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Chul Ki Ko
University College, Yonsei University, 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, Korea, kochulki@yonsei.ac.kr

Hyun Jae Yoo
School of Computer Engineering and Applied Mathematics, and Institute for Integrated Mathematical Sciences, Hankyong National University, 327 Jungang-ro, Anseong-si, Gyeonggi-do 17579, Korea, yoohj@hknu.ac.kr

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QUANTUM MARKOV CHAINS ASSOCIATED WITH UNITARY QUANTUM WALKS

CHUL KI KO AND HYUN JAE YOO*

Dedicated to Professor Leonard Gross on the occasion of his 88th birthday

Abstract. In this paper we discuss the quantum Markov chains of unitary quantum walks. The construction of the quantum Markov chain associated with a unitary quantum walk serves as a good example in the view point of quantum Markov chains. On the other hand, the method of quantum Markov chain provides a tool for the investigation of dynamical properties of the unitary quantum walks. We discuss the reducibility/irreducibility and the recurrence/transience properties. Comparing with the results known in other literature and in classical random walks, we will see some similarity as well as some differences.

1. Introduction

The purpose of this paper is to construct quantum Markov chains (QMCs here after) associated with unitary quantum walks (UQWs shortly). The aim is two folds: one is to give a nontrivial example of QMCs and the other is to investigate the dynamical properties of the UQWs.

The QMC has been introduced by Accardi [1, 2, 3] and found many applications [4, 5, 6, 7, 9, 8, 10, 11]. Recently, Dhahri and Mukhamedov, and Dhahri and the present authors constructed QMCs associated with open quantum random walks (OQRWs shortly) and investigated recurrence and accessibility [19], and reducibility and irreducibility of the OQRWs [18]. So, it is natural to ask whether it is possible to investigate the dynamical properties of UQWs via QMCs. The paper answers this question.

The UQWs, which will be briefly introduced in the next section, was developed for some applications in quantum computation, e.g., to speed up the search algorithm, see [22] and references therein. The most big difference between UQWs and OQRWs is, to the best knowledge of the authors, that after one evolution, the UQW adds up the probability amplitudes, on the other hand the OQRW adds up the probability densities. This difference results apparently in the limits of the distributions. The UQWs reveal the Konno distribution [26, 27], but the OQRWs show the central limit theorems [13, 23]. This difference also requires us to use a

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* Corresponding author.

different method to construct the QMCs for the UQWs from the construction of QMCs for OQRWs. Anyway, we have successively constructed the QMCs associated with the UQWs in the sense that when the constructed QMC is restricted to the local observables at time n it recovers the original dynamics of the UQW at time n (see eq. (3.16)). Then we can investigate the dynamical properties of the UQWs in the scheme of the QMCs.

The paper is organized as follows. In section 2 we introduce the UQWs. In section 3, we construct the QMCs for the UQWs. In section 4, we investigate the reducibility and the irreducibility of the UQWs by QMCs. In the final section we discuss the recurrence and transience of UQWs using the associated QMCs. We will see in particular that the recurrence/transience property of UQWs is typically different from that of the classical random walks.

2. Unitary Quantum Walks

2.1. Evolution of states. We briefly introduce the 1-dimensional unitary quantum walks (UQWs hereafter). For the details we refer to the references [12, 20, 22, 24, 25, 26, 27]. A quantum particle has an intrinsic degree of freedom, called "chirality", which is represented by a 2-dimensional vector: we represent them in $\mathbb{C}^2$ and call the vectors $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$ and $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$ the left and right chirality, respectively. Let $\mathfrak{h} := l^2(\mathbb{Z}, \mathbb{C}^2)$ be the Hilbert space of sequences of $\mathbb{C}^2$-vectors. $\mathfrak{h}$ consists of the vectors $\psi = (\psi_i)_{i\in\mathbb{Z}}$, where $\psi_i = \begin{bmatrix} \psi_i(1) \\ \psi_i(2) \end{bmatrix} \in \mathbb{C}^2$ satisfies $\sum_{i\in\mathbb{Z}} \|\psi_i\|^2 < \infty$. We can think of $\mathfrak{h} = \oplus_{i\in\mathbb{Z}}\mathbb{C}^2$ by denoting $\psi = \oplus_{i\in\mathbb{Z}}\psi_i$. A physical meaning of the state ψ is as follows. A measurement of the position of a quantum particle in the state ψ will result in the position i with a probability $\|\psi_i\|^2$. A UQW is an evolution of pure states on $\mathfrak{h}$. More precisely, let

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix} =: P + Q \tag{2.1}$$

be a unitary matrix. Given a pure state, i.e., a unit vector $\psi = \oplus_{i\in\mathbb{Z}}\psi_i \in \mathfrak{h}$, the UQW operates on ψ giving a new pure state defined by

$$\mathcal{U}(\psi) := \oplus_{i\in\mathbb{Z}}(P\psi_{i+1} + Q\psi_{i-1}) \in \mathfrak{h}. \tag{2.2}$$

2.2. UQW: a completely positive map on the pure states. In this subsection, we will see the UQWs in a slightly different point of view. Given a unit vector $\psi = \oplus_{i\in\mathbb{Z}}\psi_i \in \mathfrak{h}$, we will also look at it as a pure state $\rho_\psi := |\psi\rangle\langle\psi|$ on $\mathcal{B}(\mathfrak{h})$, the space of all bounded linear operators on $\mathfrak{h}$. Let P_i be the projection onto the ith position space, defined by

$$P_i(\cdots \oplus \psi_{i-1} \oplus \psi_i \oplus \psi_{i+1} \oplus \cdots) = \cdots \oplus 0 \oplus \psi_i \oplus 0 \oplus \cdots .$$

If we measure the position of the particle in the state ψ, it will result in the site $i \in \mathbb{Z}$ with a probability

$$\mathrm{Tr}(\rho_\psi P_i) = \mathrm{Tr}(|\psi\rangle\langle\psi|P_i) = \langle\psi, P_i\psi\rangle = \|\psi_i\|^2.$$

We define the operators $\widetilde{P}$ and $\widetilde{Q}$ in $\mathcal{B}(\mathfrak{h})$ by

$$\widetilde{P}(\xi) = \oplus_{i\in\mathbb{Z}}(P\xi_{i+1}), \quad \widetilde{Q}(\xi) = \oplus_{i\in\mathbb{Z}}(Q\xi_{i-1}), \quad \text{for } \xi = \oplus_{i\in\mathbb{Z}}\xi_i \in \mathfrak{h}. \tag{2.3}$$

Let us define $\widetilde{U} := \widetilde{P} + \widetilde{Q}$. The following can be easily checked.

Lemma 2.1. *The operator $\widetilde{U} \in \mathcal{B}(\mathfrak{h})$ is a unitary operator. In particular, it holds that*

$$\big(\widetilde{P}\big)^*\widetilde{P} + \big(\widetilde{Q}\big)^*\widetilde{Q} = I = \widetilde{P}\big(\widetilde{P}\big)^* + \widetilde{Q}\big(\widetilde{Q}\big)^*,$$

and

$$\big(\widetilde{Q}\big)^*\widetilde{P} = 0,\ \big(\widetilde{P}\big)^*\widetilde{Q} = 0,\ \widetilde{P}\big(\widetilde{Q}\big)^* = 0,\ \widetilde{Q}\big(\widetilde{P}\big)^* = 0.$$

Proposition 2.2. *The UQW is a completely positive map on the pure states defined by*

$$\mathcal{U}(|\psi\rangle\langle\psi|) = \widetilde{U}|\psi\rangle\langle\psi|(\widetilde{U})^*. \tag{2.4}$$

Proof. It follows from the definitions (2.2) and (2.3). □

3. Quantum Markov Chains of Unitary Quantum Walks

3.1. Quantum Markov chains. In this section we briefly recall the definition of the quantum Markov chains [6, 7, 19, 28]. Here we recall the setting used in [18].

Let $\mathbb{Z}_+$ be the set of all nonnegative integers. Let $\mathcal{B}$ be a von Neumann subalgebra of $\mathcal{B}(\mathfrak{h})$, the space of all bounded linear operators on a separable Hilbert space $\mathfrak{h}$. For any bounded $\Lambda \subset \mathbb{Z}_+$, let

$$\mathcal{A}_\Lambda := \bigotimes_{i\in\Lambda}\mathcal{A}_i,\ \mathcal{A}_i = \mathcal{B}, \tag{3.1}$$

be the finite tensor product of von Neumann algebras and

$$\mathcal{A} := \bigotimes_{i\in\mathbb{Z}_+}\mathcal{A}_i \tag{3.2}$$

be the infinite tensor product of von Neumann algebras [16, 30, 32]. For each $i \in \mathbb{Z}_+$, let J_i be the embedding homomorphism

$$J_i : \mathcal{B} \hookrightarrow I_0 \otimes I_1 \otimes \cdots \otimes I_{i-1} \otimes \mathcal{B} \otimes I_{i+1} \otimes \cdots =: I_{i-1]} \otimes \mathcal{B} \otimes I_{[i+1}$$

defined by

$$J_i(a) = I_{i-1]} \otimes a \otimes I_{[i+1}, \quad a \in \mathcal{B}.$$

For each $\Lambda \subset \mathbb{Z}_+$, we identify $\mathcal{A}_\Lambda$ as a subalgebra of $\mathcal{A}$. We denote $\mathcal{A}_{n]}$ the subalgebra of $\mathcal{A}$, generated by the first $(n+1)$ factors, i.e., by the elements of the form

$$a_{n]} = a_0 \otimes a_1 \otimes \cdots \otimes a_n \otimes I_{[n+1} = J_0(a_0)J_1(a_1)\cdots J_n(a_n)$$

with $a_0, a_1, \cdots, a_n \in \mathcal{B}$.

A bilinear map $\mathcal{E}$ from $\mathcal{B} \otimes \mathcal{B}$ to $\mathcal{B}$ is called a transition expectation if it is completely positive and sub-Markovian in the sense that [11]

$$\mathcal{E}(I \otimes I) \leq I. \tag{3.3}$$

Given a (sub-)Markovian transition expectation, one can define a (unique) completely positive map

$$E_{m]} : \mathcal{A} \to \mathcal{A}_{m]}. \tag{3.4}$$

Formally, it is defined for $a = a_0 \otimes a_1 \otimes \cdots \in \mathcal{A}$ as

$$E_{m]}(a) := \lim_{n\to\infty} E_{m]}(a_{n]}), \tag{3.5}$$

where

$$\begin{aligned} E_{m]}(a_{n]}) := \lim_{k\to\infty} \Big[a_0 \otimes \cdots \otimes a_{m-1} \otimes \mathcal{E}^{(m)}(a_m \otimes \mathcal{E}^{(m+1)}(a_{m+1} \otimes \cdots \\ \otimes \mathcal{E}^{(n)}(a_n \otimes \mathcal{E}^{(n+1)}(I \otimes \cdots \otimes \mathcal{E}^{(n+k)}(I \otimes I))))) \Big]. \end{aligned} \tag{3.6}$$

See [1, 2, 3, 11]. For the Markovian transition expectations, the limit in (3.6) is trivial but for the sub-Markovian transition expectations, however, it is a little bit delicate to show the existence. In [18], we have shown that for each $m \geq 0$, there exists a (unique) completely positive map $E_{m]}$ in (3.4) defined by (3.5)-(3.6), which is sub-Markovian.

Suppose that a sequence of transition expectations $(\mathcal{E}^{(n)})_{n\geq 0}$ and a state ϕ_0 on $\mathcal{B}$ are given. We define a positive definite functional ϕ on $\mathcal{A}$ by

$$\phi(a) := \phi_0(E_{0]}(a)), \quad a \in \mathcal{A}. \tag{3.7}$$

Notice that since $E_{0]}$ is sub-Markovian, ϕ is also sub-Markovian, meaning that $\phi(I \otimes I \otimes \cdots) \leq 1$.

Definition 3.1. (i) A pair $\big(\phi_0, (\mathcal{E}^{(n)})_{n\geq 0}\big)$ of a state ϕ_0 on $\mathcal{B}$ and a sequence of transition expectations $(\mathcal{E}^{(n)})_{n\geq 0}$ is called a *Markov pair* if the positive definite functional ϕ in (3.7) defines a state on $\mathcal{A}$, i.e., it is Markovian in the sense that

$$\phi(I \otimes I \otimes \cdots) = 1.$$

(ii) A Markov pair $\big(\phi_0, (\mathcal{E}^{(n)})_{n\geq 0}\big)$, or alternatively the state ϕ in (3.7) defined by the pair, is called a *nonhomogeneous* QMC with initial state ϕ_0. When $\mathcal{E}^{(n)} = \mathcal{E}$ for all n, we say that the QMC is homogeneous.

3.2. QMCs associated with UQWs. Let $\mathcal{U}$ be a UQW on $\mathbb{Z}$ with a defining unitary matrix $U = P + Q$ in (2.1). We let $\mathfrak{h} := \oplus_{j\in\mathbb{Z}}\mathbb{C}^2 \cong \mathcal{K} \otimes \mathbb{C}^2$, where $\mathcal{K} := l^2(\mathbb{Z})$, and let $\mathcal{B} := \mathcal{B}(\mathfrak{h})$. Given any initial state $\psi^{(0)} \in \mathfrak{h}$, let $\psi^{(n)} := \mathcal{U}^n(\psi^{(0)})$ be the state at time n. $\psi^{(n)}$ can be written as

$$\psi^{(n)} = \oplus_{j\in\mathbb{Z}}\psi_j^{(n)} \quad \text{or} \quad \psi^{(n)} = \sum_{j\in\mathbb{Z}} \psi_j^{(n)} \otimes |j\rangle.$$

For any vector $0 \neq \xi \in \mathbb{C}^2$, we let $\widehat{\xi} := \xi/\|\xi\|$ be the unit vector in the direction ξ. For each $n \geq 0$, and $i, j \in \mathbb{Z}$, let $A_{ij}^{(n)}$ and $M_{ij}^{(n)}$ be the linear operators on $\mathfrak{h}$

defined as follows:

$$A_{ij}^{(n)} \quad := \quad \begin{cases} |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |i\rangle\langle j|, & \psi_j^{(n)} \neq 0 \\ 0, & \psi_j^{(n)} = 0, \end{cases} \tag{3.8}$$

$$M_{ij}^{(n)} \quad := \quad \begin{cases} \|\psi_i^{(n+1)}\| |\widehat{\psi_i^{(n+1)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |i\rangle\langle j|, & \psi_j^{(n)} \neq 0,\ \psi_i^{(n+1)} \neq 0 \\ 0, & \text{otherwise}. \end{cases} \tag{3.9}$$

Using these operators, for each $n \geq 0$ and $i, j \in \mathbb{Z}$, we define also the linear operators $K_{ij}^{(n)}$ on $\mathfrak{h} \otimes \mathfrak{h}$ by

$$K_{ij}^{(n)} := A_{ij}^{(n)} \otimes M_{ij}^{(n)^*}. \tag{3.10}$$

Notice that $K_{ij}^{(n)} \in \mathcal{B} \otimes \mathcal{B}$ for any $i, j \in \mathbb{Z}$ and $n \in \mathbb{Z}_+$. Below, $\mathrm{Tr}_1(\cdot)$ means a partial trace on $\mathcal{B} \otimes \mathcal{B}$ defined by $\mathrm{Tr}_1(a \otimes b) = \mathrm{Tr}(a)b$ for trace class operators $a \otimes b \in \mathcal{B} \otimes \mathcal{B}$.

Proposition 3.2. *It holds that*

$$\sum_{i,j \in \mathbb{Z}} \mathrm{Tr}_1 \left(K_{ij}^{(n)} K_{ij}^{(n)^*} \right) \leq I_{\mathfrak{h}}.$$

Proof. By definition

$$\begin{aligned} \sum_{i,j \in \mathbb{Z}} \mathrm{Tr}_1 \left(K_{ij}^{(n)} K_{ij}^{(n)^*} \right) \quad &= \quad {\sum_j}' \sum_i \mathrm{Tr}\Big(|\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |i\rangle\langle i| \Big) \\ &\qquad \times \|\psi_i^{(n+1)}\|^2 |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |j\rangle\langle j| \\ &= \quad {\sum_j}' |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |j\rangle\langle j| \leq I_{\mathfrak{h}}. \end{aligned}$$

Here ${\sum_j}'$ means $\sum_{j:\psi_j^{(n)} \neq 0}$ and in the last we have used $|\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \leq I_{\mathbb{C}^2}$. This completes the proof. □

Now let us define for each $n \geq 0$ and $x, y \in \mathcal{B}$,

$$\mathcal{E}^{(n)}(x \otimes y) := \sum_{i,j \in \mathbb{Z}} \mathrm{Tr}_1 \Big(K_{ij}^{(n)} (x \otimes y) K_{ij}^{(n)^*} \Big). \tag{3.11}$$

Then, by Proposition 3.2, the sequence $(\mathcal{E}^{(n)})_{n \geq 0}$ becomes a (non-homogeneous) transition expectation.

Lemma 3.3. *It holds that*

$$\mathcal{E}^{(n)}(x \otimes y) = \psi^{(n+1)}(y) \sum_{j:\psi_j^{(n)} \neq 0} \langle \widehat{\psi_j^{(n)}}, x_j \widehat{\psi_j^{(n)}} \rangle |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}| \otimes |j\rangle\langle j|. \tag{3.12}$$

Proof. By definition, we see that

$$\begin{aligned}
\mathcal{E}^{(n)}(x\otimes y) &= \sum_{i,j\in\mathbb{Z}} \mathrm{Tr}_1\left(K_{ij}^{(n)}(x\otimes y)K_{ij}^{(n)^*}\right)\\
&= \sum_{j:\psi_j^{(n)}\neq 0} \langle \widehat{\psi_j^{(n)}}, x_j\widehat{\psi_j^{(n)}}\rangle \sum_i M_{ij}^{(n)^*} y M_{ij}^{(n)}\\
&= \psi^{(n+1)}(y)\sum_{j:\psi_j^{(n)}\neq 0} \langle \widehat{\psi_j^{(n)}}, x_j\widehat{\psi_j^{(n)}}\rangle |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}|\otimes|j\rangle\langle j|.
\end{aligned}$$

The proof is completed. □

Remark 3.4. In the definition of the operators $M_{ij}^{(n)}$ in (3.9), or in the definition of the transition expectation $\mathcal{E}^{(n)}$ in the above, the state at time $n+1$ was used. But, notice that $\psi_i^{(n+1)} = P\psi_{i+1}^{(n)} + Q\psi_{i-1}^{(n)}$. Therefore, we see that the transition expectation at time n is totally determined by the state at the present, $\psi^{(n)}$, and the matrices P and Q.

Lemma 3.5. *For any $n\geq 0$, $k\geq 1$, and $x\in\mathcal{B}$,*

$$\mathcal{E}^{(n)}(x\otimes\mathcal{E}^{(n+1)}(I\otimes\cdots\otimes\mathcal{E}^{(n+k)}(I\otimes I))) = \mathcal{E}^{(n)}(x\otimes I).$$

Proof. First we show that for any $n\geq 0$,

$$\mathcal{E}^{(n)}(I\otimes\mathcal{E}^{(n+1)}(I\otimes I)) = \mathcal{E}^{(n)}(I\otimes I).$$

In fact, by (3.12),

$$\mathcal{E}^{(n+1)}(I\otimes I) = \sum_{j:\psi_j^{(n+1)}\neq 0} |\widehat{\psi_j^{(n+1)}}\rangle\langle\widehat{\psi_j^{(n+1)}}|\otimes|j\rangle\langle j|.$$

Thus, by again (3.12),

$$\begin{aligned}
\mathcal{E}^{(n)}(I\otimes\mathcal{E}^{(n+1)}(I\otimes I)) &= \psi^{(n+1)}\Big(\sum_{l:\psi_l^{(n+1)}\neq 0} |\widehat{\psi_l^{(n+1)}}\rangle\langle\widehat{\psi_l^{(n+1)}}|\otimes|l\rangle\langle l|\Big)\\
&\qquad\times\sum_{j:\psi_j^{(n)}\neq 0} |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}|\otimes|j\rangle\langle j|\\
&= \sum_{j:\psi_j^{(n)}\neq 0} |\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}|\otimes|j\rangle\langle j| = \mathcal{E}^{(n)}(I\otimes I).
\end{aligned}$$

From this we see that

$$\begin{aligned}
&\mathcal{E}^{(n)}(x\otimes\mathcal{E}^{(n+1)}(I\otimes\cdots\otimes\mathcal{E}^{(n+k)}(I\otimes I)))\\
=\;&\mathcal{E}^{(n)}(x\otimes\mathcal{E}^{(n+1)}(I\times I))\\
=\;&\mathcal{E}^{(n)}\Big(x\otimes\Big(\sum_{l:\psi_l^{(n+1)}\neq 0}|\widehat{\psi_l^{(n+1)}}\rangle\langle\widehat{\psi_l^{(n+1)}}|\otimes|l\rangle\langle l|\Big)\Big)\\
=\;&\psi^{(n+1)}\Big(\sum_{l:\psi_l^{(n+1)}\neq 0}|\widehat{\psi_l^{(n+1)}}\rangle\langle\widehat{\psi_l^{(n+1)}}|\otimes|l\rangle\langle l|\Big)\\
&\quad\times\sum_{j:\psi_j^{(n)}\neq 0}\langle\widehat{\psi_j^{(n)}},x_j\widehat{\psi_j^{(n)}}\rangle|\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}|\otimes|j\rangle\langle j|\\
=\;&\sum_{j:\psi_j^{(n)}\neq 0}\langle\widehat{\psi_j^{(n)}},x_j\widehat{\psi_j^{(n)}}\rangle|\widehat{\psi_j^{(n)}}\rangle\langle\widehat{\psi_j^{(n)}}|\otimes|j\rangle\langle j|=\mathcal{E}^{(n)}(x\otimes I).
\end{aligned}$$

The proof is completed. □

By the consistency given in Lemma 3.5, we can define for $a_{n]}=a_0\otimes\cdots\otimes a_n\otimes I_{[n+1}\in\mathcal{A}_{n]}$, the completely positive map

$$E_{0]}(a_{n]}):=\mathcal{E}^{(0)}(a_0\otimes\mathcal{E}^{(1)}(a_1\otimes\cdots\otimes\mathcal{E}^{(n)}(a_n\otimes I))),\tag{3.13}$$

and for $a=a_0\otimes a_1\otimes\cdots\in\mathcal{A}$,

$$E_{0]}(a):=\lim_{n\to\infty}E_{0]}(a_{n]}).\tag{3.14}$$

Proposition 3.6. *For $a_{n]}=a_0\otimes\cdots\otimes a_n\otimes I_{[n+1}\in\mathcal{A}_{n]}$,*

$$E_{0]}(a_{n]})=\prod_{k=1}^{n}\psi^{(k)}(a_k)\sum_{i_0:\psi_{i_0}^{(0)}\neq 0}\langle\widehat{\psi_{i_0}^{(0)}},a_0(i_0)\widehat{\psi_{i_0}^{(0)}}\rangle|\widehat{\psi_{i_0}^{(0)}}\rangle\langle\widehat{\psi_{i_0}^{(0)}}|\otimes|i_0\rangle\langle i_0|.$$

Therefore,

$$\psi^{(0)}(E_{0]}(a_{n]}))=\prod_{k=0}^{n}\psi^{(k)}(a_k).$$

Proof. This follows from (3.13) and (3.12). □

Let us define a functional $\varphi:\mathcal{A}\to\mathbb{C}$ by

$$\varphi(a):=\psi^{(0)}(E_{0]}(a)).\tag{3.15}$$

Corollary 3.7. *The functional φ in (3.15) is a QMC. In other words, the pair $(\psi^{(0)},(\mathcal{E}^{(n)})_{n\geq 0})$ is a Markov pair.*

Proof. From Proposition 3.6, it follows that

$$\varphi(I\otimes I\otimes\cdots\otimes I\otimes\overset{n\text{th}}{x}\otimes I_{[n+1})=\psi^{(n)}(x).\tag{3.16}$$

In particular, we have $\varphi(I\otimes I\otimes\cdots)=1$. Therefore, φ, or the pair $(\psi^{(0)},(\mathcal{E}^{(n)})_{n\geq 0})$, is a QMC. □

In the sequel, we write $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ and call it a QMC associated with the UQW with initial state $\psi^{(0)}$.

4. Reducibility and Irreducibility of QMCs Associated With UQWs

4.1. Definition and properties. For a projection $p \in \mathcal{B}$, we let

$$p_{[n} := I \otimes \cdots I \otimes \overset{n\text{th}}{p} \otimes p \otimes \cdots .$$

Let us define

$$\mathcal{P}_0 := \{p_{[n} : p,\ \text{a projection in } \mathcal{B},\ n \geq 0\}.$$

As in [18], we define the reducibility and irreducibility of the QMC as follows.

Definition 4.1. The QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ associated with a UQW is called reducible if there is a nontrivial projection $p_{[n_0} \in \mathcal{P}_0$ such that

$$E_{0]}(p_{[n_0} a p_{[n_0}) = E_{0]}(a) \text{ for all } a \in \mathcal{A}.$$

Otherwise, it is called irreducible.

The following property can be shown as in [18, Theorem 3.7].

Lemma 4.2. *The QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ associated with a UQW is reducible if and only if there is a $p_{[n_0} \in \mathcal{P}_0$ such that $E_{0]}(p_{[n_0}) = I$.*

Theorem 4.3. *The QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ associated with a UQW is reducible if and only if there is a projection $p \in \mathcal{B}$ and $n_0 \in \mathbb{N}$ such that $\psi^{(n)}(p) = 1$ for all $n \geq n_0$.*

Proof. We may assume $n_0 \geq 1$. Notice that by Proposition 3.6,

$$E_{0]}(I \otimes I \otimes \cdots) = \sum_{i_0 : \psi^{(0)}_{i_0} \neq 0} |\widehat{\psi^{(0)}_{i_0}}\rangle\langle\widehat{\psi^{(0)}_{i_0}}| \otimes |i_0\rangle\langle i_0|,$$

and

$$E_{0]}(p_{[n_0,n]}) = \prod_{k=n_0}^{n} \psi^{(k)}(p) \sum_{i_0 : \psi^{(0)}_{i_0} \neq 0} |\widehat{\psi^{(0)}_{i_0}}\rangle\langle\widehat{\psi^{(0)}_{i_0}}| \otimes |i_0\rangle\langle i_0|.$$

From this and the fact that $E_{0]}(p_{[n_0}) = \lim_{n\to\infty} E_{0]}(p_{[n_0,n]})$, we see that $E_{0]}(p_{[n_0})$ $= E_{0]}(I \otimes I \otimes \cdots)$ if and only if $\psi^{(n)}(p) = 1$ for all $n \geq n_0$. This completes the proof. $\square$

Example 4.4 (Reducible UQW)**.** Let us consider the unitary matrix

$$U = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

It is easy to check that $\mathcal{U}^2(\psi) = \psi$ for any state $\psi \in \mathfrak{h}$. Moreover, if $\psi = (\psi_i)_{i\in\mathbb{Z}}$ is supported in $\Lambda := [-n_0, n_0]$, in the sense that $\psi_i = 0$ for $i \notin \Lambda$, then $\mathcal{U}(\psi)$ is supported in $\overline{\Lambda} := [-(n_0 + 1), n_0 + 1]$. Now suppose that the initial state $\psi^{(0)}$ is locally supported, say $\mathrm{supp}(\psi^{(0)}) \subset \Lambda = [-n_0, n_0]$. Let $q \in \mathcal{B}(\mathcal{H})$ be any nontrivial projection and define a projection $p = \oplus_{i\in\mathbb{Z}} p_i$ by

$$p_i = \begin{cases} I, & i \in \overline{\Lambda}, \\ q, & i \notin \overline{\Lambda}. \end{cases}$$

By the above observation, we see that $\psi^{(n)}(p) = 1$ for all $n \geq 0$. By Theorem 4.3, the QMC for this UQW is reducible.

4.2. A sufficient condition for the irreducibility. In this subsection, we provide with a meaningful class of irreducible QMCs for UQWs.

Let $\mathcal{U}$ be the UQW with a generating unitary matrix U in (2.1), and let $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ be the QMC associated with $\mathcal{U}$.

Theorem 4.5. *Suppose that the unitary matrix U in* (2.1) *has nonzero components: $abcd \neq 0$. Then, for any initial state $\psi^{(0)}$ supported on the origin, the QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ associated with $\mathcal{U}$ is irreducible.*

The main ingredient of the proof is to use the path-wise computation of the probability density of the UQW developed by Konno [26, 27]. Let $\phi = [\alpha, \beta]^T \in \mathbb{C}^2$ be a unit vector and let

$$\psi^{(0)} := \phi \otimes |0\rangle \in \mathfrak{h}$$

be the initial state. As in [27], in addition to the matrices P and Q in (2.1), let us define

$$R := \begin{bmatrix} c & d \\ 0 & 0 \end{bmatrix}, \quad S := \begin{bmatrix} 0 & 0 \\ a & b \end{bmatrix}.$$

Konno introduced a transition kernel to determine the state at any time and any position in the following way. The state at time n and at the position $k \in \mathbb{Z}$ is $\psi_k^{(n)} \equiv \psi_k^{(n)}(\phi)$, which can be written by using the transition kernel:

$$\psi_k^{(n)}(\phi) = \Xi(l,m)\phi, \tag{4.1}$$

where $l, m \in \mathbb{N}$ are such that $l + m = n$ and $-l + m = k$, and

$$\Xi(l,m) = \sum_{\substack{l_j, m_j \geq 0; \\ l_1+\cdots+l_n = l,\, m_1+\cdots+m_n = m}} P^{l_1} Q^{m_1} \cdots P^{l_n} Q^{m_n}. \tag{4.2}$$

Konno has concretely computed the kernel [27, Lemma 2]:

Lemma 4.6. *Suppose $abcd \neq 0$. Then, for $l \wedge m \geq 1$,*

$$\begin{aligned} & \Xi(l,m) \\ = \quad & a^l \overline{a}^m \Delta^m \sum_{r=1}^{l\wedge m} \left(-\frac{|b|^2}{|a|^2}\right)^r \binom{l-1}{r-1}\binom{m-1}{r-1} \left[\frac{l-r}{ar}P + \frac{m-r}{\Delta\overline{a}r}Q - \frac{1}{\Delta\overline{b}}R + \frac{1}{b}S\right] \\ =: \quad & p_n(l,m)P + q_n(l,m)Q + r_n(l,m)R + s_n(l,m)S, \end{aligned} \tag{4.3}$$

where $\Delta := \det U$.

Proof of Theorem 4.5. Suppose on the contrary the QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\ge 0})$ is reducible for some initial state $\psi^{(0)} = \phi \otimes |0\rangle$. Then, it means that there is a one-dimensional projection $|\xi\rangle\langle\xi|$ for some unit vector $\xi \in \mathbb{C}^2$ and a position $k \in \mathbb{Z}$ such that $|\xi\rangle\langle\xi|\psi_k^{(n)} = \psi_k^{(n)}$ for all $n \ge n_0$ for some n_0, or equivalently, there is a constant $c \in \mathbb{C}$ such that the vector $\psi_k^{(n)} = [\psi_k^{(n)}(1), \psi_k^{(n)}(2)]^T$ satisfies $\psi_k^{(n)}(1) = c\psi_k^{(n)}(2)$ for all $n \ge n_0$. Assume first that $\phi = [a,b]^T$. Then, for $l, m \in \mathbb{N}$ such that $l+m = n$ and $-l+m = k$, since $\left\langle \begin{bmatrix} c \\ d \end{bmatrix}, \begin{bmatrix} a \\ b \end{bmatrix} \right\rangle = 0$, we have

$$\psi_k^{(n)} = \Xi(l,m)\phi = \begin{bmatrix} p_n(l,m) \\ s_n(l,m) \end{bmatrix}, \tag{4.4}$$

with $p_n(l,m)$ and $s_n(l,m)$ defined in (4.3). Following the notations in [27], let us define for $\nu, \mu > -1$ and $x \in [-1,1]$,

$$P_n^{\nu,\mu}(x) := \frac{\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(\nu+1)}\, {}_2F_1(-n, n+\nu+\mu+1; \nu+1; (1-x)/2),$$

where $\Gamma(z)$ is the Gamma function and ${}_2F_1(a,b;c;z)$ is the hypergeometric function:

$${}_2F_1(a,b;c;z) = \sum_{n=0}^{\infty} \frac{\Gamma(a+n)}{\Gamma(a)} \frac{\Gamma(b+n)}{\Gamma(b)} \frac{\Gamma(c)}{\Gamma(c+n)} \cdot \frac{z^n}{n!}.$$

Define for $i = 0, 1$,

$$\rho_{n,k,i} := P_{k-1}^{i, n-2k}(2|a|^2 - 1). \tag{4.5}$$

Then Konno has obtained the following relations:

$$\sum_{r=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{r-1} \frac{1}{r} \binom{k-1}{r-1} \binom{n-k-1}{r-1} = \frac{1}{k} |a|^{-2(k-1)} \rho_{n,k,1} \tag{4.6}$$

$$\sum_{r=1}^{k} \left(-\frac{|b|^2}{|a|^2}\right)^{r-1} \binom{k-1}{r-1} \binom{n-k-1}{r-1} = |a|^{-2(k-1)} \rho_{n,k,0}. \tag{4.7}$$

(see [27, page 1190].) Without loss of generality we may assume $k \ge 0$. Then, from (4.3), (4.4), (4.6) and (4.7), we see that

$$\frac{p_n(l,m)}{s_n(l,m)} = \frac{b}{a}\left(\frac{\rho_{n,l,1}}{\rho_{n,l,0}} - 1\right).$$

Therefore, $\frac{p_n(l,m)}{s_n(l,m)} = \text{const.}$ if and only if $\frac{\rho_{n,l,1}}{\rho_{n,l,0}} = \text{const.}$, but the latter is far from the case by definition of $\rho_{n,k,i}$'s in (4.5). We conclude that the QMC $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\ge 0})$ is not reducible. The same conclusion holds if we assume $\phi = [c,d]^T$. Finally, for any unit vector $\phi = [\alpha, \beta]^T \in \mathbb{C}^2$, since $\{[a,b]^T, [c,d]^T\}$ is a basis of $\mathbb{C}^2$, we can write

$$\begin{bmatrix} \alpha \\ \beta \end{bmatrix} = c_1 \begin{bmatrix} a \\ b \end{bmatrix} + c_2 \begin{bmatrix} c \\ d \end{bmatrix},$$

for some constants c_1 and c_2. Applying the above arguments, we see that the QMC $(\psi^{(0)}, (\mathcal{E}^{(n)})_{n\ge 0})$ can not be reducible with $\psi^{(0)} = \phi \otimes |0\rangle$. This completes the proof. $\square$

5. Recurrence of QMCs Associated With UQWs

5.1. Recurrence and transience. We recall the definition of stopping times from [7].

Given a projection $e \in \mathcal{B}$, the stopping times associated with e are defined as follows.

$$\begin{aligned}
\tau_0 &= e \otimes I_{[1} = J_0(e), \\
\tau_1 &= e^{\perp} \otimes e \otimes I_{[2} = J_0(e^{\perp})J_1(e), \\
&\cdots \\
\tau_k &= (e^{\perp})^{\otimes k} \otimes e \otimes I_{[k+1} = J_0(e^{\perp}) \cdots J_{k-1}(e^{\perp})J_k(e). \qquad (5.1)
\end{aligned}$$

We also define

$$\tau_\infty^n := (e^{\perp})^{\otimes(n+1)} \otimes I_{[n+1} \qquad (5.2)$$

$$\tau_\infty := \lim_{n\to\infty} \tau_\infty^n = \otimes_{\mathbb{Z}_+} e^{\perp}. \qquad (5.3)$$

In this subsection we discuss the recurrence and transience of the QMCs associated with UQWs. We start with a definition following [7].

Definition 5.1. Let $\varphi = (\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ be a QMC associated with a UQW. A projection $e \in \mathcal{B}$ with $\psi^{(0)}(e) > 0$ is called recurrent if

$$\sum_{n\geq 1} \varphi\Big(e \otimes \big(\otimes e^{\perp}\big)^{(n-1)} \otimes e \otimes I_{[n+1}\Big) = \psi^{(0)}(e). \qquad (5.4)$$

A projection e is called transient if it is not recurrent.

Remark 5.2. The above definition of recurrence was named as the φ-recurrence in [19].

Proposition 5.3. *Let $\varphi = (\psi^{(0)}, (\mathcal{E}_n)_{n\geq 0})$ be the QMC associated with the UQW with initial state $\psi^{(0)}$. Then a projection e with $\psi^{(0)}(e) > 0$ is recurrent if and only if*

$$\lim_{n\to\infty} \varphi\left(e \otimes (e^{\perp})^{\otimes n} \otimes I_{[n+1}\right) = 0.$$

Proof. We see that

$$\begin{aligned}
E_{0]}(e \otimes I_{[1}) &= E_{0]}(e \otimes e \otimes I_{[2}) + E_{0]}(e \otimes e^{\perp} \otimes I_{[2}) \\
&= E_{0]}(e \otimes e \otimes I_{[2}) + E_{0]}(e \otimes e^{\perp} \otimes e \otimes I_{[3}) + E_{0]}(e \otimes e^{\perp} \otimes e^{\perp} \otimes I_{[3}) \\
&= \cdots \\
&= \sum_{k=1}^{n} E_{0]}(e \otimes (e^{\perp})^{\otimes(k-1)}) \otimes e \otimes I_{[k+1} + E_{0]}(e \otimes (e^{\perp})^{\otimes n} \otimes I_{[n+1}).
\end{aligned}$$

Taking the expectation w.r.t. the initial state $\psi^{(0)}$ on both sides and letting n go to infinity we get

$$\begin{aligned}
\psi^{(0)}(e) &= \psi^{(0)}\Big(E_{0]}\Big[\sum_{n\geq 1} e \otimes \big(\otimes e^{\perp}\big)^{(n-1)} \otimes e \otimes I_{[n+1}\Big]\Big) \\
&\qquad + \lim_{n\to\infty} \psi^{(0)}\left(E_{0]}(e \otimes (e^{\perp})^{\otimes n} \otimes I_{[n+1})\right).
\end{aligned}$$

Noticing $\varphi(\cdot) = \psi^{(0)}(E_{0]}(\cdot))$, we get the result. $\square$

Theorem 5.4. *Let $e \in \mathcal{B}$ be a projection with $\psi^{(0)}(e) > 0$. Then the following conditions are equivalent.*

(i) *e is recurrent.*
(ii) $\prod_{n=1}^{\infty} \psi^{(n)}(e^{\perp}) = 0$. *(Or, equivalently $\sum_{n=1}^{\infty} \psi^{(n)}(e) = \infty$).*

Proof. By Proposition 5.3, using the computation in Proposition 3.6, e is recurrent if and only if

$$\left(\lim_{n\to\infty} \prod_{k=1}^{n} \psi^{(k)}(e^{\perp})\right) \psi^{(0)}(e) = 0.$$

Since $\psi^{(0)}(e) > 0$, the result follows. $\square$

5.2. SJK-recurrence. In [17], the authors discussed some other type of recurrences for the unitary and open quantum walks, namely the monitored recurrence and SJK-recurrence. The former is based on the monitoring procedure introduced in [15, 21] and the latter uses the concept of Pólya number and is named after the work of Štefaňák, Jex, and Kiss [31]. In this subsection, we compare the SJK-recurrence and the concept introduced here by QMCs. For it we first introduce the SJK-recurrence of UQWs following [17, 31]. Let $|\psi\rangle \in \mathbb{C}^2$ be a unit vector. Starting from the initial state $|\psi\rangle \otimes |0\rangle \in \mathfrak{h}$, let $p_0(n) \equiv p_0(n;\psi)$ denote the probability of reaching site $|0\rangle$ at time n. Let

$$\overline{p}_k := \prod_{n=1}^{k} [1 - p_0(n)]$$

denote the probability of not finding the particle at the origin in the first k trials. We define

$$\overline{p} \equiv \overline{p}(\psi) := \prod_{n=1}^{\infty} [1 - p_0(n)].$$

The number $p \equiv p(\psi) := 1 - \overline{p}$ is called the Pólya number of the UQW.

Definition 5.5. We say that a UQW is SJK-*recurrent* with respect to the state ψ if $p = p(\psi) = 1$.

Proposition 5.6. *Let $\psi \in \mathbb{C}^2$ be a unit vector. Then a UQW is SJK-recurrent with respect to the state ψ if and only if the projection $e := |\psi\rangle\langle\psi| \otimes |0\rangle\langle 0| \in \mathcal{B}$ is recurrent for the QMC $(\psi^{(0)}, (\mathcal{E}^{(n)})_{n\geq 0})$ associated with the UQW, where $\psi^{(0)}$ is the initial state $|\psi\rangle \otimes |0\rangle \in \mathfrak{h}$.*

Proof. Let e be the projection given in the statement of the proposition. By Theorem 5.4, e is recurrent if and only if

$$\prod_{n=1}^{\infty} \psi^{(n)}(e^{\perp}) = 0. \tag{5.5}$$

On the other hand, we see that $p_0(n) = p_0(n;\psi) = \psi^{(n)}(e)$, and hence (5.5) is equivalent to $\overline{p} = \overline{p}(\psi) = 0$. This completes the proof. $\square$

5.3. Example: Hadamard walk. In this subsection we discuss the recurrence and transience problem for the concrete model of Hadamard walk. The generating unitary matrix U in (2.1) for the Hadamard walk, denoted by H, is given by

$$H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{5.6}$$

Proposition 5.7. *The projection $e := I \otimes |0\rangle\langle 0| \in \mathcal{B}$ is recurrent for the QMC associated with the Hadamard walk starting from the origin.*

For the proof, we will use the Fourier transform for the quantum walk, which was developed in several literature (see [24] and references therein).

For any vector $\psi = (\psi_x)_{x\in\mathbb{Z}} \in \mathfrak{h} = l^2(\mathbb{Z}, \mathbb{C}^2)$, its Fourier transform is defined by

$$\widehat{\psi}(k) := \sum_{x\in\mathbb{Z}} e^{ikx}\psi_x, \quad k \in [0, 2\pi].$$

For the generating unitary matrix U in (2.1), define

$$U(k) := \begin{bmatrix} e^{-ik}a & e^{-ik}b \\ e^{ik}c & e^{ik}d \end{bmatrix}.$$

Then the evolution of the quantum walk in the Fourier transform space is given by ([24, eq. (2.16)])

$$\widehat{\psi^{(n)}}(k) = U(k)^n \widehat{\psi^{(0)}}(k). \tag{5.7}$$

Let $\gamma(k)$ be the function such that

$$\cos\gamma(k) = |a|\cos k, \quad k \in [0, 2\pi],$$

and θ_1, θ_2 be the phases of a and b:

$$a = |a|e^{i\theta_1}, \quad b = |b|e^{i\theta_2}.$$

Then $U(k)$ is diagonalized as (see [24])

$$U(k) = S(k-\theta_1) \begin{bmatrix} e^{i\gamma(k-\theta_1)} & 0 \\ 0 & e^{-i\gamma(k-\theta_1)} \end{bmatrix} S(k-\theta_1)^*,$$

where the unitary matrix $S(k)$ is given by

$$S(k) = \begin{bmatrix} \frac{1}{\sqrt{1+|\alpha_+(k)|^2}} & \frac{1}{\sqrt{1+|\alpha_-(k)|^2}} \\ \frac{\alpha_+(k)}{\sqrt{1+|\alpha_+(k)|^2}} & \frac{\alpha_-(k)}{\sqrt{1+|\alpha_-(k)|^2}} \end{bmatrix}$$

with

$$\alpha_\pm(k) = ie^{i(k+\theta_1-\theta_2)} \left(|a|/|b|\, \sin k \pm \sqrt{1 + (|a|/|b|\, \sin k)^2} \right).$$

Finally we state so called the method of stationary phase:

Lemma 5.8. ([14, p220]) *Suppose that $f \in C[a, b]$ and $\alpha \in C^2[a, b]$ with α real. Consider the integral of the form:*

$$I(n) := \int_a^b \exp\{in\alpha(t)\} f(t)dt. \tag{5.8}$$

Suppose further that $\alpha'(c) = 0$ *in a unique point* $c \in [a, b]$ *and* $\alpha''(c) \neq 0$. *Then as* $n \to \infty$, *we have the asymptotic behavior of* $I(n)$*:*

$$I(n) = \exp\{in\alpha(c)\} f(c) \sqrt{\frac{2}{n|\alpha''(c)|}} \exp\left\{\frac{i\pi\mu}{4}\right\} + \mathrm{o}(n^{-1/2}), \qquad (5.9)$$

where $\mu = \operatorname{sign} \alpha''(c)$.

Proof of Proposition 5.7. For the Hadamard walk with $U = H$ in (5.6), we have $\theta_1 = \theta_2 = 0$ and $\gamma(k) = \cos^{-1}(\frac{1}{\sqrt{2}} \cos k)$. The function $\gamma(k)$ satisfies $\gamma'(k) = 0$ at two points $k = 0 \equiv 2\pi$ and $k = \pi$. Moreover, $S(k)$ is continuous and $\gamma''(0) = 1$ and $\gamma''(\pi) = -1$. Therefore, by (5.7) and Lemma 5.8, we see that for any $x \in \mathbb{Z}$, the vector

$$\psi_x^{(n)} = \frac{1}{2\pi} \int_0^{2\pi} e^{-ixk} \widehat{\psi^{(n)}}(k) dk$$

has its components of order $1/\sqrt{n}$ when n is large. So, we have $\sum_{n=1}^{\infty} \psi^{(n)}(e) = \sum_{n=1}^{\infty} \|\psi_0^{(n)}\|^2 = \infty$, and hence e is recurrent by Theorem 5.4. □

Remark 5.9. Following the same method of the proof of Proposition 5.7, the statement of Proposition 5.7 can be extended to the general walk with unitary matrix U in (2.1) such that $abcd \neq 0$.

5.4. Example: multi-dimensional walk. In this subsection we discuss the recurrence/transience for the QMC associated with the multi-dimensional UQWs. As we have seen in the previous subsection, both the classical and (unitary) quantum walks are recurrent for 1-dimensional walks. However, for the multi-dimensional walks, we will see a big difference between the quantum walks and the classical walks. We start with the definition of multi-dimensional UQWs and their Fourier transforms.

Let $d \geq 1$ be any integer and we consider UQWs on $\mathbb{Z}^d$. Let U be a $2d \times 2d$ unitary matrix and for $i = 1, \cdots, d$, let $E_i^{(\pm)}$ be the rank one projections defined by

$$\begin{aligned} E_i^{(-)}(l, m) &= \begin{cases} 1, & \text{for } (l, m) = (2i-1, 2i-1) \\ 0, & \text{otherwise} \end{cases}, \\ E_i^{(+)}(l, m) &= \begin{cases} 1, & \text{for } (l, m) = (2i, 2i) \\ 0, & \text{otherwise} \end{cases}. \end{aligned}$$

Define

$$U_i^{(\pm)} := E_i^{(\pm)} U, \quad i = 1, \cdots, d. \qquad (5.10)$$

The d-dimensional UQW is an evolution on $\mathfrak{h} = l^2(\mathbb{Z}^d, \mathbb{C}^{2d})$ defined by

$$\psi_x^{(n+1)} = \sum_{i=1}^{d} \left(U_i^{(-)} (T_i \psi^{(n)})_x + U_i^{(+)} (T_i^* \psi^{(n)})_x \right), \quad x \in \mathbb{Z}^d, \qquad (5.11)$$

where T_i, $i = 1, \cdots, d$ is the translation in the ith axis:

$$(T_i \psi)_x = \psi_{x + \mathbf{e}_i}, \qquad (5.12)$$

with $\mathbf{e}_i$ the unit vector in the ith axis. As in the 1-dimensional walk, we can represent the walk in Fourier transform space:

$$\widehat{\psi^{(n)}}(k) = U(k)^n \widehat{\psi^{(0)}}(k), \quad k = (k_1, \cdots, k_d) \in [0, 2\pi]^d, \tag{5.13}$$

where $U(k)$ is the unitary matrix given by

$$\begin{aligned} U(k) &= \sum_{j=1}^{d} \left(e^{-ik_j} E_j^{(-)} + e^{ik_j} E_j^{(+)} \right) U \\ &= \begin{bmatrix} e^{-ik_1} & & & & \\ & e^{ik_1} & & 0 & \\ & & \ddots & & \\ & 0 & & e^{-ik_d} & \\ & & & & e^{ik_d} \end{bmatrix} U. \end{aligned} \tag{5.14}$$

Let

$$U(k) = S(k) \begin{bmatrix} e^{i\gamma_1^{(+)}(k)} & & & & \\ & e^{i\gamma_1^{(-)}(k)} & & 0 & \\ & & \ddots & & \\ & 0 & & e^{i\gamma_d^{(+)}(k)} & \\ & & & & e^{i\gamma_d^{(-)}(k)} \end{bmatrix} S(k)^*, \tag{5.15}$$

be a diagonalization of $U(k)$, where $S(k)$ is a unitary matrix whose columns consist of the eigenvectors of $U(k)$.

One of the simplest way to construct a d-dimensional walk is to use a block-diagonal unitary from a 2×2 unitary matrix, namely to consider a unitary of the form:

$$U = \begin{bmatrix} U_1 & 0 & \cdots & 0 \\ 0 & U_2 & \cdots & 0 \\ & & \ddots & \\ 0 & \cdots & & 0 \\ 0 & \cdots & 0 & U_d \end{bmatrix}, \tag{5.16}$$

where $U_1, \cdots, U_d$ are 2×2 unitary matrices.

Once a d-dimensional UQW is defined, it is easy to construct the associated QMC following the method given in Subsection 3.2. We skip, however, the tedious procedure.

In order to investigate the recurrence/transience problem for multi-dimensional quantum walks, we will use the multi-dimensional stationary phase method, as in the 1-dimensional walk. We state it for a reference. Consider the following integral

$$I(n) = \int_D g(x) e^{inf(x)} dx, \quad x \in \mathbb{R}^d, \tag{5.17}$$

where $D \subset \mathbb{R}^d$ is a bounded domain and f and g are C^∞-functions in D. Then as n goes to infinity

$$I(n) \sim g(x_0) |\det A|^{-1/2} \exp\left\{ inf(x_0) + i\frac{1}{4}\pi\sigma \right\} \left(\frac{2\pi}{n} \right)^{d/2}, \tag{5.18}$$

where x_0 is a stationary point of f (i.e., $\nabla f(x_0) = 0$), A is the Hessian of f defined by

$$A = \left[\frac{\partial^2 f}{\partial x_i \partial x_j}\right]\Big|_{x=x_0},$$

and σ is the signature of the matrix A, i.e., the number of the positive eigenvalues minus the number of negative eigenvalues of A. This approximation is valid only when x_0 is nondegenerate (i.e., $\det A \neq 0$) and lies in the interior of D (see [29] and references therein).

Theorem 5.10. *Consider the UQW on $\mathbb{Z}^d$, $d \geq 2$, defined by* (5.11) *from a $2d \times 2d$ unitary matrix U. (i) Suppose that $\gamma_i^{(\pm)}(k)$, $i = 1, \cdots, d$, and $S(k)$ in* (5.15) *are C^∞-functions on $(0, 2\pi)^d$ and at least one of $\gamma_i^{(\pm)}(k)$ has finitely many isolated nondegenerate stationary points. Then with a certain initial condition, the projection $e := I \otimes |0\rangle\langle 0|$ is transient for the QMC associated with the UQW. (ii) Suppose that the generating unitary matrix U is of the block diagonal form as in* (5.16)*, where the components of U_i, $i = 1, \cdots, d$, are all non-zero. Then, for all $d \geq 2$ (and hence for all $d \geq 1$), the projection $e := I \otimes |0\rangle\langle 0|$ is recurrent for the associated QMC.*

Proof. (i) For $e := I \otimes |0\rangle\langle 0|$, $\psi^{(n)}(e) = \|\psi_0^{(n)}\|^2$ and

$$\begin{aligned} \psi_0^{(n)} &= \frac{1}{(2\pi)^d} \int_0^{2\pi} \widehat{\psi^{(n)}}(k) dk \\ &= \frac{1}{(2\pi)^d} \int_0^{2\pi} U(k)^n \widehat{\psi^{(0)}}(k) dk. \end{aligned} \tag{5.19}$$

Let $X(k) \in \mathbb{C}^d$ be a normalized eigenvector of $U(k)$ with eigenvalue $e^{i\gamma(k)}$ such that $\gamma(k)$ has finitely many isolated nondegenerate stationary points. We take the initial state $\widehat{\psi^{(0)}}(k) := X(k)$. Then, we get from (5.19)

$$\psi_0^{(n)} = \frac{1}{(2\pi)^d} \int_0^{2\pi} e^{in\gamma(k)} X(k) dk.$$

By the hypotheses and by using the stationary phase method in (5.17)-(5.18), we see that $\psi_0^{(n)}$ is of order $1/n^{d/2}$ when n is large. So, $\sum_{n=1}^\infty \|\psi_0^{(n)}\|^2 < \infty$ for $d \geq 2$, and the conclusion follows.
(ii) If U is of the block diagonal form as in (5.16), the matrices $D(k)$ and $S(k)$ in (5.15) have also the same block diagonal form. Each block $S(k)D(k)^n S(k)^*$ contains a single variable from $k_1, \cdots, k_n$ and thus by the same method done in the previous subsection for 1-dimensional walk, we see that $\psi_0^{(n)}$ is of order $1/\sqrt{n}$ no matter how the dimension is. Therefore $\sum_{n=1}^\infty \|\psi_0^{(n)}\|^2 = \infty$ and the conclusion follows. $\square$

Example 5.11. Let us consider 2-dimensional Grover walk whose generating unitary matrix is

$$U = \frac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}. \tag{5.20}$$

Then the corresponding unitary matrix

$$U(k_1, k_2) := \frac{1}{2}\begin{bmatrix} -e^{-ik_1} & e^{-ik_1} & e^{-ik_1} & e^{-ik_1} \\ e^{ik_1} & -e^{ik_1} & e^{ik_1} & e^{ik_1} \\ e^{-ik_2} & e^{-ik_2} & -e^{-ik_2} & e^{-ik_2} \\ e^{ik_2} & e^{ik_2} & e^{ik_2} & -e^{ik_2} \end{bmatrix}$$

has the eigenvalues $\{1, -1, e^{i\gamma(k_1,k_2)}, e^{-i\gamma(k_1,k_2)}\}$ and the corresponding orthonormal (in $\mathbb{C}^4$) eigenvectors:

$$\left\{ c(k_1, k_2) \left[\frac{1}{1+e^{i(\gamma+k_1)}}, \frac{1}{1+e^{i(\gamma-k_1)}}, \frac{1}{1+e^{i(\gamma+k_2)}}, \frac{1}{1+e^{i(\gamma-k_2)}} \right]^T \right\},$$

for $\gamma = 0,\ \pi,\ \pm\gamma(k_1, k_2)$. Here $\gamma(k_1, k_2)$ is defined by

$$\cos\gamma(k_1, k_2) = \frac{1}{2}(\cos k_1 + \cos k_2)$$

and $c(k_1, k_2)$ is the normalization constant given by

$$c(k_1, k_2) = \sqrt{\frac{(1+\cos(\gamma+k_1))(1+\cos(\gamma+k_2))}{(1+\cos(\gamma+k_1)) + (1+\cos(\gamma+k_2))}}, \quad \gamma = 0,\ \pi,\ \pm\gamma(k_1, k_2).$$

Let us take the initial condition

$$\widehat{\psi^{(0)}}(k_1, k_2) := c\left[e^{-ik_1} - \cos k_2, e^{ik_1} - \cos k_2, i\sin k_2, -i\sin k_2\right]^T,$$

where c is the normalization constant such that $\|\widehat{\psi^{(0)}}\|_{L^2([0,2\pi]^2)} = 1$. When $\widehat{\psi^{(0)}}(k_1, k_2)$ is expanded in the basis (in $\mathbb{C}^4$) consisting of the eigenvectors of $U(k_1, k_2)$, it has zero components in the direction of the eigenvectors corresponding to the eigenvalues ± 1. By Theorem 5.10, we conclude that the projection $e := I \otimes |0\rangle\langle 0|$ is transient for the QMC.

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Chul Ki Ko: University College, Yonsei University, 85 Songdogwahak-ro, Yeonsu-gu, Incheon 21983, Korea
E-mail address: kochulki@yonsei.ac.kr

Hyun Jae Yoo: School of Computer Engineering and Applied Mathematics, and Institute for Integrated Mathematical Sciences, Hankyong National University, 327 Jungang-ro, Anseong-si, Gyeonggi-do 17579, Korea
E-mail address: yoohj@hknu.ac.kr