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Quantum walks and elliptic integrals

NORIO KONNO†

Department of Applied Mathematics, Faculty of Engineering,
Yokohama National University,
Hodogaya, Yokohama 240-8501, Japan
Email: konno@ynu.ac.jp

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Pólya showed in his 1921 paper that the generating function of the return probability for a two-dimensional random walk can be written in terms of an elliptic integral. In this paper we present a similar expression for a one-dimensional quantum walk.

1. Introduction

The classical random walk (RW) is one of the most popular models for analysing many problems in various fields. The quantum walk (QW) is viewed as a counterpart of the RW in quantum systems. The intensive study of QWs has only a short history, about ten years, but the attention paid to it is increasing within the scientific community, including physicists, mathematicians and computer scientists. Recently, a book and lecture notes on the QW have been published (Venegas-Andraca 2008; Konno 2008). For excellent reviews, see Kempe (2003) and Kendon (2007). There are two types of QWs, namely, discrete- and continuous-time walks. The relation between them has been investigated in Strauch (2006) and Childs (2010). Ambainis *et al.* (2001) studied the one-dimensional discrete-time case intensively using Fourier analysis and a path counting method. Recently, Cantero *et al.* (2010) showed how the theory of CMV matrices provides a natural tool for studying one-dimensional discrete-time QW – see, for instance, Cantero *et al.* (2003) and Simon (2007) for more on the CMV matrix. In this paper we consider the one-dimensional discrete-time QW, which is determined by a 2×2 unitary matrix. We prove that the generating function of the return probability for the one-dimensional QW can be written in terms of an elliptic integral by a path counting method. A similar expression for a two-dimensional RW was presented in Pólya (1921). The return probability of a three-dimensional RW is also given by an elliptic integral and was evaluated in Watson (1939). It is known that elliptic integrals and their inverses, that is, elliptic functions, arise in many branches of mathematics and physics. Our result for the generating function in terms of the elliptic integral may just be the tip of an iceberg. Pursuing the study along these line would provide interesting future problems on the QW.

The rest of this paper is organised as follows. Section 2 describes the definition of the QW. In Section 3, we present our main result (Theorem 3.1), and in Section 4 we

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prove Proposition 3.1, on which the main result relies. Several methods may be used for the analysis of the QW: specifically, Fourier analysis, path counting and the CMV matrix-based method. In our proof, we use a path counting method, as in the classical two-dimensional RW case described in Section 3. Finally, we give conclusions in Section 5.

2. Model

In this section we define the discrete-time QW on $\mathbb{Z}$ that we will consider here, where $\mathbb{Z}$ is the set of integers. In general, the time evolution of the QW is determined by a 2×2 unitary matrix:

$$U = \begin{bmatrix} a & b \\ c & d \end{bmatrix},$$

where $a, b, c, d \in \mathbb{C}$ and $\mathbb{C}$ is the set of complex numbers. The QW defined by the Hadamard gate $U = H$ with $a = b = c = -d = 1/\sqrt{2}$ is often called the *Hadamard walk*, and has been extensively investigated in the study of the QW:

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

In the present paper, we will focus on the Hadamard walk. The discrete-time QW is a quantum version of the random walk with an additional degree of freedom called chirality. The chirality takes values left and right, and represents the direction of motion of the walker. At each time step, if the walker has left chirality, it moves one step to the left, and if it has right chirality, it moves one step to the right. We define

$$|L\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$
$$|R\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

where L and R refer to the left and right chirality states, respectively. To define the dynamics of our model, we divide U into two matrices:

$$P = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}$$
$$Q = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}$$

with $U = P + Q$. The important point in the following is that P and Q represent the fact that the walker moves to the left or right, respectively, at position x at each time step. We let $\Xi_n(l, m)$ denote the sum of all paths starting from the origin in the trajectory consisting of l steps left and m steps right at time n with $l + m = n$. For example, we have $\Xi_2(1, 1) = QP + PQ$ and

$$\Xi_4(2, 2) = Q^2P^2 + P^2Q^2 + QPQP + PQPQ + PQ^2P + QP^2Q. \tag{2.1}$$

In this paper, we take $\varphi_* = {}^T[1/\sqrt{2}, i/\sqrt{2}]$ as the initial qubit state, where T is the transposed operator. Then the probability distribution of the walk starting from φ_* at the

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origin is symmetric. The probability that our quantum walker is in position x at time n starting from the origin with φ_* is defined by

$$P(X_n = x) = ||\Xi_n(l, m)\varphi_*||^2,$$

where $n = l + m$ and $x = -l + m$. Then the return probability at the origin at time n is given by

$$p_n(0) = P(X_n = 0).$$

By definition, $p_{2n+1}(0) = 0$ for $n \geqslant 0$, so we only need to consider even times $2n$.

3. Result

In this section we present our results. By the definition of the Hadamard walk, we can directly compute

$$\begin{aligned} p_0(0) &= 1 \\ p_2(0) &= \frac{1}{2} = 0.5 \\ p_4(0) = p_6(0) &= \frac{1}{8} = 0.125 \\ p_8(0) = p_{10}(0) &= \frac{9}{128} = 0.07031\ldots \\ p_{12}(0) = p_{14}(0) &= \frac{25}{512} = 0.04882\ldots \\ p_{16}(0) = p_{18}(0) &= \frac{1225}{32768} = 0.03738\ldots. \end{aligned} \tag{3.2}$$

In general, $p_{2n}(0)$ can be written in terms of Legendre polynomials, $P_n(x)$, as follows – see Andrews *et al.* (1999) for special functions.

Proposition 3.1. $p_0(0) = 1$ and

$$p_{2n}(0) = \frac{1}{2}\left[\{P_{n-1}(0)\}^2 + \{P_n(0)\}^2\right] \quad (n \geqslant 1).$$

The proof appears in the next section. By Proposition 3.1, $P_{2n+1}(0) = 0$ and

$$P_{2n}(0) = \frac{1}{2^{2n}}\binom{2n}{n}. \tag{3.3}$$

We get

$$p_{4m}(0) = p_{4m+2}(0) = \frac{1}{2}\{P_{2m}(0)\}^2 = \frac{1}{2^{4m+1}}\binom{2m}{m}^2 \quad (m \geqslant 1). \tag{3.4}$$

So (3.2) can also be obtained using (3.4). We will now derive our main result (Theorem 3.1) from Proposition 3.1. We begin with

$$\sum_{n=0}^{\infty} p_n(0)z^n = \sum_{n=0}^{\infty} p_{2n}(0)z^{2n} = \frac{1}{2}\left[(1+z^2)\sum_{n=0}^{\infty}\{P_n(0)\}^2 z^{2n} + 1\right].$$

Therefore, by (3.3),

$$\begin{aligned}\sum_{n=0}^{\infty} \{P_n(0)\}^2 z^{2n} &= \sum_{n=0}^{\infty} \{P_{2n}(0)\}^2 z^{4n} \\ &= \sum_{n=0}^{\infty} \binom{2n}{n}^2 \left(\frac{z^2}{4}\right)^{2n} \\ &= \frac{2}{\pi} K(z^2),\end{aligned}$$

where $K(k)$ is the complete elliptic integral (see Andrews *et al.* (1999)), that is, for $0 \leqslant k < 1$

$$\begin{aligned}K(k) &= \int_0^{\pi/2} \frac{d\theta}{\sqrt{1-k^2\sin^2\theta}} \\ &= \int_0^1 \frac{dx}{\sqrt{(1-x^2)(1-k^2x^2)}}.\end{aligned}$$

So the generating function of the return probability for the one-dimensional Hadamard walk can be expressed by $K(k)$, as follows.

Theorem 3.1.

$$\sum_{n=0}^{\infty} p_n(0) z^n = \frac{1+z^2}{\pi} K(z^2) + \frac{1}{2}.$$

We now consider the generating function for the classical case: the d-dimensional classical (simple) RW whose transition probability from the origin to x is given by $1/2d$ for any $x = (x_1, \ldots, x_d) \in \mathbb{Z}^d$ with $\sum_{k=1}^d |x_k| = 1$. Let $p_n^{(c,d)}(0)$ denote the return probability for the RW starting from the origin at time n. In the one-dimensional RW case, it is well known that for $n \geqslant 0$

$$\begin{aligned}p_{2n}^{(c,1)}(0) &= \frac{1}{2^{2n}}\binom{2n}{n} \\ p_{2n+1}^{(c,1)}(0) &= 0.\end{aligned}$$

So we get

$$\sum_{n=0}^{\infty} p_n^{(c,1)}(0) z^n = \frac{1}{\sqrt{1-z^2}}.$$

For the two-dimensional RW, we find that for $n \geqslant 0$

$$\begin{aligned}p_{2n}^{(c,2)}(0) &= \left\{p_{2n}^{(c,1)}(0)\right\}^2 = \frac{1}{4^{2n}}\binom{2n}{n}^2 \\ p_{2n+1}^{(c,2)}(0) &= 0.\end{aligned}$$

(See, for instance, Durrett (2004) for the derivation.) Therefore, we have

$$\sum_{n=0}^{\infty} p_n^{(c,2)}(0) z^n = \frac{2}{\pi} K(z).$$

This result was given in Pólya (1921, page 160). In addition, the above expression is very similar to that for the one-dimensional Hadamard walk (see Theorem 3.1). The probability that the three-dimensional RW returns to its starting point, $F = 1 - G^{-1} = 0.34053\ldots$, is given by $K(k)$ in the following (Spitzer 1976, page 103):

$$G = \frac{1}{\pi^2} \int_{-\pi}^{\pi} K\left(\frac{2}{3-\cos\theta}\right) d\theta.$$

Note that the definition of the complete elliptic integral given in Spitzer (1976) is $(2/\pi) \times K(k)$ in our notation. This integral was first evaluated in Watson (1939):

$$\begin{aligned} G &= 3(18 + 12\sqrt{2} - 10\sqrt{3} - 7\sqrt{6})\,\{K(2\sqrt{3} + \sqrt{6} - 2\sqrt{2} - 3)\}^2 \times (2/\pi)^2 \\ &= 1.51638\ldots. \end{aligned}$$

4. Proof of Proposition 3.1

In this section we will prove Proposition 3.1 by a path counting method. First we introduce some useful matrices for computing $\Xi_n(l,m)$:

$$R = \begin{bmatrix} c & d \\ 0 & 0 \end{bmatrix}$$

$$S = \begin{bmatrix} 0 & 0 \\ a & b \end{bmatrix}$$

where $a = b = c = -d = 1/\sqrt{2}$. In general, products of the matrices P, Q, R and S are given in Table 1. From this table and (2.1), we obtain

$$\Xi_4(2,2) = bcdP + abcQ + b(ad+bc)R + c(ad+bc)S.$$

Note that P, Q, R and S form an orthonormal basis of the vector space of complex 2×2 matrices with respect to the trace inner product $\langle A|B\rangle = \mathrm{tr}(A^*B)$, where $*$ means the adjoint operator. So $\Xi_n(l,m)$ has the following form:

$$\Xi_n(l,m) = p_n(l,m)P + q_n(l,m)Q + r_n(l,m)R + s_n(l,m)S.$$

The explicit forms of $p_n(l,m), q_n(l,m), r_n(l,m)$ and $s_n(l,m)$ can be computed as follows (see, for instance, Konno (2002; 2005)).

	P	Q	R	S
P	aP	bR	aR	bP
Q	cS	dQ	cQ	dS
R	cP	dR	cR	dP
S	aS	bQ	aQ	bS

Table 1. *Products of P, Q, R, S. For example, $PQ = bR$.*

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Lemma 4.1. When $l \wedge m (:= \min\{l, m\}) \geqslant 1$, we obtain

$$p_n(l,m) = \left(\frac{1}{\sqrt{2}}\right)^{n-1} \sum_{\gamma=1}^{(l-1)\wedge m} (-1)^{m-\gamma} \binom{l-1}{\gamma} \binom{m-1}{\gamma-1}$$

$$q_n(l,m) = \left(\frac{1}{\sqrt{2}}\right)^{n-1} \sum_{\gamma=1}^{l\wedge(m-1)} (-1)^{m-\gamma-1} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma}$$

$$r_n(l,m) = s_n(l,m) = \left(\frac{1}{\sqrt{2}}\right)^{n-1} \sum_{\gamma=1}^{l\wedge m} (-1)^{m-\gamma} \binom{l-1}{\gamma-1} \binom{m-1}{\gamma-1}.$$

Using Lemma 4.1, we have

$$\begin{aligned} \Xi_{2n}(n,n)\varphi_* &= \left(\frac{1}{\sqrt{2}}\right)^{2n} (-1)^n \sum_{\gamma=1}^{n} (-1)^{\gamma} \binom{n-1}{\gamma-1}^2 \begin{bmatrix} \frac{n}{\gamma} & \frac{n}{\gamma}-2 \\ -\frac{n}{\gamma}+2 & \frac{n}{\gamma} \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ i \end{bmatrix} \\ &= \left(\frac{1}{\sqrt{2}}\right)^{2n+1} (-1)^n \sum_{\gamma=1}^{n} \frac{(-1)^{\gamma}}{\gamma} \binom{n-1}{\gamma-1}^2 \begin{bmatrix} n+(n-2\gamma)i \\ -(n-2\gamma)+ni \end{bmatrix}. \end{aligned}$$

Since $p_{2n}(0) = ||\Xi_{2n}(n,n)\varphi_*||^2$, we get

$$\begin{aligned} p_{2n}(0) &= \left(\frac{1}{2}\right)^{2n} \left[\left\{ \sum_{\gamma=1}^{n} \frac{(-1)^{\gamma}}{\gamma} \binom{n-1}{\gamma-1}^2 n \right\}^2 + \left\{ \sum_{\gamma=1}^{n} \frac{(-1)^{\gamma}}{\gamma} \binom{n-1}{\gamma-1}^2 (n-2\gamma) \right\}^2 \right] \\ &= \left(\frac{1}{2}\right)^{2n} \Bigg[2n^2 \left\{ \sum_{\gamma=1}^{n} \frac{(-1)^{\gamma}}{\gamma} \binom{n-1}{\gamma-1}^2 \right\}^2 \\ &\qquad - 4n \sum_{\gamma=1}^{n} \sum_{\delta=1}^{n} \frac{(-1)^{\gamma+\delta}}{\gamma} \binom{n-1}{\gamma-1}^2 \binom{n-1}{\delta-1}^2 \\ &\qquad + 4 \sum_{\gamma=1}^{n} \sum_{\delta=1}^{n} (-1)^{\gamma+\delta} \binom{n-1}{\gamma-1}^2 \binom{n-1}{\delta-1}^2 \Bigg]. \end{aligned}$$

Furthermore, we will rewrite $p_{2n}(0)$ using the Jacobi polynomial $P_n^{\nu,\mu}(x)$, which is orthogonal on $[-1,1]$ with respect to $(1-x)^{\nu}(1+x)^{\mu}$ with $\nu, \mu > -1$. The following relation then holds:

$$P_n^{\nu,\mu}(x) = \frac{\Gamma(n+\nu+1)}{\Gamma(n+1)\Gamma(\nu+1)}\, {}_2F_1(-n, n+\nu+\mu+1; \nu+1; (1-x)/2), \tag{4.5}$$

where $\Gamma(z)$ is the gamma function. Therefore,

$$\begin{aligned} \sum_{\gamma=1}^{n} \frac{(-1)^{\gamma-1}}{\gamma} \binom{n-1}{\gamma-1}^2 &= {}_2F_1(-(n-1), -(n-1); 2; -1) \\ &= 2^{n-1}{}_2F_1(-(n-1), n+1; 2; 1/2) \\ &= \frac{2^{n-1}}{n} P_{n-1}^{(1,0)}(0). \end{aligned} \tag{4.6}$$

The first equality is given by the definition of the hypergeometric series, the second equality comes from the relation

$${}_2F_1(a,b;c;z) = (1-z)^{-a}{}_2F_1(a,c-b;c;z/(z-1))$$

and the final equality follows from (4.5). In a similar way,

$$\sum_{\gamma=1}^{n} (-1)^{\gamma-1} \binom{n-1}{\gamma-1}^2 = 2^{n-1} P_{n-1}^{(0,0)}(0). \tag{4.7}$$

Using (4.6) and (4.7), we get

$$\begin{aligned} p_{2n}(0) &= \left(\frac{1}{2}\right)^{2n} \left[2n^2 \times \frac{2^{2(n-1)}}{n^2} \left\{P_{n-1}^{(1,0)}(0)\right\}^2 \right. \\ &\qquad \left. - 4n \times \frac{2^{2(n-1)}}{n} P_{n-1}^{(1,0)}(0)\, P_{n-1}^{(0,0)}(0) + 4 \times 2^{2(n-1)} \left\{P_{n-1}^{(0,0)}(0)\right\}^2\right] \\ &= \frac{\left\{P_{n-1}^{(1,0)}(0)\right\}^2}{2} - P_{n-1}^{(1,0)}(0)\, P_{n-1}^{(0,0)}(0) + \left\{P_{n-1}^{(0,0)}(0)\right\}^2 \\ &= \frac{1}{2}\left[\left\{P_{n-1}^{(1,0)}(0) - P_{n-1}^{(0,0)}(0)\right\}^2 + \left\{P_{n-1}^{(0,0)}(0)\right\}^2\right]. \end{aligned} \tag{4.8}$$

From Andrews *et al.* (1999, 6.4.20),

$$(n+\alpha+1)P_n^{(\alpha,\beta)}(x) - (n+1)P_{n+1}^{(\alpha,\beta)}(x) = \frac{(2n+\alpha+\beta+2)(1-x)}{2} P_n^{(\alpha+1,\beta)}(x),$$

and we have

$$P_n^{(0,0)}(0) - P_{n+1}^{(0,0)}(0) = P_n^{(1,0)}(0). \tag{4.9}$$

Combining (4.8) with (4.9) yields

$$p_{2n}(0) = \left\{P_n^{(0,0)}(0)\right\}^2 + \left\{P_{n-1}^{(0,0)}(0)\right\}^2.$$

Since $P_n(0) = P_n^{(0,0)}(0)$, this completes the proof of Proposition 3.1.

5. Conclusion

In the present paper, we have shown that the generating function of the return probability for the one-dimensional Hadamard walk can be written in terms of an elliptic integral. Our expression corresponds to the result for the classical two-dimensional RW given by Pólya in 1921. Indeed, his expression is also written in terms of an elliptic integral. An interesting problem for future work is to find similar expressions for general one-dimensional and higher dimensional QWs. Recent study on the relation between discrete- and continuous-time QWs, such as Strauch (2006) and Childs (2010), may provide us with new perspectives on the relationship between our result and the corresponding one for the continuous-time case.

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