Interdisciplinary Information Sciences Vol. 24, No. 2 (2018) 185–188

ISSN 1340-9050 print/1347-6157 online
DOI 10.4036/iis.2018.S.03

SHORT COMMUNICATION

Probability Distributions and Weak Limit Theorems of Quaternionic Quantum Walks in One Dimension

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The discrete-time quantum walk (QW) is determined by a unitary matrix whose components are complex numbers. Konno (2015) extended the QW to the quaternionic quantum walk (QQW) whose components are quaternions and presented some properties of the QQW. Furthermore, Konno (2015) presented the question of whether or not the dynamics of a QQW is exactly the same as that of the corresponding QW. We give an answer to the problem by calculating the probability distribution and the weak limit density function of some classes of the QQW.

KEYWORDS: quantum walks, quaternionic quantum walks, quaternion, probability distribution, weak limit theorem

1. Introduction

The discrete-time quantum walk (QW) is a quantum dynamics defined as a quantization of the classical random walk. The study of QWs has recently begun to attract the concern of various research fields such as information science and quantum physics. Moreover, QW is powerful method for developing new quantum algorithms and protocols [6]. The discrete-time 2-state QW on $\mathbb{Z}$ has been largely investigated [2–4], where $\mathbb{Z}$ is the set of integers. As a natural quaternionic extension of this model, the quaternionic quantum walk (QQW) on $\mathbb{Z}$ is introduced by Konno [1].

In this paper, we treat the QQWs in five cases, Cases 1 to 5. We will give the definitions of Cases 1 to 4 and Case 5 in Sections 3.1 and 3.2, respectively. Our results present an equivalence of the probability distribution of QQWs to that of the 2-state QW in Case 1–4, and the weak limit theorem of QQWs in Case 5 which produces a different form of the weak limit density function from that of the QW with some appropriate parameters. The QQWs in Cases 1 to 4 include a QQW introduced as an example in [1]. In addition, we clarify that the probability distributions of the QQWs in these cases have exactly the same expression as that of the 2-state QW. However, in general, the expression does not always correspond to that of the QW. For instance, a numerical simulation suggests that the probability distribution of a QQW is different from that of the 2-state QW (see Fig. 1). As one of the main results, we clarify a concrete expression of the limit density function of the QQW in Case 5, which is different from that of the QW. The range of limit density function of the QW is determined only by the modulus of a component of unitary matrix called coin operator which gives the dynamics of the QW. However, that of the QQW in Case 5 is not determined only by the modulus of the component (see Fig. 2). Moreover, this weak limit density function for a special model in Case 5 becomes that of the QW.

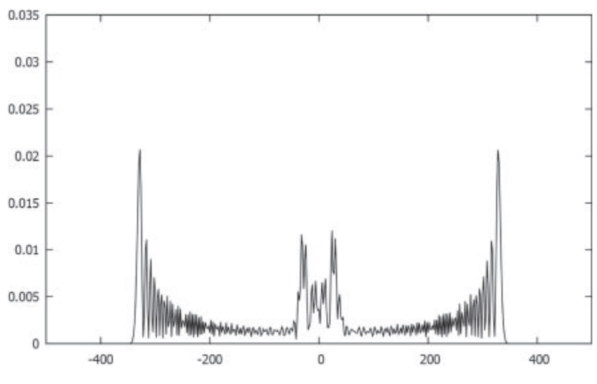

Fig. 1. The distribution of a QQW.

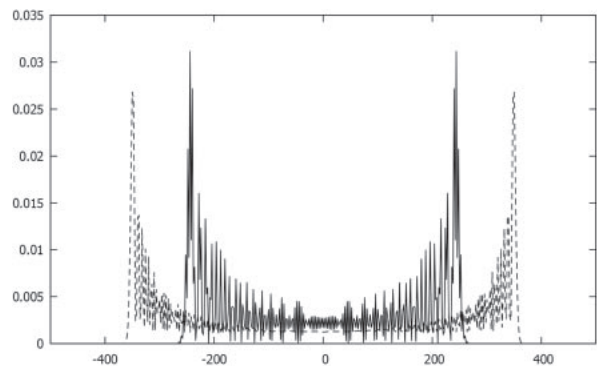

Fig. 2. The distributions of a QW (dotted line) and a QQW in Case 5 (solid line).

Received April 6, 2018; Accepted August 31, 2018; J-STAGE Advance published September 28, 2018
2010 Mathematics Subject Classification: Primary 60F05, Secondary 81P68
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2. Preliminaries

2.1 Quaternion

Let $\mathbb{R}$, $\mathbb{C}$ and $\mathbb{H}$ be the sets of the real numbers, the complex numbers and the quaternions, respectively. Then $x \in \mathbb{H}$ is expressed as $x = x_0 + x_1 i + x_2 j + x_3 k$, where $i^2 = j^2 = k^2 = -1$, $ij = -ji = k$, $jk = -kj = i$, $ki = -ik = j$, and $x_0, x_1, x_2, x_3 \in \mathbb{R}$. Throughout this paper, for any quaternion $q \in \mathbb{H}$, the coefficients of basis $1, i, j, k$ are denoted by $q_0, q_1, q_2, q_3 \in \mathbb{R}$, respectively, that is, $q = q_0 + q_1 i + q_2 j + q_3 k$. Here, x is decomposed by the real part as $\Re(x) = x_0$, and the imaginary part as $\Im(x) = x_1 i + x_2 j + x_3 k$. Moreover, for the above x, let $\overline{x}$ be the conjugate of x whose form is given by $\overline{x} = x_0 - x_1 i - x_2 j - x_3 k$. Then the modulus of x is given by $|x| = \sqrt{x\overline{x}} = \sqrt{\overline{x}x} = \sqrt{x_0^2 + x_1^2 + x_2^2 + x_3^2}$.

Let $\mathrm{M}(n, \mathbb{C})$ and $\mathrm{M}(n, \mathbb{H})$ be the sets of all $n \times n$ matrices with complex number and quaternion components, respectively. For $A = (a_{st}) \in \mathrm{M}(n, \mathbb{H})$, we put $\overline{A} = (\overline{a}_{st})$ and $A^* = {}^T(\overline{A})$. Here, T denotes the transpose operator. As with the complex components, A is a unitary matrix, if $AA^* = A^*A = I$, where I is the identity matrix. Let $\mathrm{U}(n, \mathbb{C})$ and $\mathrm{U}(n, \mathbb{H})$ be the sets of all $n \times n$ unitary matrices with complex number and quaternionic components, respectively.

Moreover, x is uniquely expressed as a direct sum of complex numbers: $x = x' + x'' j \in \mathbb{H}$ ($x' = x_0 + x_1 i$, $x'' = x_2 + x_3 i \in \mathbb{C}$). Here, x' and x'' are called simplex and perplex parts, respectively. By using this, we can express the quaternion as the isomorphic complex matrix with a homomorphism $\chi : \mathrm{M}(n, \mathbb{H}) \to \mathrm{M}(2n, \mathbb{C})$. Such a homomorphism is not uniquely determined. In this paper, we define $\chi(A) = (\chi(a_{st})) \in \mathrm{M}(2n, \mathbb{C})$ for $A = (a_{st}) \in \mathrm{M}(n, \mathbb{H})$, with

$$\chi(x) = \begin{bmatrix} x' & -x'' \\ \overline{x''} & \overline{x'} \end{bmatrix} \in \mathrm{M}(2, \mathbb{C}).$$

2.2 QQW

The QQW on $\mathbb{Z}$ is determined by the unitary matrix $U \in \mathrm{U}(2, \mathbb{H})$ which is called coin operator. The walker of QQW has two chiralities, left and right, corresponding to the direction of the motion. Then we adapt each chirality to the vector $|L\rangle = {}^T\begin{bmatrix} 1 & 0 \end{bmatrix}$ and $|R\rangle = {}^T\begin{bmatrix} 0 & 1 \end{bmatrix}$, where L and R refer to the left and right chirality states, respectively. Let the coin operator $U \in \mathrm{U}(2, \mathbb{H})$ be

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2, \mathbb{H}).$$

Then the evolution of the quaternion version amplitude on position x at time n, $\Psi_n(x) = {}^T\begin{bmatrix} \Psi_n^L(x) & \Psi_n^R(x) \end{bmatrix} \in \mathbb{H}^2$, is defined by $\Psi_{n+1}(x) = P\Psi_n(x+1) + Q\Psi_n(x-1)$, where two matrices which represent the direction of the walker P and Q are defined by $|L\rangle\langle L|U$ and $|R\rangle\langle R|U$, respectively. Here, the probability that the walker X_n exists on position x at time n is defined by $P(X_n = x) = \|\Psi_n(x)\|^2$. In this paper, we treat the model starting from only the origin. That is, we put the initial state $\Psi_0(x) = \delta_0(x)^T\begin{bmatrix} \alpha & \beta \end{bmatrix}$, with $\alpha, \beta \in \mathbb{H}$ and $|\alpha|^2 + |\beta|^2 = 1$. Here, Kronecker's delta $\delta_0(x)$ equals to 1 if $x = 0$, equals to 0 otherwise.

2.3 Fourier transform for the QQW

We should remark that since $\Psi_n(x) \in \mathbb{H}^2$ is isomorphic to $\chi(\Psi_n(x))\ {}^T\begin{bmatrix} 1 & 0 \end{bmatrix} \in \mathbb{C}^4$, from now on we use the expression of $\mathbb{C}^4$. Let $\Phi_n(x)$ be the $\mathbb{C}^4$ expression of $\Psi_n(x)$, and its Fourier transform is given by

$$\hat{\Phi}_n(\theta) = \sum_{x \in \mathbb{Z}} e^{-i\theta x} \Phi_n(x), \quad \Phi_n(x) = \int_{-\pi}^{\pi} e^{i\theta x} \hat{\Phi}_n(\theta) \frac{d\theta}{2\pi}.$$

Noting that $\Phi_n(x)$ is isomorphic to $\Psi_n(x)$, the following lemma holds.

Lemma 2.1.

$$(1) \quad P(X_n = x) = \|\Phi_n(x)\|^2. \qquad (2) \quad \Phi_{n+1}(x) = \chi(P)\Phi_n(x+1) + \chi(Q)\Phi_n(x-1).$$

We remark that this lemma implies the QQW is essentially equivalent to the corresponding 4-state QW on $\mathbb{Z}$ [5]. Here, Lemma 2.1 suggests that the time evolution of $\hat{\Phi}_n(\theta)$ is described by $U(\theta) \in \mathrm{U}(4, \mathbb{C})$:

$$U(\theta) = \begin{bmatrix} e^{i\theta}\chi(a) & e^{i\theta}\chi(b) \\ e^{-i\theta}\chi(c) & e^{-i\theta}\chi(d) \end{bmatrix} = \begin{bmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & e^{i\theta} & 0 & 0 \\ 0 & 0 & e^{-i\theta} & 0 \\ 0 & 0 & 0 & e^{-i\theta} \end{bmatrix} \begin{bmatrix} \chi(a) & \chi(b) \\ \chi(c) & \chi(d) \end{bmatrix}.$$

We can formulate the evolution by $\hat{\Phi}_n(\theta) = U(\theta)^n \hat{\Phi}_0(\theta)$. Then the probability distribution is expressed as

$$P(X_n = x) = \|\Phi_n(x)\|^2 = \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} e^{i(\theta'-\theta)x}(\hat{\Phi}_0^*(\theta)U^*(\theta)^n)(U(\theta')^n\hat{\Phi}_0(\theta'))\frac{d\theta}{2\pi}\frac{d\theta'}{2\pi}.$$

2.4 Weak limit theorem

The weak limit theorem for the 2-state QW on $\mathbb{Z}$ was given in [2, 3] by a path counting method.

Theorem 2.2 (Konno [2, 3]). *For QW, X_n, whose coin operator is $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2, \mathbb{C})$ with $abcd \neq 0$, $\Psi_0(x) = \delta_0(x)^T\begin{bmatrix} \alpha & \beta \end{bmatrix} \in \mathbb{C}^2$, we see that X_n/n converges weakly to the random variable Y as $n \to \infty$ whose density function $f(y)$ is given by*

$$f(y) = f(y; {}^T[\alpha, \beta]) = \{1 - C(a, b; \alpha, \beta)y\}f_K(y; |a|),$$

$$\text{where} \quad C(a, b; \alpha, \beta) = |\alpha|^2 - |\beta|^2 - \frac{2\Re(\alpha\,\overline{a}b\beta)}{|a|^2}, \quad f_K(y; r) = \frac{\sqrt{1 - r^2}}{\pi(1 - y^2)\sqrt{r^2 - y^2}} I_{(-r,r)}(y) \quad (0 < r < 1).$$

Here, $I_{(-r,r)}(y) = 1$, if $y \in (-r, r)$, $= 0$, otherwise.

We should note that the parameter r means the range of support of the limit density function. This weak limit theorem was also obtained by Grimmett, Janson, and Scudo [4] via the Fourier transform, which is called the *GJS method* in this paper. The GJS method showed that the limit density function of the QW can be expressed by eigenvalues $e^{i\lambda}$, eigenvectors $|v(\theta)\rangle$ of $U(\theta)$, and the change of variable $y = \frac{d}{d\theta}\lambda$. As in the case of QW, we apply the GJS method to our QQWs. Here, the characteristic polynomial of $U(\theta)$ is

$$|Ix - U(\theta)| = x^4 - 2(a_0e^{i\theta} + d_0e^{-i\theta})x^3 + 2(2a_0d_0 - \Re(bc) + |a|^2\cos(2\theta))x^2 - 2(d_0e^{i\theta} + a_0e^{-i\theta})x + 1$$

and the eigenvector associated with $e^{i\lambda}$ is

$$|v(\theta)\rangle = \begin{bmatrix} |b|^2(1 + C_1) \\ -|b|^2(C_2i + C_3) \\ -l((\overline{b}a)', -\overline{b'})(1 + C_1) - l((\overline{b}a)'', b'')(C_2i + C_3) \\ -l(\overline{(\overline{b}a)''}, \overline{b''})(1 + C_1) + l(\overline{(\overline{b}a)'}, -b')(C_2i + C_3) \end{bmatrix}, \tag{2.1}$$

where

$$C = \frac{1}{|B|^2}\Im(2a|b|^2\sin(\lambda - \theta) + (bd\overline{b} + \overline{c}dc)\sin(\lambda + \theta) + bc\sin(2\lambda) - b\overline{d^2}c\sin(2\theta)), \quad l(x, y) = x + ye^{i(\lambda-\theta)}.$$

Here, $|B|^2$ is normalized coefficient for C and given by

$$|B|^2 = |a|^2|b|^2(\sin^2(\lambda - \theta) + \sin^2(\lambda + \theta)) - 2|b|^2(a_0\sin(\lambda + \theta) + d_0\sin(\lambda - \theta))\sin(2\lambda)$$
$$- 2\Re(\overline{a^2}bc)\sin(\lambda - \theta)\sin(\lambda + \theta) + |b|^2\sin^2(2\lambda).$$

3. Results

Our main results give the probability distribution or the weak limit theorem for the QQWs in five cases. Firstly, we show that the probability distribution of the QQW in Cases 1 to 4 are formulated as exact same as that of the 2-state QW (concrete expression is presented in Konno [2]). Secondly, in contrast to Cases 1 to 4, we prove that the dynamics of the QQW in Case 5 is different from the 2-state QW by the weak limit theorem. Moreover, if $\Re(bc) = bc$, then its limit density function is the same as that of the QW, $f_K(y; |a|)$. On the other hand, if $\Re(bc) = 0$, then the limit density function becomes $f_K(y; |a|^2)$. We should remark that this range $|a|^2$ is different from that of the traditional QW. Therefore, these results give an answer to the problem of clarifying the difference between the 2-state QW and QQW.

3.1 Probability distributions (Cases 1 to 4)

Theorem 3.1. *For QQW in Cases 1 to 4 whose coin operator is $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2, \mathbb{H})$ defined as follows, probability distribution of the QQW is described by the exact same expression as the corresponding QW [2].*

$$\textit{Case 1}: \quad b = c = 0 \qquad\qquad \textit{Case 2}: \quad a = d = 0$$
$$\textit{Case 3}: \quad a, d \in \mathbb{R}, \quad b, c \in \mathbb{H} \qquad \textit{Case 4}: \quad a, d \in \mathbb{C}, \quad b, c \in \mathbb{C}j$$

Here, we assume $abcd \neq 0$ in Case 3 and Case 4.

The proof is based on a path counting method as with [2]. Especially, the walker in Case 1 (resp. Case 2) can not hop to the different (resp, same) direction of the previous step, since $PQ = QP = O$ (resp. $P^2 = Q^2 = O$). Therefore, the probability distributions of these cases of QQW are given straightforwardly.

3.2 Weak limit theorem (Case 5)

This section presents the weak limit theorem of the QQW in which components of U satisfy $\Re(a) = \Re(d) = 0$ and $abcd \neq 0$. Then eigenvalues of $U(\theta)$ are $\pm e^{i\lambda}, \pm e^{-i\lambda}$, where

$$\cos\lambda = \sqrt{\frac{1 - \Re(bc) + |a|^2 \cos 2\theta}{2}}, \quad \sin\lambda = \sqrt{\frac{1 + \Re(bc) - |a|^2 \cos 2\theta}{2}}.$$

Here, the parameter C of the eigenvector associated with $e^{i\lambda}$ in (2.1) is

$$C = \frac{1}{|B|^2} \Im(2|b|^2 a \sin(\lambda - \theta) + (bd\overline{b} + \overline{c}dc)\sin(\lambda + \theta) + bc(\sin(2\lambda) + |a|^2 \sin(2\theta)),$$

where $|B|^2 = 2|a|^2 \Re(bc)\cos(2\theta) + G - 2|a|^4$ and $G = 1 + |a|^4 - \Re(bc)^2$.

Then we have $\|v(\theta)\|^2 = \frac{4|b|^4}{|B|^2}(1 + C_1)(\sin(2\lambda) + |a|^2 \sin(2\theta)\sin(2\lambda))$. For $y = \frac{d}{d\theta}\lambda$, we get

$$\cos(2\theta) = \begin{cases} \dfrac{-\Re(bc)y^2 + \sqrt{y^4 - Gy^2 + |a|^4}}{|a|^2(1 - y^2)} & \left(\frac{-\Re(bc)r^2}{|a|^2(1-r^2)} \le \cos(2\theta) \le 1\right) \\ \dfrac{-\Re(bc)y^2 - \sqrt{y^4 - Gy^2 + |a|^4}}{|a|^2(1 - y^2)} & \left(-1 \le \cos(2\theta) < \frac{-\Re(bc)r^2}{|a|^2(1-r^2)}\right) \end{cases},$$

where $r = \sqrt{\frac{G - \sqrt{G^2 - 4|a|^4}}{2}} = \frac{\sqrt{(1 + |a|^2)^2 - \Re(bc)^2} - \sqrt{(1 - |a|^2)^2 - \Re(bc)^2}}{2}$. By using the GJS method, we obtain the following weak limit theorem in Case 5.

Theorem 3.2. *For QQW, X_n, in Case 5 whose coin operator is $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2, \mathbb{H})$, we see that X_n/n converges weakly to the random variable Y as $n \to \infty$ whose density function $f(y)$ is given by*

$$f(y) = f(y; {}^T[\alpha, \beta]) = \{1 - C(a, b; \alpha, \beta)y\} f_{QQW}(y; r),$$

where

$$f_{QQW}(y; r) = \frac{\sqrt{2}}{2\pi(1 - y^2)\sqrt{r^2 - y^2}} \frac{\sqrt{(G - 2)y^2 + G - 2|a|^4 + (1 - y^2)\sqrt{G^2 - 4|a|^4}}}{\sqrt{\frac{G + \sqrt{G^2 - 4|a|^4}}{2} - y^2}} I_{(-r,r)}(y),$$

$$r = \sqrt{\frac{G - \sqrt{G^2 - 4|a|^4}}{2}} = \frac{\sqrt{(1 + |a|^2)^2 - \Re(bc)^2} - \sqrt{(1 - |a|^2)^2 - \Re(bc)^2}}{2} \quad \textit{and} \quad G = 1 + |a|^4 - \Re(bc)^2.$$

Here, $C(a, b; \alpha, \beta)$ is the same as that in Theorem 2.2. Furthermore, it is easily checked that if $\Re(bc) = 0$ (resp. $\Re(bc) = bc$), then $f_{QQW}(y; r) = f_K(y; |a|^2)$ (resp. $f_{QQW}(y; r) = f_K(y; |a|)$), where $f_K(y; r)$ with $y \in \mathbb{Z}$ and $0 < r < 1$ is a weak limit density function of the QW. In other words, an essential difference between the QQW in Case 5 and the traditional QW is given by the parameter $\Re(bc)$ which is directly related to the range of the limit density function. Remark that when $\Re(bc) = bc$, the limit density function of the QQW in Case 5 reproduces that of the QW for $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in \mathrm{U}(2, \mathbb{C})$.

Acknowledgements

The author would like to thank Norio Konno for useful comments.

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