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INTERACTING FOCK SPACES AND THE MOMENTS OF THE LIMIT DISTRIBUTIONS FOR QUANTUM RANDOM WALKS

CHUL KI KO

University College, Yonsei University,
134 Shinchon-dong, Seodaemun-gu, Seoul 120-749, Korea
kochulki@yonsei.ac.kr

HYUN JAE YOO*

Department of Applied Mathematics, Hankyong National University,
327 Jungang-ro, Anseong-si, Gyeonggi-do 456-749, Korea
yoohj@hknu.ac.kr

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We investigate the limit distributions of the discrete time quantum random walks on lattice spaces via a spectral analysis of concretely given self-adjoint operators. We discuss the interacting Fock spaces associated with the limit distributions. Thereby, we represent the moments of the limit distribution by vacuum expectation of the monomials of the Fock operator. We get formulas not only for one-dimensional walks but also for high-dimensional walks.

Keywords: Quantum random walks; limit distribution; interacting Fock spaces; vacuum expectation; high-dimensional walks.

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1. Introduction

The purpose of this paper is to investigate the limit distributions of quantum random walks (QRW's) on lattice spaces via spectral analysis. The QRW's initiated by Meyer,[18] have been mathematically developed by many people.[5,8,12,14–16,18] Particularly, QRW's is a tool for quantum algorithms in quantum computations. We refer to Ref. 21 for comprehensive introduction for QRW's. In relevance with quantum information, Accardi and Fidaleo introduced entangled Markov chain for

*Corresponding author

a model of QRW's.[3] See also Refs. 4 and 19. Konno obtained the limit distributions by the so-called path integral approach[14,15] (see also Ref. 8 and Katori *et al.*[11]). On the other hand, the present authors also obtained the limit distributions by using the Schrödinger approach,[13] which was introduced by Ambainis *et al.*[5,20] In particular, in Ref. 13 the generator for the evaluation of the QRW was achieved. In this paper, we illustrate further applications of such a generator.

After getting the limit distributions, we study their moments using spectral analysis of self-adjoint operators. We define 1-mode type interacting Fock spaces which are associated with the limit distributions of the QRW's. Thereby, the characteristic function as well as the moments of the limit distribution are represented by vacuum expectations of the exponential and monomials of the Fock operator. This result parallels that of Grimmett *et al.*[8] and Katori *et al.*[11] in nature. As a byproduct, we get a variety of integral transforms. The study for the moments of the limit distributions of one-dimensional walks naturally leads to high-dimensional walks. We will show not only the existence of limit distributions but also the formula for the characteristic functions and the moments of the limit distributions for high-dimensional QRW's.

This paper is organized as follows. In Sec. 2, we briefly review the QRW's and the theory of the 1-mode type interacting Fock spaces, especially for the aspects related to the moments problem and the orthogonal polynomials for the probability distributions. In Sec. 3, we develop the spectral analysis associated with the one-dimensional QRW's. In Sec. 4, we investigate the limit theory for high-dimensional walks.

2. Preliminaries

In this section, we briefly introduce the one-dimensional QRW's and interacting Fock spaces.

2.1. *One-dimensional QRW's*

We first introduce the definition of one-dimensional QRW's following Refs. 5, 8, 14, 15 and 20. Then we represent the evolution via a generator. A detailed description can be found in Ref. 13.

A quantum particle has an intrinsic degree of freedom, called "chirality", which is represented by a two-dimensional vector: we can look at it as an element of $\mathbb{C}^2$ and call the vectors $\binom{1}{0}$ and $\binom{0}{1}$ the left and right chirality, respectively. At time $n \in \mathbb{N}_0 = \{0, 1, 2, \ldots\}$, the probability amplitude of finding the particle at site $x \in \mathbb{Z}$ with chirality state being left or right is given by a two-component vector

$$\psi_n(x) = \begin{pmatrix} \psi_n(1; x) \\ \psi_n(2; x) \end{pmatrix} \in \mathbb{C}^2. \qquad (2.1)$$

After one unit of time the chirality is rotated by an *a priori* given unitary matrix U. According to the final chirality state, if the particle ends up with left chirality, then it moves one step to the left, and if it ends up with right chirality, it moves one step to the right. The concrete dynamics is given in the following way: let

$$U = \begin{pmatrix} l_1 & l_2 \\ r_1 & r_2 \end{pmatrix} \tag{2.2}$$

be a unitary matrix and define

$$L = \begin{pmatrix} l_1 & l_2 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad R = \begin{pmatrix} 0 & 0 \\ r_1 & r_2 \end{pmatrix}. \tag{2.3}$$

Then the dynamics for $\psi_n = (\psi_n(x))_{x\in\mathbb{Z}}$ is given by

$$\psi_{n+1}(x) = L\psi_n(x+1) + R\psi_n(x-1). \tag{2.4}$$

We can represent the dynamics in the Fourier transform space. For each $x \in \mathbb{Z}$, let $\mathcal{H}_x := \mathbb{C}^2$ be a copy of the chirality space. Let

$$\mathcal{H} := \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x \approx l^2(\mathbb{Z}, \mathbb{C}^2) \approx l^2(\mathbb{Z}) \otimes \mathbb{C}^2 \tag{2.5}$$

be the direct sum Hilbert space, on which the evolutions of QRW's will be developed. For each $x \in \mathbb{Z}$, let

$$e_x(k) := \frac{1}{\sqrt{2\pi}} e^{ixk}, \quad k \in \mathbb{K} := (-\pi, \pi], \tag{2.6}$$

$\mathbb{K}$ being understood as a unit circle in $\mathbb{R}^2$. The set $\{e_x\}_{x\in\mathbb{Z}}$ defines an orthonormal basis in $L^2(\mathbb{K})$. For each $k \in \mathbb{K}$, let h_k be a copy of $\mathbb{C}^2$ and let

$$\widehat{\mathcal{H}} := \int_{\mathbb{K}}^{\oplus} \mathsf{h}_k \, dk \approx L^2(\mathbb{K}, \mathbb{C}^2) \approx L^2(\mathbb{K}) \otimes \mathbb{C}^2 \tag{2.7}$$

be the direct integral of Hilbert spaces. The Fourier transform between $l^2(\mathbb{Z})$ and $L^2(\mathbb{K})$ naturally extends to a unitary map from $\mathcal{H}$ to $\widehat{\mathcal{H}}$ by

$$\psi = \left\{ \begin{pmatrix} \psi(1;x) \\ \psi(2;x) \end{pmatrix} \right\}_{x\in\mathbb{Z}} \in \mathcal{H} \mapsto \widehat{\psi} = \left\{ \begin{pmatrix} \widehat{\psi}(1;k) \\ \widehat{\psi}(2;k) \end{pmatrix} \right\}_{k\in\mathbb{K}} \in \widehat{\mathcal{H}}, \tag{2.8}$$

where

$$\widehat{\psi}(i;k) = \sum_{x\in\mathbb{Z}} \psi(i;x) e_x(k), \quad i = 1, 2. \tag{2.9}$$

Let us denote by T the left translation in $l^2(\mathbb{Z})$:

$$(Ta)(x) = a(x+1), \quad \text{for } a = (a(x))_{x\in\mathbb{Z}}. \tag{2.10}$$

T is a unitary map whose adjoint is the right translation:

$$(T^*a)(x) = a(x-1), \quad \text{for } a = (a(x))_{x\in\mathbb{Z}}. \tag{2.11}$$

The operator T naturally extends to $\mathcal{H} = \bigoplus_{x\in\mathbb{Z}} \mathcal{H}_x$ and for the sake of simplicity we use the same notation T for the extension. Given an operator (2×2 matrix) B

on $\mathbb{C}^2$, we let

$$\widetilde{B} := \bigoplus_{x\in\mathbb{Z}} B \tag{2.12}$$

be the bounded direct sum operator acting on $\mathcal{H}$.

It is easily seen that the dynamics of one-dimensional QRW's is given by

$$\psi_n = (\widetilde{L}T + \widetilde{R}T^*)^n\psi_0, \quad \psi_0 \in \mathcal{H}. \tag{2.13}$$

If we represent the evolution (2.13) in Fourier transform space it readily reads as

$$\widehat{\psi}_n(k) = U(k)^n\widehat{\psi}_0(k), \tag{2.14}$$

where

$$U(k) := \begin{pmatrix} e^{-ik}l_1 & e^{-ik}l_2 \\ e^{ik}r_1 & e^{ik}r_2 \end{pmatrix} \tag{2.15}$$

and for each $k \in \mathbb{K}$ it is a unitary matrix in $\mathbb{C}^2$.[5,8,11,13,20] The probability density to find out the particle at a site $x \in \mathbb{Z}$ at time n is

$$\begin{aligned} \|\psi_n(x)\|^2 &= |\psi_n(1;x)|^2 + |\psi_n(2;x)|^2 \qquad (2.16)\\ &= \left\|\int_{-\pi}^{\pi} \frac{1}{\sqrt{2\pi}} e^{-ixk}\widehat{\psi}_n(k)\,dk\right\|^2 \\ &= \frac{1}{2\pi}\left\{\left|\int_{-\pi}^{\pi} e^{-ixk}\widehat{\psi}_n(1;k)\,dk\right|^2 + \left|\int_{-\pi}^{\pi} e^{-ixk}\widehat{\psi}_n(2;k)\,dk\right|^2\right\}. \qquad (2.17) \end{aligned}$$

Next we discuss the limit distribution of the QRW's under a suitable scaling. Let $\{X_n^{(U;\psi_0)}\}_{n\geq 0}$ be the random variables distributed on the integer space $\mathbb{Z}$ according to the QRW whose evolution is given by (2.13). That is,

$$\mathbb{P}(X_n^{(U;\psi_0)} = x) = \|\psi_n(x)\|^2. \tag{2.18}$$

For a technical reason, we assume that

$$\det U = 1. \tag{2.19}$$

Here we remark that given a unitary matrix U we first adjust it by multiplying some phase factor so that (2.19) is satisfied. The distribution (2.18) is not altered by such an adjustment. The following theorem was first shown by Konno by path integral method,[14,15] that is in a combinatorial way. Grimmett *et al.*[8] and Katori *et al.*[11] discussed the limit distributions by the method of moments. We refer to Ref. 13 for a derivation by a Schrödinger approach.

Theorem 2.1. *There is a random variable* $Z^{(U;\psi_0)}$ *on the real line such that in distribution*

$$\lim_{n\to\infty} \frac{X_n^{(U;\psi_0)}}{n} = Z^{(U;\psi_0)}. \tag{2.20}$$

If $l_1 l_2 r_1 r_2 \neq 0$, *the distribution* $\mu^{(U;\psi_0)}$ *of* $Z^{(U;\psi_0)}$ *has a density function: it is supported on* $(-|l_1|, |l_1|)$ *and has the form:*

$$\rho^{(U;\psi_0)}(y) = \frac{\sqrt{1-|l_1|^2}}{\pi(1-y^2)\sqrt{|l_1|^2-y^2}} g^{(U;\psi_0)}(y), \tag{2.21}$$

where $g^{(U;\psi_0)}(y)$ *depends on the initial condition. On the other hand, if one of* l_1 *or* l_2 *is zero, then the distribution* $\mu^{(U;\psi_0)}$ *is a point mass: for* $\psi_0 = \{\binom{\psi_0(1;x)}{\psi_0(2;x)}\}_{x\in\mathbb{Z}}$,

$$\mu^{(U;\psi_0)} = \begin{cases} \left(\sum_{x\in\mathbb{Z}} |\psi_0(1;x)|^2\right)\delta_{-1} + \left(\sum_{x\in\mathbb{Z}} |\psi_0(2;x)|^2\right)\delta_1 & \text{if } l_2 = 0, \\ \delta_0 & \text{if } l_1 = 0. \end{cases} \tag{2.22}$$

When the particle is initially located at the origin, we get a more concrete form of the limit density function.

Proposition 2.2. *Suppose that the initial condition is a qubit state* $\binom{a}{b}, a, b \in \mathbb{C}, |a|^2 + |b|^2 = 1$, *located at the origin. Then the density of the limit distribution in Theorem* 2.1 *in the case* $l_1 l_2 r_1 r_2 \neq 0$ *is given by the following formula.*

$$\rho^{(U;\psi_0)}(y) = \frac{\sqrt{1-|l_1|^2}}{\pi(1-y^2)\sqrt{|l_1|^2-y^2}}(1-\beta^{(U;\psi_0)}y)1_{(-|l_1|,|l_1|)}(y)$$

with

$$\beta^{(U;\psi_0)} = |a|^2 - |b|^2 + \frac{\overline{l_1} l_2 \overline{a} b + l_1 \overline{l_2} a \overline{b}}{|l_1|^2}.$$

2.2. *Moments of probability distributions and interacting fock spaces*

In this subsection, we briefly introduce the theory of interacting Fock spaces which is related to the moments of probability distributions via Jacobi coefficients appearing in the orthogonal polynomials for the distribution. In this paper, we only consider 1-mode type interacting Fock spaces and we will omit "1-mode type" hereafter for simplicity. For a profound understanding of the interacting Fock spaces, we refer to Refs. 1, 2, 6, 7 and 17. Here we adopt the notations in Ref. 10.

In quantum probability theory, a real random variable is decomposed into creation, annihilation, and conservation operators in the sense of stochastic equivalence.[10] To say more concretely, let $(\mathcal{A}, \varphi)$ be an algebraic probability space, i.e. $\mathcal{A}$ is a $*$-algebra over $\mathbb{C}$ and φ is a state, a positive definite linear functional on $\mathcal{A}$ with norm one. Let $a \in \mathcal{A}$ be a real random variable, i.e. $a = a^*$. Then there is a probability distribution μ on the real line such that

$$\varphi(a^m) = \int_{-\infty}^{\infty} x^m \mu(dx), \quad m = 1, 2, \ldots. \tag{2.23}$$

Let $(\{\omega_n\}, \{\alpha_n\})_{n=1}^{\infty}$ be the Jacobi coefficients of μ satisfying the three-term recurrence relation: for the orthogonal polynomial $\{P_n(x)\}_{n=0}^{\infty}$ associated with μ,

$$\begin{gathered} P_0(x) = 1, \quad P_1(x) = x - \alpha_1, \quad \text{and} \\ xP_n(x) = P_{n+1}(x) + \alpha_{n+1}P_n(x) + \omega_n P_{n-1}(x), \quad n = 1, 2, \ldots. \end{gathered} \tag{2.24}$$

By using these coefficients we can define the associated interacting Fock space $(\Gamma, \{\Phi_n\}, B^+, B^-, B^\circ)$. More precisely, Γ is a separable Hilbert space and $\{\Phi_n\}_{n=0}^{\infty}$ is an orthonormal basis for Γ. The operators $B^\varepsilon, \varepsilon = +, -, \circ$, are defined in the following way:

$$\begin{aligned} &B^+\Phi_n = \sqrt{\omega_{n+1}}\Phi_{n+1}, && n = 0, 1, 2, \ldots, \\ &B^-\Phi_0 = 0, \quad B^-\Phi_n = \sqrt{\omega_n}\Phi_{n-1}, && n = 1, 2, \ldots, \\ &B^\circ\Phi_n = \alpha_{n+1}\Phi_n, && n = 0, 1, 2, \ldots. \end{aligned} \tag{2.25}$$

They are called the creation, annihilation, and conservation operators in that order. In particular, they satisfy

$$(B^+)^* = B^-, \quad (B^\circ)^* = B^\circ.$$

The vector Φ_0 is called the vacuum vector. It is known that (see Ref. 10)

$$\langle \Phi_0, (B^+ + B^- + B^\circ)^m \Phi_0 \rangle = \int_{-\infty}^{\infty} x^m \mu(dx), \quad m = 1, 2, \ldots. \tag{2.26}$$

Thus we have the relation

$$\varphi(a^m) = \langle \Phi_0, (B^+ + B^- + B^\circ)^m \Phi_0 \rangle \tag{2.27}$$

and a and $B^+ + B^- + B^\circ$ are said to be stochastically equivalent. By writing

$$a = B^+ + B^- + B^\circ \tag{2.28}$$

we call it the quantum decomposition of a.[10]

3. Interacting Fock Spaces for QRW's

In this section, we will construct the interacting Fock space associated with the limit distribution of QRW's in Sec. 2.1. Then, we will characterize the "real operator" which has the corresponding decomposition. In Ref. 9, Hamada *et al.* investigated the Stieltjes transform and orthogonal polynomials for the limit distribution of the QRW's. They computed the Jacobi coefficients and particularly in the case of symmetric distribution, they found the concrete form of the coefficients (see Corollary 3.2 of Ref. 9). More concretely, for the unitary matrix $U = \left(\begin{smallmatrix} l_1 & l_2 \\ r_1 & r_2 \end{smallmatrix}\right)$, in the case $l_1 l_2 r_1 r_2 \neq 0$ with $\beta^{(U;\psi_0)} = 0$ in Proposition 2.2, they obtained

$$\begin{aligned} &\alpha_n = 0, \quad n = 1, 2, \ldots, \quad \text{and} \\ &\omega_1 = 1 - \sqrt{1 - |l_1|^2}, \quad \omega_2 = \frac{\sqrt{1 - |l_1|^2}(1 - \sqrt{1 - |l_1|^2})}{2}, \\ &\omega_n = \frac{|l_1|^2}{4}, \quad n \geq 3. \end{aligned} \tag{3.1}$$

Let $(\Gamma, \{\Phi_n\}, B^+, B^-, B^\circ)$ be the interacting Fock space associated with the limit distribution $\mu^{(U;\psi_0)}$ in Theorem 2.1. By spectral analysis and the relation (2.26) we see that for any real number $\xi \in \mathbb{R}$,

$$\langle \Phi_0, e^{i\xi(B^+ + B^- + B^\circ)}\Phi_0\rangle = \int_{-\infty}^{\infty} e^{i\xi x}\mu^{(U;\psi_0)}(dx). \tag{3.2}$$

Our aim is to characterize the self-adjoint operator $B := B^+ + B^- + B^\circ$. Let $U = \begin{pmatrix} l_1 & l_2 \\ r_1 & r_2 \end{pmatrix}$ be the unitary matrix for the one-dimensional QRW. We assume $l_1 l_2 r_1 r_2 \neq 0$. Recall the unitary matrix $U(k)$ in (2.15). Let us diagonalize $U(k)$. Let $\theta_1 \in \mathbb{K}$ and $\theta_2 \in \mathbb{K}$ be the unique numbers satisfying

$$l_1 = |l_1|e^{i\theta_1} \quad \text{and} \quad l_2 = |l_2|e^{i\theta_2}. \tag{3.3}$$

Then the characteristic equation for $U(k)$ reads:

$$\lambda^2 - 2|l_1|\cos(k-\theta_1)\lambda + 1 = 0. \tag{3.4}$$

Let $\gamma(k)$ be the nonnegative symmetric function defined on $\mathbb{K} = (-\pi, \pi]$ such that

$$\cos\gamma(k) = |l_1|\cos k, \quad k \in \mathbb{K}. \tag{3.5}$$

In the sequel $\gamma(k)$ is also naturally understood as a periodic function of period 2π defined on $\mathbb{R}$. Then the solutions to (3.4), i.e. the eigenvalues of $U(k)$ are

$$\lambda_+(k) := e^{i\gamma(k-\theta_1)} \quad \text{and} \quad \lambda_-(k) := e^{-i\gamma(k-\theta_1)}. \tag{3.6}$$

The corresponding (normalized) eigenvectors are

$$\begin{pmatrix} \dfrac{1}{\sqrt{1+|\alpha_+(k-\theta_1)|^2}} \\ \dfrac{\alpha_+(k-\theta_1)}{\sqrt{1+|\alpha_+(k-\theta_1)|^2}} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \dfrac{1}{\sqrt{1+|\alpha_-(k-\theta_1)|^2}} \\ \dfrac{\alpha_-(k-\theta_1)}{\sqrt{1+|\alpha_-(k-\theta_1)|^2}} \end{pmatrix}, \tag{3.7}$$

respectively, where

$$\alpha_\pm(k) = ie^{i(k+\theta_1-\theta_2)}(|l_1|/|l_2|\sin k \pm \sqrt{1+(|l_1|/|l_2|\sin k)^2}). \tag{3.8}$$

Then $U(k)$ is diagonalized as

$$U(k) = S(k-\theta_1)\begin{pmatrix} e^{i\gamma(k-\theta_1)} & 0 \\ 0 & e^{-i\gamma(k-\theta_1)} \end{pmatrix} S(k-\theta_1)^{-1}, \tag{3.9}$$

where

$$S(k) = \begin{pmatrix} \dfrac{1}{\sqrt{1+|\alpha_+(k)|^2}} & \dfrac{1}{\sqrt{1+|\alpha_-(k)|^2}} \\ \dfrac{\alpha_+(k)}{\sqrt{1+|\alpha_+(k)|^2}} & \dfrac{\alpha_-(k)}{\sqrt{1+|\alpha_-(k)|^2}} \end{pmatrix}, \tag{3.10}$$

which is a unitary matrix itself. Thus we have a representation

$$U(k) = e^{iH(k)}, \tag{3.11}$$

where $H(k)$ is a self-adjoint operator defined by

$$H(k) = S(k-\theta_1)\begin{pmatrix}\gamma(k-\theta_1) & 0 \\ 0 & -\gamma(k-\theta_1)\end{pmatrix} S(k-\theta_1)^{-1}. \tag{3.12}$$

The evolution of the QRW can now be denoted by

$$\widehat{\psi}_n(k) = e^{inH(k)}\widehat{\psi}_0(k). \tag{3.13}$$

Because $\cos^{-1}|l_1| \leq \gamma(k) \leq \pi - \cos^{-1}|l_1|$ uniformly for $k \in \mathbb{K}$, the operator norm $\|H(k)\|$ (as an operator on $\mathbb{C}^2$) is bounded by $\pi - \cos^{-1}|l_1|$ uniformly for $k \in \mathbb{K}$. Thus the operator

$$H := \int_{\mathbb{K}}^{\oplus} H(k)\, dk \tag{3.14}$$

is a bounded self-adjoint operator on $\widehat{\mathcal{H}}$, which we call the generator of the QRW. Let $\mathcal{M} \subset \mathcal{B}(\widehat{\mathcal{H}})$ be a Banach subalgebra consisting of the operators of the form

$$A := \int_{\mathbb{K}}^{\oplus} A(k)\, dk, \tag{3.15}$$

where $A(k)$ is a 2×2 matrix for each $k \in \mathbb{K}$ and they satisfy

$$\sup_k \|A(k)\| < \infty.$$

Then H belongs to $\mathcal{M}$. Let us recall the Pauli matrices $\{\sigma_l\}_{l=0}^3$:

$$\sigma_0 = \begin{pmatrix}1 & 0 \\ 0 & 1\end{pmatrix}, \quad \sigma_1 = \begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix}, \quad \sigma_2 = \begin{pmatrix}0 & -i \\ i & 0\end{pmatrix}, \quad \sigma_3 = \begin{pmatrix}1 & 0 \\ 0 & -1\end{pmatrix}.$$

By a direct computation, we can rewrite $H(k)$ as

$$\begin{aligned} H(k) &= \gamma(k-\theta_1)S(k-\theta_1)\sigma_3 S(k-\theta_1)^* \\ &= \gamma(k-\theta_1)\sum_{l=1}^{3} h_l(k-\theta_1)\sigma_l, \end{aligned} \tag{3.16}$$

with

$$\begin{aligned} h_1(k) &= \frac{1}{\sqrt{1+(|l_1|/|l_2|\sin k)^2}}(-\sin(k+\theta_1-\theta_2)), \\ h_2(k) &= \frac{1}{\sqrt{1+(|l_1|/|l_2|\cos k)^2}}(\cos(k+\theta_1-\theta_2)), \\ h_3(k) &= \frac{1}{\sqrt{1+(|l_1|/|l_2|\sin k)^2}}(-|l_1|/|l_2|\sin k). \end{aligned} \tag{3.17}$$

The following is a main theorem of this paper.

Theorem 3.1. *Let U be a unitary matrix as above. There is a self-adjoint operator $B \in \mathcal{M}$ such that for all $n = 0, 1, 2, \ldots,$*

$$\int_{-\infty}^{\infty} x^n \mu^{(U;\psi_0)}(dx) = \langle \widehat{\psi}_0, B^n \widehat{\psi}_0 \rangle_{\widehat{\mathcal{H}}}. \tag{3.18}$$

The operator B is given by

$$B = \int_{\mathbb{K}}^{\oplus} \gamma'(k - \theta_1) B(k)\, dk, \tag{3.19}$$

where $B(k) = S(k - \theta_1)\sigma_3 S(k - \theta_1)^*$. We notice that

$$B(k)^n = \begin{cases} \sigma_0 & \text{if } n \text{ is even,} \\ B(k) & \text{if } n \text{ is odd.} \end{cases} \tag{3.20}$$

Furthermore, we can directly express the operators by the components of U: we have $\gamma'(k - \theta_1) = \frac{|l_1|/|l_2| \sin(k-\theta_1)}{\sqrt{1+(|l_1|/|l_2| \sin(k-\theta_1))^2}}$ and $B(k)$ has an expansion in Pauli matrices as $B(k) = \sum_{l=1}^{3} h_l(k - \theta_1)\sigma_l$, where the coefficients $h_l(k), k = 1, 2, 3,$ are given in (3.17).

Remark 3.2. The formula (3.18) is another expression for the moments obtained by Grimmett *et al.* (see Eq. (19) in Ref. 8) and Katori *et al.*[11]

For the Hadamard walk, since $\theta_1 = 0, \theta_2 = \pi$, and $|l_1| = |l_2|$, we have a simpler form.

Corollary 3.3. *Let $U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$ be the unitary matrix for the Hadamard walk. Then the operator B in* (3.19) *is given by*

$$B = \int_{\mathbb{K}}^{\oplus} \gamma'(k) B(k)\, dk, \tag{3.21}$$

where $B(k) = a(k)\frac{\sigma_1 - \sigma_3}{\sqrt{2}} - b(k)\sigma_2$ with $a(k) = \frac{\sqrt{2}\sin k}{\sqrt{1+\sin^2 k}}, b(k) = \frac{\cos k}{\sqrt{1+\sin^2 k}}$, and we have $\gamma'(k) = \frac{\sin k}{\sqrt{1+\sin^2 k}}$. Here again $B(k)$ satisfies the relation (3.20).

Remark 3.4. Since the operator B in (3.18) has a quantum decomposition by the operators $B^\varepsilon, \varepsilon = +, -, \circ$, we can expand the right-hand side of (3.19) to get

$$M_m = \sum_{\varepsilon} \langle \widehat{\psi}_0, B^{\varepsilon_m} \cdots B^{\varepsilon_1} \widehat{\psi}_0 \rangle_{\widehat{\mathcal{H}}}, \tag{3.22}$$

where $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_m)$ runs over $\{+, -, \circ\}^m$. Thus we can interpret M_m by a random walk in a graph. Let $G = (V, E)$ be a weighted graph whose vertex set consists of $\{\Phi_n\}_{n=0}^{\infty} (\Phi_0 \equiv \widehat{\psi}_0)$ and the edges consist of $\{E_i := \{\Phi_i, \Phi_{i+1}\}\}_{i=0}^{\infty}$ and self loops $\{E_i^\circ\}_{i=0}^{\infty}$. The edges E_i has weight ω_{i+1} and E_i° has weight α_{i+1}. For a path, we say that it has a weight given by the product of the weights of the edges that it consists of. Then, M_m is the total sum of the weights of the paths of length m that start from Φ_0 and arrives at the same point. This combinatoric evaluation can be obtained by Accardi–Bożejko formula (see Refs. 1 and 10).

The remaining of this section is devoted to the proof of Theorem 3.1. First we need the following.

Lemma 3.5. *There is a uniform constant $M > 0$ such that for any k_1 and k_2 in $\mathbb{K}$ we have*

$$\|S(k_1) - S(k_2)\| \le M|k_1 - k_2|.$$

Proof. By mean value theorem, it is enough to show that $\|S'(k)\| \le M$ uniformly for $k \in \mathbb{K}$. We will see the components of $S(k)$ have uniformly bounded derivatives. We just show the property for $S(k)_{2,2}$, the (2,2)-component of $S(k)$. The other components can be done similarly. We have $S(k)_{2,2} = \frac{\alpha_-(k)}{\sqrt{1+|\alpha_-(k)|^2}}$. From (3.8), it is enough to show that the derivative of the function $k \mapsto \frac{x(k)}{\sqrt{1+x(k)^2}}$ with $x(k) := a\sin k - \sqrt{1 + a^2 \sin^2 k}$ (we have put $a \equiv |l_1|/|l_2|$) is uniformly bounded, and in fact it is bounded by $2a$. □

Proof of Theorem 3.1. Recall the random variables $\{X_n^{(U;\psi_0)}\}_{n\ge0}$ in (2.18). We start with the computation of the characteristic functions:

$$\begin{aligned}\mathbb{E}(e^{i\xi X_n^{(U;\psi_0)}}) &= \sum_{x\in\mathbb{Z}} e^{i\xi x}\|\psi_n(x)\|^2 \\ &= \langle \psi_n, e^{i\xi\cdot}\psi_n\rangle_{l^2(\mathbb{Z},\mathbb{C}^2)} \\ &= \langle \widehat{\psi}_n, \widehat{e^{i\xi\cdot}\psi_n}\rangle_{\widehat{\mathcal{H}}}.\end{aligned} \tag{3.23}$$

We see that $\widehat{e^{i\xi\cdot}\psi_n}(k) = \widehat{\psi}_n(k+\xi)$ by understanding $\widehat{\psi}_n(k)$ as a periodic function of period 2π on the real line. Therefore, we have

$$\begin{aligned}\mathbb{E}(e^{i\xi X_n^{(U;\psi_0)}}) &= \int_{-\pi}^{\pi} \langle \widehat{\psi}_n(k), \widehat{\psi}_n(k+\xi)\rangle_{\mathbb{C}^2}\, dk \\ &= \int_{-\pi}^{\pi} \langle \widehat{\psi}_0(k), e^{-inH(k)}e^{inH(k+\xi)}\widehat{\psi}_0(k+\xi)\rangle_{\mathbb{C}^2}\, dk,\end{aligned} \tag{3.24}$$

where we have used (3.13) in the second line. Notice that $\mathbb{E}(e^{i\xi/nX_n^{(U;\psi_0)}})$ converges to the right-hand side of (3.2) as n goes to infinity. Thus we need to compute the limit

$$\begin{aligned}&\lim_{n\to\infty} \mathbb{E}(e^{i\xi/nX_n^{(U;\psi_0)}}) \\ &\quad = \lim_{n\to\infty}\int_{-\pi}^{\pi} \langle \widehat{\psi}_0(k), e^{-inH(k)}e^{inH(k+\xi/n)}\widehat{\psi}_0(k+\xi/n)\rangle_{\mathbb{C}^2}\, dk.\end{aligned} \tag{3.25}$$

Since $H(k) = \gamma(k-\theta_1)S(k-\theta_1)\sigma_3 S(k-\theta_1)^*$, we have

$$\begin{aligned}e^{-inH(k)}e^{inH(k+\xi/n)} &= S(k-\theta_1)e^{-in\gamma(k-\theta_1)\sigma_3}S(k-\theta_1)^*S(k-\theta_1+\xi/n) \\ &\quad \times e^{in\gamma(k-\theta_1+\xi/n)\sigma_3}S(k-\theta_1+\xi/n)^*.\end{aligned} \tag{3.26}$$

We use Lemma 3.5 to (3.26) and by dominated convergence theorem we get the limit in (3.25) as

$$\lim_{n\to\infty} \mathbb{E}(e^{i\xi/n X_n^{(U;\psi_0)}}) = \int_{-\pi}^{\pi} \langle \widehat{\psi}_0(k), e^{i\xi\gamma'(k-\theta_1)S(k-\theta_1)\sigma_3 S(k-\theta_1)^*} \widehat{\psi}_0(k)\rangle_{\mathbb{C}^2}\, dk. \quad (3.27)$$

Thus we have for the weak limit $Z^{(U;\psi_0)}$ of $X_n^{(U;\psi_0)}/n$

$$\mathbb{E}(e^{i\xi Z^{(U;\psi_0)}}) = \langle \widehat{\psi}_0, e^{i\xi B}\widehat{\psi}_0\rangle_{\widehat{\mathcal{H}}}, \quad (3.28)$$

with B defined in (3.19). The first part is now obvious because

$$\int_{-\infty}^{\infty} x^n \mu^{(U;\psi_0)}(dx) = (-i)^n \frac{d^n}{d\xi^n}\mathbb{E}(e^{i\xi Z^{(U;\psi_0)}})\bigg|_{\xi=0}.$$

We easily see from the relation $\cos\gamma(k) = |l_1|\cos k$ that

$$\gamma'(k) = \frac{|l_1|/|l_2|\sin k}{\sqrt{1+(|l_1|/|l_2|\sin k)^2}}. \quad (3.29)$$

We have already noted in (3.16) that

$$S(k-\theta_1)\sigma_3 S(k-\theta_1)^* = \sum_{l=1}^{3} h_l(k-\theta_1)\sigma_l.$$

This gives the second part of the theorem. □

Example 3.6. We consider the Hadamard walk by taking the unitary operator U in Corollary 3.3. Take an initial condition $\psi_0 = \{\binom{0}{1}\delta_0(x)\}_{x\in\mathbb{Z}}$, or $\widehat{\psi}_0(k) = \frac{1}{\sqrt{2\pi}}\binom{0}{1}$. Then by Proposition 2.2, we have $\mu^{(U;\psi_0)}(dx) = \rho^{(U;\psi_0)}(x)dx$ with

$$\rho^{(U;\psi_0)}(x) = \frac{1}{\pi(1-x)\sqrt{1-2x^2}} 1_{(-\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})}(x). \quad (3.30)$$

Denote by $M_m \equiv M_m(\mu^{(U;\psi_0)}) := \int_{-1/\sqrt{2}}^{1/\sqrt{2}} x^m \mu^{(U;\psi_0)}(dx)$ the mth moment of $\mu^{(U;\psi_0)}$. On the other hand from Corollary 3.3, we have also the representation $M_m = \langle\widehat{\psi}_0, B^m\widehat{\psi}_0\rangle_{\widehat{\mathcal{H}}}$, and thus obtaining

$$M_m = \frac{1}{2\pi}\int_{-\pi}^{\pi} c_m(k)\, dk, \quad (3.31)$$

where

$$c_m(k) = \begin{cases} \left(\dfrac{\sin k}{\sqrt{1+\sin^2 k}}\right)^m & \text{if } m \text{ is even,} \\ \left(\dfrac{\sin k}{\sqrt{1+\sin^2 k}}\right)^{m+1} & \text{if } m \text{ is odd.} \end{cases}$$

Numerical computations give for both integrals

$$M_1 = M_2 = 0.292893, \quad M_3 = M_4 = 0.116117,$$
$$M_5 = M_6 = 0.049825, \ldots. \quad (3.32)$$

Remark 3.7. In the above example, we have seen the following integral transform:

$$\frac{1}{\pi}\int_{-1/\sqrt{2}}^{1/\sqrt{2}} \frac{x^m}{(1-x)\sqrt{1-2x^2}}\,dx = \frac{1}{2\pi}\int_{-\pi}^{\pi} c_m(k)\,dk, \quad m = 0, 1, 2, \ldots. \tag{3.33}$$

In this way, by changing the unitary matrix U and the initial condition ψ_0, we have variety of such integral transforms, which might be useful in some numerical analysis. Katori *et al.* found a change of variable formula to connect such transforms.[11]

4. High-dimensional QRW's

In this section, we summarize the arguments of the last sections to develop the theory of high-dimensional QRW's. Let $d \geq 1$ be any integer and we consider QRW's on $\mathbb{Z}^d$. The chiral states are $2d$-dimensional vectors and they are rotated by a $2d \times 2d$ unitary matrix U. For $i = 1, \ldots, d$, let $E_i^{(\pm)}$ be the $2d \times 2d$ matrices defined by

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

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

Define

$$U_i^{(\pm)} := E_i^{(\pm)} U, \quad i = 1, \ldots, d. \tag{4.1}$$

Notice that for $d = 1, U_1^{(-)}$ and $U_1^{(+)}$ correspond to L and R, respectively, in (2.3). The quantum walker in $\mathbb{Z}^d$ moves one step left or right, down or up, bottom or top, etc. at every unit time according to its chiral state. The d-dimensional QRW's are represented as evolutions on the Hilbert space

$$\mathcal{H} := l^2(\mathbb{Z}^d, \mathbb{C}^{2d}) \approx \bigoplus_{x \in \mathbb{Z}^d} \mathcal{H}_x, \tag{4.2}$$

where $\mathcal{H}_x$ is a copy of $\mathbb{C}^{2d}$, or equivalently on its Fourier transform space

$$\widehat{\mathcal{H}} := L^2(\mathbb{K}^d, \mathbb{C}^{2d}) \approx \int_{\mathbb{K}^d}^{\oplus} \mathsf{h}_\mathsf{k}\, dk, \tag{4.3}$$

where h_k is a copy of $\mathbb{C}^{2d}$. The transform between (4.2) and (4.3) is given by

$$\begin{aligned} \psi = (\psi(x))_{x \in \mathbb{Z}^d} &\mapsto \widehat{\psi} = (\widehat{\psi}(k))_{k \in \mathbb{K}^d}; \\ \widehat{\psi}(k) &= \sum_{x \in \mathbb{Z}^d} e_x(k)\psi(x), \end{aligned} \tag{4.4}$$

where $e_x(k) = (2\pi)^{-d/2} e^{i\kappa \cdot x}$. The one-dimensional evolution of QRW given in (2.4) extends now as

$$\psi_{n+1}(x) = \sum_{i=1}^{d} (U_i^{(-)}(T_i\psi_n)(x) + U_i^{(+)}(T_i^*\psi_n)(x)), \quad x \in \mathbb{Z}^d, \tag{4.5}$$

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

$$(T_i\psi)(x) = \psi(x + u_i), \tag{4.6}$$

with u_i the unit vector in the ith axis. As in (2.13), Eq. (4.5) has a solution

$$\psi_n = \left(\sum_{i=1}^{d}(\widetilde{U_i^{(-)}}T_i + \widetilde{U_i^{(+)}}T_i^*)\right)^n \psi_0, \tag{4.7}$$

where $\widetilde{U_i^{(\pm)}}$ is the extension of $U_i^{(\pm)}$ to $\mathcal{H}$. If we represent (4.7) in the Fourier transform space $\widehat{\mathcal{H}}$ we get

$$\widehat{\psi}_n(k) = U(k)^n \widehat{\psi}_0(k), \quad k \in \mathbb{K}^d, \tag{4.8}$$

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

$$\begin{aligned} U(k) &= \sum_{j=1}^{d}(e^{-ik_j}E_j^{(-)} + e^{ik_j}E_j^{(+)})U \\ &= \begin{pmatrix} e^{-ik_1} & & & & \\ & e^{ik_1} & & 0 & \\ & & \ddots & & \\ & 0 & & e^{-ik_d} & \\ & & & & e^{ik_d} \end{pmatrix} U. \end{aligned} \tag{4.9}$$

Under a mild condition the techniques of Sec. 3 extend to any higher-dimensional QRW's. Let $H(k)$ be the self-adjoint matrix that generates the QRW, i.e. it satisfies the relation:

$$U(k) = e^{iH(k)}. \tag{4.10}$$

Our basic Hypothesis is the following:

(H) The eigenvalues and eigenvectors of $H(k)$ are continuously differentiable on the compact set $\mathbb{K}^d$.

In the sequel we assume the Hypothesis (H). Let $H(k)$ be diagonalized as

$$H(k) = S(k)\Gamma(k)S(k)^*, \tag{4.11}$$

where

$$\Gamma(k) = \begin{pmatrix} \gamma_1^{(+)}(k) & & & & \\ & \gamma_1^{(-)}(k) & & 0 & \\ & & \ddots & & \\ & 0 & & \gamma_d^{(+)}(k) & \\ & & & & \gamma_d^{(-)}(k) \end{pmatrix} \tag{4.12}$$

is the diagonal matrix of eigenvalues and $S(k)$ is a unitary matrix whose columns consist of the eigenvectors of $H(k)$. Theorem 3.1 then extends to the d-dimensional QRW's. Let $X_n^{(U;\psi_0)}$ be the random variable on $\mathbb{Z}^d$ whose distribution is that of QRW at time n with initial condition $\psi_0 \in \mathcal{H}$.

Theorem 4.1. *Assume the Hypothesis* (H). *Then the sequence of random variables* $\{X_n^{(U;\psi_0)}/n\}$ *converges weakly to a limit* $Z^{(U;\psi_0)}$ *whose characteristic function is given by the formula*:

$$\mathbb{E}(e^{i\xi\cdot Z^{(U;\psi_0)}}) = \langle\widehat{\psi}_0, e^{i\xi\cdot B}\widehat{\psi}_0\rangle_{\widehat{\mathcal{H}}}. \tag{4.13}$$

For any $\xi \in \mathbb{R}^d$, *the operator* $\xi \cdot B \in \mathcal{B}(\widehat{\mathcal{H}})$ *is given by*

$$\xi \cdot B = \int_{\mathbb{K}^d}^{\oplus} S(k)\xi \cdot \nabla\Gamma(k)S(k)^* \, dk, \tag{4.14}$$

where

$$\xi \cdot \nabla\Gamma(k) = \begin{pmatrix} \xi\cdot\nabla\gamma_1^{(+)}(k) & & & & \\ & \xi\cdot\nabla\gamma_1^{(-)}(k) & & 0 & \\ & & \ddots & & \\ & 0 & & \xi\cdot\nabla\gamma_d^{(+)}(k) & \\ & & & & \xi\cdot\nabla\gamma_d^{(-)}(k) \end{pmatrix}. \tag{4.15}$$

Corollary 4.2. *Let* $Z^{(U;\psi_0)} = (Z_1^{(U;\psi_0)}, \ldots, Z_d^{(U;\psi_0)})$. *Then for any* $m = (m_1, \ldots, m_d) \in \mathbb{N}_0^d$,

$$\mathbb{E}\left(\prod_{i=1}^{d}(Z_i^{(U;\psi_0)})^{m_i}\right) = \langle\widehat{\psi}_0, B^{(m)}\widehat{\psi}_0\rangle_{\widehat{\mathcal{H}}}, \tag{4.16}$$

where

$$B^{(m)} = \int_{\mathbb{K}^d}^{\oplus} S(k)D^{(m)}\Gamma(k)S(k)^* \, dk, \tag{4.17}$$

with

$$D^{(m)}\Gamma(k) = \prod_{i=1}^{d}\left(\frac{\partial\Gamma(k)}{\partial k_i}\right)^{m_i}. \tag{4.18}$$

Proof. It follows from Theorem 4.1 using the relation:

$$\mathbb{E}\left(\prod_{i=1}^{d}(Z_i^{(U;\psi_0)})^{m_i}\right) = (-i)^{|m|}\frac{\partial^{|m|}}{\partial\xi_1^{m_1}\cdots\partial\xi_d^{m_d}}\mathbb{E}(e^{i\xi\cdot Z^{(U;\psi_0)}})\bigg|_{\xi=0}, \tag{4.19}$$

where $|m| = m_1 + \cdots + m_d$. $\square$

Proof of Theorem 4.1. The method of the proof is identical to that of Theorem 3.1. As in (3.25) we have

$$\mathbb{E}(e^{i\xi/n\cdot X_n^{(U;\psi_0)}}) = \int_{\mathbb{K}^d} \langle\widehat{\psi}_0(k), e^{-inH(k)}e^{inH(k+\xi/n)}\widehat{\psi}_0(k+\xi/n)\rangle_{\mathbb{C}^{2d}}\, dk. \quad (4.20)$$

By (4.11) we have

$$\begin{aligned} e^{-inH(k)}e^{inH(k+\xi/n)} &= S(k)e^{-in\Gamma(k)}S(k)^*S(k+\xi/n) \\ &\quad \times e^{in\Gamma(k+\xi/n)}S(k+\xi/n)^*. \end{aligned} \quad (4.21)$$

From the Hypothesis (H) we see that there is an $M > 0$ such that

$$\|S(k+\xi/n) - S(k)\| \le M\|\xi\|/n \quad \text{for all } k \in \mathbb{K}^d. \quad (4.22)$$

Using this, by dominated convergence theorem we have

$$\lim_{n\to\infty} \mathbb{E}(e^{i\xi/n\cdot X_n^{(U;\psi_0)}}) = \int_{\mathbb{K}^d} \langle\widehat{\psi}_0(k), e^{iS(k)\xi\cdot\nabla\Gamma(k)S(k)^*}\widehat{\psi}_0(k)\rangle_{\mathbb{C}^{2d}}\, dk. \quad (4.23)$$

The conclusion now immediately follows. □

Example 4.3. (1) In the last section for the one-dimensional QRW, we have seen in the proof of Lemma 3.5 that if the matrix U satisfies $l_1 l_2 r_1 r_2 \neq 0$ then the Hypothesis (H) is satisfied.

(2) In Ref. 22, Watabe *et al.* considered two-dimensional QRW with unitary matrix

$$U = \begin{pmatrix} -p & q & \sqrt{pq} & \sqrt{pq} \\ q & -p & \sqrt{pq} & \sqrt{pq} \\ \sqrt{pq} & \sqrt{pq} & -q & p \\ \sqrt{pq} & \sqrt{pq} & p & -q \end{pmatrix}, \quad p \in (0,1), \quad q = 1-p, \quad (4.24)$$

which generalizes the Grover model. They showed that the eigenvalues of $U(k)$ are $\lambda_1 = 1, \lambda_2 = -1, \lambda_3 = e^{i\gamma(k)}, \lambda_4 = e^{-i\gamma(k)}$ with $\gamma(k)$ satisfying

$$\cos\gamma(k) = -(p\cos k_1 + q\sin k_2). \quad (4.25)$$

The corresponding normalized eigenvectors are

$$u_j(k) = N_j \begin{pmatrix} q(e^{ik_2}\lambda_j+1)(e^{ik_1}\lambda_j+1)(e^{-ik_2}\lambda_j+1) \\ q(e^{ik_2}\lambda_j+1)(e^{-ik_1}\lambda_j+1)(e^{-ik_2}\lambda_j+1) \\ \sqrt{pq}(e^{ik_2}\lambda_j+1)(e^{-ik_1}\lambda_j+1)(e^{ik_1}\lambda_j+1) \\ \sqrt{pq}(e^{-ik_1}\lambda_j+1)(e^{ik_1}\lambda_j+1)(e^{-ik_2}\lambda_j+1) \end{pmatrix}, \quad j = 1,2,3,4, \quad (4.26)$$

where N_j is the normalization constant. Thus, the generator $H(k)$ has the following eigenvalues:

$$\gamma_1^{(+)}(k) = 0, \quad \gamma_1^{(-)}(k) = \pi, \quad \gamma_2^{(+)}(k) = \gamma(k), \quad \gamma_2^{(-)}(k) = -\gamma(k), \quad (4.27)$$

and the unitary matrix $S(k)$ consists of the four column vectors $u_j(k)$, $j = 1,2,3,4$. Obviously, this model satisfies the Hypothesis (H). Thus by Theorem 4.1, we can compute the characteristic function and the mixed moments of the limit distribution. The detailed computation of the mixed moments was done in Ref. 22.

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