Orthogonal Polynomials Induced by Discrete-Time Quantum Walks in One Dimension

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In this paper we obtain some properties of orthogonal polynomials given by a weight function which is a limit density of a rescaled discrete-time quantum walk on the line.

KEYWORDS: quantum walk, orthogonal polynomial, Hadamard walk

1. Introduction

A quantum walk is the quantum analog of a classical random walk. Quantum walks are expected to play an important role in the field of quantum algorithms. A number of benefits for such walks are already known. Reviews and books on quantum walks are Kempe [6], Kendon [7], Konno [10, 11], Venegas-Andraca [15], for examples. There are two types of quantum walks. One is the discrete-time walk and the other is the continuous-time one. Here we focus on the case of a discrete-time walk on \( \mathbb{Z} \), where \( \mathbb{Z} \) is the set of integers. Ambainis et al. [3] investigated the quantum walk intensively.

In the present paper, we consider some properties of orthogonal polynomials given by a weight function which is a limit density of a rescaled discrete-time quantum walk on \( \mathbb{Z} \). Recently Cantero et al. [4] showed that the theory of matrix-valued orthogonal polynomials associated with a certain kind of unitary matrices, i.e., the CMV matrices, is a natural tool to study the discrete-time quantum walk on the line. It would be interesting to know a relation between their approach and our results.

The rest of the paper is organized as follows. In Sect. 2, we define the quantum walk and explain the weak limit theorem. Section 3 treats a symmetric quantum walk. In Sect. 4, we give a result for an asymmetric case. Section 5 is devoted to a general case.

2. Quantum Walk

First we give a definition of one-dimensional discrete-time quantum walk. The time evolution of the quantum walk is defined by the following matrix:

\[
U = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \in U(2),
\]

where \( a, b, c, d \in \mathbb{C} \) and \( U(2) \) is the set of \( 2 \times 2 \) unitary matrices. Here \( \mathbb{C} \) is the set of complex numbers. The unitarity of \( U \) gives

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

where \( \bar{z} \) is the complex conjugate of \( z \in \mathbb{C} \) and \( \Delta = ad - bc \). The quantum walk is a quantum version of the classical random walk with additional degree of freedom called chirality. The chirality takes values left and right, and it means the direction of the motion of the particle. At each time step, if the particle has the left chirality, it moves one step to the left, and if it has the right chirality, it moves one step to the right. Let define

\[
|L\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |R\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix},
\]

so \( U \) acts on two chiralities as follows:

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Theorem 2.1. If \( abcd \neq 0 \), then
\[
\lim_{n \to \infty} P(u \leq X_n/n \leq v) = \int_u^v [1 - c(a, b, \psi)x] k(x : |a|) \, dx,
\]
where
\[
k(x : r) = \frac{\sqrt{1 - r^2}}{\pi(1 - x^2)\sqrt{r^2 - x^2}} I_{-r, r}(x), \quad c(a, b, \psi) = |\alpha|^2 - |\beta|^2 + \frac{a \overline{ab} \beta + \overline{a} \overline{ab} \beta}{|\alpha|^2},
\]
and \( \psi = \gamma [\alpha, \beta] \). Here \( I_{-r, r}(x) = 1 \, (x \in A), = 0 \, (x \notin A) \). In other words, the limit density of \( X_n/n \) is \( f_{\infty}(x) \equiv [1 - c(a, b, \psi)x] k(x : |a|) \).

3. Symmetric Case

In this section we consider the symmetric case of the limit density \( f_{\infty}(x) \), i.e., \( c(a, b, \psi) = 0 \). Let \( \mu \) be the probability measure on the real line \( \mathbb{R} \), with the density \( k(x : r) \), where \( 0 < r < 1 \).

Theorem 3.1. Let \( G_{\mu}(z) := \int_{\mathbb{R}} \frac{d\mu(t)}{z-t} \) be the Stieltjes transform of \( \mu \). Then
\[
G_{\mu}(z) = \frac{z(z^2 - r^2) - \sqrt{1 - r^2}\sqrt{z^2 - r^2}}{(z^2 - 1)(z^2 - r^2)}.
\]
Moreover, \( G_{\mu} \) admits the following expansion as continued fraction:
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\[ G_\mu(z) = \frac{1}{z - \frac{1 - \sqrt{1 - r^2}}{(\sqrt{1 - r^2} - 1 + r^2)/2}}. \]

Before the proof we will derive some consequences.

**Corollary 3.2.** The monic orthogonal polynomials for \( \mu \) are given by: \( P_0(x) = 1, \)
\[ xP_n(x) = P_{n+1}(x) + \gamma_{n-1}P_{n-1}(x), \]
where
\[ \gamma_0 = 1 - \sqrt{1 - r^2}, \quad \gamma_1 = \frac{\sqrt{1 - r^2}(1 - \sqrt{1 - r^2})}{2}, \quad \gamma_n = \frac{r^2}{4} \quad \text{for} \ n \geq 2, \]
under convention that \( P_{-1}(x) = 0 \) and \( \gamma_{-1} = 0. \)

In particular, for the Hadamard walk case \( (r = 1/\sqrt{2}) \) we have
\[ \gamma_0 = \frac{2 - \sqrt{2}}{2}, \quad \gamma_1 = \frac{\sqrt{2} - 1}{4}, \quad \gamma_n = \frac{1}{8} \quad \text{for} \ n \geq 2. \]

Then we can compute a few first orthogonal polynomials:
\[
\begin{align*}
P_0(x) &= 1, \quad P_1(x) = x, \\
P_2(x) &= x^2 + \frac{-2 + \sqrt{2}}{2}, \\
P_3(x) &= x^3 + \frac{-3 + \sqrt{2}}{2^2}x, \\
P_4(x) &= x^4 + \frac{-7 + 2\sqrt{2}}{2^3}x^2 + \frac{2 - \sqrt{2}}{2^4}, \\
P_5(x) &= x^5 + \frac{-4 + \sqrt{2}}{2^2}x^3 + \frac{7 - 3\sqrt{2}}{2^5}x, \\
P_6(x) &= x^6 + \frac{-9 + 2\sqrt{2}}{2^3}x^4 + \frac{21 - 8\sqrt{2}}{2^6}x^2 + \frac{-2 + \sqrt{2}}{2^7}. \end{align*}
\]

From Corollary 3.2, we can easily compute the following generating function:
\[ Q(x, z) = \sum_{n=0}^{\infty} P_n(x)z^n. \]

**Corollary 3.3.**
\[ (4 - 4xz + r^2z^2)Q(x, z) = 4 + (r^2 - 4 + 4\sqrt{1 - r^2})z^2 + (2 - 2\sqrt{1 - r^2} - r^2)xz^3. \]

In particular, for the Hadamard walk
\[ \left(4 - 4xz + \frac{1}{2}z^2\right)Q(x, z) = 4 + \left(-\frac{7}{2} + 2\sqrt{2}\right)z^2 + \left(\frac{3}{2} - \frac{1}{\sqrt{2}}\right)xz^3. \]

The following fact is useful for computing \( G_\mu(z) \).

**Lemma 3.4.** Define a function \( A : \mathbb{C}^+ \to \mathbb{C}^- \), where \( \mathbb{C}^+ = \{ z \in \mathbb{C} : \Re z > 0 \}, \mathbb{C}^- = \{ z \in \mathbb{C} : \Re z < 0 \} \), given by the continued fraction
\[ A(z) = \frac{1}{z - \frac{r^2/4}{z - \frac{r^2/4}{z - \ddots}}}. \]
Then, under appropriate choice of the square root, we have
\[ A(z) = \frac{2z}{r^2} - \frac{2}{r^2} \sqrt{z^2 - r^2}. \]

**Proof.** The definition of \( A(z) \) yields
\[ A(z) = \frac{1}{z - r^2A(z)/4}, \]
so we have
\[ r^2A(z)^2 - 4zA(z) + 4 = 0. \]
This leads to the desired formula. \( \Box \)

**Proof of Theorem 3.1.** Denoting the continued fraction by \( G(z) \) we have
\[
G(z) = \frac{1}{z - \frac{1 - \sqrt{1 - r^2}}{z - \frac{(\sqrt{1 - r^2} - 1 + r^2)/2}{z - A(z)r^2/4}}}
\]
\[
= \frac{1}{z - \frac{1 - \sqrt{1 - r^2}}{z - \frac{\sqrt{1 - r^2} - 1 + r^2}{z + \sqrt{z^2 - r^2}}}}
\]
\[
= \frac{1}{z - \frac{(1 - \sqrt{1 - r^2})/(z - \sqrt{z^2 - r^2})}{r^2}}
\]
\[
= \frac{z^2 - r^2 + z\sqrt{1 - r^2}\sqrt{z^2 - r^2}}{(z^2 - 1)(z^2 - r^2)},
\]
which is equal to the right hand side of the first formula. Now, using the standard technique (see [2,5]) one can verify that \( G(z) \) is Stieltjes transform for \( \mu \), which concludes the proof of Theorem 3.1. \( \Box \)

Next we consider the \( n \)th moment of the measure \( \mu \):
\[ s_n(\mu) := \int_{\mathbb{R}} x^n k(x; \gamma) \, dx = \int_{-\gamma}^{\gamma} \frac{x^n \sqrt{1 - r^2}}{\pi(1 - x^2)^{\sqrt{r^2} - x^2}} \, dx. \]

**Theorem 3.5.** For \( m \geq 0 \) we have \( s_{2m+1}(\mu) = 0 \) and
\[ s_{2m}(\mu) = 1 - \sqrt{1 - r^2} \sum_{k=0}^{m-1} \binom{2k}{k} \left( \frac{r^2}{4} \right)^k. \]

The moment generating function is equal to
\[ M_\mu(z) := \sum_{m=0}^{\infty} s_m(\mu)z^m = \frac{1 - r^2z^2 - z^2\sqrt{1 - r^2}\sqrt{1 - r^2z^2}}{(z^2)^2(1 - r^2z^2)}. \]

We note that this result for the Hadamard walk case appeared in Konno et al. [13].

**Proof.** First we note that
\[ M_\mu(z) = G_\mu(1/z) = \frac{1 - r^2z^2 - z^2\sqrt{1 - r^2}\sqrt{1 - r^2z^2}}{(1 - z^2)(1 - r^2z^2)}. \]

Now denoting the sequence given in theorem by \( s_m \), and its generating function by \( M(z) \), we have
Theorem 4.1. From this we obtain the Stieltjes transform

\[ M(z) = \sum_{n=0}^{\infty} \left( 1 - \sqrt{1 - r^2} \sum_{k=0}^{n-1} \frac{2k}{k} \left( \frac{r}{4} \right)^k \right) z^n \]

\[ = \frac{1}{1 - z^2} - \sqrt{1 - r^2} \sum_{k=0}^{\infty} \sum_{n=k+1}^{\infty} \frac{2k}{k} \left( \frac{r}{4} \right)^k z^{2n} \]

\[ = \frac{1}{1 - z^2} - \sqrt{1 - r^2} \left( 2k \right) \left( \frac{r^2}{4} \right)^k z^{2k+2} \frac{1}{1 - z^2} \]

\[ = \frac{1}{1 - z^2} - \frac{z^2 \sqrt{1 - r^2}}{(1 - z^2)(1 - 4z^2)} \]

\[ = \frac{1 - r^2 z^2 - z^2 \sqrt{1 - r^2} \sqrt{1 - r^2 z^2}}{(1 - z^2)(1 - r^2 z^2)} , \]

which is equal to \( M_p(z) \). We used the well known formula:

\[ \sum_{k=0}^{\infty} \left( \frac{2k}{k} \right) x^k = \frac{1}{\sqrt{1 - 4x}}. \]

4. Asymmetric Case

In this section, we consider an asymmetric case of the limit density \( f_{\infty}(x) \). Denote by \( \mu(r, c) \) the probability measure on \( \mathbb{R} \) which has density \((1 + cx)k(x,r)\), where \( r \in (0, 1) \) and \( c \in [-1/r, 1/r] \). We note that \( c = 0 \) leads to the symmetric case.

Theorem 4.1. For the moment generating function and the Stieltjes transform of \( \mu(r, c) \) we have

\[ M_{\mu(r,c)}(z) = \frac{(1 - r^2 z^2)(1 + cz) - (z + c)z\sqrt{1 - r^2} \sqrt{1 - r^2 z^2}}{(1 - z^2)(1 - r^2 z^2)}, \]

\[ G_{\mu(r,c)}(z) = \frac{(z^2 - r^2)(z + c) - (1 + cz)\sqrt{1 - r^2} \sqrt{z^2 - r^2}}{(z^2 - 1)(z^2 - r^2)}. \]

Proof. First we note that for the moments of \( \mu(r, c) \) we have

\[ s_n(\mu(r, c)) = \int_{-r}^{r} x^n \sqrt{1 - r^2}(1 + cx) \frac{dx}{\pi(1 - x^2)\sqrt{r^2 - x^2}} \]

\[ = \int_{-r}^{r} \frac{x^n \sqrt{1 - r^2}}{\pi(1 - x^2)\sqrt{r^2 - x^2}} dx + c \int_{-r}^{r} \frac{x^{n+1} \sqrt{1 - r^2}}{\pi(1 - x^2)\sqrt{r^2 - x^2}} dx \]

\[ = s_n(\mu(r, 0)) + c \cdot s_{n+1}(\mu(r, 0)). \]

Hence we can use Theorem 3.5 to get:

\[ M_{\mu(r,c)}(z) = \sum_{n=0}^{\infty} s_n(\mu(r, c)) z^n = M_{\mu(r,0)}(z) + \frac{c}{z} (M_{\mu(r,0)}(z) - 1) \]

\[ = \frac{(1 - r^2 z^2)(1 + cz) - (z + c)z\sqrt{1 - r^2} \sqrt{1 - r^2 z^2}}{(1 - z^2)(1 - r^2 z^2)} . \]

From this we obtain the Stieltjes transform \( G_{\mu(r,c)}(z) = M_{\mu(r,c)}(1/z)/z \) of \( \mu(r, c) \).

Denote by \( \beta_0(r, c), \gamma_i(r, c) \) the Jacobi coefficients of \( \mu(r, c) \), so that

\[ G_{\mu(r,c)}(z) = \frac{1}{z - \beta_0(r, c) - \frac{\gamma_0(r, c)}{z - \beta_1(r, c) - \frac{\gamma_1(r, c)}{z - \beta_2(r, c) - \frac{\gamma_2(r, c)}{z - \beta_3(r, c) - \ldots}}}} . \]
Since $\mu(r, -c)$ is the reflection of $\mu(r, c)$ we have $\beta_n(r, -c) = -\beta_n(r, c)$ and $\gamma_n(r, -c) = \gamma_n(r, c)$, so we can assume that $c \geq 0$. Using combinatorial relations between moments and Jacobi coefficients (see [1, 16]) one can check that

\[
\beta_0(r, c) = c(1 - s),
\]

\[
\gamma_0(r, c) = (1 - s)(1 - c^2 + c^2 s),
\]

\[
\beta_1(r, c) = -c(1 - s)(2 - 2c^2 - s + 2c^2 s) / 2(1 - c^2 + c^2 s),
\]

\[
\gamma_1(r, c) = s(1 - s)(2 - 2c^2 + c^2 s + c^2 s^2) / 4(1 - c^2 + c^2 s)^2,
\]

where $s := \sqrt{1 - r^2}$, and these coefficients are getting more and more complicated. It is possible however to find them in particular cases.

**Proposition 4.2.**

\[
\beta_n(r, 1) = \begin{cases} 
1 & n = 0, \\
-(1 - \sqrt{1 - r^2})/2 & n = 1, \\
0 & n \geq 2,
\end{cases} \quad \gamma_n(r, 1) = \begin{cases} 
\sqrt{1 - r^2}(1 - \sqrt{1 - r^2}) & n = 0, \\
\sqrt{r^2}/4 & n \geq 1.
\end{cases}
\]

**Proof.** We have

\[
\frac{1} {z - (1 - \sqrt{1 - r^2})} = \frac{\sqrt{1 - r^2}(1 - \sqrt{1 - r^2})} {z + (1 - \sqrt{1 - r^2})/2 - r^2/4} - \frac{r^2/4} {z - r^2/4} = \ldots
\]

In a similar way one can prove

**Proposition 4.3.**

\[
\beta_n(r, 1/r) = \begin{cases} 
(1 - \sqrt{1 - r^2)/r} & n = 0, \\
-(1 - \sqrt{1 - r^2})^2/(2r) & n = 1, \\
0 & n \geq 2,
\end{cases} \quad \gamma_n(r, 1/r) = \begin{cases} 
\sqrt{1 - r^2}(1 - \sqrt{1 - r^2})^2 & n = 0, \\
\sqrt{r^2}/4 & n \geq 1.
\end{cases}
\]

### 5. General Case

In the first half of this section, we consider a general symmetric case (i.e., $\beta_n = 0$) with the Jacobi coefficients $\{\gamma_n\}_{n=0}^{\infty}$ which are given by
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We note that if Corollary 5.2.

Applying the Stieltjes inverse formula, we have the following absolutely continuous part of the corresponding

where

In particular,

Applying the Stieltjes inverse formula, we have the following absolutely continuous part of the corresponding probability measure.

Corollary 5.2.

We illustrate \( \rho^{(2)}(x) \) for \((p_0, p_1, p)\)-case in Figs. 1–4.

For \( n = 1 \) case, see Obata [14]. In particular, when \( p_0 = 2N \) and \( p = 2N - 1 \), \( \rho^{(1)}(x) \) is a constant multiple of the density function of a Kesten distribution.

Finally we consider the following asymmetric case:

In a similar way, we obtain

We note that if \( q_0 = q = 0 \), then \( G^{2, \text{asy}}(z) \) (resp. \( \rho^{2, \text{asy}}(x) \)) becomes \( G^2(z) \) (resp. \( \rho^2(x) \)).
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