Parameterization of quantum walks on cycles

Shuji Kuriki^{*}, Md Sams Afif Nirjhor[†], Hiromichi Ohno^{*}

Abstract

This study investigate the unitary equivalence classes of quantum walks on cycles. We show that unitary equivalence classes of quantum walks on a cycle with N vertices are parameterized by 2N real parameters. Moreover, the ranges of two of the parameters are restricted, and the ranges depend on the parity of N.

1 Introduction

Quantum walks are analogous to classical random walks. They have been studied in various fields, such as quantum information theory and quantum probability theory. A quantum walk is defined by a pair $(U, \{H_x\}_{x \in V})$, in which V is a countable set, $\{H_x\}_{x \in V}$ is a family of separable Hilbert spaces, and U is a unitary operator on $\mathcal{H} = \bigoplus_{x \in V} \mathcal{H}_x$ [10]. In this paper, we discuss quantum walks on a cycle, in which $V = \{1, 2, \ldots, N\}$ and $\mathcal{H}_x = \mathbb{C}^2$. These have been the subject of some previous studies [1, 2, 4, 5].

It is important to clarify when two quantum walks are unitarily equivalent in the sense of [7,10]. If two quantum walks are unitarily equivalent, many properties of their quantum walks are the same. For example, digraphs, dimensions of Hilbert spaces, spectrums of unitary operators, probability distributions of quantum walks, etc. would be the same for each quantum walk. The aim of this paper is to determine the unitary equivalence classes of quantum walks on cycles. Then, we only need to study representatives of unitary equivalence classes to know the above properties.

In the previous papers [7–9], we considered unitary equivalence classes of one-dimensional and two-dimensional quantum walks. Unitary equivalence classes of translation-invariant one-dimensional quantum walks were also investigated in [3].

In Sect. 2, we show a natural expression of quantum walks with some conditions. After that, we consider unitary equivalence of such quantum walks. The results in Sect. 2 are similar to those in [6,7], but improved a little.

In Sect. 3, we prove that unitary equivalence classes of quantum walks on a cycle with N vertices are parameterized by 2N real numbers. This parameterization is similar to that of one-dimensional quantum walks, because we need two parameters for each vertex to parameterize the unitary equivalence classes of one-dimensional quantum walks [8]. On the other hand, ranges of two of the parameters are restricted, and the two parameters go to zero when N goes to infinity. Moreover, the ranges depend on the parity of N. These properties are not seen in the cases of one-dimensional and two-dimensional quantum walks.

^{*}Department of Mathematics, Faculty of Engineering, Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

[†]Graduate School of Information Sciences, Tohoku University, Aoba-ku, Sendai, 980-8579, Japan

Natural expression of quantum walks 2

In this section, we present a natural expression of quantum walks with some conditions. We also consider unitary equivalence of such quantum walks.

Let V be a countable set. For each $x \in V$, $\mathcal{H}_x = \mathbb{C}^{k_x}$ is a finite dimensional Hilbert space, and P_x is a projection from $\mathcal{H} = \bigoplus_{y \in V} \mathcal{H}_y$ onto \mathcal{H}_x . A unitary U on \mathcal{H} is called a quantum walk [7,10]. Given a quantum walk U on \mathcal{H} , we can construct a multidigraph $G_U = (V, D_U)$. For vertices $x, y \in V$, the number of directed edges from y to x is denoted by card(x, y); i.e.,

$$\operatorname{card}(x, y) = \operatorname{card}\{\mathbf{a} \in D_U \colon t(\mathbf{a}) = x, o(\mathbf{a}) = y\},\$$

where $o(\mathbf{a})$ and $t(\mathbf{a})$ are the origin and terminus of the directed edge \mathbf{a} , respectively, and card indicates the cardinal number of a set. We define the number of directed edges from yto x by

$$\operatorname{card}(x, y) = \operatorname{rank} P_x U P_y.$$

Then, a multidigraph $G_U = (V, D_U)$ is called a multidigraph of the quantum walk U. We will write $G = G_U$ and $D = D_U$, when there is no confusion.

We consider quantum walks which satisfy one of the following conditions: for all $x \in V$,

$$\operatorname{card}\{\mathbf{a} \in D \colon o(\mathbf{a}) = x\} = \dim \mathcal{H}_x,$$
(1)

$$\operatorname{card}\{\mathbf{a} \in D \colon t(\mathbf{a}) = x\} = \dim \mathcal{H}_x.$$
 (2)

We prepare two lemmas.

Lemma 2.1 If a quantum walk U satisfies (1), then for each $x \in V$, $\operatorname{Ran}(UP_x) = \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x)$. Moreover, $U|_{\mathcal{H}_x}$ is a unitary from \mathcal{H}_x onto $\bigoplus_{y \in V} \operatorname{Ran}(P_y U P_x)$.

Proof. For any $UP_x\psi \in \operatorname{Ran}(UP_x)$,

$$UP_x\psi = \sum_{y\in V} P_y UP_x\psi \in \bigoplus_{y\in V} \operatorname{Ran}(P_y UP_x).$$

Therefore, $\operatorname{Ran}(UP_x) \subset \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x)$. This implies $\operatorname{rank}UP_x \leq \sum_{y \in V} \operatorname{rank}P_y UP_x$. By definitions and (1),

$$\dim \mathcal{H}_x = \dim U\mathcal{H}_x = \operatorname{rank} UP_x \le \sum_{y \in V} \operatorname{rank} P_y UP_x = \sum_{y \in V} \operatorname{card}(y, x)$$
$$= \operatorname{card}\{\mathbf{a} \in D \colon o(\mathbf{a}) = x\} = \dim \mathcal{H}_x.$$

Hence, rank $UP_x = \sum_{y \in V} \operatorname{rank} P_y UP_x$ and therefore,

$$\dim \operatorname{Ran}(UP_x) = \sum_{y \in V} \dim \operatorname{Ran}(P_y UP_x) = \dim \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x).$$

Since $\operatorname{Ran}(UP_x) \subset \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x)$, we obtain $\operatorname{Ran}(UP_x) = \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x)$. By the equation $U\mathcal{H}_x = \operatorname{Ran}(UP_x) = \bigoplus_{y \in V} \operatorname{Ran}(P_y UP_x)$, $U|_{\mathcal{H}_x}$ is a unitary from \mathcal{H}_x onto $\bigoplus_{y \in V} \operatorname{Ran}(P_y U P_x)$

Lemma 2.2 If a quantum walk U satisfies (2), then U^* satisfies (1).

Proof. By the equation $\operatorname{rank} P_x U P_y = \operatorname{rank} P_y U^* P_x$ and (2),

$$\dim \mathcal{H}_x = \operatorname{card}\{\mathbf{a} \in D_U \colon t(\mathbf{a}) = x\} = \sum_{y \in V} \operatorname{card}(x, y) = \sum_{y \in V} \operatorname{rank} P_x U P_y$$
$$= \sum_{y \in V} \operatorname{rank} P_y U^* P_x = \operatorname{card}\{\mathbf{a} \in D_{U^*} \colon o(\mathbf{a}) = x\}.$$

Hence, U^* satisfies (1).

The next theorem shows a natural expression of a quantum walk with the condition (1) or (2). This result is similar to that in [6,7], but improved a little.

Theorem 2.3 If a quantum walk U satisfies (1) or (2), there exist orthonormal bases $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D}$ and $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D}$ of the Hilbert space \mathcal{H} with $\xi_{\mathbf{a}}\in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}}\in \mathcal{H}_{o(\mathbf{a})}$ such that

$$U = \sum_{\mathbf{a} \in D} |\xi_{\mathbf{a}}\rangle \langle \zeta_{\mathbf{a}}|.$$

Proof. First, we assume that U satisfies (1). Since dim $\operatorname{Ran}(P_y U P_x) = \operatorname{rank} P_y U P_x = \operatorname{card}(y, x)$ for all $x, y \in V$, an orthonormal basis of $\operatorname{Ran}(P_y U P_x)$ is indexed by directed edges $\{\mathbf{a} : \mathbf{a} \in D, t(\mathbf{a}) = y, o(\mathbf{a}) = x\}$. Hence, there is an orthonormal basis $\{\xi_{\mathbf{a}} : \mathbf{a} \in D, t(\mathbf{a}) = y, o(\mathbf{a}) = x\}$ of $\operatorname{Ran}(P_y U P_x)$. Note that $\xi_{\mathbf{a}} \in \mathcal{H}_y = \mathcal{H}_{t(\mathbf{a})}$. Then, the union

$$\bigcup_{y \in V} \{\xi_{\mathbf{a}} \colon \mathbf{a} \in D, t(\mathbf{a}) = y, o(\mathbf{a}) = x\} = \{\xi_{\mathbf{a}} \colon \mathbf{a} \in D, o(\mathbf{a}) = x\}$$

is an orthonormal basis of $\bigoplus_{y \in V} \operatorname{Ran}(P_y U P_x)$. Define $\zeta_{\mathbf{a}} = U^* \xi_{\mathbf{a}}$. By Lemma 2.1, $\{\zeta_{\mathbf{a}} : \mathbf{a} \in D, o(\mathbf{a}) = x\}$ is an orthonormal basis of $\mathcal{H}_x = \mathcal{H}_{o(\mathbf{a})}$. Then, the union

$$\bigcup_{x \in V} \{ \zeta_{\mathbf{a}} \colon \mathbf{a} \in D, o(\mathbf{a}) = x \} = \{ \zeta_{\mathbf{a}} \colon \mathbf{a} \in D \}$$

is an orthonormal basis of \mathcal{H} . Since U is unitary and $\xi_{\mathbf{a}} = U\zeta_{\mathbf{a}}, \{\xi_{\mathbf{a}} : \mathbf{a} \in D\}$ is also an orthonormal basis of \mathcal{H} . Consequently, we have orthonormal bases $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D}$ and $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D}$ of the Hilbert space \mathcal{H} with $\xi_{\mathbf{a}} \in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}} \in \mathcal{H}_{o(\mathbf{a})}$ such that

$$U = \sum_{\mathbf{a}\in D} |\xi_{\mathbf{a}}\rangle \langle \zeta_{\mathbf{a}}|.$$

Next, we assume that U satisfies (2). By Lemma 2.2, U^* satisfies (1). Therefore, there exist orthonormal bases $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D_{U^*}}$ and $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D_{U^*}}$ of the Hilbert space \mathcal{H} with $\zeta_{\mathbf{a}}\in \mathcal{H}_{t(\mathbf{a})}$ and $\{\mathbf{a}_{\mathbf{a}}\in \mathcal{H}_{o(\mathbf{a})}\}$ such that

$$U^* = \sum_{\mathbf{a} \in D_{U^*}} |\zeta_{\mathbf{a}}\rangle \langle \xi_{\mathbf{a}} |$$

The equation rank $P_x U P_y = \operatorname{rank} P_y U^* P_x$ implies $D_{U^*} = \{ \bar{\mathbf{a}} : \mathbf{a} \in D_U \}$, where $\bar{\mathbf{a}}$ is the inverse edge of \mathbf{a} . This allows us to change the index set from D_{U^*} to D_U , that is,

$$U^* = \sum_{\mathbf{a} \in D_U} |\zeta_{\mathbf{a}}\rangle \langle \xi_{\mathbf{a}}$$

with $\xi_{\mathbf{a}} \in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}} \in \mathcal{H}_{o(\mathbf{a})}$. Consequently, we have

$$U = \sum_{\mathbf{a} \in D_U} |\xi_{\mathbf{a}}\rangle \langle \zeta_{\mathbf{a}}|,$$

where $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D_U}$ and $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D_U}$ are orthonormal bases of \mathcal{H} with $\xi_{\mathbf{a}}\in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}}\in \mathcal{H}_{o(\mathbf{a})}$.

As a corollary of this theorem, we have the following.

Corollary 2.4 For a quantum walk U, the conditions (1) and (2) are equivalent.

Proof. Assume that U satisfies (1). By Theorem 2.3, there exist orthonormal bases $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D}$ and $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D}$ of the Hilbert space \mathcal{H} with $\xi_{\mathbf{a}}\in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}}\in \mathcal{H}_{o(\mathbf{a})}$ such that

$$U = \sum_{\mathbf{a} \in D} |\xi_{\mathbf{a}}\rangle \langle \zeta_{\mathbf{a}}|.$$

Since $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D}$ is an orthonormal basis of \mathcal{H} and $\xi_{\mathbf{a}}$ is in $\mathcal{H}_{t(\mathbf{a})}$, for each $x \in V$, the set

$$\{\xi_{\mathbf{a}} \colon \mathbf{a} \in D, t(\mathbf{a}) = x\}$$

is an orthonormal basis \mathcal{H}_x . Therefore, U satisfies (2).

On the other hand, assume that U satisfies (2). By Lemma 2.2, U^* satisfies (1) and therefore, U^* satisfies (2). Again, by Lemma 2.2, U satisfies (1).

Now, we consider unitary equivalence of quantum walks. We recall the definition of unitary equivalence of quantum walks.

Definition 2.5 Quantum walks U_1 and U_2 on $\mathcal{H} = \bigoplus_{x \in V} \mathcal{H}_x$ are unitarily equivalent if there exists a unitary $W = \bigoplus_{x \in V} W_x$ on \mathcal{H} such that

$$WU_1W^* = U_2.$$

In a natural expression in Theorem 2.3, we need two orthonormal bases $\{\xi_{\mathbf{a}}\}\$ and $\{\zeta_{\mathbf{a}}\}$. Considering unitary equivalence of quantum walks with the conditions (1) and (2), we can disappear one of them. $\{\mathbf{e}_i^x\}_{i=1}^{k_x}$ denotes a canonical basis of $\mathcal{H}_x = \mathbb{C}^{k_x}$.

Theorem 2.6 If U satisfies (1) or (2), there exists an orthonormal basis $\{\zeta_i^x : i = 1, ..., k_x, x \in V\}$ of \mathcal{H} such that U is unitarily equivalent to

$$U_{\zeta} = \sum_{x \in V} \sum_{i=1}^{k_x} |\mathbf{e}_i^x\rangle \langle \zeta_i^x |,$$

and ζ_i^x is in \mathcal{H}_y for some y which satisfies $(x, y) \in D$.

Proof. By Theorem 2.3, there exist orthonormal bases $\{\xi_{\mathbf{a}}\}_{\mathbf{a}\in D}$ and $\{\zeta_{\mathbf{a}}\}_{\mathbf{a}\in D}$ of \mathcal{H} with $\xi_{\mathbf{a}}\in \mathcal{H}_{t(\mathbf{a})}$ and $\zeta_{\mathbf{a}}\in \mathcal{H}_{o(\mathbf{a})}$ such that

$$U = \sum_{\mathbf{a}\in D} |\xi_{\mathbf{a}}\rangle \langle \zeta_{\mathbf{a}}|.$$

Since $\operatorname{card} \{ \mathbf{a} \in D : t(\mathbf{a}) = x \} = \dim \mathcal{H}_x = k_x$, we can write

$$\{\xi_{\mathbf{a}}: \mathbf{a} \in D, t(\mathbf{a}) = x\} = \{\xi_i^x\}_{i=1}^{k_x} \text{ and } \{\zeta_{\mathbf{a}}: \mathbf{a} \in D, t(\mathbf{a}) = x\} = \{\eta_i^x\}_{i=1}^{k_x}.$$

Note that $\{\xi_i^x\}_{i=1}^{k_x}$ is an orthonormal basis of \mathcal{H}_x . Then, U can be written as

$$U = \sum_{x \in V} \sum_{i=1}^{k_x} |\xi_i^x\rangle \langle \eta_i^x|.$$

Define a unitary W by

$$W = \bigoplus_{x \in V} \sum_{i=1}^{k_x} |\mathbf{e}_i^x\rangle \langle \xi_i^x|.$$
(3)

Then,

$$WUW^* = \sum_{x \in V} \sum_{i=1}^{k_x} |W\xi_i^x\rangle \langle W\eta_i^x| = \sum_{x \in V} \sum_{i=1}^{k_x} |\mathbf{e}_i^x\rangle \langle \zeta_i^x|$$

where $\zeta_i^x = W \eta_i^x$. By definition, ζ_i^x is in \mathcal{H}_y for some y which satisfies $(x, y) \in D$.

3 Unitary equivalence classes of quantum walks on cycles

In this section, we consider unitary equivalence classes of quantum walks on cycles. The vertex set is $V = \{1, 2, ..., N\}$ $(N \ge 3)$. For each $x \in V$, $\mathcal{H}_x = \mathbb{C}^2$. We define $\mathcal{H} = \bigoplus_{x=1}^N \mathcal{H}_x$. P_x is a projection from \mathcal{H} onto \mathcal{H}_x , and $\{\mathbf{e}_1^x, \mathbf{e}_2^x\}$ is a canonical basis of $\mathcal{H}_x = \mathbb{C}^2$.

Definition 3.1 A unitary U on \mathcal{H} is called a quantum walk on a cycle if

$$\operatorname{rank} P_y U P_x = \begin{cases} 1 & y = x \pm 1 \\ 0 & \text{otherwise} \end{cases}$$

for all $x \in V$, where we define N + 1 = 1 and 0 = N with respect to $x \pm 1$.

By definition, a quantum walk U on a cycle satisfies (1). Hence, by Theorem 2.6, there exists an orthonormal basis $\{\zeta_1^x, \zeta_2^x\}_{x \in V}$ of \mathcal{H} such that U is unitarily equivalent to

$$U_{\zeta} = \sum_{x \in V} \left(|\mathbf{e}_1^x \rangle \langle \zeta_1^x | + |\mathbf{e}_2^x \rangle \langle \zeta_2^x | \right).$$

Here, ζ_i^x is in \mathcal{H}_y for some y which satisfies $(x, y) \in D$. For any $x \in V$, (x, y) is in D if and only if $y = x \pm 1$ by definition. Therefore, ζ_i^x is in \mathcal{H}_{x+1} or \mathcal{H}_{x-1} . We assume that $\zeta_1^x \in \mathcal{H}_{x-1}$ and $\zeta_2^x \in \mathcal{H}_{x+1}$ without loss of generality. We set $\zeta_1^{x+1} = \eta_1^x$ and $\zeta_2^{x-1} = \eta_2^x$. Then, $\{\eta_1^x, \eta_2^x\}$ is an orthonormal basis of \mathcal{H}_x , and

$$U_{\zeta} = \sum_{x \in V} \left(|\mathbf{e}_1^x \rangle \langle \eta_1^{x-1}| + |\mathbf{e}_2^x \rangle \langle \eta_2^{x+1}| \right) = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1} \rangle \langle \eta_1^x| + |\mathbf{e}_2^{x-1} \rangle \langle \eta_2^x| \right).$$
(4)

Since $\{\eta_1^x, \eta_2^x\}$ is an orthonormal basis of \mathcal{H}_x , we can write

$$\eta_1^x = r_x e^{ia_x} \mathbf{e}_1^x + \sqrt{1 - r_x^2} e^{ib_x} \mathbf{e}_2^x, \quad \eta_2^x = \sqrt{1 - r_x^2} e^{ic_x} \mathbf{e}_1^x + r_x e^{id_x} \mathbf{e}_2^x$$

for some $0 \le r_x \le 1$ and $a_x, b_x, c_x, d_x \in \mathbb{R}$ with $a_x - c_x = b_x - d_x + \pi \pmod{2\pi}$, where $i = \sqrt{-1}$. We will use $s_x = \sqrt{1 - r_x^2}$ for short, and omit (mod 2π) if there is no confusion.

We prepare three lemmas to get the unitary equivalence classes of quantum walks on cycles.

Lemma 3.2 The set $\frac{4\pi}{N}\mathbb{Z}$ is equal to the following set in modulo 2π :

$$\begin{cases} \frac{4\pi m}{N} \colon 0 \le m \le \frac{N}{2} - 1 \\ \begin{cases} \frac{2\pi m}{N} \colon 0 \le m \le N - 1 \end{cases} & \text{(when } N \text{ is even),} \\ \end{cases}$$

Proof. When N is even,

$$\frac{4\pi}{N}\mathbb{Z} = \frac{2\pi}{N/2}\mathbb{Z} = \left\{\frac{2\pi m}{N/2}: 0 \le m \le \frac{N}{2} - 1\right\} = \left\{\frac{4\pi m}{N}: 0 \le m \le \frac{N}{2} - 1\right\}$$

in modulo 2π .

When N is odd,

$$\frac{4\pi}{N} \cdot \frac{N+1}{2} = \frac{2\pi}{N} \pmod{2\pi}.$$

This implies

$$\frac{4\pi}{N}\mathbb{Z} = \frac{2\pi}{N}\mathbb{Z} = \left\{\frac{2\pi m}{N}: 0 \le m \le N-1\right\}$$

in modulo 2π .

Lemma 3.3 For any $\beta, \gamma, \delta \in \mathbb{R}$, there exist real numbers α and l which satisfy $N\alpha = \beta \pmod{2\pi}$, $Nl = \gamma \pmod{2\pi}$, $0 \le \delta + \alpha + 2l < \frac{2\pi}{N}$ in modulo 2π and

$$0 \le \alpha < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha < \frac{2\pi}{N}$ (when N is odd).

Proof. For the conditions $N\alpha = \beta$ and $Nl = \gamma$, α and l should be

$$\alpha = \frac{\beta}{N} + \frac{2\pi m_1}{N}, \qquad l = \frac{\gamma}{N} + \frac{2\pi m_2}{N}$$

for some $m_1, m_2 \in \mathbb{Z}$. Here,

$$\delta + \alpha + 2l = \delta + \frac{\beta + 2\gamma}{N} + \frac{2\pi m_1}{N} + \frac{4\pi m_2}{N}$$

When N is odd, there exists $m_1 \in \mathbb{Z}$ such that

$$0 \le \frac{\beta}{N} + \frac{2\pi m_1}{N} < \frac{2\pi}{N}.$$

Moreover, by the previous lemma, there exists $m_2 \in \mathbb{Z}$ such that

$$0 \le \delta + \frac{\beta + 2\gamma}{N} + \frac{2\pi m_1}{N} + \frac{4\pi m_2}{N} < \frac{2\pi}{N}$$

in modulo 2π .

When N is even, there exists $m_3 \in \mathbb{Z}$ such that

$$0 \le \frac{\beta}{N} + \frac{2\pi m_3}{N} < \frac{2\pi}{N} \le \frac{\beta}{N} + \frac{2\pi (m_3 + 1)}{N} < \frac{4\pi}{N}.$$

Moreover, by the previous lemma, there exists $m_2 \in \mathbb{Z}$ such that

$$-\frac{2\pi}{N} \le \delta + \frac{\beta + 2\gamma}{N} + \frac{2\pi m_3}{N} + \frac{4\pi m_2}{N} =: t < \frac{2\pi}{N}$$

in modulo 2π . If $-\frac{2\pi}{N} \leq t < 0$, we set $m_1 = m_3 + 1$. If $0 \leq t < \frac{2\pi}{N}$, we set $m_1 = m_3$. Then, we obtain the assertion.

Lemma 3.4 Let *l* be a real number which satisfies $lN = 0 \pmod{2\pi}$. When N is even,

$$2l = \frac{4\pi m}{N}$$

for some $m \in \{0, 1, \ldots, N/2 - 1\}$ in modulo 2π . When N is odd,

$$2l = \frac{2\pi m}{N}$$

for some $m \in \{0, 1, \dots, N-1\}$ in modulo 2π .

Proof. By the assumption, $l \in \frac{2\pi}{N}\mathbb{Z}$. Hence, $2l \in \frac{4\pi}{N}\mathbb{Z}$. Then, we have the assertion by Lemma 3.2.

In quantum mechanics, a state ψ in a Hilbert space is identified with $e^{il}\psi$. Moreover, almost all properties of $e^{il}U$, such as the spectrum and the distribution for an initial state, can be obtained from those of U. Thus, we also identify a quantum walk U with $e^{il}U$.

Theorem 3.5 A quantum walk U on a cycle is unitarily equivalent to

$$U_{r,\theta,\alpha} = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle r_x \mathbf{e}_1^x + s_x e^{\mathrm{i}\theta_x} \mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle -s_x e^{\mathrm{i}(-\theta_x + \alpha)} \mathbf{e}_1^x + r_x e^{\mathrm{i}\alpha} \mathbf{e}_2^x| \right)$$
(5)

for some $0 \le r_x \le 1$, $s_x = \sqrt{1 - r_x^2}$, $\theta_1 = 0$, $0 \le \theta_2 < \frac{2\pi}{N}$, $0 \le \theta_x < 2\pi$ $(x = 3, 4, \dots N)$ and

$$0 \le \alpha < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha < \frac{2\pi}{N}$ (when N is odd).

Proof. We already show that U is unitarily equivalent to

$$U_{\zeta} = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle r_x e^{\mathbf{i}a_x} \mathbf{e}_1^x + s_x e^{\mathbf{i}b_x} \mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle s_x e^{\mathbf{i}c_x} \mathbf{e}_1^x + r_x e^{\mathbf{i}d_x} \mathbf{e}_2^x| \right).$$

Let α be a real number which satisfies

$$N\alpha = \sum_{k=1}^{N} d_k - \sum_{k=1}^{N} a_k \pmod{2\pi},$$
 (6)

and let l be a real number which satisfies

$$Nl = \sum_{k=1}^{N} a_k \pmod{2\pi}.$$
(7)

Define a unitary W_x on \mathcal{H}_x by

$$W_x = \begin{bmatrix} e^{\mathrm{i}p_x} & 0\\ 0 & e^{\mathrm{i}q_x} \end{bmatrix} = e^{\mathrm{i}p_x} |\mathbf{e}_1^x\rangle \langle \mathbf{e}_1^x| + e^{\mathrm{i}q_x} |\mathbf{e}_2^x\rangle \langle \mathbf{e}_2^x|,$$

where

$$p_1 = 0, \quad p_x = \sum_{k=1}^{x-1} a_k - (x-1)l \quad (2 \le x \le N),$$

$$q_1 = a_1 - b_1, \quad q_x = -\sum_{k=2}^{x} d_k + (x-1)(\alpha+l) + a_1 - b_1 \quad (2 \le x \le N).$$

Then, $W = \bigoplus_{x \in V} W_x$ is a unitary on $\mathcal{H} = \bigoplus \mathcal{H}_x$. By simple calculation,

$$e^{il}WU_{\zeta}W^{*} = e^{il}\sum_{x\in V} \left(|W\mathbf{e}_{1}^{x+1}\rangle\langle r_{x}e^{ia_{x}}W\mathbf{e}_{1}^{x} + s_{x}e^{ib_{x}}W\mathbf{e}_{2}^{x}| + |W\mathbf{e}_{2}^{x-1}\rangle\langle s_{x}e^{ic_{x}}W\mathbf{e}_{1}^{x} + r_{x}e^{id_{x}}W\mathbf{e}_{2}^{x}| \right)$$
$$= \sum_{x\in V} \left(|\mathbf{e}_{1}^{x+1}\rangle\langle r_{x}e^{i(a_{x}+p_{x}-p_{x+1}-l)}\mathbf{e}_{1}^{x} + s_{x}e^{i(b_{x}+q_{x}-p_{x+1}-l)}\mathbf{e}_{2}^{x}| + |\mathbf{e}_{2}^{x-1}\rangle\langle s_{x}e^{i(c_{x}+p_{x}-q_{x-1}-l)}\mathbf{e}_{1}^{x} + r_{x}e^{i(d_{x}+q_{x}-q_{x-1}-l)}\mathbf{e}_{2}^{x}| \right).$$
(8)

By paying attention to the cases x = 1 and x = N, we have

$$a_x + p_x - p_{x+1} - l = 0 \quad (1 \le x \le N),$$

$$d_x + q_x - q_{x-1} - l = \alpha \quad (1 \le x \le N).$$

We set $\theta_x = b_x + q_x - p_{x+1} - l$. Then, $\theta_1 = 0$ and

$$\theta_x = -\sum_{k=2}^x a_k - \sum_{k=2}^x d_k + b_x - b_1 + (x-1)(\alpha+2l) \quad (2 \le x \le N).$$
(9)

In particular, $\theta_2 = -a_2 - d_2 + b_2 - b_1 + \alpha + 2l$. By lemma 3.3, there exist real numbers α and l such that $N\alpha = \sum_{k=1}^{N} d_k - \sum_{k=1}^{N} a_k$, $Nl = \sum_{k=1}^{N} a_k$,

$$0 \le -a_2 - d_2 + b_2 - b_1 + \alpha + 2l < \frac{2\pi}{N}$$

in modulo 2π and

$$0 \le \alpha < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha < \frac{2\pi}{N}$ (when N is odd)

Since the vectors

 $r_{x}e^{i(a_{x}+p_{x}-p_{x+1}-l)}\mathbf{e}_{1}^{x}+s_{x}e^{i(b_{x}+q_{x}-p_{x+1}-l)}\mathbf{e}_{2}^{x} \quad \text{and} \quad s_{x}e^{i(c_{x}+p_{x}-q_{x-1}-l)}\mathbf{e}_{1}^{x}+r_{x}e^{i(d_{x}+q_{x}-q_{x-1}-l)}\mathbf{e}_{2}^{x}$ in (8) make an orthonormal basis of \mathcal{H}_{x} ,

$$c_x + p_x - q_{x-1} - l = -\theta_x + \alpha + \pi.$$

Consequently,

$$e^{\mathrm{i}l}WU_{\zeta}W^* = \sum_{x\in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle r_x \mathbf{e}_1^x + s_x e^{\mathrm{i}\theta_x} \mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle -s_x e^{\mathrm{i}(-\theta_x+\alpha)} \mathbf{e}_1^x + r_x e^{\mathrm{i}\alpha} \mathbf{e}_2^x| \right) = U_{r,\theta,\alpha}.$$

Therefore, we conclude that a quantum walk U is unitary equivalent to $U_{r,\theta,\alpha}$ for some $0 \le r_x \le 1, \ \theta_1 = 0, \ 0 \le \theta_2 < \frac{2\pi}{N}, \ 0 \le \theta_x < 2\pi \ (x = 3, 4, \dots N)$ and

$$0 \le \alpha < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha < \frac{2\pi}{N}$ (when N is odd).

Theorem 3.6 Quantum walks $U_{r,\theta,\alpha}$ and $U_{r',\theta',\alpha'}$ with $0 < r_x, r'_x < 1$, $\theta_1 = \theta'_1 = 0$, $0 \le \theta_2, \theta'_2 < \frac{2\pi}{N}, 0 \le \theta_x, \theta'_x < 2\pi$ $(x = 3, 4, \ldots N)$ and

$$0 \le \alpha, \alpha' < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha, \alpha' < \frac{2\pi}{N}$ (when N is odd)

are unitarily equivalent if and only if, for all $1 \le x \le N$,

$$r_x = r'_x, \quad \theta_x = \theta'_x \quad \text{and} \quad \alpha = \alpha'.$$
 (10)

Proof. If (10) holds, then $U_{r,\theta,\alpha} = U_{r',\theta',\alpha'}$. Therefore, $U_{r,\theta,\alpha}$ and $U_{r',\theta',\alpha'}$ are unitarily equivalent.

Conversely, we assume that $U_{r,\theta,\alpha}$ and $U_{r',\theta',\alpha'}$ are unitarily equivalent, that is, there exist a unitary $W = \bigoplus_{x \in V} W_x$ on \mathcal{H} and a real number l such that

$$e^{il}WU_{r,\theta,\alpha}W^* = U_{r',\theta',\alpha'}.$$

First, we consider the equation

$$P_{x\pm 1}e^{il}WU_{r,\theta,\alpha}W^*P_x = P_{x\pm 1}U_{r',\theta',\alpha'}P_x.$$

By (5),

$$P_{x+1}e^{il}WU_{r,\theta,\alpha}W^*P_x = e^{il}|W\mathbf{e}_1^{x+1}\rangle\langle W(r_x\mathbf{e}_1^x + s_xe^{i\theta_x}\mathbf{e}_2^x)|$$

and

$$P_{x+1}U_{r',\theta',\alpha'}P_x = |\mathbf{e}_1^{x+1}\rangle\langle r'_x\mathbf{e}_1^x + s'_xe^{\mathrm{i}\theta'_x}\mathbf{e}_2^x|$$

Therefore, $\operatorname{Ran}(P_{x+1}e^{il}WU_{r,\theta,\alpha}W^*P_x) = \mathbb{C}W\mathbf{e}_1^{x+1}$ and $\operatorname{Ran}(P_{x+1}U_{r',\theta',\alpha'}P_x) = \mathbb{C}\mathbf{e}_1^{x+1}$, so that $W\mathbf{e}_1^{x+1} \in \mathbb{C}\mathbf{e}_1^{x+1}$. Similarly, the equations

$$P_{x-1}e^{\mathrm{i}l}WU_{r,\theta,\alpha}W^*P_x = e^{\mathrm{i}l}|W\mathbf{e}_2^{x-1}\rangle\langle W(-s_xe^{\mathrm{i}(-\theta_x+\alpha)}\mathbf{e}_1^x + r_xe^{\mathrm{i}\alpha}\mathbf{e}_2^x)|$$
$$P_{x-1}U_{r',\theta',\alpha'}P_x = |\mathbf{e}_2^{x-1}\rangle\langle -s'_xe^{\mathrm{i}(-\theta'_x+\alpha')}\mathbf{e}_1^x + r'_xe^{\mathrm{i}\alpha'}\mathbf{e}_2^x|$$

imply $W \mathbf{e}_2^{x-1} \in \mathbb{C} \mathbf{e}_2^{x-1}$. Since $W = \bigoplus_{x \in V} W_x$ is unitary, W_x can be written as

$$W_x = \begin{bmatrix} e^{\mathbf{i}p_x} & 0\\ 0 & e^{\mathbf{i}q_x} \end{bmatrix} = e^{\mathbf{i}p_x} |\mathbf{e}_1^x\rangle \langle \mathbf{e}_1^x| + e^{\mathbf{i}q_x} |\mathbf{e}_2^x\rangle \langle \mathbf{e}_2^x|$$

for some $p_x, q_x \in \mathbb{R}$.

Now, we consider the equation $e^{il}WU_{r,\theta,\alpha}W^* = U_{r',\theta',\alpha'}$. Because $(e^{it}W)U_{r,\theta,\alpha}(e^{it}W)^* = WU_{r,\theta,\alpha}W^*$ for any $t \in \mathbb{R}$, we can assume that $p_1 = 0$. By simple calculation, we have

$$\begin{split} e^{\mathrm{i}l}WU_{r,\theta,\alpha}W^* \\ &= e^{\mathrm{i}l}\sum_{x\in V} \left(|W\mathbf{e}_1^{x+1}\rangle\langle r_xW\mathbf{e}_1^x + s_x e^{\mathrm{i}\theta_x}W\mathbf{e}_2^x| + |W\mathbf{e}_2^{x-1}\rangle\langle -s_x e^{\mathrm{i}(-\theta_x+\alpha)}W\mathbf{e}_1^x + r_x e^{\mathrm{i}\alpha}W\mathbf{e}_2^x|\right) \\ &= \sum_{x\in V} \left(|\mathbf{e}_1^{x+1}\rangle\langle r_x e^{\mathrm{i}(p_x-p_{x+1}-l)}\mathbf{e}_1^x + s_x e^{\mathrm{i}(\theta_x+q_x-p_{x+1}-l)}\mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle\langle -s_x e^{\mathrm{i}(-\theta_x+\alpha+p_x-q_{x-1}-l)}\mathbf{e}_1^x + r_x e^{\mathrm{i}(\alpha+q_x-q_{x-1}-l)}\mathbf{e}_2^x|\right). \end{split}$$

On the other hand,

$$U_{r',\theta',\alpha'} = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle r'_x \mathbf{e}_1^x + s'_x e^{i\theta'_x} \mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle -s'_x e^{i(-\theta'_x + \alpha')} \mathbf{e}_1^x + r_x e^{i\alpha'} \mathbf{e}_2^x| \right).$$

Therefore, we get $r_x = r'_x$ and the equations

$$p_x - p_{x+1} - l = 0, \quad \theta_x + q_x - p_{x+1} - l = \theta'_x$$
$$-\theta_x + \alpha + p_x - q_{x-1} - l = -\theta'_x + \alpha', \quad \alpha + q_x - q_{x-1} - l = \alpha'$$

in modulo 2π . By $p_1 = 0$ and the first equation,

$$p_x = -l(x-1) \quad (1 \le x \le N).$$

Moreover, $p_N - p_0 - l = 0$ implies lN = 0. By the second equation with x = 1, we have $q_1 = 0$, because $\theta_1 = \theta'_1 = 0$. Then, by the fourth equation,

$$q_x = (l - \alpha + \alpha')(x - 1) \quad (1 \le x \le N).$$

Furthermore, $\alpha + q_1 - q_N - l = \alpha'$ implies $(l - \alpha + \alpha')N = 0$. The second equation is calculated as

$$\theta_x + (2l - \alpha + \alpha')(x - 1) = \theta'_x \quad (1 \le x \le N).$$

$$\tag{11}$$

In particular,

$$\theta_2 + 2l - \alpha + \alpha' = \theta'_2. \tag{12}$$

Since lN = 0 and $(l - \alpha + \alpha')N = 0$,

$$(\theta_2 - \theta_2')N = 0.$$

By the assumption $0 \le \theta_2, \theta'_2 < \frac{2\pi}{N}$, we obtain $\theta_2 = \theta'_2$. Then, (12) is

$$2l - \alpha + \alpha' = 0.$$

Here, α and α' satisfy

$$-\frac{4\pi}{N} < \alpha - \alpha' < \frac{4\pi}{N} \quad \text{(when } N \text{ is even}\text{)}, \quad -\frac{2\pi}{N} < \alpha - \alpha' < \frac{2\pi}{N} \quad \text{(when } N \text{ is odd)}.$$

Therefore, we obtain $\alpha - \alpha' = 2l = 0$ by Lemma 3.4, and hence, $\alpha = \alpha'$. Moreover, by (11), $\theta_x = \theta'_x$ for all $1 \le x \le N$. Consequently, we conclude $\alpha = \alpha'$, $r_x = r'_x$ and $\theta_x = \theta'_x$ for all $1 \le x \le N$.

Theorem 3.5 and 3.6 say that the unitary equivalence classes of quantum walks on a cycle are parametrized by α , r_x and θ_x . As N goes to infinity, the limits of α and θ_2 are 0. On the other hand, a one-dimensional quantum walk is unitarily equivalent to

$$\sum_{x \in \mathbb{Z}} \left(|\mathbf{e}_1^{x+1}\rangle \langle r_x \mathbf{e}_1^x + e^{\mathrm{i}\theta_x} s_x \mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle -e^{-\mathrm{i}\theta_x} s_x \mathbf{e}_1^x + r_x \mathbf{e}_2^x| \right)$$

where $0 \leq r_x \leq 1$, $\theta_0 = \theta_1 = 0$ and $0 \leq \theta_x < 2\pi$ ($x \neq 0, 1$). Therefore, the parametrization of the unitary equivalence classes of one-dimensional quantum walks is similar to that of quantum walks on a cycle with $N \to \infty$.

There is a natural shift operator S on \mathcal{H} , that is,

$$S\mathbf{e}_i^x = \mathbf{e}_i^{x+1}$$

for i = 1, 2 and $x \in V$. A quantum walk U on a cycle is called translation-invariant if

$$SUS^* = U.$$

By the next theorem, unitary equivalence classes of translation-invariant quantum walk on a cycle are parametrized by two real numbers.

Corollary 3.7 A translation-invariant quantum walk on a cycle is unitarily equivalent to

$$U_{r,\alpha} = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle r\mathbf{e}_1^x + s\mathbf{e}_2^x| + |\mathbf{e}_2^{x-1}\rangle \langle -se^{\mathrm{i}\alpha}\mathbf{e}_1^x + re^{\mathrm{i}\alpha}\mathbf{e}_2^x| \right)$$

for some $0 \le r \le 1$, $s = \sqrt{1 - r^2}$ and

$$0 \le \alpha < \frac{4\pi}{N}$$
 (when N is even), $0 \le \alpha < \frac{2\pi}{N}$ (when N is odd).

Moreover, $U_{r,\alpha}$ and $U_{r',\alpha'}$ with $r, r' \neq 0, 1$ are unitarily equivalent if and only if r = r' and $\alpha = \alpha'$.

Proof. We need to consider Theorem 2.3 and 2.6, again. By Theorem 2.3, U can be written as

$$U = \sum_{x \in V} \sum_{i=1}^{2} |\xi_i^x\rangle \langle \zeta_i^x|.$$

Since U is translation-invariant, there exist ξ_i and ζ_i (i = 1, 2) in \mathbb{C}^2 such that $\xi_i^x = \xi_i$ and $\zeta_i^x = \zeta_i$ for all $x \in V$. Hence, the unitary W in (3) is described as

$$W = \bigoplus_{x \in V} \sum_{i=1}^{2} |\mathbf{e}_{i}^{x}\rangle \langle \xi_{i}^{x}|$$

and is translation-invariant. Therefore, $U_{\zeta} = WUW^*$ in Theorem 2.6 is also translation-invariant and is written as

$$U_{\zeta} = \sum_{x \in V} \left(|\mathbf{e}_1^{x+1}\rangle \langle \eta_1^x| + |\mathbf{e}_2^{x-1}\rangle \langle \eta_2^x| \right),$$

where $\eta_1^x = \eta_1$ and $\eta_2^x = \eta_2$ for some $\eta_1, \eta_2 \in \mathbb{C}^2$, as we see in (4). This implies that there exist $0 \leq r \leq 1$ and $a, b, c, d \in \mathbb{R}$ such that, for all $x \in V$, $r_x = r$, $a_x = a$ and so on. Then, θ_x in (9) is

$$\theta_x = (x - 1)(-a - d + \alpha + 2l) = (x - 1)\theta_2.$$

By (6) and (7), $N\theta_2 = 0 \pmod{2\pi}$. Since $0 \le \theta_2 < \frac{2\pi}{N}$, $\theta_2 = 0$, and hence, $\theta_x = 0$ ($1 \le x \le N$). Consequently, U_{ζ} is unitarily equivalent to $U_{r,\alpha}$.

The remaining assertion follows from Theorem 3.6, immediately.

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