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Skeleton structure inherent in quantum walks

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Abstract—This paper demonstrates that a common underlying structure, or a skeleton structure, is present behind quantum walks with a homogeneous coin matrix. More specifically, we examine the transition probabilities of random walks that replicate the probability distribution of quantum walks. We show that the transition probability contains a skeleton structure by considering the weak limit that excludes the oscillatory behavior. Remarkably, the skeleton structure does not depend on the coin matrix or the initial condition of the quantum walk.

► We use the following descriptions:

- $\mathbb{N} := \{n \in \mathbb{Z} \,|\, n \geq 1\}$.
- $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$.
- i is the imaginary unit.
- For $a \in \mathbb{R}$, the function $\delta_a : \mathbb{R} \to \{0, 1\}$ is given by

$$\delta_a(x) = \begin{cases} 1 & (x = a) \\ 0 & (x \neq a) \end{cases}.$$

- For a matrix A, A^{T} and A^* are the transpose and the adjoint matrix of A, respectively.
- The symbols "$\langle \cdot |$" and "$| \cdot \rangle$" are often used as description of row vectors and column vectors, respectively. For a column vector $|x\rangle$, $\langle x| = |x\rangle^*$. When we take inner products or norms of vectors, we often omit them: $\langle x| \, |y\rangle = \langle x|y\rangle$, $\| \, |x\rangle \, \| = \| \, \langle x| \, \| = \|x\|$.
- $\mathbf{L}^2(\mathbb{R})$ is a set of functions square-integrable on $\mathbb{R}$.

1. Introduction

A quantum walk (QW) is known as the quantum counterpart of the classical random walk [1, 2, 3, 4], which extends by including the effects of quantum superposition and complex probability amplitudes. QWs were first introduced in the field of quantum information theory [5, 6, 7]. After that, the characteristic structure of quantum walks mentioned above was intensively studied by mathematicians

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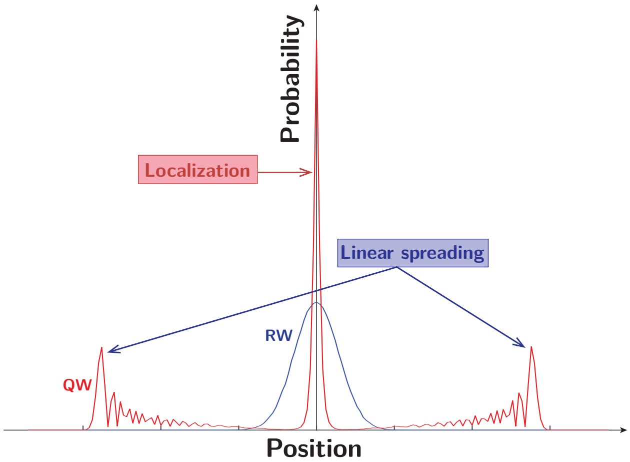

Figure 1: Comparison of the probability distributions between quantum walk (QW) and random walk (RW).

[8, 9], and since then, quantum walks have been an important topic in both fundamental and applied research.

The main properties of the quantum walk are *linear spreading* and *localization*. The former means that the standard deviation about the distribution of the observation probability of walkers grows proportionally to the run time n. The latter implies that probability can be distributed at a particular position no matter how long the walker runs. Quantum walks have both or either of these properties, which results in the probability distribution that is totally different from those of random walks which weakly converge to normal distributions, as represented in Fig. 1.

Meanwhile, generating distributions of quantum walks via time- and site-dependent random walks are examined [10, 11], which we call *quantum-walk-replicating random walk* (QWRW). Especially, Yamagami *et al.* [12] showed that linear spreading and localization appear for the behavior of individual walkers, which obeys the discrete-time QWRW on one-dimensional lattice $\mathbb{Z}$. In [12], the directivity of QWRWs is investigated by introducing the notion of transition probability of QWRWs.

In this paper, we analyze the transition probabilities of QWRW in the case of the homogeneous coin matrix. We show that the transition probability accompanies a skeleton structure by considering the weak limit that excludes the oscillatory behavior. It is noteworthy that the skeleton structure does *not* depend on the coin matrix nor the initial condition of the quantum walk, although the transition probability including oscillatory terms differs significantly depending on the coin matrix and the initial condition of the quantum walk.

2. Preliminaries

2.1. Quantum walk (QW)

We introduce the following matrix:

$$C = \begin{bmatrix} a & b \\ -\varDelta\bar{b} & \varDelta\bar{a} \end{bmatrix}, \tag{1}$$

with the conditions $|a|^2 + |b|^2 = 1$ and $|\varDelta| = 1$ being satisfied where $a, b, \varDelta \in \mathbb{C}$. Here, C is a unitary matrix and called a *coin matrix*. In particular, since C is independent of time n and the position x, C is called *homogeneous coin matrix*. Let $|\mathrm{L}\rangle$ and $|\mathrm{R}\rangle$ be the vectors given by $|\mathrm{L}\rangle = [1 \;\; 0]^{\mathsf{T}}$ and $|\mathrm{R}\rangle = [0 \;\; 1]^{\mathsf{T}}$, respectively. Then, we define the matrices

$$P = |\mathrm{L}\rangle\langle\mathrm{L}|\, C \quad \text{and} \quad Q = |\mathrm{R}\rangle\langle\mathrm{R}|\, C. \tag{2}$$

Note that P and Q are the decomposition elements of C: $P + Q = C$.

Here, we consider the state of quantum walk on the position $x \in \mathbb{Z}$ at time $n \in \mathbb{N}_0$ denoted by a vector $|\varPsi_n(x)\rangle \in \mathbb{C}^2$. First, we set the state $|\varPsi_0(x)\rangle$, called the initial state, as

$$|\varPsi_0(x)\rangle = \delta_0(x)\, |\varphi\rangle\,, \tag{3}$$

where $|\varphi\rangle \in \mathbb{C}^2$ satisfies $\||\varphi\rangle\| = 1$. In addition, we define time evolution of $|\varPsi_n(x)\rangle$ as

$$|\varPsi_{n+1}(x)\rangle = P\,|\varPsi_n(x+1)\rangle + Q\,|\varPsi_n(x-1)\rangle\,. \tag{4}$$

Moreover, the probability that a quantum walker is measured on the position x after time evolution until time n, denoted by $\mu_n(x)$, is defined as

$$\mu_n(x) := \|\varPsi_n(x)\|^2. \tag{5}$$

2.2. Quantum-walk-replicating random walk (QWRW)

We define the random walk that replicates the probability distribution of a quantum walk (quantum-walk-replicating random walk; QWRW) [12]. For a pair $(n, x) \in \mathbb{N}_0 \times \mathbb{Z}$ that satisfies $\mu_n(x) > 0$, we define the transition probabilities to the left and right side as

$$p_n(x) = \frac{\|P\varPsi_n(x)\|^2}{\mu_n(x)} \quad \text{and} \quad q_n(x) = \frac{\|Q\varPsi_n(x)\|^2}{\mu_n(x)}, \tag{6}$$

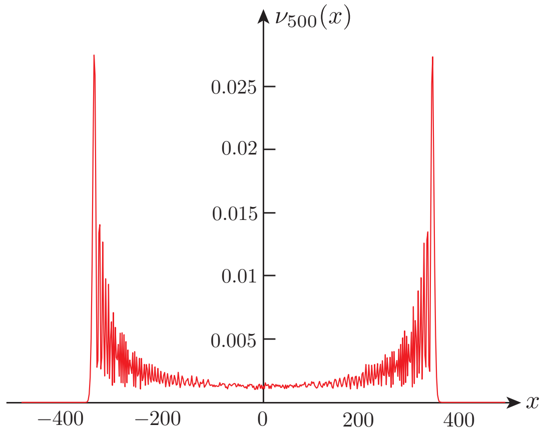

Figure 2: The distribution of QWRW in the case of $a = b = 1/\sqrt{2}$, $\varDelta = -1$, and $|\varphi_0\rangle = [1 \;\; i]^{\mathsf{T}}/\sqrt{2}$ (Setting A), at time $n = 500$. The number of walkers is $K = 100,000$.

respectively. Note that $p_n(x)$ and $q_n(x)$ satisfy $0 \leq p_n(x), q_n(x) \leq 1$ and $p_n(x) + q_n(x) = 1$. Furthermore, the probability that a walker following QWRW exists on the position x at time n, denoted by $\nu_n(x)$, has the following equation:

$$\nu_{n+1}(x) = p_n(x+1)\nu_n(x+1) + q_n(x-1)\nu_n(x-1). \tag{7}$$

On the other hand, the equation

$$\mu_{n+1}(x) = p_n(x+1)\mu_n(x+1) + q_n(x-1)\mu_n(x-1) \tag{8}$$

holds by the definitions of the transition probabilities (6). Based on Eqs. (7) and (8), we have the following result:

Theorem 2.1 ([12]). *$\nu_0 = \mu_0 \iff \nu_n = \mu_n$ for all n.*

This indicates that the probability distribution of QWRW is identical to that of QW, assuming that both of the initial states match.

Figure 2 shows the probability distribution of QWRW in case of $a = b = 1/\sqrt{2}$, $\varDelta = -1$, and $|\varphi\rangle = [1 \;\; i]^{\mathsf{T}}/\sqrt{2}$ (we call this case *Setting A*), and this distribution is identical to that of the corresponding quantum walk, shown in [9], for example. With homogeneous coin matrix, we observe linear spreading, but not localization.

Figure 3 represents the transition probabilities $p_n(x)$ and $q_n(x)$ as a function of the position x when the time n is specified by 500. In the following sections, we analyze transition probabilities and consider their observation based on this analysis.

3. Skeleton structure of the transition probability on QWRW

We show the mathematical statements regarding the transition probabilities and define the skeleton structure.

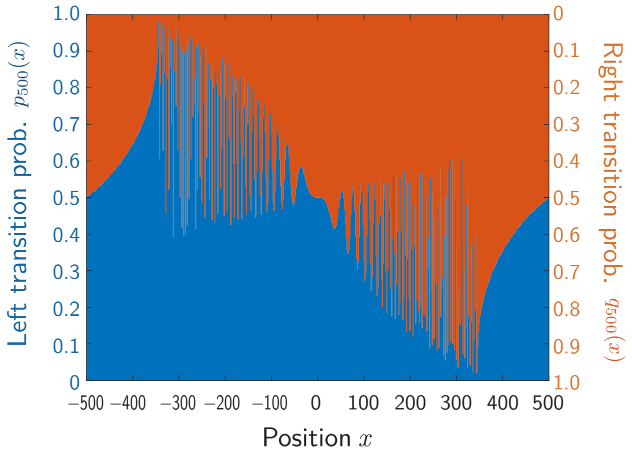

Figure 3: The transition probabilities $p_{500}(x)$ and $q_{500}(x)$ for QWRWs in Setting A. The relationship $p_{500}(x) + q_{500}(x) = 1$ holds , so left ($p_{500}(x)$, blue) and right ($q_{500}(x)$, orange) transition probabilities are expressed as a stacked bar graph.

3.1. Underlying statements

As we can observe from Fig. 3, the transition probabilities can be divided into two kinds of regions: oscillatory and non-oscillatory regions. The boundaries of these parts correspond to the peaks of the probability distribution of the QWRW on $x = \pm n|a|$ at run time n. Therefore, we refer to the oscillatory region as being *inside the peaks*, and the non-oscillatory region as being *outside the peaks*.

Inside the peaks, oscillations do not decay with time n, and thus $p_n(x)$ does not converge with increasing n. We can characterize the transition probabilities in the following form with the notion of a weak limit.

Theorem 3.1. *Let $x_n \in \mathbb{Z}$ and $s \in (-|a|, |a|)$ satisfy*

$$x_n = ns + O\left(\frac{1}{n}\right) \quad \text{as } n \to \infty.$$

Then, $p_n(x_n)$ and $q_n(x_n)$ can be described as

$$p_n(x_n) = \frac{\tau_1(s) + \xi_n(s)}{1 + \eta_n(s)} \quad \text{and} \quad q_n(x_n) = \frac{(1 - \tau_1(s)) + \zeta_n(s)}{1 + \eta_n(s)},$$

where

$$\tau_1(s) = \frac{1-s}{2} \quad \text{and}$$
$$\operatorname*{wlim}_{n\to\infty} \xi_n(s) = \operatorname*{wlim}_{n\to\infty} \eta_n(s) = \operatorname*{wlim}_{n\to\infty} \zeta_n(s) = 0.$$

Here, for the sequence $\{f_n\}_{n\in\mathbb{N}_0} \subset \mathbf{L}^2(\mathbb{R})$, there exists $f \in \mathbf{L}^2(\mathbb{R})$ such that $\operatorname*{wlim}_{n\to\infty} f_n(s) = f(s)$ ($f_n(s)$ weakly converges to $f(s)$) iff for any function $g(s) \in \mathbf{L}^2(\mathbb{R})$ and $y \in \mathbb{R}$,

$$\lim_{n\to\infty} \int_{-\infty}^{y} f_n(s)g(s)\,\mathrm{d}s = \int_{-\infty}^{y} f(s)g(s)\,\mathrm{d}s.$$

The forms represented in Theorem 3.1 are the decomposition of the numerator and denominator of $p_n(x_n)$ and $q_n(x_n)$ into the terms dependent on or independent of run time n. The functions ξ_n, η_n and ζ_n correspond to the former terms; they include a term that oscillates and one that decays with the growth of n on the order of $1/n$. Although these terms do not converge to specific values, weak convergence holds. In contrast, the function $\tau_1(s)$ corresponds to the latter term, meaning that $\tau_1(s)$ does not depend on n. In other words, it represents the invariant structure of $p_n(x_n)$ inside the peaks. Similarly, $1 - \tau_1(s)$ is the invariant structure of $q_n(x_n)$.

Congruently, we obtain the following fact about the transition probabilities outside the peaks:

Theorem 3.2. *For $s \in \mathbb{R}$ that satisfies $|a| \le |s| < 1$, $p_n(ns)$ and $q_n(ns)$ can be described as*

$$\lim_{n\to\infty} p_n(ns) = \tau_2(s) := \frac{s - |a|^2 + |b|\sqrt{s^2 - |a|^2}}{2s} \quad \text{and}$$
$$\lim_{n\to\infty} q_n(ns) = 1 - \tau_2(s).$$

Herein, $\tau_2(s)$ does not depend on n and contains no oscillations in time nor space.

The final statement regards the area *around the peaks*, or the boundaries between the regions inside and outside the peaks.

Theorem 3.3. *Let a sequence $\{x_n^\pm\}$ satisfy*

$$x_n^\pm = \pm n|a| + d_n^\pm,$$

where $\{d_n^\pm\}$ is a sequence that satisfies $d_n^\pm = \gamma n^{1/3} + o(n^{1/3})$ with any $\gamma \ge 0$. Then, it follows that

$$\lim_{j\to\infty} p_n(x_n^\pm) = \tau_\circ^\pm \quad \text{and} \quad \lim_{j\to\infty} q_n(x_n^\pm) = 1 - \tau_\circ^\pm.$$

3.2. Skeleton structure

The skeleton structure of QWRW is defined by combining the functions introduced in the Theorems 3.1 and 3.2:

Definition 3.4. *Define the function $\tau : (-1, 1) \to [0, 1]$ as*

$$\tau(s) = \begin{cases} \tau_1(s) = \dfrac{1-s}{2} & (0 \le |s| < |a|) \\ \tau_2(s) = \dfrac{s - |a|^2 + |b|\sqrt{s^2 - |a|^2}}{2s} & (|a| \le |s| < 1) \end{cases},$$

and call it the skeleton structure of the transition probability $p_n(ns)$. Equally, $1 - \tau(s)$ is the skeleton structure of $q_n(ns)$.

The function $\tau(s)$ defined above is independent of the initial state $|\varphi\rangle$, i.e., the skeletal structure is only determined by the parameters of the coin matrix. In addition, on the straight part inside the peaks, the range is determined by the parameters of the coin matrix, but the gradient is always $-1/2$, regardless of the setting of QWRW, as long as the coin matrix is time- and site-homogeneous. Moreover, $\tau(s)$ is continuous around the peaks $s = \pm|a|$; that is,

$$\lim_{s\to\pm|a|\mp 0} \tau_1(s) = \lim_{s\to\pm|a|\pm 0} \tau_2(s) = \tau_\circ^\pm. \tag{9}$$

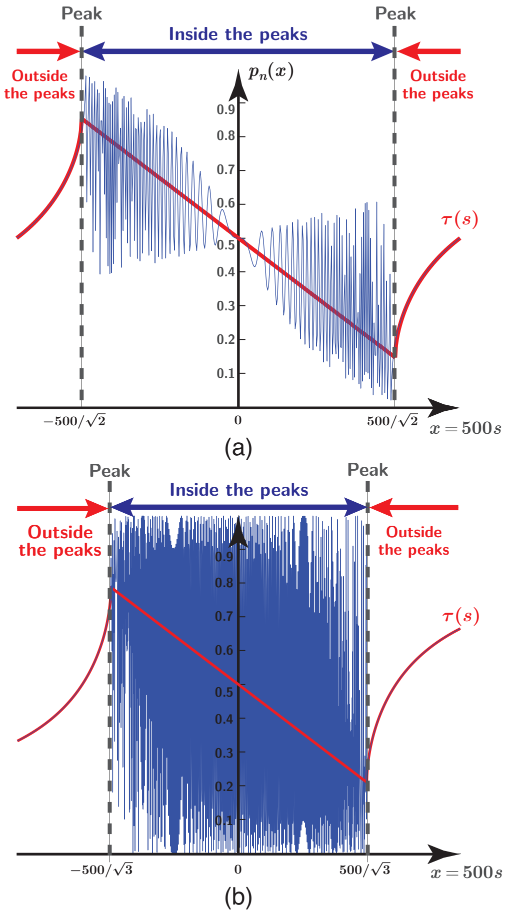

Figure 4: The relationship between $p_{500}(x)$ (blue line) and its skeleton structure $\tau(s)$ (red line). (a) Parameters of Setting A; (b) $a = 1/\sqrt{3}$, $b = 2/\sqrt{3}$, $\varDelta = 1$, $|\varphi_0\rangle = [1 \;\; 0]^{\mathsf{T}}$.

The graph of this skeleton structure $\tau(s)$ fits with that of $p_n(x)$ by stretching the s-axis n times. As examples, we show the case of Setting A and $(a, b, \varDelta, |\varphi\rangle) = (1/\sqrt{3}, 2/\sqrt{3}, 1, [1 \;\; 0]^{\mathsf{T}})$ in Figs. 4(a) and (b), respectively. Inside the peaks, these two cases seemingly exhibit different oscillatory behavior. However, the skeleton structure of these two cases are the same. Outside the peaks, both cases follow the same no-oscillatory curves. This is the visualization of the convergence stated in Theorem 3.2.

4. Summary

In this paper, we analyzed the transition probabilities of quantum-walk-replicating random walks. First, we presented a mathematical statement regarding the transition probabilities, and then we defined the skeleton structure. This skeleton structure is completely independent of the initial state of the quantum walk; additionally, the straight part inside the peaks has the same shape regardless of the setting of QWRW, except for its range.

Acknowledgments

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References

[1] N. Konno, "Quantum walks," in *Quantum potential theory*, pp. 309–452, Springer, 2008.

[2] J. Kempe, "Quantum random walks: an introductory overview," *Contemporary Physics*, vol. 44, no. 4, pp. 307–327, 2003.

[3] S. E. Venegas-Andraca, "Quantum walks: a comprehensive review," *Quantum Information Processing*, vol. 11, no. 5, pp. 1015–1106, 2012.

[4] V. Kendon, "Decoherence in quantum walks–a review," *Mathematical Structures in Computer Science*, vol. 17, no. 6, pp. 1169–1220, 2007.

[5] S. P. Gudder, *Quantum Probability*. Elsevier Science, 1988.

[6] Y. Aharonov, L. Davidovich, and N. Zagury, "Quantum random walks," *Phys. Rev. A*, vol. 48, pp. 1687–1690, Aug 1993.

[7] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, "One-dimensional quantum walks," in *Proceedings of the thirty-third annual ACM symposium on Theory of computing*, pp. 37–49, 2001.

[8] N. Konno, "Quantum random walks in one dimension," *Quantum Information Processing*, vol. 1, no. 5, pp. 345–354, 2002.

[9] N. Konno, "A new type of limit theorems for the one-dimensional quantum random walk," *Journal of the Mathematical Society of Japan*, vol. 57, no. 4, pp. 1179–1195, 2005.

[10] M. G. Andrade, F. de Lima Marquezino, and D. R. Figueiredo, "On the equivalence between quantum and random walks on finite graphs," *Quantum Information Processing*, vol. 19, no. 11, pp. 1–20, 2020.

[11] M. Montero, "Quantum and random walks as universal generators of probability distributions," *Physical Review A*, vol. 95, no. 6, p. 062326, 2017.

[12] T. Yamagami, E. Segawa, N. Chauvet, A. Röhm, R. Horisaki, and M. Naruse, "Directivity of quantum walk via its random walk replica," arXiv preprint arXiv:2201.08067, 2022 (accepted for publication in *Complexity*).