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Absorption problems for quantum walks in one dimension

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Abstract

This paper treats absorption problems for the one-dimensional quantum walk determined by a 2×2 unitary matrix U on a state space $\{0, 1, \dots, N\}$ where N is finite or infinite by using a new path integral approach based on an orthonormal basis P , Q , R and S of the vector space of complex 2×2 matrices. Our method studied here is a natural extension of the approach in the classical random walk.

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1. Introduction

In this paper we consider absorption problems for quantum walks located on the sets $\{0, 1, \dots, N\}$ or $\{0, 1, \dots\}$. Before we move to a quantum case, first we describe the classical random walk on a finite set $\{0, 1, \dots, N\}$ with two absorbing barriers at locations 0 and N (see, for example, Grimmett and Stirzaker (1992) and Durrett (1999)). The particle moves at each step either one unit to the left with probability p or one unit to the right with probability $q = 1 - p$ until it hits one of the absorbing barriers. The directions of different steps are independent of each other. The classical random walk starting from $k \in \{0, 1, \dots, N\}$ at time n is denoted by S_n^k here. Let

$$T_m = \min \{n \geq 0 : S_n^k = m\}$$

be the time of the first visit to $m \in \{0, 1, \dots, N\}$. Using the subscript k to indicate $S_0^k = k$, we let

$$P_k^{(N)} = P_k(T_0 < T_N)$$

be the probability that the particle hits 0 starting from k before it arrives at N . The absorption problem is well known as the gambler's ruin problem.

Recently, in quantum walks, various problems including absorption have been widely investigated by a number of groups in connection with quantum computing. Examples include Aharonov *et al* (2001), Ambainis *et al* (2001), Bach *et al* (2002), Childs *et al* (2002), Dür *et al* (2002), Kempe (2002), Konno *et al* (2002), Konno (2002a, 2002b), Mackay *et al* (2002), Moore and Russell (2001), Travaglione and Milburn (2002) and Yamasaki *et al* (2002). For a more general setting including quantum cellular automata, see Meyer (1996). A more mathematical point of view can be found in Brylinsky and Chen (2002).

The study of absorption problems in the classical case is important in many fields including physics, biology and computer science. The behaviour of quantum walks differs from that of classical random walks in several striking ways. Let X_n^φ be the quantum walk on a line with no absorbing boundaries at time n starting from initial qubit state φ . In the symmetric classical case the distribution of the scaled position S_n^0/\sqrt{n} converges to $N(0, 1)$, the standard normal, as $(n \rightarrow \infty)$. However, a differently rescaled quantum walk X_n^φ/n converges to a random variable Z^φ , which has a density $1/\pi(1-x^2)\sqrt{1-2x^2}$ for $x \in (-\sqrt{2}/2, \sqrt{2}/2)$ (see Konno (2002a, 2002b)). As a corollary, it is shown that, whereas the standard deviation σ_n at time n in the classical case is \sqrt{n} , in the quantum case it is $\sqrt{(2-\sqrt{2})} \times n$ ($\approx 0.5412 \times n$) for large n . It is hoped that quantum walks may have many new applications as in the classical case. The main interest of our paper is in studying quantum walks with one or two absorbing boundaries.

This paper is organized as follows. The quantum walk considered here is determined by a 2×2 unitary matrix U . In section 2, we give a definition of the quantum walk and introduce a new path integral approach based on an orthonormal basis P , Q , R and S of the vector space of complex 2×2 matrices which is called the PQRS method here. Section 3 provides some known results on absorption problems for classical and quantum cases. Section 4 is devoted to our new results. We summarize this paper in section 5, which mentions a direction for further study.

2. Definition and PQRS method

The time evolution of the one-dimensional quantum walk studied here is given by the following unitary matrix (see, for example, Nielsen and Chuang (2000) and Brylinsky and Chen (2002)):

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

where $a, b, c, d \in \mathbb{C}$ and \mathbb{C} is the set of complex numbers. So we have

$$|a|^2 + |b|^2 = |c|^2 + |d|^2 = 1 \quad a\bar{c} + b\bar{d} = 0 \quad c = -\Delta\bar{b} \quad d = \Delta\bar{a}$$

where \bar{z} is a complex conjugate of $z \in \mathbb{C}$ and $\Delta = \det U = ad - bc$. We should note that the unitarity of U gives $|\Delta| = 1$.

The quantum walk is a quantum generalization of the classical random walk with an additional degree of freedom called the chirality. The chirality takes values left and right, and means the direction of the motion of the particle. The evolution of the quantum walk is given in the following way. At each time step, if the particle has left chirality, it moves one unit to the left, and if it has right chirality, it moves one unit to the right.

The unitary matrix U acts on two chirality states $|L\rangle$ and $|R\rangle$:

$$|L\rangle \rightarrow a|L\rangle + c|R\rangle \quad |R\rangle \rightarrow b|L\rangle + d|R\rangle$$

where L and R refer to the left and right chirality states, respectively. In fact, define

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

so we have

$$U|L\rangle = a|L\rangle + c|R\rangle \quad U|R\rangle = b|L\rangle + d|R\rangle.$$

More precisely, at any time n , the amplitude of the location of the particle is defined by a 2-vector $\in \mathbb{C}^2$ at each location $\{0, 1, \dots, N\}$. The probability that the particle is at location j is given by the square of the modulus of the vector at j . If $|\Psi_j(n)\rangle$ define the amplitude at time n at location j where

$$|\Psi_j(n)\rangle = \begin{bmatrix} \psi_j^L(n) \\ \psi_j^R(n) \end{bmatrix}$$

with the chirality being left (upper component) or right (lower component), then the dynamics for $|\Psi_j(n)\rangle$ in quantum walks is given by the following transformation:

$$|\Psi_j(n+1)\rangle = |L\rangle\langle L|U|\Psi_{j+1}(n)\rangle + |R\rangle\langle R|U|\Psi_{j-1}(n)\rangle.$$

The above equation can be rewritten as

$$|\Psi_j(n+1)\rangle = P|\Psi_{j+1}(n)\rangle + Q|\Psi_{j-1}(n)\rangle \quad (2.1)$$

where

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

We see that $U = P + Q$. The unitarity of U ensures that the amplitude always defines a probability distribution for the location.

The simplest and well-studied example of a quantum walk is the Hadamard walk whose unitary matrix U is defined by

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

The dynamics of this walk corresponds to that of the symmetric random walk in the classical case. In general, the following unitary matrices can also lead to symmetric walks:

$$U_{\eta, \phi, \psi} = \frac{e^{i\eta}}{\sqrt{2}} \begin{bmatrix} e^{i(\phi+\psi)} & e^{-i(\phi-\psi)} \\ e^{i(\phi-\psi)} & -e^{-i(\phi+\psi)} \end{bmatrix}$$

where η , ϕ and ψ are real numbers (see, for example, Nielsen and Chuang (2000), pp 175–6). In particular, we see that $U_{0,0,0} = H$.

However, symmetry of the Hadamard walk depends heavily on the initial qubit state, see Konno *et al* (2002). Another extension of the Hadamard walk is

$$H(\rho) = \begin{bmatrix} \sqrt{\rho} & \sqrt{1-\rho} \\ \sqrt{1-\rho} & -\sqrt{\rho} \end{bmatrix}$$

where $0 \leq \rho \leq 1$. Note that $\rho = 1/2$ is the Hadamard walk, that is $H = H(1/2)$.

In the present paper, the study of the dependence of some important quantities (e.g., absorption probability) on initial qubit state is one of the essential parts, so we define the collection of initial qubit states as follows:

$$\Phi = \left\{ \varphi = \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \in \mathbb{C}^2 : |\alpha|^2 + |\beta|^2 = 1 \right\}.$$

Let X_n^φ be the quantum walk at time n starting from initial qubit state $\varphi \in \Phi$ with $X_0^\varphi = 0$. In contrast with classical random walks, X_n^φ cannot be written as $X_n^\varphi = Y_1 + \dots + Y_n$, where Y_1, Y_2, \dots are independent and identically distributed random variables. In our treatment of quantum walks, as well as the matrices P and Q , it is convenient to introduce

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

We should remark that P, Q, R and S form an orthonormal basis of the vector space of complex 2×2 matrices $M_2(\mathbb{C})$ with respect to the trace inner product $\langle A|B \rangle = \text{tr}(A^*B)$. Therefore we can express any 2×2 matrix A conveniently in the form

$$A = \text{tr}(P^*A)P + \text{tr}(Q^*A)Q + \text{tr}(R^*A)R + \text{tr}(S^*A)S. \tag{2.2}$$

We call the analysis based on P, Q, R and S the PQRS method.

The $n \times n$ unit and zero matrices are written as I_n and O_n , respectively. For instance, if $A = I_2$, then

$$I_2 = \bar{a}P + \bar{d}Q + \bar{c}R + \bar{b}S. \tag{2.3}$$

The following table of products of P, Q, R and S is very useful in computing some quantities:

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

where $PQ = bR$, for example.

Now we describe the evolution and measurement of quantum walks starting from location k on $\{0, 1, \dots, N\}$ with absorbing boundaries (see, for example, Ambainis *et al* (2001), Bach *et al* (2002) and Kempe (2002) for more detailed information).

First we consider the $N = \infty$ case. In this case, an absorbing boundary is present at location 0. The evolution mechanism is described as follows:

- Step 1. Initialize the system $\varphi \in \Phi$ at location k .
- Step 2. (a) Apply equation (2.1) to one step time evolution. (b) Measure the system to see whether it is at location 0 or not.
- Step 3. If the result of measurement revealed that the system was at location 0, then terminate the process, otherwise repeat step 2.

In this setting, let $\Xi_k^{(N)}(n)$ be the sum over possible paths for which the particle first hits 0 at time n starting from k before it arrives at N . For example,

$$\Xi_1^{(3)}(5) = P^2QPQ = ab^2cR. \tag{2.4}$$

The probability that the particle first hits 0 at time n starting from k before it arrives at N is

$$P_k^{(N)}(n; \varphi) = |\Xi_k^{(N)}(n)\varphi|^2. \tag{2.5}$$

So the probability that the particle first hits 0 starting from k before it arrives at N is

$$P_k^{(N)}(\varphi) = \sum_{n=0}^{\infty} P_k^{(N)}(n; \varphi).$$

Next we consider the $N < \infty$ case. This case is similar to the $N = \infty$ case, except that two absorbing boundaries are presented at locations 0 and N as follows:

Step 1. Initialize the system $\varphi \in \Phi$ at location k .

Step 2. (a) Apply equation (2.1) to one step time evolution. (b) Measure the system to see whether it is at location 0 or not. (c) Measure the system to see whether it is at location N or not.

Step 3. If the result of either measurement revealed that the system was either at location 0 or at location N , then terminate the process, otherwise repeat step 2.

Let $\Xi_k^{(\infty)}(n)$ be the sum over possible paths for which the particle first hits 0 at time n starting from k . For example,

$$\Xi_1^{(\infty)}(5) = P^2 Q P Q + P^3 Q^2 = (ab^2c + a^2bd)R.$$

In a similar way, we can define $P_k^{(\infty)}(n; \varphi)$ and $P_k^{(\infty)}(\varphi)$.

3. Facts for the classical and quantum cases

In this section we review some results and conjectures on absorption problems related to this paper for both classical and quantum walks in one dimension.

First we review the classical case. As we described in the introduction, $P_k^{(N)} = P_k(T_0 < T_N)$ denotes the probability that the particle hits 0 starting from k before it arrives at N . We may use conditional probabilities to see that $P_k^{(N)}$ satisfies the following difference equation:

$$P_k^{(N)} = pP_{k-1}^{(N)} + qP_{k+1}^{(N)} \quad (1 \leq k \leq N-1) \quad (3.6)$$

with boundary conditions

$$P_0^{(N)} = 1 \quad P_N^{(N)} = 0. \quad (3.7)$$

The solution of such a difference equation is given by

$$P_k^{(N)} = 1 - \frac{k}{N} \quad \text{if } p = 1/2 \quad (3.8)$$

$$P_k^{(N)} = \frac{(p/q)^k - (p/q)^N}{1 - (p/q)^N} \quad \text{if } p \neq 1/2 \quad (3.9)$$

for any $0 \leq k \leq N$. Therefore, when $N = \infty$, we see that

$$P_k^{(\infty)} = 1 \quad \text{if } 1/2 \leq p \leq 1 \quad (3.10)$$

$$P_k^{(\infty)} = (p/q)^k \quad \text{if } 0 \leq p < 1/2. \quad (3.11)$$

Furthermore,

$$\lim_{k \rightarrow \infty} P_k^{(\infty)} = 1 \quad \text{if } 1/2 \leq p \leq 1 \quad (3.12)$$

$$\lim_{k \rightarrow \infty} P_k^{(\infty)} = 0 \quad \text{if } 0 \leq p < 1/2. \quad (3.13)$$

Let T_0 be the first hitting time to 0. We consider the conditional expectation of T_0 starting from $k = 1$ given the event $\{T_0 < \infty\}$, that is $E_1^{(\infty)}(T_0 | T_0 < \infty) = E_1^{(\infty)}(T_0; T_0 < \infty) / P_1^{(\infty)}(T_0 < \infty) = E_1^{(\infty)}(T_0; T_0 < \infty) / P_1^{(\infty)}$,

$$E_1^{(\infty)}(T_0 | T_0 < \infty) = \frac{2p}{\sqrt{1-4pq}} - 1 \quad \text{if } 1/2 < p \leq 1$$

$$E_1^{(\infty)}(T_0 | T_0 < \infty) = \infty \quad \text{if } p = 1/2$$

$$E_1^{(\infty)}(T_0 | T_0 < \infty) = \frac{2q}{\sqrt{1-4pq}} - 1 \quad \text{if } 0 \leq p < 1/2.$$

Next we review the quantum case. In the case of $U = H$ (the Hadamard walk), when $N = \infty$, that is when the state space is the $\{0, 1, \dots\}$ case, Ambainis *et al* (2001) proved

$$P_1^{(\infty)}({}^t[0, 1]) = P_1^{(\infty)}({}^t[1, 0]) = \frac{2}{\pi} \tag{3.14}$$

and Bach *et al* (2002) showed

$$\lim_{k \rightarrow \infty} P_k^{(\infty)}(\varphi) = \left(\frac{1}{2}\right) |\alpha|^2 + \left(\frac{2}{\pi} - \frac{1}{2}\right) |\beta|^2 + 2 \left(\frac{1}{\pi} - \frac{1}{2}\right) \text{Re}(\bar{\alpha}\beta)$$

for any initial qubit state $\varphi = {}^t[\alpha, \beta] \in \Phi$. Furthermore, in the case of $U = H(\rho)$, Bach *et al* (2002) gave

$$\begin{aligned} \lim_{k \rightarrow \infty} P_k^{(\infty)}({}^t[0, 1]) &= \frac{\rho}{1 - \rho} \left(\frac{\cos^{-1}(1 - 2\rho)}{\pi} - 1 \right) + \frac{2}{\pi \sqrt{1/\rho - 1}} \\ \lim_{k \rightarrow \infty} P_k^{(\infty)}({}^t[1, 0]) &= \frac{\cos^{-1}(1 - 2\rho)}{\pi}. \end{aligned}$$

The second result was conjectured by Yamasaki *et al* (2002).

When N is finite the following conjecture by Ambainis *et al* (2001) is still open for the $U = H$ case:

$$P_1^{(N+1)}({}^t[0, 1]) = \frac{2P_1^{(N)}({}^t[0, 1]) + 1}{2P_1^{(N)}({}^t[0, 1]) + 2} \quad (N \geq 1) \quad P_1^{(1)}({}^t[0, 1]) = 0.$$

Solving the above recurrence gives

$$P_1^{(N)}({}^t[0, 1]) = \frac{1}{\sqrt{2}} \times \frac{(3 + 2\sqrt{2})^{N-1} - 1}{(3 + 2\sqrt{2})^{N-1} + 1} \quad (N \geq 1). \tag{3.15}$$

However, in contrast with $P_1^{(\infty)}({}^t[0, 1]) = 2/\pi$, Ambainis *et al* (2001) proved

$$\lim_{N \rightarrow \infty} P_1^{(N)}({}^t[0, 1]) = 1/\sqrt{2}.$$

It should be noted that $P_k^{(\infty)} = \lim_{N \rightarrow \infty} P_k^{(N)}$ for any $0 \leq k \leq N$ in the classical case (see equations (3.8)–(3.11)).

We are not aware of results concerning $E_1^{(\infty)}(T_0|T_0 < \infty)$ having been published; however, we will give such a result in the next section.

4. Our results

In the first half of this section, we consider a general setting including a hitting time to N before it arrives at 0 or a hitting time to 0 before it arrives at N , when N is finite. In the case of $N = \infty$, a similar argument holds, so we will omit it here.

Noting that $\{P, Q, R, S\}$ is a basis of $M_2(\mathbb{C})$, $\Xi_k^{(N)}(n)$ can be written as

$$\Xi_k^{(N)}(n) = p_k^{(N)}(n)P + q_k^{(N)}(n)Q + r_k^{(N)}(n)R + s_k^{(N)}(n)S.$$

Therefore equation (2.5) implies

$$P_k^{(N)}(n; \varphi) = |\Xi_k^{(N)}(n)\varphi|^2 = C_1(n)|\alpha|^2 + C_2(n)|\beta|^2 + 2\text{Re}(C_3(n)\bar{\alpha}\beta)$$

where $\text{Re}(z)$ is the real part of $z \in \mathbb{C}$, $\varphi = {}^t[\alpha, \beta] \in \Phi$ and

$$\begin{aligned} C_1(n) &= |ap_k^{(N)}(n) + cr_k^{(N)}(n)|^2 + |as_k^{(N)}(n) + cq_k^{(N)}(n)|^2 \\ C_2(n) &= |bp_k^{(N)}(n) + dr_k^{(N)}(n)|^2 + |bs_k^{(N)}(n) + dq_k^{(N)}(n)|^2 \\ C_3(n) &= \overline{(ap_k^{(N)}(n) + cr_k^{(N)}(n))} (bp_k^{(N)}(n) + dr_k^{(N)}(n)) \\ &\quad + \overline{(as_k^{(N)}(n) + cq_k^{(N)}(n))} (bs_k^{(N)}(n) + dq_k^{(N)}(n)). \end{aligned}$$

From now on we assume $N \geq 3$. Noting the definition of $\Xi_k^{(N)}(n)$, we see that for $1 \leq k \leq N-1$,

$$\Xi_k^{(N)}(n) = \Xi_{k-1}^{(N)}(n-1)P + \Xi_{k+1}^{(N)}(n-1)Q.$$

The above equation is a quantum version of the difference equation, i.e. equation (3.6) for the classical random walk. As an example, see equation (2.4). Then we have

$$\begin{aligned} p_k^{(N)}(n) &= ap_{k-1}^{(N)}(n-1) + cr_{k-1}^{(N)}(n-1) \\ q_k^{(N)}(n) &= dq_{k+1}^{(N)}(n-1) + bs_{k+1}^{(N)}(n-1) \\ r_k^{(N)}(n) &= bp_{k+1}^{(N)}(n-1) + dr_{k+1}^{(N)}(n-1) \\ s_k^{(N)}(n) &= cq_{k-1}^{(N)}(n-1) + as_{k-1}^{(N)}(n-1). \end{aligned}$$

Next we consider the boundary condition related to equation (3.7) in the classical case. When $k = N$,

$$P_N^{(N)}(0; \varphi) = |\Xi_N^{(N)}(0)\varphi|^2 = 0$$

for any $\varphi \in \Phi$. So we take $\Xi_N^{(N)}(0) = O_2$, i.e.

$$p_N^{(N)}(0) = q_N^{(N)}(0) = r_N^{(N)}(0) = s_N^{(N)}(0) = 0.$$

If $k = 0$, then

$$P_0^{(N)}(0; \varphi) = |\Xi_0^{(N)}(0)\varphi|^2 = 1$$

for any $\varphi \in \Phi$. So we choose $\Xi_0^{(N)}(0) = I_2$. From equation (2.3), we have

$$p_0^{(N)}(0) = \bar{a} \quad q_0^{(N)}(0) = \bar{d} \quad r_0^{(N)}(0) = \bar{c} \quad s_0^{(N)}(0) = \bar{b}.$$

Let

$$v_k^{(N)}(n) = \begin{bmatrix} p_k^{(N)}(n) \\ r_k^{(N)}(n) \end{bmatrix} \quad w_k^{(N)}(n) = \begin{bmatrix} q_k^{(N)}(n) \\ s_k^{(N)}(n) \end{bmatrix}.$$

Then we see that for $n \geq 1$ and $1 \leq k \leq N-1$,

$$v_k^{(N)}(n) = \begin{bmatrix} a & c \\ 0 & 0 \end{bmatrix} v_{k-1}^{(N)}(n-1) + \begin{bmatrix} 0 & 0 \\ b & d \end{bmatrix} v_{k+1}^{(N)}(n-1) \quad (4.16)$$

$$w_k^{(N)}(n) = \begin{bmatrix} 0 & 0 \\ c & a \end{bmatrix} w_{k-1}^{(N)}(n-1) + \begin{bmatrix} d & b \\ 0 & 0 \end{bmatrix} w_{k+1}^{(N)}(n-1) \quad (4.17)$$

and for $1 \leq k \leq N$,

$$\begin{aligned} v_0^{(N)}(0) &= \begin{bmatrix} \bar{a} \\ \bar{c} \end{bmatrix} & v_N^{(N)}(0) &= \begin{bmatrix} 0 \\ 0 \end{bmatrix} \\ w_0^{(N)}(0) &= \begin{bmatrix} \bar{d} \\ \bar{b} \end{bmatrix} & w_N^{(N)}(0) &= \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \end{aligned}$$

Moreover,

$$v_0^{(N)}(n) = v_N^{(N)}(n) = w_0^{(N)}(n) = w_N^{(N)}(n) = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (n \geq 1).$$

From now on we focus on the $1 \leq k \leq N-1$ case. So we consider only the $n \geq 1$ case. Moreover, from the definition of $\Xi_k^{(N)}(n)$, it is easily shown that there exist only two types of paths, that is $P \dots P$ and $P \dots Q$. Therefore, we see that $q_k^{(N)}(n) = s_k^{(N)}(n) = 0$ ($n \geq 1$). So we have

Lemma 1.

$$P_k^{(N)}(\varphi) = \sum_{n=1}^{\infty} P_k^{(N)}(n; \varphi) \quad P_k^{(N)}(n; \varphi) = C_1(n)|\alpha|^2 + C_2(n)|\beta|^2 + 2\text{Re}(C_3(n)\bar{\alpha}\beta)$$

where $\varphi = {}^t[\alpha, \beta] \in \Phi$ and

$$\begin{aligned} C_1(n) &= |ap_k^{(N)}(n) + cr_k^{(N)}(n)|^2 \\ C_2(n) &= |bp_k^{(N)}(n) + dr_k^{(N)}(n)|^2 \\ C_3(n) &= \overline{(ap_k^{(N)}(n) + cr_k^{(N)}(n))} (bp_k^{(N)}(n) + dr_k^{(N)}(n)). \end{aligned}$$

To solve $P_k^{(N)}(\varphi)$, we introduce generating functions of $p_k^{(N)}(n)$ and $r_k^{(N)}(n)$ as follows:

$$p_k^{(N)}(z) = \sum_{n=1}^{\infty} p_k^{(N)}(n)z^n \quad r_k^{(N)}(z) = \sum_{n=1}^{\infty} r_k^{(N)}(n)z^n.$$

By equation (4.16), we have

$$p_k^{(N)}(z) = azp_{k-1}^{(N)}(z) + czr_{k-1}^{(N)}(z) \quad r_k^{(N)}(z) = bzp_{k+1}^{(N)}(z) + dzr_{k+1}^{(N)}(z).$$

Solving these, we see that both $p_k^{(N)}(z)$ and $r_k^{(N)}(z)$ satisfy the same recurrence

$$\begin{aligned} dp_{k+2}^{(N)}(z) - \left(\Delta z + \frac{1}{z}\right) p_{k+1}^{(N)}(z) + ap_k^{(N)}(z) &= 0 \\ dr_{k+2}^{(N)}(z) - \left(\Delta z + \frac{1}{z}\right) r_{k+1}^{(N)}(z) + ar_k^{(N)}(z) &= 0. \end{aligned}$$

From the characteristic equations with respect to the above recurrences, we have the same roots: if $a \neq 0$, then

$$\lambda_{\pm} = \frac{\Delta z^2 + 1 \mp \sqrt{\Delta^2 z^4 + 2\Delta(1 - 2|a|^2)z^2 + 1}}{2\Delta a z}$$

where $\Delta = \det U = ad - bc$.

From now on we consider mainly the $U = H$ (the Hadamard walk) case with $N = \infty$. Remark that the definition of $\Xi_1^{(\infty)}(n)$ gives $p_1^{(\infty)}(n) = 0$ ($n \geq 2$) and $p_1^{(\infty)}(1) = 1$. So we have $p_1^{(\infty)}(z) = z$. Moreover, noting $\lim_{k \rightarrow \infty} p_k^{(\infty)}(z) < \infty$, the following explicit form is obtained:

$$p_k^{(\infty)}(z) = z\lambda_+^{k-1} \quad r_k^{(\infty)}(z) = \frac{-1 + \sqrt{z^4 + 1}}{z} \lambda_+^{k-1}$$

where

$$\lambda_{\pm} = \frac{z^2 - 1 \pm \sqrt{z^4 + 1}}{\sqrt{2}z}.$$

Therefore for $k = 1$,

$$r_1^{(\infty)}(z) = \frac{-1 + \sqrt{z^4 + 1}}{z}.$$

From the above equation and the definition of the hypergeometric series ${}_2F_1(a, b; c; z)$, we have

$$\sum_{n=1}^{\infty} (r_1^{(\infty)}(n))^2 z^n = \sum_{n=1}^{\infty} \binom{1/2}{n}^2 z^{4n-1} = \frac{{}_2F_1(-1/2, -1/2; 1; z^4) - 1}{z}.$$

On the other hand, it should be noted that

$${}_2F_1(a, b; c; 1) = \frac{\Gamma(c)\Gamma(c-a-b)}{\Gamma(c-a)\Gamma(c-b)} \quad (\operatorname{Re}(a+b-c) < 0)$$

where $\Gamma(z)$ is the gamma function defined by

$$\Gamma(z) = \int_0^\infty e^{-t} t^{z-1} dt \quad (\operatorname{Re}(z) > 0).$$

Therefore

$$\sum_{n=1}^{\infty} (r_1^{(\infty)}(n))^2 = \frac{\Gamma(1)\Gamma(2)}{\Gamma(3/2)^2} - 1 = \frac{4}{\pi} - 1$$

since $\Gamma(1) = \Gamma(2) = 1$ and $\Gamma(3/2) = \sqrt{\pi}/2$. By lemma 1

$$P_1^{(\infty)}(\varphi) = \sum_{n=1}^{\infty} \left[\frac{1}{2} \{ (p_1^{(\infty)}(n))^2 + (r_1^{(\infty)}(n))^2 \} + p_1^{(\infty)}(n)r_1^{(\infty)}(n)(|\alpha|^2 - |\beta|^2) \right. \\ \left. + \frac{1}{2} \{ (p_1^{(\infty)}(n))^2 - (r_1^{(\infty)}(n))^2 \} (\alpha\bar{\beta} + \bar{\alpha}\beta) \right].$$

Note that $p_1^{(\infty)}(n)r_1^{(\infty)}(n) = 0$ ($n \geq 1$), since $p_1^{(\infty)}(n) = 0$ ($n \geq 2$), $p_1^{(\infty)}(1) = 1$ and $r_1^{(\infty)}(1) = 0$. So we have

$$P_1^{(\infty)}(\varphi) = \frac{2}{\pi} + 2 \left(1 - \frac{2}{\pi} \right) \operatorname{Re}(\bar{\alpha}\beta) \quad (4.18)$$

for any initial qubit state $\varphi = {}^t[\alpha, \beta] \in \Phi$. This result is a generalization of equation (3.14) given by Ambainis *et al* (2001). From equation (4.18), we get the range of $P_1^{(\infty)}(\varphi)$,

$$\frac{4-\pi}{\pi} \leq P_1^{(\infty)}(\varphi) \leq 1$$

the equality holds in the following cases:

$$P_1^{(\infty)}(\varphi) = 1 \quad \text{iff} \quad \varphi = \frac{e^{i\theta}}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \quad \text{and} \quad P_1^{(\infty)}(\varphi) = \frac{4-\pi}{\pi} \quad \text{iff} \quad \varphi = \frac{e^{i\theta}}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

where $0 \leq \theta < 2\pi$.

Moreover, we consider the conditional expectation of the first hitting time to 0 starting from $k = 1$ given an event $\{T_0 < \infty\}$, that is $E_1^{(\infty)}(T_0 | T_0 < \infty) = E_1^{(\infty)}(T_0; T_0 < \infty) / P_1^{(\infty)}(T_0 < \infty)$. Let

$$f(z) = \sum_{n=1}^{\infty} (r_1^{(\infty)}(n))^2 z^n \left(= \frac{{}_2F_1(-1/2, -1/2; 1; z^4) - 1}{z} \right).$$

In this case we have to know the value of $f'(1)$. It should be noted that

$$\frac{d}{dz} ({}_2F_1(a, b; c; g(z))) = \left(\frac{ab}{c} \right) {}_2F_1(a+1, b+1; c+1; g(z))g'(z).$$

The above formula gives

$$f'(z) = \frac{z^4 {}_2F_1(1/2, 1/2; 2; z^4) - {}_2F_1(-1/2, -1/2; 1; z^4) + 1}{z^2}.$$

Moreover noting

$${}_2F_1(-1/2, -1/2; 1; 1) = {}_2F_1(1/2, 1/2; 2; 1) = \frac{4}{\pi}$$

we have $f'(1) = 1$. Therefore the desired conclusion is obtained

$$E_1^{(\infty)}(T_0|T_0 < \infty) = \frac{\sum_{n=1}^{\infty} n P_1^{(\infty)}(T_0 = n)}{\sum_{n=1}^{\infty} P_1^{(\infty)}(T_0 = n)} = \frac{1}{P_1^{(\infty)}(\varphi)}$$

since

$$\begin{aligned} \sum_{n=1}^{\infty} n P_1^{(\infty)}(T_0 = n) &= \sum_{n=1}^{\infty} n \left[\frac{1}{2} \{ (p_1^{(\infty)}(n))^2 + (r_1^{(\infty)}(n))^2 \} \right. \\ &\quad \left. + \frac{1}{2} \{ (p_1^{(\infty)}(n))^2 - (r_1^{(\infty)}(n))^2 \} (\alpha \bar{\beta} + \bar{\alpha} \beta) \right] \\ &= \frac{1}{2} \{ 1 + f'(1) \} + \frac{1}{2} \{ 1 - f'(1) \} (\alpha \bar{\beta} + \bar{\alpha} \beta) = 1. \end{aligned}$$

In a similar way we see that $f''(1) = \infty$ implies

$$E_1^{(\infty)}((T_0)^2|T_0 < \infty) = \infty$$

so the m th moment $E_1^{(\infty)}((T_0)^m|T_0 < \infty)$ diverges for $m \geq 2$.

Next we consider the finite N case. Then $p_k^{(N)}(z)$ and $r_k^{(N)}(z)$ satisfy

$$p_k^{(N)}(z) = A_z \lambda_+^{k-1} + B_z \lambda_-^{k-1} \quad r_k^{(N)}(z) = C_z \lambda_+^{k-N+1} + D_z \lambda_-^{k-N+1}$$

since $\lambda_+ \lambda_- = -1$. All we have to do is to determine the coefficients A_z, B_z, C_z, D_z by using boundary conditions: $p_1^{(N)}(z) = z$ and $r_{N-1}^{(N)}(z) = 0$ come from the definition of $\Xi_k^{(N)}(n)$. The boundary conditions imply $C_z + D_z = 0$ and $A_z + B_z = z$, so we see

$$p_k^{(N)}(z) = \left(\frac{z}{2} + E_z\right) \lambda_+^{k-1} + \left(\frac{z}{2} - E_z\right) \lambda_-^{k-1} \tag{4.19}$$

$$r_k^{(N)}(z) = C_z (\lambda_+^{k-N+1} - \lambda_-^{k-N+1}) \tag{4.20}$$

where $E_z = A_z - z/2 = z/2 - B_z$. To obtain E_z and C_z , we use $r_1^{(N)}(z) = (p_2^{(N)}(z) - r_2^{(N)}(z))z/\sqrt{2}$ and $r_{N-2}^{(N)}(z) = (p_{N-1}^{(N)}(z) - r_{N-1}^{(N)}(z))z/\sqrt{2} = p_{N-1}^{(N)}(z)z/\sqrt{2}$. Therefore

$$\begin{aligned} C_z (\lambda_+ - \lambda_-) &= \frac{z}{\sqrt{2}} \left\{ \left(\frac{z}{2} + E_z\right) \lambda_+^{N-2} + \left(\frac{z}{2} - E_z\right) \lambda_-^{N-2} \right\} \\ C_z (\lambda_+^{N-2} - \lambda_-^{N-2}) &= \frac{z}{\sqrt{2}} \left\{ \left(\frac{z}{2} + E_z\right) (-1)^{N-1} \lambda_+ + \left(\frac{z}{2} - E_z\right) (-1)^{N-1} \lambda_- \right. \\ &\quad \left. + C_z (\lambda_+^{N-3} - \lambda_-^{N-3}) \right\}. \end{aligned}$$

Solving the above equations gives

$$\begin{aligned} C_z &= \frac{z^2}{\sqrt{2}} (-1)^{N-2} (\lambda_+^{N-3} - \lambda_-^{N-3}) \left\{ (\lambda_+^{N-2} - \lambda_-^{N-2})^2 \right. \\ &\quad \left. - \frac{z}{\sqrt{2}} (\lambda_+^{N-2} - \lambda_-^{N-2}) (\lambda_+^{N-3} - \lambda_-^{N-3}) - (-1)^{N-3} (\lambda_+ - \lambda_-)^2 \right\}^{-1} \end{aligned} \tag{4.21}$$

$$\begin{aligned} E_z &= -\frac{z}{2 (\lambda_+^{N-2} - \lambda_-^{N-2})} \left[2 (-1)^{N-3} (\lambda_+ - \lambda_-) (\lambda_+^{N-3} - \lambda_-^{N-3}) \left\{ (\lambda_+^{N-2} - \lambda_-^{N-2})^2 \right. \right. \\ &\quad \left. \left. - \frac{z}{\sqrt{2}} (\lambda_+^{N-2} - \lambda_-^{N-2}) (\lambda_+^{N-3} - \lambda_-^{N-3}) - (-1)^{N-3} (\lambda_+ - \lambda_-)^2 \right\}^{-1} \right. \\ &\quad \left. + (\lambda_+^{N-2} + \lambda_-^{N-2}) \right]. \end{aligned} \tag{4.22}$$

By lemma 1, we obtain

Theorem 2.

$$P_k^{(N)}(\varphi) = C_1|\alpha|^2 + C_2|\beta|^2 + 2\operatorname{Re}(C_3\bar{\alpha}\beta)$$

where $\varphi = {}^t[\alpha, \beta] \in \Phi$ and

$$\begin{aligned} C_1 &= \frac{1}{2\pi} \int_0^{2\pi} |ap_k^{(N)}(e^{i\theta}) + cr_k^{(N)}(e^{i\theta})|^2 d\theta \\ C_2 &= \frac{1}{2\pi} \int_0^{2\pi} |bp_k^{(N)}(e^{i\theta}) + dr_k^{(N)}(e^{i\theta})|^2 d\theta \\ C_3 &= \frac{1}{2\pi} \int_0^{2\pi} \overline{(ap_k^{(N)}(e^{i\theta}) + cr_k^{(N)}(e^{i\theta}))} (bp_k^{(N)}(e^{i\theta}) + dr_k^{(N)}(e^{i\theta})) d\theta. \end{aligned}$$

Here $p_k^{(N)}(z)$ and $r_k^{(N)}(z)$ satisfy equations (4.19) and (4.20) and C_z and E_z satisfy equations (4.21) and (4.22).

Therefore to compute $P_k^{(N)}(\varphi)$, we need to obtain both $p_k^{(N)}(z)$ and $r_k^{(N)}(z)$, and calculate the above C_i ($i = 1, 2, 3$) explicitly.

Here we consider $U = H$ (the Hadamard walk), $\varphi = {}^t[\alpha, \beta]$ and $k = 1$. From theorem 2, noting that $p_1^{(N)}(z) = z$ for any $N \geq 2$, we have

Corollary 3. For $N \geq 2$,

$$P_1^{(N)}(\varphi) = \frac{1}{2} \left(1 + \frac{1}{2\pi} \int_0^{2\pi} |r_1^{(N)}(e^{i\theta})|^2 d\theta \right) (1 + 2\operatorname{Re}(\bar{\alpha}\beta))$$

where $r_1^{(2)}(z) = 0$, $r_1^{(3)}(z) = z^3/(2 - z^2)$,

$$\begin{aligned} r_1^{(4)}(z) &= \frac{z^3(1 - z^2)}{2 - 2z^2 + z^4} & r_1^{(5)}(z) &= \frac{z^3(2 - 3z^2 + 2z^4)}{4 - 6z^2 + 5z^4 - 2z^6} \\ r_1^{(6)}(z) &= \frac{2z^3(1 - z^2)(1 - z^2 + z^4)}{4 - 8z^2 + 9z^4 - 6z^6 + 2z^8} \end{aligned}$$

and in general for $N \geq 4$

$$r_1^{(N)}(z) = -\frac{z^2 J_{N-3}(z) J_{N-4}(z)}{\sqrt{2}(J_{N-3}(z))^2 - z J_{N-3}(z) J_{N-4}(z) - \sqrt{2}(-1)^{N-3}}$$

with

$$J_n(z) = \sum_{k=0}^n \lambda_+^k \lambda_-^{n-k} \quad \lambda_+ + \lambda_- = \sqrt{2} \left(z - \frac{1}{z} \right) \quad \lambda_+ \lambda_- = -1.$$

In particular, when $\varphi = {}^t[0, 1] = |R\rangle$, $k = 1$ and $N = 2, \dots, 6$ cases, the above corollary gives

$$\begin{aligned} P_1^{(2)}({}^t[0, 1]) &= \frac{1}{2} & P_1^{(3)}({}^t[0, 1]) &= \frac{2}{3} & P_1^{(4)}({}^t[0, 1]) &= \frac{7}{10} \\ P_1^{(5)}({}^t[0, 1]) &= \frac{12}{17} & P_1^{(6)}({}^t[0, 1]) &= \frac{41}{58}. \end{aligned}$$

It is easily checked that the above values $P_1^{(N)}({}^t[0, 1])$ ($N = 2, \dots, 6$) satisfy the conjecture given by equation (3.15).

5. Summary

In this paper we consider absorption problems for quantum walks on $\{0, 1, \dots, N\}$ for both $N < \infty$ and $N = \infty$ cases by using the PQRS method. Here we summarize our main results.

First we describe the $N = \infty$ case. In this case, we have

$$P_1^{(\infty)}(\varphi) = \frac{2}{\pi} + 2 \left(1 - \frac{2}{\pi}\right) \operatorname{Re}(\bar{\alpha}\beta)$$

and

$$E_1^{(\infty)}(T_0 | T_0 < \infty) = \frac{1}{P_1^{(\infty)}(\varphi)} \quad E_1^{(\infty)}((T_0)^m | T_0 < \infty) = \infty \quad (m \geq 2)$$

for any initial qubit state $\varphi = {}^t[\alpha, \beta] \in \Phi$, where $P_1^{(\infty)}(\varphi)$ is the probability that the particle first hits location 0 starting from location 1, and $E_1^{(\infty)}((T_0)^m | T_0 < \infty)$ is the conditional m th moment of T_0 starting from location 1 given an event $\{T_0 < \infty\}$ with T_0 being the first hitting time to location 0.

Next we describe the $N < \infty$ case. In this case, we obtain the following explicit expression of $P_1^{(N)}(\varphi)$:

$$P_1^{(N)}(\varphi) = \frac{1}{2} \left(1 + \frac{1}{2\pi} \int_0^{2\pi} |r_1^{(N)}(e^{i\theta})|^2 d\theta\right) (1 + 2\operatorname{Re}(\bar{\alpha}\beta))$$

for any initial qubit state $\varphi = {}^t[\alpha, \beta] \in \Phi$, where $P_1^{(N)}(\varphi)$ is the probability that the particle first hits location 0 starting from location 1 before it arrives at location N and $r_1^{(N)}(z)$ is given by corollary 3.

The above result guarantees that the conjecture presented by Ambainis *et al* (see equation (3.15)) is true for $N = 2, \dots, 6$. However, their conjecture is still open for any N . So one of the future interesting problems is to find and prove an explicit form such as equation (3.15) for any $N (\leq \infty)$, $k \in \{1, \dots, N - 1\}$, and $\varphi \in \Phi$.

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