Deterministic discrete-time quantum walk search on complete bipartite graphs

Fangjie Peng, Meng Li,* and Xiaoming Sun

State Key Laboratory of Processors, Institute of Computing Technology, Chinese Academy of Sciences, Beijing 100190, China and School of Computer Science and Technology, University of Chinese Academy of Sciences, Beijing 100049, China

(Received 9 January 2024; accepted 11 June 2024; published 9 July 2024)

Searching via quantum walk is a topic that has been extensively studied. Most previous results provide approximate solutions, while in this paper we prove an algorithm that can find a marked vertex certainly. We adopt the coined discrete-time quantum walk (DTQW) model with adjusted operators and prove that, on complete bipartite graphs, when parameters are set properly, coined DTQW can deterministically find a marked vertex, i.e., the success probability is exactly 1. Before this paper there have been results of an alternating continuous-time quantum walk method that achieve deterministic spatial search, but this paper provides a deterministic quantum spatial search result via DTQW, while maintaining a quadratic speedup compared to classical algorithms. We also provide the quantum circuit implementation.

DOI: 10.1103/PhysRevResearch.6.033042

I. INTRODUCTION

Quantum computation has drawn a lot of attention in computer science since it can provide efficient algorithms in many problems [1–4]. The quantum walk, the quantum analog of random walk, is a widely used model in quantum algorithm design. Applications of quantum walk include search [5–8], state transfer [9,10], element distinctness [11], triangle finding [12], etc. There are two kinds of quantum walk: continuous-time quantum walk (CTQW) and discrete-time quantum walk (DTQW). In CTQW, the Childs and Goldstone algorithm [5,6] is often used, which define the walk with the Schrödinger equation and the Hamiltonian could be Laplacion or the adjacency matrix of the graph [13]. Foulger *et al.* present analysis of CTQW on graphene lattice based on spectral gap [14,15]. A variant of CTQW is the alternating CTQW [16], which alternatively uses two Hamiltonians. For DTQW, many models have been brought up, such as the coined DTQW [17], Szegedy's quantum walk [18], and the staggered quantum walk [19].

Quantum walk has been applied on the spatial search problem, i.e., finding a marked vertex on a given graph. Both CTQW [5,6,8] and DTQW [7,20,21] have been used for spatial search, and all these results have a quadratic speedup compared with classical algorithms. However, these algorithms are probabilistic, i.e., performing these algorithms does not guarantee to output a marked vertex.

The study of deterministic search begins with deterministic Grover search. The original Grover's algorithm can find a marked vertex with high probability but still has a small probability to fail. Grover's algorithm is based on reflection operators about the initial state and the marked state [2], while researchers have found that, if we could replace the reflection operators with rotation operators, we can achieve a deterministic search while still maintaining a quadratic speedup compared to classical algorithms [22–24]. In recent years, further improvements on deterministic Grover's algorithm have been proposed, claiming that either the rotations about the initial state or the rotations about the marked state can have a fixed angle, so we may choose to only adjust parameters in one side [25,26].

Naturally, we are also interested in the deterministic spatial search. In 2021, Marsh and Wang proposed an algorithm called the alternating CTQW and proved that it can deterministically find the marked vertex on a class of complete identity interdependent networks (CIIN) [16]. Then in 2022, Qu *et al.* performed research on star graphs and give an experimental demonstration for deterministic spatial search via alternating CTQW [27]. In 2023, Wang *et al.* proved a rather strong result, claiming that if eigenvalues of the adjacency matrix of a graph are all integers, then alternating CTQW can find the marked vertex deterministically [28]. See Table I for a summary.

Until now all previous results on deterministic spatial search are based on the alternating CTQW model. It is natural to ask: can we perform a deterministic spatial search with other models, especially DTQW? This paper explores this topic.

In this paper, we propose a deterministic search algorithm on complete bipartite graphs based on the coined DTQW framework, maintaining a quadratic speedup compared to classical algorithms. Typically the coined DTQW uses the Grover coin and the reflection oracle about marked vertices, while in this work we assume that we are accessible to the

*Contact author: limeng2021@ict.ac.cn

TABLE I. Comparison of previous results and our result on the deterministic spatial search.

Author	Graph	Model
Marsh & Wang [16]	CIIN	CTQW
Qu *et al.* [27]	Star graph	CTQW
Wang *et al.* [28]	Integer eigenvalue	CTQW
Our result	Complete bipartite graph	DTQW

generalized Grover coin and phase oracle, then by setting proper parameters, a marked vertex is guaranteed to be found. See Theorem 1 for our main result.

In practice, approximate search is enough in most situations, but deterministic quantum search still has theoretical significance, because it is related to a key problem about quantum computation: is quantum computation essentially probabilistic? Our results indicate that the answer may be no. Besides its own interest, when it is used as a subprocess, being deterministic makes the error analysis simpler because the error of search process can be eliminated.

This paper is organized as follows. Section II illustrates some basic settings about the graph and quantum walk model. Our algorithm is put in Sec. III, then in Secs. IV and V, the correctness of our algorithm is proved, and a key lemma is proved in Sec. VI using Bloch sphere. Section VII provides a quantum circuit implementation of our algorithm. Finally, Sec. VIII summarizes our work.

II. PRELIMINARY

A. Graph definition

This article works on complete bipartite graphs. Let $G = (V, E)$ be a bipartite graph, then vertices of G are divided into two parts, $V = V_1 \cup V_2$ and $V_1 \cap V_2 = \emptyset$. The complete bipartite graph is defined by $E = \{\{v, u\} \mid v \in V_1 \text{ and } u \in V_2\}$, i.e., every vertex in V_1 is connected to each vertex in V_2. Let N_1 and N_2 be the number of vertices in V_1 and V_2, $N_1 > 0$ and $N_2 > 0$, let $N \triangleq |V| = N_1 + N_2$. Suppose there are some marked vertices which we want to find, let M be the set of marked vertices and n_1, n_2 be the number of marked vertices in V_1 and V_2, i.e., $n_1 \triangleq |V_1 \cap M|$, $n_2 \triangleq |V_2 \cap M|$, let $n \triangleq |M| = n_1 + n_2$. Figure 1 shows an example of complete bipartite graphs.

In this paper, we use $v \sim u$ to denote $\{v, u\} \in E$. Let d_v be the degree of v, i.e., the number of vertices connected to v, then for $v \in V_1$, $d_v = N_2$; for $v \in V_2$, $d_v = N_1$.

B. Discrete-time quantum walk

In this paper, the coined DTQW model is adopted. The state space is

$$\mathcal{H} = \text{span}\{|v, u\rangle \mid v \in V, u \sim v\}.$$

For the basis state $|v, u\rangle$, v represents the current position of the walker and u represents the next position that the walker will go to.

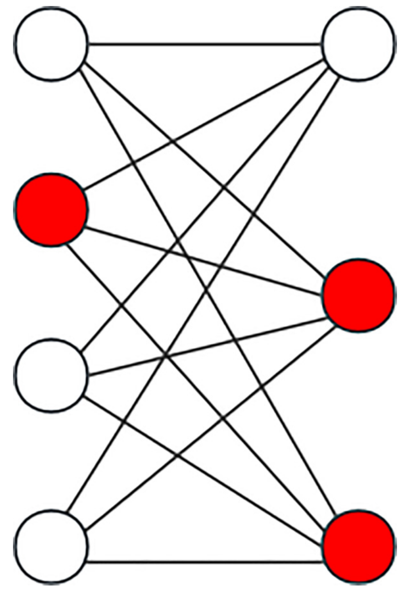

FIG. 1. An example of complete bipartite graphs. Red dots represent marked vertices. Here $N_1 = 4$, $N_2 = 3$, $n_1 = 1$, $n_2 = 2$.

Next we define the walk operator. Let

$$U(\alpha, \beta) = SC(\alpha)Q(\beta). \tag{1}$$

The shift operator S is defined as

$$S\,|v, u\rangle = |u, v\rangle\,;$$

the coin operator $C(\alpha)$ is

$$C(\alpha)\,|v, u\rangle = |v\rangle \otimes G_v(\alpha)\,|u\rangle\,,$$

where $G_v(\alpha) = (1 - e^{-i\alpha})\,|s_v\rangle\,\langle s_v| - I$ and $|s_v\rangle = \frac{1}{\sqrt{d_v}} \sum_{w\sim v} |w\rangle$; the oracle operator $Q(\beta)$ is defined as

$$Q(\beta)\,|v, u\rangle = \begin{cases} e^{i\beta}\,|v, u\rangle & \text{if } v \in M \\ |v, u\rangle & \text{if } v \notin M \end{cases}.$$

The initial state is the uniform superposition of all basis states in $\mathcal{H}$, i.e.,

$$|\Psi_0\rangle = \frac{1}{\sqrt{2N_1N_2}} \sum_{v\in V, u\sim v} |v, u\rangle\,.$$

After performing the quantum walk t steps $U(\alpha_1, \beta_1), U(\alpha_2, \beta_2), \cdots, U(\alpha_t, \beta_t)$, the state becomes

$$|\Psi_t\rangle = U(\alpha_t, \beta_t) \cdots U(\alpha_1, \beta_1)\,|\Psi_0\rangle\,.$$

Then, we measure the state $|\Psi_t\rangle$. In this paper both registers are measured, then the probability of finding a marked vertex is

$$P_t = \sum_{v\in M \text{ or } u\in M, u\sim v} |\langle v, u|\Psi_t\rangle|^2.$$

A global phase on a quantum state can be ignored. We write $|\psi\rangle \sim |\phi\rangle$ when $|\psi\rangle = e^{i\gamma}\,|\phi\rangle$. For quantum operators A and B, we also write $A \sim B$ iff they only differ on a global phase, i.e., $A = e^{i\gamma} B$.

III. ALGORITHM

In this section, we show an algorithm that can deterministically find a marked vertex in complete bipartite graphs, which can be seen in Algorithm 1.

ALGORITHM 1: Deterministic search.

Input: A complete bipartite graph $G = (V, E)$, an oracle operator $Q(\beta)$ marking a set $M \subseteq V$, N_1, N_2, n_1 with $n_1 > 0$.
Output: A marked vertex $v \in M$.
//**calculate parameters**
$\omega_1 \leftarrow 2 \arcsin \sqrt{\frac{n_1}{N_1}}$
set p be the smallest odd integer in $[\frac{\pi}{3\omega_1}, \frac{\pi}{\omega_1}]$
$x \leftarrow \frac{\cos^3 \frac{\omega_1}{2} - \cos \frac{\pi}{2p}}{\cos \frac{\omega_1}{2} \sin^2 \frac{\omega_1}{2}}$, $\phi_2 \leftarrow \arccos(\frac{x-1}{2})$, $t \leftarrow 3p + 1$
For $i = 1$ to p **do**
  set $\varphi_{3i-2}, \varphi_{3i}, \psi_{3i-2}, \psi_{3i}$ to be 0
  set $\varphi_{3i-1}, \psi_{3i-1}$ to be ϕ_2
$\psi_{t+1} \leftarrow -\frac{\pi}{2}$, $\psi_t \leftarrow \frac{\pi}{2}$
$\alpha_1 \leftarrow 0$, $\alpha_2 \leftarrow \pi - \psi_3 + \psi_2$
For $i = 2$ to $t/2$ **do**
  $\alpha_{2i-1} \leftarrow \pi - \varphi_{2i-1} + \varphi_{2i-2}$
  $\alpha_{2i} \leftarrow \pi - \psi_{2i+1} + \psi_{2i}$
For $i = 1$ to $t/2 - 1$ **do**
  $\beta_{2i-1} \leftarrow -\pi - \psi_{2i} + \psi_{2i-1}$
  $\beta_{2i} \leftarrow -\pi - \varphi_{2i} + \varphi_{2i-1}$
$\beta_{t-1} \leftarrow -\pi - \psi_t + \psi_{t-1}$, $\beta_t \leftarrow 0$
//**perform quantum walk**
construct the initial state:
$|\Psi_0\rangle \leftarrow \frac{1}{\sqrt{2N_1N_2}} \sum_{v \in V, u \sim v} |v, u\rangle$
perform quantum walk with operator (1):
$|\Psi_t\rangle \leftarrow U(\alpha_t, \beta_t) \cdots U(\alpha_1, \beta_1) |\Psi_0\rangle$
measure $|\Psi_t\rangle$ and get $|v, u\rangle$
If $v \in M$ **then**
  Return v
else
  Return u

Our main result is as follows:

Theorem 1. In the complete bipartite graph, let N_1, N_2 be the number of vertices in each part and n_1, n_2 be the number of marked vertices in each part. If $n_1 > 0$ and n_1 is known, Algorithm 1 outputs a marked vertex with certainty and the number of steps t is $O(\sqrt{\frac{N_1}{n_1}})$.

Remark. If $n_2 > 0$ and n_2 is known, by symmetry we can also deterministically find a marked vertex in $O(\sqrt{\frac{N_2}{n_2}})$ rounds. Furthermore, if both n_1 and n_2 are greater than 0 and known, we can find a marked vertex in $\min\{O(\sqrt{\frac{N_1}{n_1}}), O(\sqrt{\frac{N_2}{n_2}})\} = O(\sqrt{\frac{N}{n}})$ steps, where $n = n_1 + n_2$ is the number of marked vertices.

We believe that knowing n_1 or n_2 is necessary. Indeed for deterministic Grover's algorithm it has been proved that knowing n is necessary to deterministically find a marked vertex with quadratic speedup [29].

Theorem 1 is proved with two separate cases. When all marked vertices are in one part, it is proven in Sec. IV; otherwise it is proven in Sec. V. Combining two cases together, Theorem 1 is proven.

IV. CASE 1: ALL MARKED VERTICES IN ONE PART

The first case is when all marked vertices are in one part. Without loss of generality, we assume that $n_1 > 0, n_1$ is known and $n_2 = 0$, i.e., all marked vertices are in V_1.

Suppose $n_1 < N_1$, otherwise the initial state already satisfies $P_0 = 1$. The quantum walk can be analyzed in an invariant subspace of the walk operator $U(\alpha, \beta)$. The four basis vector are defined as

$$|\psi_1\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v \in M, u \in V_2} |v, u\rangle ,$$

$$|\psi_2\rangle = \frac{1}{\sqrt{(N_1 - n_1)N_2}} \sum_{v \in V_1 \setminus M, u \in V_2} |v, u\rangle ,$$

$$|\psi_3\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v \in V_2, u \in M} |v, u\rangle ,$$

$$|\psi_4\rangle = \frac{1}{\sqrt{(N_1 - n_1)N_2}} \sum_{v \in V_2, u \in V_1 \setminus M} |v, u\rangle .$$

Then, it can be verified that the subspace spanned by $|\psi_i\rangle$ $(i = 1, 2, 3, 4)$ is an invariant subspace of $S, C(\alpha), Q(\beta)$, thus is also an invariant subspace of $U(\alpha, \beta)$. With the base $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle, |\psi_4\rangle$, we could compute the matrix representation of these operators as follows. For the computation of $C(\alpha)$, see Appendix A. We get

$$S = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad Q(\beta) = \begin{pmatrix} e^{i\beta} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$C(\alpha) = \begin{pmatrix} -e^{-i\alpha} & 0 & 0 & 0 \\ 0 & -e^{-i\alpha} & 0 & 0 \\ 0 & 0 & (1 - e^{-i\alpha}) \sin^2 \frac{\omega}{2} - 1 & (1 - e^{-i\alpha}) \sin \frac{\omega}{2} \cos \frac{\omega}{2} \\ 0 & 0 & (1 - e^{-i\alpha}) \sin \frac{\omega}{2} \cos \frac{\omega}{2} & (1 - e^{-i\alpha}) \cos^2 \frac{\omega}{2} - 1 \end{pmatrix},$$

where $\omega = 2 \arcsin \sqrt{\frac{n_1}{N_1}}$.

Inspired by Ref. [30], we can decompose $C(\alpha)$ and use some equations to make the expression of $|\Psi_t\rangle$ easier to calculate and analyze.

Lemma 1 (Ref. [30]). Define

$$A(\theta)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&\cos\frac{\omega}{2}&-ie^{i\theta}\sin\frac{\omega}{2}\\0&0&-ie^{-i\theta}\sin\frac{\omega}{2}&\cos\frac{\omega}{2}\end{pmatrix}$$

and

$$R(\theta)=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&e^{i\theta}&0\\0&0&0&1\end{pmatrix},$$

then the following equations can be used to decompose our walk operators:

$$C(\alpha)\sim A\Big(\frac{\pi}{2}\Big)R(\alpha)A\Big(-\frac{\pi}{2}\Big), \tag{2}$$

$$Q(\beta)=SR(\beta)S, \tag{3}$$

$$I=SS=R(0)=A\Big(-\frac{\pi}{2}\Big)A\Big(\frac{\pi}{2}\Big), \tag{4}$$

$$A(\alpha+\beta)=R(\beta)A(\alpha)R(-\beta), \tag{5}$$

$$R(\alpha)R(\beta)=R(\alpha+\beta). \tag{6}$$

The initial state $|\Psi_0\rangle$ can also be expressed as

$$|\Psi_0\rangle=A\Big(\frac{\pi}{2}\Big)SA\Big(\frac{\pi}{2}\Big)|\bar{0}\rangle, \tag{7}$$

where $|\bar{0}\rangle=\frac{1}{\sqrt{2}}(0,1,0,1)^T$.

An observation is that suppose $D_1=\prod_{i=1}^{l_1}E_{1i}$ and $D_2=\prod_{i=1}^{l_2}E_{2i}$, where l_1,l_2 are arbitrary positive integers and $E_{1i},E_{2i}\in\{A(\theta),R(\theta)\mid\theta\in\mathbb{R}\}$, then

$$SD_1SD_2S=D_2SD_1. \tag{8}$$

Using Lemma 1, $|\Psi_t\rangle$ can be reduced to a neater form. Without loss of generality, we always let t be even, then inspired by Ref. [30], we have the following lemma:

Lemma 2. Given an even integer t and parameters $\varphi_1,\varphi_2,\cdots,\varphi_{t-1}$ and $\psi_1,\psi_2,\cdots,\psi_{t+1}$, there exists a set of parameters α_i,β_i $(i=1,2,\cdots,t)$ such that

$$\begin{aligned}|\Psi_t\rangle&=SC(\alpha_t)Q(\beta_t)\cdots SC(\alpha_1)Q(\beta_1)|\Psi_0\rangle\\&\sim R(*)[A(\varphi_{t-1})\cdots A(\varphi_1)]R(*)SR(*)\\&\quad\times[A(\psi_{t+1})\cdots A(\psi_1)]R(*)|\bar{0}\rangle,\end{aligned}$$

where $R(*)$ means the argument may be arbitrary.

Furthermore, the following is one solution of parameters:

$$\alpha_i=\begin{cases}\text{arbitrary}&i=1\\\pi-\varphi_i+\varphi_{i-1}&i\text{ is odd and }i>1,\\\pi-\psi_{i+1}+\psi_i&i\text{ is even}\end{cases}$$

$$\beta_i=\begin{cases}-\pi-\psi_{i+1}+\psi_i&i\text{ is odd}\\-\pi-\varphi_i+\varphi_{i-1}&i\text{ is even and }i<t.\\\text{arbitrary}&i=t\end{cases}$$

Since Lemma 2 is a little different from Ref. [30], for the completeness of the article, the proof of Lemma 2 is given in Appendix B.

In order to achieve deterministic search, a key lemma is needed.

Lemma 3. Let $\omega\in(0,\pi)$,

$$B(\theta)=\begin{pmatrix}\cos\frac{\omega}{2}&-ie^{i\theta}\sin\frac{\omega}{2}\\-ie^{-i\theta}\sin\frac{\omega}{2}&\cos\frac{\omega}{2}\end{pmatrix},$$

then there is an odd integer $t'=O(\frac{1}{\omega})$ and parameters $\varphi_1,\varphi_2,\cdots,\varphi_{t'}$ such that

$$B(\varphi_{t'})B(\varphi_{t'-1})\cdots B(\varphi_1)\begin{pmatrix}0\\1\end{pmatrix}\sim\begin{pmatrix}1\\0\end{pmatrix}.$$

Lemma 3 is proved in Sec. VI. The $B(\theta)$ in Lemma 3 is the right-bottom part of $A(\theta)$, so with a set of carefully designed parameters, successively applying $A(\theta)$ can map $(0,0,0,1)^T$ to $(0,0,1,0)^T$. This is the key component of our deterministic searching algorithm.

Now we can prove the main result of case 1.

Theorem 2. Suppose $M\subseteq V_1$ and $n_1>0$, n_1 is known. There are a number $t=O(\sqrt{\frac{N_1}{n_1}})$ and parameters α_i,β_i $(i=1,2,\cdots,t)$ such that after t steps, the success probability P_t is exactly 1.

Proof. Recall that from Lemma 2, $|\Psi_t\rangle$ can be reduced to

$$\begin{aligned}|\Psi_t\rangle\sim R(*)[A(\varphi_{t-1})\cdots A(\varphi_1)]R(*)SR(*)\\ [A(\psi_{t+1})\cdots A(\psi_1)]R(*)|\bar{0}\rangle.\end{aligned}$$

Let $\varphi_1,\varphi_2,\cdots,\varphi_{t-1}$ be the parameters in Lemma 3 ($t'=t-1$). Notice that

$$A(\theta)=\begin{pmatrix}I&O\\O&B(\theta)\end{pmatrix},$$

so

$$A(\varphi_{t-1})\cdots A(\varphi_1)=\begin{pmatrix}I&O\\O&B(\varphi_{t-1})\cdots B(\varphi_1)\end{pmatrix}. \tag{9}$$

Define

$$B_{\text{com}}\triangleq B(\varphi_{t-1})B(\varphi_{t-2})\cdots B(\varphi_1), \tag{10}$$

then from Eqs. (9) and (10),

$$A(\varphi_{t-1})A(\varphi_{t-2})\cdots A(\varphi_1)=\begin{pmatrix}I&O\\O&B_{\text{com}}\end{pmatrix}. \tag{11}$$

From Lemma 3,

$$B_{\text{com}}\begin{pmatrix}0\\1\end{pmatrix}=\begin{pmatrix}e^{i\theta_1}\\0\end{pmatrix}$$

for some θ_1. Here $t=O(\frac{1}{\omega})$, and since $\omega=\Theta(\sqrt{\frac{n_1}{N_1}})$, $t=O(\sqrt{\frac{N_1}{n_1}})$.

Set $\psi_i=\varphi_i,\forall i=1,2,\cdots,t-1$, and set $\psi_{t+1}=-\frac{\pi}{2}$, $\psi_t=\frac{\pi}{2}$. Since $B(-\frac{\pi}{2})B(\frac{\pi}{2})=I$, we have

$$B_{\text{com}}=B(\psi_{t+1})B(\psi_t)B(\psi_{t-1})\cdots B(\psi_1).$$

Therefore,

$$A(\psi_{t+1})A(\psi_t)\cdots A(\psi_1)=\begin{pmatrix}I&O\\O&B_{\text{com}}\end{pmatrix}. \tag{12}$$

According to Lemma 2, Eqs. (11) and (12), the final state $|\Psi_t\rangle$ can be derived by the following process:

$$\begin{pmatrix}0\\1\\0\\1\end{pmatrix} \xrightarrow{R(*)} \begin{pmatrix}0\\1\\0\\1\end{pmatrix} \xrightarrow{A(\psi_{t+1})\cdots A(\psi_1)} \begin{pmatrix}0\\1\\e^{i\theta_1}\\0\end{pmatrix} \xrightarrow{R(*)SR(*)} \begin{pmatrix}e^{i\theta_2}\\0\\0\\1\end{pmatrix} \xrightarrow{A(\varphi_{t-1})\cdots A(\varphi_1)} \begin{pmatrix}e^{i\theta_2}\\0\\e^{i\theta_1}\\0\end{pmatrix} \xrightarrow{R(*)} \begin{pmatrix}e^{i\theta_2}\\0\\e^{i\theta_3}\\0\end{pmatrix}. \tag{13}$$

We can verify each step of Eq. (13), where the θ_2 and θ_3 comes from $R(*)$. Therefore, $|\Psi_t\rangle = \frac{1}{\sqrt{2}}(e^{i\theta_2}|\psi_1\rangle + e^{i\theta_3}|\psi_3\rangle)$ and the success probability is exactly 1.

V. CASE 2: MARKED VERTICES IN BOTH PARTS

The second case is when both parts have marked vertices. Suppose $n_1 < N_1$ and $n_2 < N_2$, otherwise the initial state already satisfies $P_0 = 1$. The quantum walk can be analysed in an invariant subspace of the walk operator $U(\alpha, \beta)$. Define $M_1 \triangleq M \cap V_1 \neq \emptyset$, $M_2 \triangleq M \cap V_2 \neq \emptyset$, the eight basis vector are defined as

$$|\psi_1\rangle = \frac{1}{\sqrt{n_1 n_2}} \sum_{v\in M_1, u\in M_2} |v, u\rangle,$$

$$|\psi_2\rangle = \frac{1}{\sqrt{n_1(N_2 - n_2)}} \sum_{v\in M_1, u\in V_2\setminus M_2} |v, u\rangle,$$

$$|\psi_3\rangle = \frac{1}{\sqrt{(N_1 - n_1)n_2}} \sum_{v\in V_1\setminus M_1, u\in M_2} |v, u\rangle,$$

$$|\psi_4\rangle = \frac{1}{\sqrt{(N_1 - n_1)(N_2 - n_2)}} \sum_{v\in V_1\setminus M_1, u\in V_2\setminus M_2} |v, u\rangle,$$

$$|\psi_5\rangle = \frac{1}{\sqrt{n_1 n_2}} \sum_{v\in M_2, u\in M_1} |v, u\rangle,$$

$$|\psi_6\rangle = \frac{1}{\sqrt{(N_1 - n_1)n_2}} \sum_{v\in M_2, u\in V_1\setminus M_1} |v, u\rangle,$$

$$|\psi_7\rangle = \frac{1}{\sqrt{n_1(N_2 - n_2)}} \sum_{v\in V_2\setminus M_2, u\in M_1} |v, u\rangle,$$

$$|\psi_8\rangle = \frac{1}{\sqrt{(N_1 - n_1)(N_2 - n_2)}} \sum_{v\in V_2\setminus M_2, u\in V_1\setminus M_1} |v, u\rangle.$$

Then, it can be verified that the subspace spanned by $|\psi_i\rangle$ $(i = 1, 2, \cdots, 8)$ is an invariant subspace of $S, C(\alpha), Q(\beta)$, thus is also an invariant subspace of $U(\alpha, \beta)$. With the base $|\psi_1\rangle, |\psi_2\rangle, \cdots, |\psi_8\rangle$, we could compute the matrix representation of these operators as follows. We get

$$S = \begin{pmatrix}0&0&0&0&1&0&0&0\\0&0&0&0&0&0&1&0\\0&0&0&0&0&1&0&0\\0&0&0&0&0&0&0&1\\1&0&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&1&0&0&0&0&0&0\\0&0&0&1&0&0&0&0\end{pmatrix},$$

$$Q(\beta) = \begin{pmatrix}e^{i\beta}&0&0&0&0&0&0&0\\0&e^{i\beta}&0&0&0&0&0&0\\0&0&1&0&0&0&0&0\\0&0&0&1&0&0&0&0\\0&0&0&0&e^{i\beta}&0&0&0\\0&0&0&0&0&e^{i\beta}&0&0\\0&0&0&0&0&0&1&0\\0&0&0&0&0&0&0&1\end{pmatrix}$$

and

$$C(\alpha) = \begin{pmatrix}C_2(\alpha)&O&O&O\\O&C_2(\alpha)&O&O\\O&O&C_1(\alpha)&O\\O&O&O&C_1(\alpha)\end{pmatrix},$$

where

$$C_1(\alpha) = \begin{pmatrix}(1-e^{-i\alpha})\sin^2\frac{\omega_1}{2} - 1 & (1-e^{-i\alpha})\sin\frac{\omega_1}{2}\cos\frac{\omega_1}{2}\\(1-e^{-i\alpha})\sin\frac{\omega_1}{2}\cos\frac{\omega_1}{2} & (1-e^{-i\alpha})\cos^2\frac{\omega_1}{2} - 1\end{pmatrix},$$

$$C_2(\alpha) = \begin{pmatrix}(1-e^{-i\alpha})\sin^2\frac{\omega_2}{2} - 1 & (1-e^{-i\alpha})\sin\frac{\omega_2}{2}\cos\frac{\omega_2}{2}\\(1-e^{-i\alpha})\sin\frac{\omega_2}{2}\cos\frac{\omega_2}{2} & (1-e^{-i\alpha})\cos^2\frac{\omega_2}{2} - 1\end{pmatrix},$$

$\omega_1 = 2\arcsin\sqrt{\frac{n_1}{N_1}}$ and $\omega_2 = 2\arcsin\sqrt{\frac{n_2}{N_2}}$.

Similar to case 1, we can decompose $C(\alpha)$ and get a different expression of $|\Psi_t\rangle$.

Lemma 4 (Ref. [30]). Define

$$B_1(\theta) = \begin{pmatrix} \cos\frac{\omega_1}{2} & -ie^{i\theta}\sin\frac{\omega_1}{2} \\ -ie^{-i\theta}\sin\frac{\omega_1}{2} & \cos\frac{\omega_1}{2} \end{pmatrix},$$

$$B_2(\theta) = \begin{pmatrix} \cos\frac{\omega_2}{2} & -ie^{i\theta}\sin\frac{\omega_2}{2} \\ -ie^{-i\theta}\sin\frac{\omega_2}{2} & \cos\frac{\omega_2}{2} \end{pmatrix},$$

$$A'(\theta) = \begin{pmatrix} B_2(\theta) & O & O & O \\ O & B_2(\theta) & O & O \\ O & O & B_1(\theta) & O \\ O & O & O & B_1(\theta) \end{pmatrix}, \quad (14)$$

$$R'(\theta) = \begin{pmatrix} e^{i\theta} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{i\theta} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{i\theta} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & e^{i\theta} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

then similar to case 1, the following equations are satisfied:

$$\begin{aligned} &C(\alpha) \sim A'\left(\frac{\pi}{2}\right)R'(\alpha)A'\left(-\frac{\pi}{2}\right), \\ &Q(\beta) = SR'(\beta)S, \\ &I = SS = R'(0) = A'\left(-\frac{\pi}{2}\right)A'\left(\frac{\pi}{2}\right), \\ &A'(\alpha+\beta) = R'(\beta)A'(\alpha)R'(-\beta), \\ &R'(\alpha)R'(\beta) = R'(\alpha+\beta), \\ &|\Psi_0\rangle = A'\left(\frac{\pi}{2}\right)SA'\left(\frac{\pi}{2}\right)|\bar{0}\rangle, \end{aligned}$$

where $|\bar{0}\rangle = \frac{1}{\sqrt{2}}(0,0,0,1,0,0,0,1)^T$.

Furthermore, let $D_1 = \prod_{i=1}^{l_1} E_{1i}$ and $D_2 = \prod_{i=1}^{l_2} E_{2i}$, where l_1, l_2 are arbitrary positive integers and $E_{1i}, E_{2i} \in \{A'(\theta), R'(\theta) \mid \theta \in \mathbb{R}\}$, then

$$SD_1SD_2S = D_2SD_1.$$

Then, $|\Psi_t\rangle$ has another expression using Lemma 4.

Lemma 5. Given an even integer t and parameters $\varphi_1, \varphi_2, \cdots, \varphi_{t-1}$ and $\psi_1, \psi_2, \cdots, \psi_{t+1}$, there exists a set of parameters α_i, β_i $(i = 1, 2, \cdots, t)$ such that

$$\begin{aligned} |\Psi_t\rangle &= SC(\alpha_t)Q(\beta_t)\cdots SC(\alpha_1)Q(\beta_1)|\Psi_0\rangle \\ &\sim R'(*)[A'(\varphi_{t-1})\cdots A'(\varphi_1)]R'(*)SR'(*) \\ &\quad\times [A'(\psi_{t+1})\cdots A'(\psi_1)]R'(*)|\bar{0}\rangle, \end{aligned}$$

where $R'(*)$ means the argument may be arbitrary.

Furthermore, the following is one solution of parameters:

$$\alpha_i = \begin{cases} \text{arbitrary} & i = 1 \\ \pi - \varphi_i + \varphi_{i-1} & i \text{ is odd and } i > 1, \\ \pi - \psi_{i+1} + \psi_i & i \text{ is even} \end{cases}$$

$$\beta_i = \begin{cases} -\pi - \psi_{i+1} + \psi_i & i \text{ is odd} \\ -\pi - \varphi_i + \varphi_{i-1} & i \text{ is even and } i < t. \\ \text{arbitrary} & i = t \end{cases}$$

The proof of Lemma 5 is in Appendix B.

Now we state our result of case 2. We will prove that when n_1 is known, we can find a marked vertex in V_1 in $O(\sqrt{\frac{N_1}{n_1}})$ steps. When n_2 is known, the proof is similar.

Theorem 3. Suppose $n_1 > 0$ and n_1 is known. There are a number $t = O(\sqrt{\frac{N_1}{n_1}})$ and parameters α_i, β_i $(i = 1, 2, \cdots, t)$ such that after t steps, the success probability P_t is exactly 1.

Proof. Let $\varphi_1, \varphi_2, \cdots, \varphi_{t-1}$ be the parameters in Lemma 3 $(t' = t - 1)$, where $\omega = \omega_1$. From Eq. (14), multiplication of $A'(\theta)$ can be reduced to multiplication of $B_1(\theta)$ and $B_2(\theta)$. Define

$$B_{\text{com}}^{(1)} \triangleq B_1(\varphi_{t-1})B_1(\varphi_{t-2})\cdots B_1(\varphi_1), \quad (15)$$

and

$$B_{\text{com}}^{(2)} \triangleq B_2(\varphi_{t-1})B_2(\varphi_{t-2})\cdots B_2(\varphi_1), \quad (16)$$

then from Lemma 3,

$$B_{\text{com}}^{(1)}\begin{pmatrix}0\\1\end{pmatrix} = \begin{pmatrix}e^{i\theta_1}\\0\end{pmatrix}$$

for some θ_1. Here $t = O(\frac{1}{\omega_1})$, and since $\omega_1 = \Theta(\sqrt{\frac{n_1}{N_1}})$, $t = O(\sqrt{\frac{N_1}{n_1}})$.

Set $\psi_i = \varphi_i, \forall i = 1, 2, \cdots, t-1$, and set $\psi_{t+1} = -\frac{\pi}{2}$, $\psi_t = \frac{\pi}{2}$, since $B_1(-\frac{\pi}{2})B_1(\frac{\pi}{2}) = I$, $B_2(-\frac{\pi}{2})B_2(\frac{\pi}{2}) = I$, we have

$$B_{\text{com}}^{(1)} = B_1(\psi_{t+1})B_1(\psi_t)\cdots B_1(\psi_1) \quad (17)$$

and

$$B_{\text{com}}^{(2)} = B_2(\psi_{t+1})B_2(\psi_t)\cdots B_2(\psi_1). \quad (18)$$

From Eqs. (14), (15), (16), (17), and (18), we get

$$A'(\varphi_{t-1})A'(\varphi_{t-2})\cdots A'(\varphi_1) = \begin{pmatrix} B_{\text{com}}^{(2)} & O & O & O \\ O & B_{\text{com}}^{(2)} & O & O \\ O & O & B_{\text{com}}^{(1)} & O \\ O & O & O & B_{\text{com}}^{(1)} \end{pmatrix} \quad (19)$$

and

$$A'(\psi_{t+1})A'(\psi_t)\cdots A'(\psi_1) = \begin{pmatrix} B_{\text{com}}^{(2)} & O & O & O \\ O & B_{\text{com}}^{(2)} & O & O \\ O & O & B_{\text{com}}^{(1)} & O \\ O & O & O & B_{\text{com}}^{(1)} \end{pmatrix}. \quad (20)$$

Set

$$\begin{pmatrix}a\\b\end{pmatrix} \triangleq B_{\text{com}}^{(2)}\begin{pmatrix}0\\1\end{pmatrix}.$$

According to Lemma 5, Eqs. (19) and (20), the final state $|\Psi_t\rangle$ can be derived by the following process:

$$\begin{pmatrix}0\\0\\0\\1\\0\\0\\0\\1\end{pmatrix} \xrightarrow{R'(*)} \begin{pmatrix}0\\0\\0\\1\\0\\0\\0\\1\end{pmatrix} \xrightarrow{A'(\psi_{t+1})\cdots A'(\psi_1)} \begin{pmatrix}0\\0\\a\\b\\0\\0\\e^{i\theta_1}\\0\end{pmatrix} \xrightarrow{R'(*)SR'(*)} \begin{pmatrix}0\\e^{i\theta_2}\\0\\0\\0\\ae^{i\theta_3}\\0\\b\end{pmatrix} \xrightarrow{A'(\varphi_{t-1})\cdots A'(\varphi_1)} \begin{pmatrix}ae^{i\theta_2}\\be^{i\theta_2}\\0\\0\\ae^{i\theta_4}\\0\\be^{i\theta_1}\\0\end{pmatrix} \xrightarrow{R'(*)} \begin{pmatrix}ae^{i\theta_5}\\be^{i\theta_2}\\0\\0\\ae^{i\theta_6}\\0\\be^{i\theta_7}\\0\end{pmatrix}. \tag{21}$$

We can verify each step of Eq. (21), where the $\theta_2, \theta_3, \theta_4, \theta_5, \theta_6$ and θ_7 comes from $R(*)$. Therefore,

$$|\Psi_t\rangle = \frac{1}{\sqrt{2}}(ae^{i\theta_5}|\psi_1\rangle + be^{i\theta_2}|\psi_2\rangle + ae^{i\theta_6}|\psi_5\rangle + be^{i\theta_7}|\psi_7\rangle)$$

and the success probability is exactly 1. ■

VI. PROOF OF LEMMA 3

In this section we prove Lemma 3, a crucial step of our work. Since in Lemma 3 we are dealing with 2×2 matrices, which is equivalent to operators in a single-qubit system, we can utilize a tool called Bloch sphere.

For a single-qubit quantum system, Bloch sphere representation is a useful tool to visualize states and operations. Let

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad |\alpha|^2 + |\beta|^2 = 1$$

be a state, then it can be rewritten as

$$|\psi\rangle = e^{i\gamma}\left(\cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle\right)$$

($\theta \in [0, \pi]$ and $\gamma, \varphi \in [0, 2\pi)$), i.e.

$$|\psi\rangle \sim \cos\frac{\theta}{2}|0\rangle + e^{i\varphi}\sin\frac{\theta}{2}|1\rangle .$$

We can treat θ, φ as parameters of spherical coordinates, then $|\psi\rangle$ corresponds to a point $(\cos\varphi\sin\theta, \sin\varphi\sin\theta, \cos\theta)$ on a unit sphere. Figure 2 illustrates the correspondence.

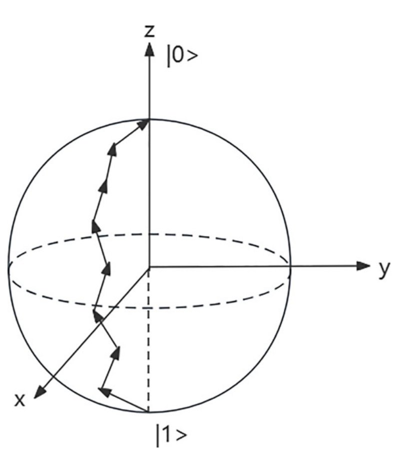

FIG. 2. Bloch sphere representation of a quantum state. The lines in the figure shows how our state moves.

Unitary operations can also be visualized by Bloch sphere. Recall that the Pauli matrices are

$$X = \begin{pmatrix}0 & 1\\1 & 0\end{pmatrix}, \quad Y = \begin{pmatrix}0 & -i\\i & 0\end{pmatrix}, \quad Z = \begin{pmatrix}1 & 0\\0 & -1\end{pmatrix},$$

then

Lemma 6 (Ref. [31]). Any unitary operation on a single-qubit quantum system can be expressed as

$$U \sim R_{\vec{n}}(\theta),$$

where $\vec{n} = (n_x, n_y, n_z)$ is a real unit vector and

$$R_{\vec{n}}(\theta) = \cos\frac{\theta}{2}I - i\sin\frac{\theta}{2}(n_xX + n_yY + n_zZ)$$

is a rotation on unit sphere with $\vec{n}$ being the rotation axis and θ being the rotation angle.

Now we have the tools to prove Lemma 3.

Proof. It can be verified that

$$B(\theta) = \begin{pmatrix}\cos\frac{\omega}{2} & -ie^{i\theta}\sin\frac{\omega}{2}\\ -ie^{-i\theta}\sin\frac{\omega}{2} & \cos\frac{\omega}{2}\end{pmatrix}$$

satisfies

$$B(\theta) = \cos\frac{\omega}{2}I - i\sin\frac{\omega}{2}(\cos\theta\cdot X - \sin\theta\cdot Y), \tag{22}$$

then from Lemma 6, $B(\theta) = R_{\vec{n}}(\omega)$ where the axis $\vec{n} = (\cos\theta, -\sin\theta, 0)$ is on the xy plane. We are to prove that

$$B(\varphi_{t'})B(\varphi_{t'-1})\cdots B(\varphi_1)\begin{pmatrix}0\\1\end{pmatrix} \sim \begin{pmatrix}1\\0\end{pmatrix}$$

with $t' = O(\frac{1}{\omega})$, which means to rotate $(0, 0, -1)$ to $(0, 0, 1)$ on Bloch sphere.

We define three parameters ϕ_1, ϕ_2, ϕ_3 and set $B^* = B(\phi_3)B(\phi_2)B(\phi_1)$. We will achieve our goal by repeatedly applying B^*. Suppose we apply B^* for p times, then B^* should be equivalent to a rotation with axis on the xy plane and angle $\frac{\pi}{p}$.

From Eq. (22), we express $B(\phi_3), B(\phi_2), B(\phi_1)$ under (I, X, Y, Z) basis. According to Lemma 6, B^* should satisfies the following conditions:

(i) the coordinate of I should be $\cos\frac{\pi}{2p}$;

(ii) the coordinate of Z should be 0.

Then we get the following equations:

$$\cos\frac{\pi}{2p} = \cos^3\frac{\omega}{2} - \cos\frac{\omega}{2}\sin^2\frac{\omega}{2}[\cos(\phi_3 - \phi_2) + \cos(\phi_3 - \phi_1) + \cos(\phi_2 - \phi_1)], \tag{23}$$

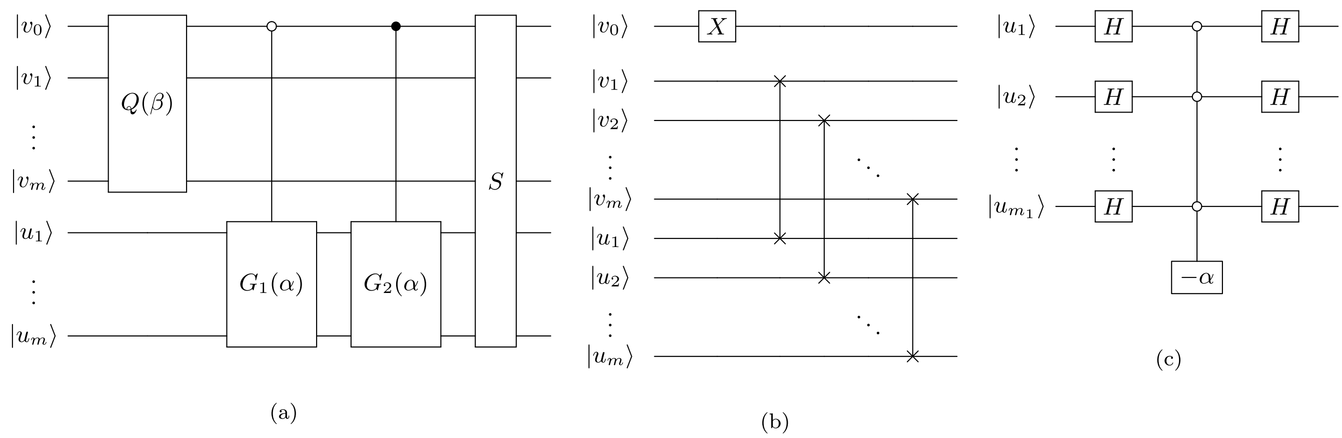

FIG. 3. Quantum circuit implementation of one-step walk. (a) is the overall circuit of the operator $U(\alpha, \beta)$; (b) is the circuit of S and (c) is the circuit of $G_1(\alpha)$, where the $-\alpha$ block means to add a phase $e^{-i\alpha}$ under the condition.

$$\sin(\phi_3 - \phi_2) + \sin(\phi_3 - \phi_1) + \sin(\phi_2 - \phi_1) = 0. \quad (24)$$

Set $\phi_1 = \phi_3 = 0$, then Eq. (24) is satisfied. Then Eq. (23) becomes

$$\cos\frac{\pi}{2p} = \cos^3\frac{\omega}{2} - \cos\frac{\omega}{2}\sin^2\frac{\omega}{2}(1 + 2\cos\phi_2).$$

As ϕ_2 varies, $1 + 2\cos\phi_2$ varies from $[-1, 3]$, then

$$\cos\frac{\pi}{2p} \in \left[\cos\frac{3\omega}{2}, \cos\frac{\omega}{2}\right].$$

Depending on the range of ω, there are two cases:

- If $\omega \in (0, \frac{2\pi}{3}]$, then $\cos x$ decreases in $[\frac{\omega}{2}, \frac{3\omega}{2}]$, it only needs $p \in [\frac{\pi}{3\omega}, \frac{\pi}{\omega}]$. There always exists an odd integer p in the interval.
- If $\omega \in (\frac{2\pi}{3}, \pi)$, then $\cos\frac{3\omega}{2} < 0$ and $\cos\frac{\omega}{2} > 0$, we simply set $p = 1$.

In both cases, $p = O(\frac{1}{\omega})$.

Now we can calculate parameters in Lemma 3. Set p as the smallest odd integer in $[\frac{\pi}{3\omega}, \frac{\pi}{\omega}]$, define $x \triangleq 1 + 2\cos\phi_2$, then

$$x = \frac{\cos^3\frac{\omega}{2} - \cos\frac{\pi}{2p}}{\cos\frac{\omega}{2}\sin^2\frac{\omega}{2}}, \quad \phi_2 = \arccos\left(\frac{x-1}{2}\right).$$

Since we repeatedly apply $B^* = B(\phi_3)B(\phi_2)B(\phi_1)$ where $\phi_1 = \phi_3 = 0$, the number of operators is

$$t' = 3p = O\left(\frac{1}{\omega}\right)$$

and

$$\forall i = 1, 2, \cdots, t', \varphi_i = \begin{cases} \phi_2 & \text{if } i \bmod 3 = 2 \\ 0 & \text{otherwise} \end{cases}.$$

■

VII. QUANTUM CIRCUIT IMPLEMENTATION

In this section, we briefly talk about the quantum circuit implementation of our algorithm. The walk operator $U(\alpha, \beta)$ consists of S, $C(\alpha)$ and $Q(\beta)$, where $Q(\beta)$ is the oracle operator assumed by the algorithm, so in this section we implement S and $C(\alpha)$.

For simplicity, in the following we assume $N_1 = 2^{m_1}$, $N_2 = 2^{m_2}$, $m = \max\{m_1, m_2\}$, then a vertex can be expressed by $m+1$ qubits. If N_1 or N_2 are not powers of 2, we could add imaginary vertices to create a complete bipartite graph in which N_1 and N_2 become powers of 2 (these imaginary vertices should not be marked). Let $|v\rangle = |v_0\rangle |v_1\rangle \cdots |v_m\rangle$ be the position register, where $|v_0\rangle$ decides which side v is in ($v_0 = 1$ means $v \in V_1$ and $v_0 = 0$ means $v \in V_2$), and $v_1, \cdots, v_m$ is the serial number of v in that side (if $v \in V_1$ and $m_1 < m$, we only use the first m_1 qubits $v_1, v_2, \cdots, v_{m_1}$ and the rest qubits are set arbitrarily; similar for $v \in V_2$). Let $|u\rangle = |u_1\rangle \cdots |u_m\rangle$ be the coin register, where $u_1, \cdots, u_m$ is the serial number of u in the opposite side. The shift operator S is quite easy to implement. Recall that $S|v, u\rangle = |u, v\rangle$, so we flip $|v_0\rangle$ to change which part v is in (thus also change which part u is in), and exchange the value of $v_1 \cdots v_m$ and $u_1 \cdots u_m$. See Fig. 3(b) for the implementation of S.

The coin operator C is a bit more complicated. Recall that

$$C(\alpha) = \sum_{v \in V} |v\rangle\langle v| \otimes G_v(\alpha).$$

For $v \in V_1$, $G_v(\alpha) = G_2(\alpha)$, where

$$G_2(\alpha) \triangleq (1 - e^{-i\alpha})|s_2\rangle\langle s_2| - I$$

and

$$|s_2\rangle \triangleq \frac{1}{\sqrt{N_2}}\sum_{u \in V_2}|u\rangle;$$

for $v \in V_2$, $G_v(\alpha) = G_1(\alpha)$, where

$$G_1(\alpha) \triangleq (1 - e^{-i\alpha})|s_1\rangle\langle s_1| - I$$

and

$$|s_1\rangle \triangleq \frac{1}{\sqrt{N_1}}\sum_{u \in V_1}|u\rangle.$$

Then $C(\alpha)$ can be simplified as

$$C(\alpha) = \left(\sum_{v \in V_1}|v\rangle\langle v|\right) \otimes G_2(\alpha) + \left(\sum_{v \in V_2}|v\rangle\langle v|\right) \otimes G_1(\alpha)$$
$$= |1\rangle_{v_0}\langle 1|_{v_0} \otimes I \otimes G_2(\alpha) + |0\rangle_{v_0}\langle 0|_{v_0} \otimes I \otimes G_1(\alpha).$$

With the promise that $u \in V_1$, G_1 acts on $|u_1\rangle |u_2\rangle \cdots |u_{m_1}\rangle$ and can be easily implemented. Notice that

$$|s_1\rangle = H^{\otimes m_1} |0\rangle^{\otimes m_1} ,$$

we get

$$G_1(\alpha) = H^{\otimes m_1}[(1 - e^{-i\alpha}) |0\rangle^{\otimes m_1} \langle 0|^{\otimes m_1} - I]H^{\otimes m_1}.$$

Then $G_1(\alpha)$ can be realized as in Fig. 3(c). The implementation of $G_2(\alpha)$ is similar.

The walk operator $U(\alpha, \beta)$ is the combination of $Q(\beta)$, $G(\alpha)$, and S, see Fig. 3(a) for the overall circuit. The number of qubits is $O(m) = O(\log N)$; for the number of gates, the cost of each step of walk is the sum of these three operators. S only takes $O(m)$ gates, with $m = O(\log N)$; $G_1(\alpha)$ and $G_2(\alpha)$ each needs a controlled phase gate, which takes $O(m^2)$ basic gates [32]; together with $O(m)$ Hadamard gates, $G(\alpha)$ needs $O(m^2) = O(\log^2 N)$ basic gates. Suppose the cost of oracle is q, then the cost of each step $U(\alpha, \beta)$ is $q + O(\log^2 N)$.

VIII. SUMMARY

In this paper, we propose a deterministic search algorithm on complete bipartite graphs by DTQW and provide the quantum circuit implementation. The calculation is reduced to a single-qubit quantum system, then Bloch sphere representation provides a tool to precisely analyze the composition of operators. This paper allows us to gain insights about the deterministic quantum algorithm, and determinacy makes error analysis easier in application. This approach exploits the specific structure of complete bipartite graphs, so we will need more inspirations if we hope to explore other classes of graphs. In the future we are interested in performing deterministic quantum search on more graphs via DTQW, and trying to find a universal pattern for various graphs.

ACKNOWLEDGMENTS

This work was supported in part by the National Natural Science Foundation of China Grants No. 62325210 and No. 62301531, the Strategic Priority Research Program of Chinese Academy of Sciences Grant No. XDB28000000, and China Postdoctoral Science Foundation Grant No. 2022M723209.

APPENDIX A: COMPUTATION OF $C(\alpha)$

This section computes the matrix representation of $C(\alpha)$ in case 1. The computation of case 2 is similar.

Recall that $C(\alpha)|v, u\rangle = |v\rangle \otimes G_v(\alpha)|u\rangle$, where $G_v(\alpha) = (1 - e^{-i\alpha})|s_v\rangle\langle s_v| - I$ and $|s_v\rangle = \frac{1}{\sqrt{d_v}} \sum_{w\sim v} |w\rangle$. For $v \in V_1$, $|s_v\rangle = \frac{1}{\sqrt{N_2}} \sum_{w\in V_2} |w\rangle$. Then,

$$C(\alpha)|\psi_1\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v\in M, u\in V_2} C(\alpha)|v, u\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v\in M} |v\rangle \otimes \left(\sum_{u\in V_2} G_v(\alpha)|u\rangle\right)$$
$$= \frac{1}{\sqrt{n_1}} \sum_{v\in M} |v\rangle \otimes G_v(\alpha)|s_v\rangle = \frac{1}{\sqrt{n_1}} \sum_{v\in M} |v\rangle \otimes (-e^{-i\alpha}|s_v\rangle) = -e^{-i\alpha}|\psi_1\rangle .$$

Similarly,

$$C(\alpha)|\psi_2\rangle = \frac{1}{\sqrt{(N_1 - n_1)N_2}} \sum_{v\in V_1\setminus M, u\in V_2} C(\alpha)|v, u\rangle = \frac{1}{\sqrt{(N_1 - n_1)N_2}} \sum_{v\in V_1\setminus M} |v\rangle \otimes \left(\sum_{u\in V_2} G_v(\alpha)|u\rangle\right)$$
$$= \frac{1}{\sqrt{N_1 - n_1}} \sum_{v\in V_1\setminus M} |v\rangle \otimes G_v(\alpha)|s_v\rangle = \frac{1}{\sqrt{N_1 - n_1}} \sum_{v\in V_1\setminus M} |v\rangle \otimes (-e^{-i\alpha}|s_v\rangle) = -e^{-i\alpha}|\psi_2\rangle .$$

For $v \in V_2$, $|s_v\rangle = \frac{1}{\sqrt{N_1}} \sum_{w\in V_1} |w\rangle$. Then,

$$C(\alpha)|\psi_3\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v\in V_2, u\in M} C(\alpha)|v, u\rangle = \frac{1}{\sqrt{n_1 N_2}} \sum_{v\in V_2} |v\rangle \otimes \left(\sum_{u\in M} G_v(\alpha)|u\rangle\right),$$

where

$$G_v(\alpha)|u\rangle = (1 - e^{-i\alpha})|s_v\rangle\langle s_v|u\rangle - |u\rangle = (1 - e^{-i\alpha})\frac{1}{\sqrt{N_1}}|s_v\rangle - |u\rangle ,$$

$$|v\rangle \otimes \left(\sum_{u\in M} G_v(\alpha)|u\rangle\right) = (1 - e^{-i\alpha})\frac{n_1}{\sqrt{N_1}}|v\rangle \otimes |s_v\rangle - \sum_{u\in M} |v, u\rangle ,$$

$$\sum_{v\in V_2} |v\rangle \otimes |s_v\rangle = \frac{1}{\sqrt{N_1}} \sum_{v\in V_2, u\in V_1} |v, u\rangle = \frac{1}{\sqrt{N_1}}(\sqrt{n_1 N_2}|\psi_3\rangle + \sqrt{(N_1 - n_1)N_2}|\psi_4\rangle),$$

$$\sum_{v\in V_2,u\in M}|v,u\rangle=\sqrt{n_1N_2}\,|\psi_3\rangle\,,$$

we get

$$\begin{aligned}C(\alpha)\,|\psi_3\rangle&=\frac{1}{\sqrt{n_1N_2}}\left[(1-e^{-i\alpha})\frac{n_1}{\sqrt{N_1}}\cdot\frac{1}{\sqrt{N_1}}(\sqrt{n_1N_2}\,|\psi_3\rangle+\sqrt{(N_1-n_1)N_2}\,|\psi_4\rangle)-\sqrt{n_1N_2}\,|\psi_3\rangle\right]\\&=\left[(1-e^{-i\alpha})\frac{n_1}{N_1}-1\right]\cdot|\psi_3\rangle+(1-e^{-i\alpha})\frac{\sqrt{n_1(N_1-n_1)}}{N_1}\,|\psi_4\rangle\,.\end{aligned}$$

Since $\sin\frac{\omega}{2}=\sqrt{\frac{n_1}{N_1}}$ and $\cos\frac{\omega}{2}=\sqrt{\frac{N_1-n_1}{N_1}}$, we have

$$C(\alpha)\,|\psi_3\rangle=\left[(1-e^{-i\alpha})\sin^2\frac{\omega}{2}-1\right]\cdot|\psi_3\rangle+(1-e^{-i\alpha})\sin\frac{\omega}{2}\cos\frac{\omega}{2}\,|\psi_4\rangle\,.$$

Similarly,

$$C(\alpha)\,|\psi_4\rangle=\frac{1}{\sqrt{(N_1-n_1)N_2}}\sum_{v\in V_2,u\in V_1\setminus M}C(\alpha)\,|v,u\rangle=\frac{1}{\sqrt{(N_1-n_1)N_2}}\sum_{v\in V_2}|v\rangle\otimes\left(\sum_{u\in V_1\setminus M}G_v(\alpha)\,|u\rangle\right),$$

where

$$|v\rangle\otimes\left(\sum_{u\in V_1\setminus M}G_v(\alpha)\,|u\rangle\right)=(1-e^{-i\alpha})\frac{N_1-n_1}{\sqrt{N_1}}\,|v\rangle\otimes|s_v\rangle-\sum_{u\in V_1\setminus M}|v,u\rangle\,,$$

$$\sum_{v\in V_2,u\in V_1\setminus M}|v,u\rangle=\sqrt{(N_1-n_1)N_2}\,|\psi_4\rangle\,,$$

we get

$$\begin{aligned}C(\alpha)\,|\psi_4\rangle&=\frac{1}{\sqrt{(N_1-n_1)N_2}}\left[(1-e^{-i\alpha})\frac{N_1-n_1}{\sqrt{N_1}}\frac{1}{\sqrt{N_1}}(\sqrt{n_1N_2}\,|\psi_3\rangle+\sqrt{(N_1-n_1)N_2}\,|\psi_4\rangle)-\sqrt{(N_1-n_1)N_2}\,|\psi_4\rangle\right]\\&=(1-e^{-i\alpha})\frac{\sqrt{n_1(N_1-n_1)}}{N_1}\,|\psi_3\rangle+\left[(1-e^{-i\alpha})\frac{N_1-n_1}{N_1}-1\right]|\psi_4\rangle\,.\end{aligned}$$

Since $\sin\frac{\omega}{2}=\sqrt{\frac{n_1}{N_1}}$ and $\cos\frac{\omega}{2}=\sqrt{\frac{N_1-n_1}{N_1}}$, we have

$$C(\alpha)\,|\psi_4\rangle=(1-e^{-i\alpha})\sin\frac{\omega}{2}\cos\frac{\omega}{2}\,|\psi_3\rangle+\left[(1-e^{-i\alpha})\cos^2\frac{\omega}{2}-1\right]|\psi_4\rangle\,.$$

Above all, the matrix representation of $C(\alpha)$ with respect to $|\psi_1\rangle\,,|\psi_2\rangle\,,|\psi_3\rangle\,,|\psi_4\rangle$ is

$$C(\alpha)=\begin{pmatrix}-e^{-i\alpha}&0&0&0\\0&-e^{-i\alpha}&0&0\\0&0&\left(1-e^{-i\alpha}\right)\sin^2\frac{\omega}{2}-1&(1-e^{-i\alpha})\sin\frac{\omega}{2}\cos\frac{\omega}{2}\\0&0&(1-e^{-i\alpha})\sin\frac{\omega}{2}\cos\frac{\omega}{2}&(1-e^{-i\alpha})\cos^2\frac{\omega}{2}-1\end{pmatrix}.$$

APPENDIX B: PROOF OF LEMMA 2 AND LEMMA 5

This section provides the proof of Lemma 2 and Lemma 5.

Proof. Recall that

$$|\Psi_t\rangle=SC(\alpha_t)Q(\beta_t)\cdots SC(\alpha_1)Q(\beta_1)\,|\Psi_0\rangle\,,$$

from Eqs. (2), (3), (7) and $SS=I$, we get

$$\begin{aligned}|\Psi_t\rangle\sim\ &SA\Big(\frac{\pi}{2}\Big)R(\alpha_t)A\Big(-\frac{\pi}{2}\Big)SR(\beta_t)A\Big(\frac{\pi}{2}\Big)R(\alpha_{t-1})A\Big(-\frac{\pi}{2}\Big)SR(\beta_{t-1})\\&\cdots A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2+1})A\Big(-\frac{\pi}{2}\Big)\Big\{SR(\beta_{t/2+1})A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2})A\Big(-\frac{\pi}{2}\Big)SR(\beta_{t/2})A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2-1})A\Big(-\frac{\pi}{2}\Big)S\Big\}R(\beta_{t/2-1})\\&\cdots A\Big(\frac{\pi}{2}\Big)R(\alpha_1)A\Big(-\frac{\pi}{2}\Big)SR(\beta_1)SA\Big(\frac{\pi}{2}\Big)SA\Big(\frac{\pi}{2}\Big)\,|\bar{0}\rangle\,,\end{aligned}$$

then by applying Eq. (8),

$$
\begin{aligned}
|\Psi_t\rangle \sim\ & SA\Big(\frac{\pi}{2}\Big)R(\alpha_t)A\Big(-\frac{\pi}{2}\Big)SR(\beta_t)A\Big(\frac{\pi}{2}\Big)R(\alpha_{t-1})A\Big(-\frac{\pi}{2}\Big)SR(\beta_{t-1})\\
&\cdots A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2+1})A\Big(-\frac{\pi}{2}\Big)\Big\{R(\beta_{t/2})A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2-1})A\Big(-\frac{\pi}{2}\Big)SR(\beta_{t/2+1})A\Big(\frac{\pi}{2}\Big)R(\alpha_{t/2})A\Big(-\frac{\pi}{2}\Big)\Big\}R(\beta_{t/2-1})\\
&\cdots A\Big(\frac{\pi}{2}\Big)R(\alpha_1)A\Big(-\frac{\pi}{2}\Big)SR(\beta_1)SA\Big(\frac{\pi}{2}\Big)SA\Big(\frac{\pi}{2}\Big)|\bar{0}\rangle\,,
\end{aligned}
$$

when t is even, by repeatedly applying Eq. (8) and using $A(-\frac{\pi}{2})A(\frac{\pi}{2}) = I$, we finally get

$$
\begin{aligned}
|\Psi_t\rangle \sim\ & R(\beta_t)A\Big(\frac{\pi}{2}\Big)R(\alpha_{t-1})A\Big(-\frac{\pi}{2}\Big)\cdots R(\beta_2)A\Big(\frac{\pi}{2}\Big)R(\alpha_1)S\\
&\times A\Big(\frac{\pi}{2}\Big)R(\alpha_t)A\Big(-\frac{\pi}{2}\Big)R(\beta_{t-1})A\Big(\frac{\pi}{2}\Big)\cdots R(\alpha_2)A\Big(-\frac{\pi}{2}\Big)R(\beta_1)A\Big(\frac{\pi}{2}\Big)|\bar{0}\rangle\,.
\end{aligned}
$$

Then, from Eq. (5), we have

$$
A\Big(\frac{\pi}{2}\Big) = R\Big(\frac{\pi}{2}-\theta\Big)A(\theta)R\Big(-\frac{\pi}{2}+\theta\Big)
$$

and

$$
A\Big(-\frac{\pi}{2}\Big) = R\Big(-\frac{\pi}{2}-\theta\Big)A(\theta)R\Big(\frac{\pi}{2}+\theta\Big)
$$

for arbitrary θ. Together with Eq. (6),

$$
\begin{aligned}
|\Psi_t\rangle \sim\ & R\Big(\beta_t+\frac{\pi}{2}-\varphi_{t-1}\Big)A(\varphi_{t-1})R(\alpha_{t-1}-\pi+\varphi_{t-1}-\varphi_{t-2})A(\varphi_{t-2})\cdots R(\beta_2+\pi+\varphi_2-\varphi_1)A(\varphi_1)R\Big(\alpha_1-\frac{\pi}{2}+\varphi_1\Big)S\\
&\times R\Big(\frac{\pi}{2}-\psi_{t+1}\Big)A(\psi_{t+1})R(\alpha_t-\pi+\psi_{t+1}-\psi_t)A(\psi_t)\cdots R(\beta_1+\pi+\psi_2-\psi_1)A(\psi_1)R\Big(-\frac{\pi}{2}+\psi_1\Big)|\bar{0}\rangle\,.
\end{aligned}
$$

By setting

$$
\alpha_i = \begin{cases} \text{arbitrary} & i = 1\\ \pi-\varphi_i+\varphi_{i-1} & i \text{ is odd and } i>1\,,\\ \pi-\psi_{i+1}+\psi_i & i \text{ is even}\end{cases}
$$

$$
\beta_i = \begin{cases} -\pi-\psi_{i+1}+\psi_i & i \text{ is odd}\\ -\pi-\varphi_i+\varphi_{i-1} & i \text{ is even and } i<t\,.\\ \text{arbitrary} & i = t\end{cases}
$$

and using $R(0) = I$, we get

$$
\begin{aligned}
|\Psi_t\rangle \sim\ & R\Big(\beta_t+\frac{\pi}{2}-\varphi_{t-1}\Big)A(\varphi_{t-1})A(\varphi_{t-2})\cdots A(\varphi_1)R\Big(\alpha_1-\frac{\pi}{2}+\varphi_1\Big)S\\
&\times R\Big(\frac{\pi}{2}-\psi_{t+1}\Big)A(\psi_{t+1})A(\psi_t)\cdots A(\psi_2)A(\psi_1)R\Big(-\frac{\pi}{2}+\psi_1\Big)|\bar{0}\rangle\,.
\end{aligned}
$$

■

Proof. Since the proof of Lemma 2 only relies on Eqs. (2)–(8) in Lemma 1 and in case 2 the same equations also hold in Lemma 4 and the proof of Lemma 2 also works for Lemma 5. ■

[1] P. W. Shor, Algorithms for quantum computation: Discrete logarithms and factoring, in *Proceedings 35th Annual Symposium on Foundations of Computer Science* (IEEE, New York, 1994), pp. 124-134.

[2] L. K. Grover, Quantum mechanics helps in searching for a needle in a haystack, Phys. Rev. Lett. **79**, 325 (1997).

[3] K. Fang, J. Zhao, X. Li, Y. Li, and R. Duan, Quantum network: From theory to practice, Sci. China Inf. Sci. **66**, 180509 (2023).

[4] X. He, X. Sun, G. Yang, and P. Yuan, Exact quantum query complexity of weight decision problems via Chebyshev polynomials, Sci. China Inf. Sci. **66**, 129503 (2023).

[5] A. M. Childs and J. Goldstone, Spatial search by quantum walk, Phys. Rev. A **70**, 022314 (2004).

[6] S. Chakraborty, L. Novo, A. Ambainis, and Y. Omar, Spatial search by quantum walk is optimal for almost all graphs, Phys. Rev. Lett. **116**, 100501 (2016).

[7] A. Ambainis, A. Gilyén, S. Jeffery, and M. Kokainis, Quadratic speedup for finding marked vertices by quantum walks, in *Proceedings of the 52nd Annual ACM SIGACT Symposium on Theory of Computing* (ACM, New York, 2020), pp. 412–424.

[8] S. Apers, S. Chakraborty, L. Novo, and J. Roland, Quadratic speedup for spatial search by continuous-time quantum walk, Phys. Rev. Lett. **129**, 160502 (2022).

[9] M. Štefaňák and S. Skoupý, Perfect state transfer by means of discrete-time quantum walk search algorithms on highly symmetric graphs, Phys. Rev. A **94**, 022301 (2016).

[10] S. Skoupý and M. Štefaňák, Quantum-walk-based state-transfer algorithms on the complete *M*-partite graph, Phys. Rev. A **103**, 042222 (2021).

[11] A. Ambainis, Quantum walk algorithm for element distinctness, SIAM J. Comput. **37**, 210 (2007).

[12] F. Magniez, M. Santha, and M. Szegedy, Quantum algorithms for the triangle problem, SIAM J. Comput. **37**, 413 (2007).

[13] T. G. Wong, L. Tarrataca, and N. Nahimov, Laplacian versus adjacency matrix in quantum walk search, Quant. Inf. Proc. **15**, 4029 (2016).

[14] I. Foulger, S. Gnutzmann, and G. Tanner, Quantum walks and quantum search on graphene lattices, Phys. Rev. A **91**, 062323 (2015).

[15] J. Böhm, M. Bellec, F. Mortessagne, U. Kuhl, S. Barkhofen, S. Gehler, H.-J. Stöckmann, I. Foulger, S. Gnutzmann, and G. Tanner, Microwave experiments simulating quantum search and directed transport in artificial graphene, Phys. Rev. Lett. **114**, 110501 (2015).

[16] S. Marsh and J. B. Wang, Deterministic spatial search using alternating quantum walks, Phys. Rev. A **104**, 022216 (2021).

[17] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, Quantum walks on graphs, in *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing* (ACM, New York, 2001), pp. 50–59.

[18] M. Szegedy, Quantum speed-up of Markov chain based algorithms, in *45th Annual IEEE Symposium on Foundations of Computer Science* (IEEE, New York, 2004), pp. 32–41.

[19] R. Portugal, R. A. M. Santos, T. D. Fernandes, and D. N. Gonçalves, The staggered quantum walk model, Quant. Inf. Proc. **15**, 85 (2016).

[20] A. Ambainis, J. Kempe, and A. Rivosh, Coins make quantum walks faster, in *Proceedings of 16th ACM-SIAM SODA* (SIAM, Philiadelphia, PA, 2005), pp. 1099–1108.

[21] V. Potoček, A. Gábris, T. Kiss, and I. Jex, Optimized quantum random-walk search algorithms on the hypercube, Phys. Rev. A **79**, 012325 (2009).

[22] G. Brassard, P. Hoyer, M. Mosca, and A. Tapp, Quantum amplitude amplification and estimation, Contemp. Math. **305**, 53 (2002).

[23] P. Høyer, Arbitrary phases in quantum amplitude amplification, Phys. Rev. A **62**, 052304 (2000).

[24] G.-L. Long, Grover algorithm with zero theoretical failure rate, Phys. Rev. A **64**, 022307 (2001).

[25] T. Roy, L. Jiang, and D. I. Schuster, Deterministic Grover search with a restricted oracle, Phys. Rev. Res. **4**, L022013 (2022).

[26] G. Li and L. Li, Deterministic quantum search with adjustable parameters: Implementations and applications, Inf. Comput. **292**, 105042 (2023).

[27] D. Qu, S. Marsh, K. Wang, L. Xiao, J. Wang, and P. Xue, Deterministic search on star graphs via quantum walks, Phys. Rev. Lett. **128**, 050501 (2022).

[28] Q. Wang, Y. Jiang, S. Feng, and L. Li, Universal approach to deterministic spatial search via alternating quantum walks, arXiv:2307.16133.

[29] R. Beals, H. Buhrman, R. Cleve, M. Mosca, and R. De Wolf, Quantum lower bounds by polynomials, J. ACM **48**, 778 (2001).

[30] Y. Xu, D. Zhang, and L. Li, Robust quantum walk search without knowing the number of marked vertices, Phys. Rev. A **106**, 052207 (2022).

[31] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2010).

[32] M. Saeedi and M. Pedram, Linear-depth quantum circuits for *n*-qubit Toffoli gates with no ancilla, Phys. Rev. A **87**, 062318 (2013).