Automatic Preparation of Uniform Quantum States Utilizing Boolean Functions

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***Abstract*—Many quantum algorithms inherently assume a specific initial state in order to perform the desired computations. The preparation of such states itself requires a computation in terms of a quantum circuit. In this paper, we investigate the automatic state preparation of a specific subset of arbitrary quantum states that are uniform superpositions over a subset of basic states. We exploit that such functions can be represented using Boolean functions, and propose an automatic compilation algorithm that finds a quantum circuit for state preparation given as input a Boolean function, which represents the desired state. The proposed method provides an upper bound on the number of quantum gates in the $\{R_y(\theta), \mathrm{CNOT}\}$ gate set. In addition, an optimization is presented that can reduce the number of quantum gates in the generated circuit.**

***Index Terms*—Quantum state preparation, Boolean functions, quantum compilation, quantum algorithms.**

I. Introduction

Quantum computing is concerned with developing computing technology based on the principles of quantum mechanics. In classical computing, a bit is a single piece of information that exists in one of the classical two states 1 and 0. In quantum computing the fundamental unit of information is a quantum bit, or qubit in short. The state of a qubit includes the two basic states $|0\rangle$ and $|1\rangle$, but unlike a classical bit, the state can also be any superposition of these states. Such state is described using two complex amplitudes α and β, which are entries in the state vector $\binom{\alpha}{\beta}$. The combined state for n qubits is described in terms of 2^n complex-valued amplitudes. In fact, each amplitude corresponds to the probability of the quantum state being in one of the 2^n possible basic states after measuring all qubits.

A quantum operation on n qubits is described in terms of quantum gates, which are modeled as $2^n \times 2^n$ unitary matrices. A combination of these gates represents a quantum circuit, which show the interaction of quantum gates with qubits in the quantum computer. A quantum algorithm is a quantum circuit that can solve a specific problem. Two well-known quantum algorithms are Grover's search algorithm [1], and Shor's algorithm [2] for period finding that can be used for prime factorization.

In general the initial quantum state is the classical basic state in which all bits are 0. Some quantum algorithms require a specific quantum state at the beginning of the computation. Consequently, an efficient quantum state preparation is an important task in quantum compilation. More precisely, in addition to the quantum circuit that performs the quantum algorithm, a specific quantum circuit is required that prepares the desired initial quantum state.

Some approaches [3]–[8] have been considered in the past to prepare arbitrary quantum states. Since these approaches can generated arbitrary quantum states, the input to such algorithms are 2^n complex-valued amplitudes, which limits their scalability drastically. Further, some of the algorithms require a rather abstract set of gates, which requires an additional compilation step in order to run it on physical quantum computers.

In this paper, we target a subset of all possible quantum states called uniform quantum states. A uniform quantum state is a quantum state that is a superposition of a nonempty subset of basic states. In other words, all nonzero amplitudes in such a state have the same value. Therefore, such states can be characterized by a Boolean function where each minterm corresponds to a nonzero amplitude. This enables a scalable quantum state preparation (QSP), since many Boolean functions of practical interest have small representations, e.g., in terms of binary decision diagrams (BDD) or logic network. Many important quantum states are uniform quantum states, such as the uniform superposition of *all* basis states, the Bell state, the W state, and the GHZ state.

We propose an automatic quantum compilation algorithm, which takes as input a Boolean function and produces a quantum circuit over the $\{R_y(\theta), \mathrm{CNOT}\}$ gate set. The algorithm is based on decomposition of the input function and a recursive procedure on smaller subfunctions.

II. Preliminaries

In this section, we introduce necessary background on Boolean functions and quantum computation.

A. Boolean Functions

A Boolean function is a function of the form $f : \mathbb{B}^n \to \mathbb{B}$, where $\mathbb{B} = \{0, 1\}$. The *on-set* and *off-set* of the function are the sets of all input assignments that map to 1 and 0, respectively. Formally, we define

$$\begin{aligned} \mathrm{on}(f) &= \{x \in \mathbb{B}^n \mid f(x) = 1\} \\ \mathrm{off}(f) &= \{x \in \mathbb{B}^n \mid f(x) = 0\} \end{aligned} \tag{1}$$

We also define $|f| = |\,\mathrm{on}(f)|$ as the number of minterms in f.

A Boolean function can be represented in terms of its truth table, which is the column vector

$$f = \big(f(0,\dots,0,0), f(0,\dots,0,1),\dots, f(1,\dots,1,0), f(1,\dots,1,1)\big)^T, \quad (2)$$

where each entry corresponds to the function value of one of the input assignments. In this paper, we use f to both refer to the function and its truth table.

The *positive* and *negative co-factors* of a Boolean function $f(x_0,\dots,x_{n-1})$ with respect to a variable x_i are obtained by assigning x_i to 1 and 0, respectively. We define

$$\begin{aligned} f_{x_i} &= f(x_0,\dots,x_{i-1},1,x_{i+1},\dots,x_{n-1}) \\ f_{\bar{x}_i} &= f(x_0,\dots,x_{i-1},0,x_{i+1},\dots,x_{n-1}) \end{aligned} \quad (3)$$

We use co-factors in this paper to compute the influence on the function's output. We define

$$p_f(x_i) = \frac{|f_{x_i}|}{|f|} \quad \text{and} \quad p_f(\bar{x}_i) = \frac{|f_{\bar{x}_i}|}{|f|}. \quad (4)$$

The intuition is that the co-factors partition the function's on-set into two halves. Note that $p_f(x_i) + p_f(\bar{x}_i) = 1$. When f is clear from the context, we simply write $p(x_i)$ and $p(\bar{x}_i)$.

B. Quantum Operations and Circuits

A quantum circuit is a diagram to represent a quantum program. A combinational quantum circuit consists of quantum operations, connected using quantum wires transmitting qubits, without fanout. This section reviews the basics of quantum computation and circuits.

Qubits: A qubit models the basic unit in quantum computing that has two basic states, represented using $|0\rangle$ and $|1\rangle$. In fact, a qubit can be any superposition of two basic states, which can be denoted as

$$|\psi\rangle = \alpha_0|0\rangle + \alpha_1|1\rangle = \begin{pmatrix}\alpha_0\\ \alpha_1\end{pmatrix} \quad (5)$$

Here, $\alpha_0, \alpha_1 \in \mathbb{C}$ with $|\alpha_0|^2 + |\alpha_1|^2 = 1$. The squared complex numbers $|\alpha_0|^2$ and $|\alpha_1|^2$ indicate the probability that the quantum state will collapse to the classical state $|0\rangle = \binom{1}{0}$ or $|1\rangle = \binom{0}{1}$ after the qubit is measured. Moreover, quantum states over n qubits are represented by

$$|\varphi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle, \quad (6)$$

a column vector of 2^n complex values α_i such that $\sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1$. Each squared amplitude $|\alpha_i|^2$ indicates the probability that after measurement the n qubits are in classical states i.

Quantum states can be combined by applying the Kronecker product to produce larger ones, e.g., $\binom{1}{0} \otimes \frac{1}{\sqrt{2}}\binom{1}{1} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$, which represents a 2-qubit state that is in the perfect superposition between the classical states 00 and 01 [9].

Quantum operations: As quantum operations in this paper we consider *quantum gates*, which are modelled as unitary operations which are applied on the qubits to alter their states. A single-qubit quantum gate acts on a single-qubit, and transforms its state into another quantum state. The single-qubit gates are represented by 2×2 unitary matrices [10], [11].

Since single-qubit states correspond to points on the Bloch sphere [11], quantum operations on a single-qubit correspond to rotations. There are three types of rotation gates R_x, R_y, and R_z regarding the three axis x, y, and z. Each rotation gate is parameterized with a continuous angle $\theta \in \mathbb{R}$:

$$\begin{aligned} R_x(\theta) &= \begin{pmatrix} \cos\frac{\theta}{2} & -\mathrm{i}\sin\frac{\theta}{2} \\ -\mathrm{i}\sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix} \\ R_y(\theta) &= \begin{pmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix} \\ R_z(\theta) &= \begin{pmatrix} 1 & 0 \\ 0 & e^{\mathrm{i}\theta}\end{pmatrix} \end{aligned} \quad (7)$$

Quantum gates that act on n qubits are represented in terms of $2^n \times 2^n$ unitary matrices. Some 2-qubit gates that we consider in this work are:

$$\text{CNOT} = \begin{pmatrix} 1&0&0&0\\0&1&0&0\\0&0&0&1\\0&0&1&0 \end{pmatrix} \text{ and SWAP} = \begin{pmatrix} 1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1 \end{pmatrix} \quad (8)$$

In fact, a CNOT gate consists of one control and one target, the target will be flipped when the control is 1. A SWAP gate changes the state of 2 qubits with each other.

Uniformly-controlled rotation gates: In this work, we make use of a family of unitaries called *uniformly-controlled rotation gates* [5]. These unitaries are $2^{n+1} \times 2^{n+1}$ block diagonal matrices of the form

$$\begin{aligned} U_\alpha &= R_a(\alpha_1) \oplus \cdots \oplus R_a(\alpha_{2^n}) \\ &= \begin{pmatrix} R_a(\alpha_1) & & \\ & \ddots & \\ & & R_a(\alpha_{2^n}) \end{pmatrix}, \end{aligned} \quad (9)$$

where $a \in \{x, y, z\}$ and $\alpha = (\alpha_1, \dots, \alpha_{2^n})$ are 2^n rotation matrices. The unitary is applied to n control qubits $|x\rangle$ and 1 target qubit $|y\rangle$. One of the 2^n rotations is applied to the target qubit depending on the value of the control lines. The action of the unitary is

$$U_\alpha : |x\rangle|y\rangle \mapsto |x\rangle R_a(\alpha_x)|y\rangle. \quad (10)$$

If $|x\rangle$ is in superposition, then a superposition of rotations is applied accordingly.

An example of a uniformly-controlled rotation gate with 2 controls is shown in Fig. 1. The figure also shows the visual representation of the uniformly-controlled rotation gate on the left-hand side.

III. Proposed Method

In this section, we introduce the problem definition and the general idea of our approach to generate uniform quantum states. We also discuss a synthesis approach and possible optimizations to generate a quantum circuit for large abstract gates.

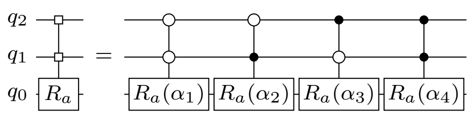

Fig. 1. A uniformly-controlled rotation gate

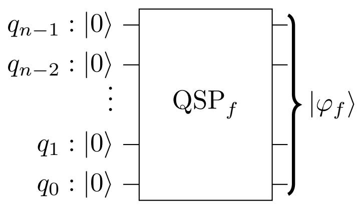

Fig. 2. The problem of quantum state preparation

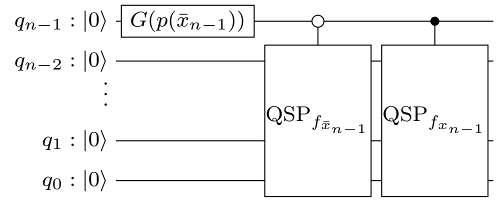

Fig. 3. The general idea

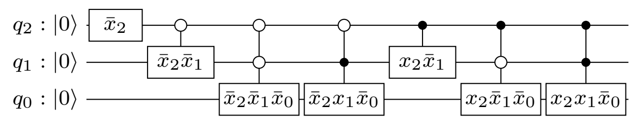

Fig. 4. The abstract quantum gates of $\mathrm{QSP}_{\langle x_0x_1x_2\rangle}$

A. *Problem Definition*

In this work, we consider n-qubit quantum states that are uniform superpositions over a nonempty subset of the basis states $|0\rangle, |1\rangle, \dots, |2^n-1\rangle$. In such quantum states all amplitudes of the state vector are either 0 or have the same value $\alpha = 1/\sqrt{s}$, where s is the size of the subset of basis states. We exploit that such states can be characterized by a Boolean function $f : \mathbb{B}^n \to \mathbb{B}$ such that $f(x) = 1$, if and only if $|x\rangle$ is in the subset of considered basis states, and therefore its corresponding amplitude is nonzero.

Example 1: The majority-of-three function $f = \langle x_0x_1x_2\rangle = x_0x_1 \vee x_0x_2 \vee x_1x_2$ has the truth table $f = (0,0,0,1,0,1,1,1)^T$. It encodes the uniform quantum state $|\varphi\rangle = \frac{1}{\sqrt{4}}\begin{pmatrix}0\\0\\0\\1\\0\\1\\1\\1\end{pmatrix}$.

In other words, we are interested in generating a quantum state $|\varphi_f\rangle$ that corresponds to the normalized truth table of f

$$|\varphi_f\rangle = \frac{f}{\sqrt{|f|}} = \frac{1}{\sqrt{|f|}} \sum_{x \in \mathrm{on}(f)} |x\rangle. \tag{11}$$

In this paper, we propose automatic algorithms to find a quantum circuit for generating such a state given as input a Boolean function f in some representation. In particular, we are looking for efficient circuit constructions for a unitary QSP_f where $\mathrm{QSP}_f|0\rangle^{\otimes n} = |\varphi_f\rangle$. Fig. 2 summarizes our problem formulation.

Note that many of the quantum states that appear in quantum algorithms are uniform quantum states, e.g., the uniform superposition of all basis states, for which $f = 1$ (tautology), the Bell state, for which $f = \bar{x}_1 \oplus x_2$, the generalized GHZ state, for which $f = \bar{x}_1\bar{x}_2 \dots \bar{x}_n \oplus x_1x_2 \dots x_n$, and the generalized W state, for which $f = [x_1 + x_2 + \cdots + x_n = 1]$.

B. *General Idea*

To prepare an n-qubit uniform quantum state $|\varphi_f\rangle$ using Boolean functions, each qubit q_i in the quantum circuit corresponds to variable x_i in f. In the remainder, we will use the function variable and the corresponding qubit interchangeably, as well as the quantum state representation with the corresponding Boolean function. We will outline our proposed algorithm based on an n-variable Boolean function $f(x_0, x_1, \dots, x_{n-1})$.

The genral idea of our proposed algorithm relies on the recursive circuit construction in Fig. 3. It can be shown that

$$\mathrm{QSP}_f|0^n\rangle = (\mathrm{QSP}_{f_{\bar{x}_i}} \oplus \mathrm{QSP}_{f_{x_i}})(G(p(\bar{x}_{n-1})) \otimes I_{2^n-1})|0\rangle,$$

where $G(p)$ is a unitary transformation gate such that

$$G(p)|0\rangle = \sqrt{p}|0\rangle + \sqrt{1-p}|1\rangle. \tag{12}$$

Fig. 3 shows the application of this property in the quantum circuit model for $i = n-1$.

Applying this procedure for all variables for the majority function $f = \langle x_1x_2x_3\rangle$ from Example 1 leads to the circuit in Fig. 4. For the sake of clarity, we only write the co-factors into the boxes, e.g., the box labeled $x_2\bar{x}_1\bar{x}_0$ refers to the quantum operation $G(p_{f_{x_2\bar{x}_1}}(\bar{x}_0))$.

Notice that the two gates with target on q_1 can be moved next to each other, since the right-most gate commutes with the two gates left of it, with target on q_0. We can do this in general, allowing us to retrieve a generic quantum circuit with n uniformly-controlled one-qubit quantum gates as shown in Fig. 5.

Given this general circuit construction, the overall cost of the circuit is upper bounded by the cost for each of the uniformly-controlled gates. Two factors have the largest influence on the cost:

- The order in which the function is decomposed
- The truth values of the function

In the remainder of the paper, we show how the order of decomposition the function affects the realization cost for the uniformly-controlled gates. We also show that better upper bounds can be achieved if the input function has special properties.

IV. Quantum Gate Realization

From the definition of $R_y(\theta)$ one can readily derive that

$$G(p) = R_y\left(2\cos^{-1}(\sqrt{p})\right). \tag{13}$$

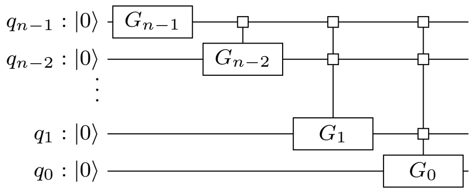

Fig. 5. The general structure of the proposed algorithm

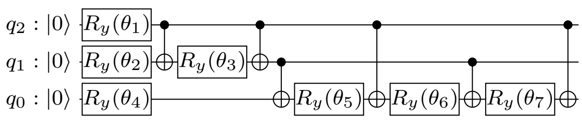

Fig. 6. The quantum circuit of $\text{QSP}_{\langle x_0 x_1 x_2 \rangle}$

Consequently, replacing all G gates by R_y gates in Fig. 5, we obtain a circuit consisting only of multiple-controlled R_y rotation gates.

The i^{th} qubit requires at most 2^{n-1-i} controlled R_y rotation gates with $n-1-i$ controls. In order to run such gates on a quantum computer synthesis is required. This is very expensive when we decompose every multiple-controlled gate separately using the well-known decomposition given in [12]. Even if we divide these gates to two single-qubit gates, and multiple-controlled Z gates (MCZ) and employ MCZ decomposition presented in [13], every MCZ includes a cost of 2^n-2 CNOTs and 2^n-1 R_z rotation gates.

Instead, we utilize the decomposition method presented in [14] to synthesize uniformly-controlled rotation gates directly into a sequence of CNOT gates and R_y rotations. The decomposition of the i^{th} qubit yields at most 2^{i-1} R_y rotation gates and 2^{i-1} CNOTs. As a result, the quantum state preparation affords at most 2^n-1 R_y rotation gates and 2^n-2 CNOTs. Given this property results the quantum circuit in Fig. 6 for the majority Boolean function.

V. Discussion and Evaluation

A. Comparison over Previous Works

It is important to note that we address the specific case of quantum state preparation in which the state is a uniform state. The main advantage of our approach compared to existing approaches that generate arbitrary quantum states is that the input state can be represented as a Boolean function in our case. As a consequence, we can exploit that a compact representation of the Boolean function is also a compact representation of the input state. The main future research question is whether one can find a compact quantum circuit, if it exists, without exploring all elements of the function's on-set.

B. The Effect of the Variable Reordering

In this section, we demonstrate an example that illustrates the influence on variable reordering when performing the decomposition. Consider the following example with two different variable orderings.

TABLE I
THE RESULTS OF QSP_f WITH 2 DIFFERENT ORDERINGS.

Ordering	#CNOTs	$\#R_y$
$x_3 < x_2 < x_1 < x_0$	14	15
$x_2 < x_0 < x_1 < x_3$	10	10

Example 2: Given the function $f(x_0, x_1, x_2, x_3) = (1,1,1,0,0,0,1,0,1,0,1,1,1,1,0,1)^T$ which encodes the uniform quantum state $|\varphi_f\rangle = \frac{1}{\sqrt{10}}(1,1,1,0,0,0,1,0,1,0,1,1,1,1,0,1)^T$. The circuit shown in Fig. 7 realizes QSP_f with the ordering $x_3 < x_2 < x_1 < x_0$, whereas the circuit in Fig. 8 realizes QSP_f with the ordering $x_2 < x_0 < x_1 < x_3$. In the circuit of Fig. 8, all rotation angles applied to qubit q_1 are the same for all four control line assignments. Therefore, these four gates can be replaced by a single-qubit rotation gate. After transforming both circuits to the elementary quantum gates, one obtains the costs summarized in Table I. This demonstrates that a good variable ordering helps to reduce the number of CNOT gates and R_y gates.

C. Comparison with Known Circuit Constructions

In this section, we want to investigate how the proposed algorithm performs for known quantum states, for which there exist efficient circuit constructions. In particular, whether the algorithm can recover these constructions for the generalized GHZ state and the generalized W state.

W state: The W state [16] is defined for 3 qubits and is the superposition of all basis states with a single '1':

$$|W\rangle = \frac{1}{\sqrt{3}}\left(|001\rangle + |010\rangle + |100\rangle\right) \quad (14)$$

The notion of a W state has been generalized for n qubits which involves the superposition of all basis states with exactly one '1':

$$|W_n\rangle = \frac{1}{\sqrt{n}}\left(|0\dots01\rangle + |0\dots10\rangle + \dots + |1\dots00\rangle\right) \quad (15)$$

To understand the circuit construction for the generalized W state, first note that if $f = \bar{x}_1\bar{x}_2\dots\bar{x}_n$, then the corresponding uniform quantum state is $|\varphi_f\rangle = |0^n\rangle$ and therefore $\text{QSP}_f = I_{2^n}$, where I is the $2^n \times 2^n$ identity matrix. In other words, the quantum circuit for QSP_f is empty.

The characteristic function for $|W_n\rangle$ is

$$\begin{aligned} f &= [x_0 + x_1 + \dots + x_{n-1} = 1] \\ &= \bar{x}_{n-1}\dots\bar{x}_1 x_0 \oplus \bar{x}_{n-1}\dots x_1\bar{x}_0 \oplus \dots \oplus x_{n-1}\dots\bar{x}_1\bar{x}_0. \end{aligned}$$

We have, that the positive co-factor $f_{x_{n-1}} = \bar{x}_{n-2}\dots\bar{x}_1\bar{x}_0$, while the negative co-factor $f_{\bar{x}_{n-1}} = [x_0 + x_1 + \dots + x_{n-2} = 1]$, which is the characteristic function for $|W_{n-1}\rangle$. Regarding Fig. 3, this means that the circuit construction recurses in the negative-controlled gate (for the negative co-factor), and that the positive-controlled gate (for the positive co-factor) can be removed, since $\text{QSP}_{f_{x_{n-1}}} = I_{2^{n-1}}$. Fig. 9 shows the resulting circuit for $|W_4\rangle$.

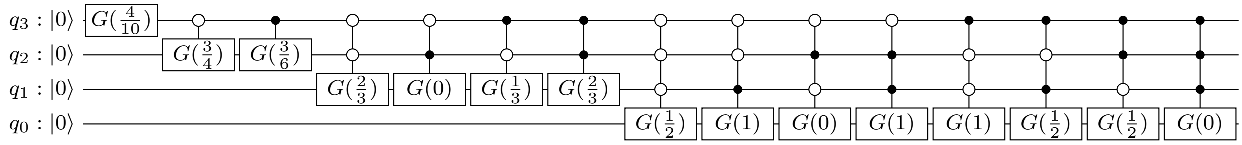

Fig. 7. The general circuit for QSP_f using $x_3 < x_2 < x_1 < x_0$ ordering

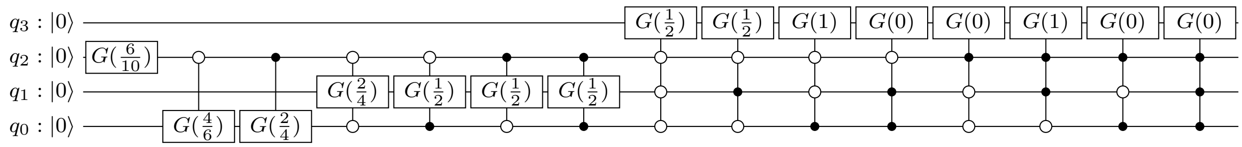

Fig. 8. The general circuit for QSP_f using $x_2 < x_0 < x_1 < x_3$ ordering

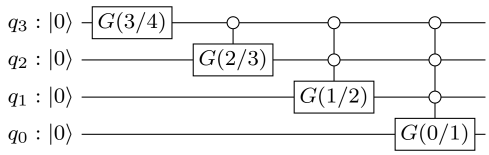

Fig. 9. QSP for the $|W_4\rangle$ state

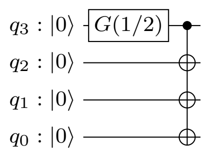

Fig. 10. QSP for the $|\text{GHZ}_4\rangle$ state

GHZ state: The Greenberger-Horne-Zeilinger (GHZ) state [15] is a generalization of the 2-qubit Bell state and consists of only two basic states. For a number of qubits n, it can be formulated as

$$|\text{GHZ}_n\rangle = \frac{1}{\sqrt{2}} \left(|0^n\rangle + |1^n\rangle\right). \tag{16}$$

In the previous section, we made use of the fact that if the characteristic $f = \bar{x}_1\bar{x}_2 \dots \bar{x}_n$, then the circuit to construct $|\varphi_f\rangle$ is empty. We now consider characteristic functions that are minterms, i.e., $|f| = 1$. We can describe such functions as $f = x_1^{p_1} x_2^{p_2} \dots x_n^{p_n}$, where the polarities $p_i \in \{0, 1\}$, with $x_i^1 = x_i$ and $x_i^0 = \bar{x}_i$. Note that the quantum circuit to prepare this state has an X gate on qubit q_i whenever $p_i = 1$.

The characteristic function for $|\text{GHZ}_n\rangle$ is $f = \bar{x}_0\bar{x}_1 \cdots \bar{x}_{n-1} \oplus x_0 x_1 \cdots x_{n-1}$. We have that its negative co-factor is $f_{\bar{x}_{n-1}} = \bar{x}_0\bar{x}_1 \cdots \bar{x}_{n-2}$ and its positive co-factor is $f_{x_{n-1}} = x_0 x_1 \cdots x_{n-2}$. These are both minterms, and therefore the circuit for QSP_f terminates after a single application of the recursive procedure in Fig. 3. The resulting circuit for $|\text{GHZ}_4\rangle$ is shown in Fig. 10. In general, our algorithm can find a quantum circuit that prepares the $|\text{GHZ}_n\rangle$ state with the expected $n-1$ CNOT gates and a single R_y gate.

VI. Conclusions

We discussed the preparation of a special family of quantum states which are uniform superpositions of a subset of basis states. We motivated this subclass by several quantum states in the literature which are uniform quantum states. The advantage of such states is that they can be characterized by a Boolean function, and therefore permit a compact representation, if the Boolean function has a compact representation—e.g., in terms of a BDD or logic network. We have shown a recursive algorithm to generate a quantum circuit based on uniformly-controlled R_y rotation gates. Our algorithm can find the same existing circuit constructions for the generalized W and GHZ states.

In future work, we want to investigate symbolic implementations of the algorithm that work directly on a BDD or logic network representation of the characteristic function. The goal is to find a compact quantum circuit—if it exists—without investigating each minterm separately. Futher, we would like to explore classes of characteristic functions that lead to small quantum circuits.

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