+\,$ $\sqrt{3} \ket{1} \ket{1}_{a_{11}} \ket{0} \ket{0}.$ • Apply a CW gate to reduce the weight on the
- outgoing edges of the v_{10} node, the state becomes: $\frac{\sqrt{11}}{2}\left|0\right\rangle\left|1\right\rangle_{a_{10}}\left|0\right\rangle\left|0\right\rangle+\sqrt{3}\left|1\right\rangle\left|1\right\rangle_{a_{11}}\left|0\right\rangle\left|0\right\rangle.$

c) Process the v_{20}^{10} Node:

- Apply two CCX gates to unmark v_{10} and v_{11} , and the state becomes: $\frac{\sqrt{11}}{2}\ket{0}\ket{0}\ket{0} + \sqrt{3}\ket{1}\ket{0}\ket{0}$.
- Apply a CM gate to reduce the weight on the outgoing edges of the v_{20} node, the state becomes: $\frac{\sqrt{23}}{2} |0\rangle |0\rangle |0\rangle.$

C. Complexity

- 1) Time Complexity: Assume that m nodes have been allocated ancilla qubits, and there are p reduced paths originating from the topmost non-terminal nodes that have not been allocated ancilla qubits. Suppose these topmost non-terminal nodes correspond to qubit q_k . The time complexity of this algorithm is $\mathcal{O}(m+kp)$.
- 2) Gate Complexity: The upper bound on the gate complexity is as follows:
 - 2p k + 1-qubit gates,
 - 3p s-qubit gates for $s \in \{4, \dots, k\}$,
 - $(3n+4)m + \frac{k(k-1)}{2}p + 3p$ 3-qubit gates,
 - m + kp + 3p 2-qubit gates,
 - n single-qubit gates.
- 3) Special Case: For decision diagrams in the tower form, the upper bound reduces to n single-qubit gates, n two-qubit gates, and $\frac{n(n-1)}{2} + 2m$ three-qubit gates.

VIII. EXPERIMENTS

We conducted experiments to compare our algorithms with many existing methods, including those implemented in Qiskit, QuICT, and ADD-based, and FBDD-based methods. Specifically, Qiskit and OuICT-which to not utilise ancilla gubits-were compared with our Alg. 1. The ADD-based method, which uses one ancilla qubit, was compared with our Alg. 2. The FBDD-based algorithm, which uses as many ancilla qubits as the number of non-terminal nodes, was compared with our Alg. 3. In addition, we evaluated the performance of our four algorithms with different numbers of ancilla qubits.

All experiments were conducted on a Linux server equipped with a 13th Gen Intel(R) Core(TM) i5-13600KF processor and 32GB RAM. The tested quantum states were generated using Clifford + T circuits, a commonly used circuit category. For each qubit number n, we generated 20 random quantum states and analysed their average performance.

We measured the running time of the algorithms and the number of multi-qubit gates in the resulting circuits (similar results were obtained when calculating the number of all gates or circuit depths). It is worth noting that the circuits generated by multiple DD-based

Algorithm 4 STATEPRE4(v, m)**Input:** The root node v of a LimTDD \mathcal{F} representing an n-qubit quantum state $|\psi\rangle$, suppose there are m ancilla qubits available **Output:** A quantum circuit C, corresponding to an unitary matrix U, such that $U|0\rangle^{\otimes m_0}|1\rangle^{\otimes m_1}|\psi\rangle = |0\rangle^{\otimes m_0}|1\rangle^{\otimes m_1}|0\rangle^{\otimes n}$, where $m_0 = \max(0, m - 2)$ and $m_1 = \min(2, m)$. 1: Directly call Alg. 2 if m = 12: $q_a \leftarrow$ a reserved ancilla qubit ⊳ for calling Alg. 2 3: $Q \leftarrow \{v\}$ \triangleright An queue initialled with the node v4: *S* ← [] 5: $E \leftarrow$ the set of all edges in \mathcal{F} 6: $cir \leftarrow QuantumCircuit(n+m)$ 7: $avi_anc \leftarrow m-1$ > Available ancilla qubit num 8: **while** Q is not empty **do** Remove a node v from Q9. Push v to the stack S10: Allocate v with an ancilla qubit q_{a_v} and set $avi_anc \leftarrow$ 11: $avi_anc - 1$, if it has not been allocated one and $avi_anc > 0$ Suppose wt $((v, high(v))) = \lambda \cdot O$ 12: Append cir with a controlled O^{\dagger} gate with the control 13: condition $|1\rangle_v |1\rangle_{a_v}$, if v has been allocated with an ancilla v'for b = 0 to 1 do 14: 15: $u \leftarrow b$ -successor of v16: Remove edge (v, u) from E17: End For Loop if u is the terminal node 18: Allocate u with an ancilla qubit q_{a_u} and set $avi_anc \leftarrow$ $avi_anc - 1$, if it has not been allocated one and $avi_anc > 0$ Add u to Q, if u has no incoming edge and has been 19: allocated with an ancilla qubit q_{a_u} Append cir with a CCX gate with control condition 20: $|b\rangle_v |1\rangle_{a_v}$, and target qubit q_{a_u} , if u has been allocated with an ancilla qubit q_{a_u} end for 21: 22: end while 23: while S is not empty do 24: Remove a node v from Sif $low(v) = high(v) \neq v_T$ and low(v) has not been 25: allocated an ancilla qubit then 26: $cir_l \leftarrow \text{STATEPRE2}(\text{low}(v), q_a)$ Append cir with cir_l with control condition $|1\rangle$ 27: 28: Continue While Loop without running lines 30-39 29: end if for b = 0 to 1 do 30: 31: $u \leftarrow b$ -successor of vEnd For Loop if u is the terminal node 32: if u has not been allocated an ancilla qubit then 33: 34: $cir_b \leftarrow \text{STATEPRE2}(u, q_a)$ 35: Append cir with cir_b with control condition $|b\rangle_v |1\rangle_{a_v}$ else 36: Append cir with a CCX gate with control condition 37: $|b\rangle_v\,|1\rangle_{a_v}$, and target qubit q_{a_u} end if 38: end for 39:

40:

41: end while

42: return cir

Do Lines 31-36 from Alg. 3

methods contain multiple-controlled gates, while circuits generated by Qiskit and QuICT only contain CX gates and single-qubit gates. For fairness, we use Qiskit to transpile the circuits generated by the DD-based methods into the set of CX gates and single-qubit gates so they can be compared under the same gate set. Both pre- and post-transpilation results for time and gate complexity are reported in our experiments, denoted as "nt"(not transpiled) or "t"(transpiled), respectively. Note that the ADD-based algorithm tools have implemented their own method of converting multi-control qubit gates into CX and single-qubit gates. Therefore, we used their native transpilation implementation instead of Qiskit.

A. Non-ancilla Algorithm (Alg. 1) compared with Qiskit and QuICT.

We first compared our no-ancilla algorithm with two widely-used quantum computing frameworks: Qiskit [27] and QuICT [28]. The algorithms used for quantum state preparation in Qiskit and QuICT are established in [14] and [15], respectively. The experiment results are shown in Fig. 9.

- Gate Complexity: Overall, our algorithm requires fewer quantum gates compared to Qiskit and QuICT, both before and after compilation. The advantage becomes more pronounced as the number of qubits increases, highlighting the scalability of our approach. For instance, for n=15 qubits, our method requires around 90 and 3510 gates before and after the transpilation, while both Qiskit and QuICT require around 130000 gates.
- Runtime Complexity: The trend of runtime complexity is consistent with that of gate complexity. Overall, when the transpilation time is excluded, our algorithm 1 requires less time. Similarly, when the number of qubits increases, the advantage becomes more pronounced and stable. For example, for n=15 qubits, our algorithm takes 0.27 seconds—not including an extra 1.68 seconds needed for transpilation—while Qiskit and QuICT take approximately 3 and 2 seconds, respectively.

B. One-ancilla Algorithm (Alg. 2) Compared with ADD-based Method

We compared our One-ancilla algorithm with the ADD-based method proposed in [24]. Fig. 10 shows the runtime and multi-qubit gate complexity of the two methods.

- Gate Complexity: Our method consistently requires fewer gates when the number of qubits exceeds 5. This improvement is attributed to the more compact representation of quantum states using LimTDD compared to ADD. For example, for n=15 qubits, our method uses approximately 80 and 200 gates before and after transpilation, while the ADD-based method uses around 2,500 and 50,000 gates before and after transpilation, respectively.
- Runtime Complexity: For small qubit numbers, the ADD-based method is faster due to its C++ implementation, while our Python implementation is slower until qubit number surpasses 15. As the number of qubits increases, our method's runtime becomes significantly shorter and exhibits better scalability, highlighting the advantage of LimTDD's compactness.

C. Sufficient Ancilla Algorithm (Alg. 3) Compared with FBDD based method

We compared our sufficient-ancilla algorithm with the FBDD-based method proposed in [25]. Note that there is no implementation provided in [25], so we implemented the algorithm using Tensor Decision Diagram (TDD), which can be seen as a type of FBDD.

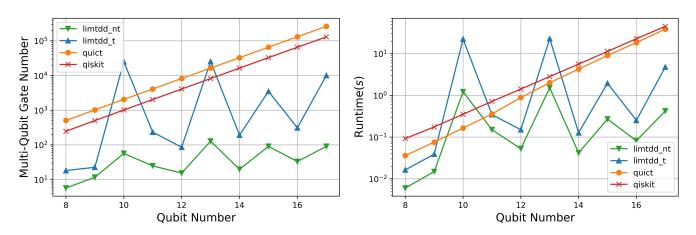


Fig. 9. Experiment results of the Alg. 1, compared with QuICT and Qiskit.

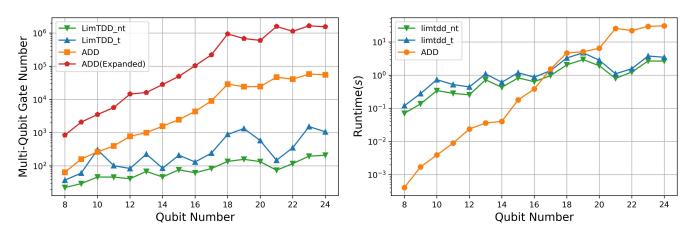


Fig. 10. Experiment results of our method against ADD-based method [24].

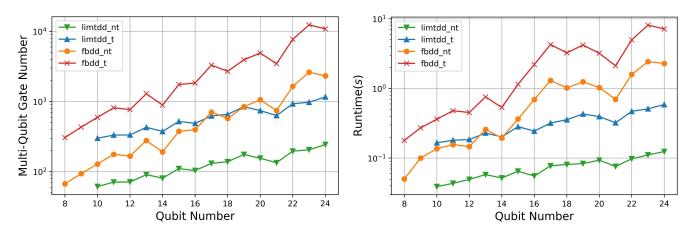


Fig. 11. Experiment results of our method (Alg. 3) against FBDD-based method [25] implemented in TDD.

Fig. 11 shows the runtime and multi-qubit gate complexity of the two methods.

- Gate Complexity: Our algorithm consistently requires fewer multi-qubit gates, and this trend remains after transpilation. The gap widens as the number of qubits increases.
- Runtime Complexity: The runtime comparison follows the same trend, further demonstrating the advantages of using LimTDD for quantum state preparation.

D. The Performance of Our Four Algorithms

Finally, we compared the performance of all four algorithms proposed in our work. For Alg. 4, we set the number of auxiliary qubits to 10. Fig. 12 shows the runtime and multi-qubit gate complexity of the algorithms. The number of gates is the one after transpilation.

- Gate Complexity: Alg. 1 exhibits unstable performance, mainly
 due to the large number of multi-control bit gates introduced
 during compilation. Excluding Alg. 1, the number of multiqubit gates required for state preparation decreases with an
 increased number of ancilla qubits. Furthermore, the trend of
 gate complexity becomes more stable and smooth as more
 ancilla qubits are utilised.
- Runtime Complexity: The runtime trend mirrors the gate complexity trend. Excluding Alg. 1, the runtime decreases with the number of ancilla qubits.

IX. CONCLUSION

In this paper, we proposed novel quantum state preparation algorithms based on the Local Invertible Map Tensor Decision Diagram (LimTDD). These algorithms significantly improve the efficiency and reduce the complexity of quantum circuits, particularly for large-scale quantum states. The compact representation of LimTDD enables substantial improvements in both time and gate complexity, achieving exponential efficiency gains in certain scenarios.

Our experiments demonstrate that the proposed methods outperform existing frameworks such as Qiskit and QuICT, especially as the number of qubits increases. The integration of LimTDD into quantum state preparation highlights its potential for handling complex or large-scale quantum states with fewer resources. This work not only advances the state-of-the-art in quantum state preparation but also provides a robust foundation for future developments in quantum computing technologies.

Future work will focus on further optimising LimTDD and exploring its applications in other quantum computing tasks. We aim to integrate our algorithms into widely used quantum computing frameworks to standardise and accelerate the quantum state preparation process. Additionally, we plan to develop more sophisticated interfaces to streamline the workflow for quantum physicists and experimentalists, enabling them to efficiently generate the quantum states required for their research.

In summary, this paper has demonstrated the potential of LimTDD in quantum state preparation, paving the way for more efficient and scalable quantum computing solutions.

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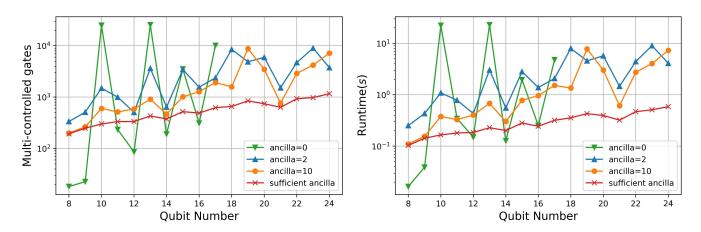


Fig. 12. Compare with other ancilla-based LimTDD algorithms.

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