MATRIX VALUED SZEGŐ POLYNOMIALS AND QUANTUM RANDOM WALKS

M. J. CANTERO, F. A. GRÜNBAUM, L. MORAL, L. VELÁZQUEZ

Abstract. We consider quantum random walks (QRW) on the integers, a subject that has been considered in the last few years in the framework of quantum computation.

We show how the theory of CMV matrices gives a natural tool to study these processes and to give results that are analogous to those that Karlin and McGregor developed to study (classical) birth-and-death processes using orthogonal polynomials on the real line.

In perfect analogy with the classical case the study of QRWs on the set of non-negative integers can be handled using scalar valued (Laurent) polynomials and a scalar valued measure on the circle. In the case of classical or quantum random walks on the integers one needs to allow for matrix valued versions of these notions.

We show how our tools yield results in the well known case of the Hadamard walk, but we go beyond this translation invariant model to analyze examples that are hard to analyze using other methods. More precisely we consider QRWs on the set of non-negative integers. The analysis of these cases leads to phenomena that are absent in the case of QRWs on the integers even if one restricts oneself to a constant coin. This is illustrated here by studying recurrence properties of the walk, but the same method can be used for other purposes.

The presentation here aims at being selfcontained, but we refrain from trying to give an introduction to quantum random walks, a subject well surveyed in the literature we quote. For two excellent reviews, see [1, 18]. See also the recent notes [19].

2000 *Mathematics Subject Classification.* 81P68, 47B36, 42C05.

Key words and phrases. Matrix valued Laurent orthogonal polynomials, Karlin-McGregor representation, CMV matrices, quantum random walks.

We thank Julia Kempe for some guidance with the literature.

The research of the second author was supported in part by NSF Grant # DMS 0603901.

The research of the rest of the authors was partly supported by the Spanish grants from the Ministry of Education and Science, project code MTM2005-08648-C02-01, and the Ministry of Science and Innovation, project code MTM2008-06689-C02-01, and by Project E-64 of Diputación General de Aragón (Spain).

1. Introduction and contents of the paper

We start with a brief look at classical random walks.

Consider, for simplicity, a discrete time random walk in a denumerable state space which we take to be the non-negative integers $i = 0, 1, 2, \ldots$.

The state of the system at time n is given by a row vector $\pi_{i,n}$. This is also called the probability distribution at time n. The i^{th} component is interpreted as the probability that a particle can be found at site i at time n.

These non-negative quantities $\pi_{i,n}$ are assumed to add up to one, for any n, when summed over i in the set of non-negative integers. This is not the only way to describe these simple processes, but this facilitates the transition to the quantum case.

The evolution of the system is given by some transition probability matrix $P = (P_{i,j})$. This means that for each state i we have a collection of "transition probabilities" $P_{i,j}$ with the condition that these non-negative numbers add up to one when summed over the index j. $P_{i,j}$ is interpreted as the probability of a transition form site i to site j in one unit of time.

The Markov nature of our process is given by the fact that at time $t = 1$ the new probability distribution gives weight

$$\sum_{j=0}^{\infty} \pi_{j,0} P_{j,i}$$

to the i^{th} site. In other words the state at time $t = 1$ is the vector obtained by multiplying the probability distribution at time 0, namely $\pi_{j,0}$, by P. The Markov property says that the process starts from scratch at any integer time, so that the probability distribution (i.e., the state of the system) at time $t = n$ is obtained by taking the product of the row vector $\pi_{j,0}$ and the matrix P^n.

Random walks with a stationary (i.e., time invariant) transition mechanism as above have been studied extensively. In some cases it is convenient to exploit some of the mathematics associated with the matrix P. We will not go into details here but it turns out that this is the case when the matrix P is either symmetric to begin with, i.e., $P_{i,j} = P_{j,i}$ or it is what is called symmetrizable, namely there exists a vector π_i such that

$$\pi_i P_{i,j} = P_{j,i} \pi_j.$$

This notion is on the one hand related to the issue of reversibility and on the other it allows one to introduce a certain inner product in

$L^2(\mathbb{Z} \geq 0)$ that makes P selfadjoint and thus one has recourse to a nice and simple spectral theory.

A new item comes in now: the idea of a "local" transition. More specifically we consider a special kind of random walks, namely those that only allow for "nearest neighbour" transitions, i.e., $P_{i,j} = 0$ if the indices i, j differ by more than one unit. In this case the matrix P is tridiagonal and this is the best of all worlds since under very simple conditions any such matrix is symmetrizable into a tridiagonal one. Here we see a physically important issue such as nearest neighbour interactions going along with a nice mathematical fact such as symmetrizability.

The consequence of the combination of these two features is that one has a powerful and natural tool to study random walks with a tridiagonal or Jacobi transition matrix, namely the classical theory of orthogonal polynomials on the real line, a subject that goes back to the beginning of the 20th century.

This idea of making explicit use of the spectral theory for selfadjoint operators in Hilbert space to study an important class of random walks on $\mathbb{Z} \geq 0$ probably appears first in [16] . The authors point out that similar ideas had been used earlier in the case of diffusion processes by W. Feller, see [10], and H. P. McKean, Jr., see [23]. One could add to this list of precursors of this fruitful line of work other papers, such as [22]. One can also handle the case of continuous time, but we do not pursue this here.

The basic idea in [16] is simple: if one is dealing with these Markov chains that only allow for a "local" transition with $P_{i,j} = 0$ if i, j differ by more than one unit (also known as birth-and-death processes) then the orthogonal polynomials that can be built out of the corresponding Jacobi matrix and the underlying orthogonality measure give all the ingredients of the spectral resolution of the matrix. In particular they allow for a simple way to compute its power P^n.

All of this can be adapted to the case when our state space is not the set of non-negative integers but the set of all integers. The fact that now we have two different ways of going to infinity calls for the use of matrix valued orthogonal polynomials, a notion introduced by M. G. Krein [20, 21] around 1950. In this case we need polynomials with values in the set of square matrices of size two, whereas up to now we were dealing with scalar valued polynomials.

In fact a larger class of random walks, known under the name of quasi-birth-and-death processes, can also be analyzed by using these matrix valued orthogonal polynomials on the real line. In many cases the orthogonality measure is not really a matrix valued measure, but an appropriate linear functional. For two papers doing just this see [9, 12].

With this background we can now move closer to the subject of our paper, namely the study of a different sort of processes that go under the name of "quantum random walks" (QRW).

The basic idea is this: a system has a (denumerable) set $\{|i\rangle\}_{i\in\mathcal{I}}$ of measurable states called "pure states". The state $|\Psi_n\rangle$ of the system at time n is a (complex) superposition $|\Psi_n\rangle = \sum_{i\in\mathcal{I}} \psi_{i,n}|i\rangle$ of pure states, so it is described by a "wave function" $\psi_{i,n}$ with i running over the pure states. Therefore, a state can be identified with its wave function.

The complex number $\psi_{i,n}$ is no longer a probability but a probability amplitude, so that the actual probability to be in the state $|i\rangle$ at time n is $|\psi_{i,n}|^2$. The total probability of finding the system at time n must be 1, thus the wave function must satisfy the condition

$$\sum_{i\in\mathcal{I}} |\psi_{i,n}|^2 = 1. \tag{1}$$

In other words, the wave function lives in the unit ball of $L^2(\mathcal{I})$, which is equivalent to consider the pure states as an orthonormal basis of a Hilbert space whose unit vectors are the states of the system.

According to the conservation of the probability, in the time invariant case the time evolution of the system is characterized by a single unitary operator $\mathfrak{U}$ on the Hilbert state space: $|\Psi_n\rangle = \mathfrak{U}^n|\Psi_0\rangle$. If $U = (U_{i,j})_{i,j\in\mathcal{I}}$ is the unitary matrix such that $\mathfrak{U}|i\rangle = \sum_{j\in\mathcal{I}} U_{i,j}|j\rangle$, the evolution of the wave function is governed by

$$\psi_n = \psi_0 U^n, \qquad \psi_n = (\psi_{i,n})_{i\in\mathcal{I}}. \tag{2}$$

That is, the evolution operator in the wave function representation is a unitary operator U on $L^2(\mathcal{I})$.

When $\mathcal{I} = \mathbb{Z}$, it is proved in [24] that all the local QRWs ($U_{i,j} = 0$ if $|i-j| > r$ for some r) which are translation invariant ($U_{i,j} = U_{i+1,j+1}$) are, up to a phase, integer powers of a simple translation, i.e., $\mathfrak{U} = e^{i\theta}T^k$, $T|j\rangle = |j+1\rangle$.

If we do not ask for translation invariance but allow only nearest neighbour transitions ($U_{i,j} = 0$ if $|i-j| > 1$) then the QRW splits into independent QRWs with no more than two pure states or, up to a change of phases of the pure states, it is a simple right or left translation, i.e., $\mathfrak{U}|j\rangle = e^{i\theta_j}|j\pm 1\rangle$. The situation is even worse in the case $\mathcal{I} = \mathbb{Z} \geq 0$, where the restriction to nearest neighbour transitions always forces the splitting. These results, less known in quantum computation, are direct consequences of [4, Lemma 3.1] and [6, Theorem 3.9].

A way to generate non-trivial QRWs on the integers or the non-negative integers, allowing at the same time only nearest neighbour transitions, is to include extra degrees of freedom. Following the analogy with a quantum physical system, the simplest way to do this is to consider that every site $i \in \mathcal{I}$ has an internal degree of freedom of spin 1/2 type, i.e, taking values $s \in \mathcal{S} = \{\uparrow, \downarrow\}$. The space state is a tensor product spanned by $\{|i\rangle \otimes |\uparrow\rangle, |i\rangle \otimes |\downarrow\rangle\}_{i\in\mathcal{I}}$.

We will be considering mostly the cases when $\mathcal{I}$ is either the set of non-negative integers or the set of all integers. The evolution of the wave function $\psi_{i,s,n}$ satisfies (1) when summing in $i \in \mathcal{I}$ and $s \in \mathcal{S}$, so its evolution is given similarly to (2) by a unitary operator U on $L^2(\mathcal{I} \times \mathcal{S})$.

Although the choice $\mathcal{I} = \mathbb{Z} \geq 0$ would be as natural as $\mathcal{I} = \mathbb{Z}$, the first one has not received too much attention in the quantum case, maybe due to the difficulties to work with a non translation invariant system. However, just as in the classical case, QRWs on the non-negative integers are more natural for an orthogonal polynomial approach. Indeed, from this point of view, QRWs on the non-negative integers will be the cornerstone for the analysis of QRWs on the integers.

We are finally ready to state the purpose of this paper. We will show that in the case of a large class of quantum random walks on the integers there is a natural tool that takes the place of the matrix valued orthogonal polynomials on the real line briefly alluded to above, namely the theory of Laurent 2×2 matrix valued orthogonal polynomials associated with a certain kind of unitary matrices, namely CMV matrices. This is a ready made tool that combines the necessary features for a quantum mechanical description of the phenomenon of nearest neighbours transitions: unitarity and a block tridiagonal shape.

In the next section we first review the standard tools to deal with a simple random walk on the integers: the first two are very well known and have been used in the case of quatum random walks. The third method, involving matrix valued polynomials on the real line is less well known as a useful tool for the study of classical random walks on the integers. To the best of our knowledge neither scalar nor matrix valued orthogonal polynomials have so far been used in the case of QRWs and they constitute the main novel point of this paper.

The contents of the paper are organized as follows:

Section 2 reviews different approaches to the study of classical random walks, with special emphasis in the methods using orthogonal polynomials. This will establish a benchmark for the development of analogous techniques in the quantum case.

Section 3 introduces CMV matrices and Szegő polynomials.

Sections 4, 5 and 6 introduce QRWs and consider two extremely simple examples to show the workings of our method.

Section 7 considers the case of a not (necessarily) constant coin. We refer to this as dealing with "distinct coins". In principle our method can handle this general case, something that the more standard methods cannot do.

Section 8 takes up the simpler case of a constant coin and one sees that the case of the integers reduces to the study of two QRWs on the non-negative integers.

Section 9 tackles in detail the case of a QRW with a constant coin on the non-negative integers. The study of this case will be used in the following section and it is of independent interest since the phases of the coin have now a strong influence on the results, and in general the orthogonality measure has a discrete mass.

Section 10 uses the results of the previous two sections and shows that when dealing with all the integers there is no mass point in the orthogonality measure and that the phases of the coin play no role.

Section 11 applies the results of the previous sections to compare in the case of two specific QRWs their behaviour when considered on $\mathbb{Z} \geq 0$ or $\mathbb{Z}$.

Section 12 is devoted to getting some large time asymptotics.

Section 13 takes up the issue of recurrence of a QRW. By using our method we see here some marked differences between the classical and the quantum case. This section exhibits very clearly the benefits of using the notions introduced in this paper to analyze QRWs.

Section 14 lists some conclusions as well as some open problems that can be treated with the methods in this paper.

2. Classical random walk on the integers, three looks at a classical subject

Consider a random walk on the integers with p, q respectively the probabilities of going right or left in one unit of time starting at any integer position i.

Denote by $P(a, b, n)$ the quantity of interest, namely the probability of going in n steps from the initial position a to the final position b.

We describe three ways to study this basic problem.

a) Path counting: we must have c steps to the right and d steps to the left with $c + d = n$ and $c - d = b - a$. One can thus solve for c, d in terms of $a - b, n$. Each such path has probability $p^c q^d$ and there is total of $\binom{n}{c}$ such paths. This gives $P(a, b, n)$.

b) Fourier methods: if for simplicity we take $p = q = 1/2$, it is clear that

$$P(a,b,n) = \frac{1}{2}(P(a,b-1,n-1) + P(a,b+1,n-1)).$$

Introduce the Fourier series

$$\widehat{P}_a^r(\theta) \equiv \sum_{b=-\infty}^{\infty} P(a,b,r)e^{ib\theta}$$

with an inverse given by

$$P(a,b,n) = \frac{1}{2\pi}\int_0^{2\pi} e^{-ib\theta}\widehat{P}_a^n(\theta)d\theta.$$

The difference equation above can be used to see that

$$\widehat{P}_a^n(\theta) = \widehat{P}_a^{n-1}(\theta)\cos\theta = \widehat{P}_a^0(\theta)(\cos\theta)^n$$

and therefore

$$P(a,b,n) = \frac{1}{2\pi}\int_0^{2\pi} \widehat{P}_a^0(\theta)(\cos\theta)^n e^{-ib\theta}d\theta.$$

In the special case when $P(i,j,0)$ is given by $\delta_{i,j}$ we get

$$P(a,b,n) = \frac{1}{2\pi}\int_0^{2\pi} (\cos\theta)^n e^{-i(b-a)\theta}d\theta.$$

This integral can be computed explicitly in terms of Bessel functions, or just as easily, it can be seen to agree with the general expression obtained earlier. For general values of p, q one simply replaces $\cos\theta$ by a weighted sum of $e^{i\theta}, e^{-i\theta}$.

These two methods have been properly adapted to study QRWs on the integers. "Path counting" was used by D. Meyer, see [24]. This analysis was pushed further along by using Jacobi polynomials in [2]. In this same paper as well as in [25] one finds expressions obtained by using "Fourier methods" to analyze the appropriate recursion relations. The reader can find a very sophisticated use of these formulas to derive some aymptotic results about the Hadamard QRW in [7]. A recent and very precise analysis of asymptotic results is given in [19]. Some interesting use of generating functions to obtain rigorous results is made in [3].

c) Using matrix valued orthogonal polynomials: since this is not too standard and since this is the way in which we analyze the quantum case we give a lengthier account of this way of tackling this problem. This method goes back, in spirit at least, to the original paper of Karlin and McGregor, [16], where the reader will find a complete discussion of the case of a random walk on the non-negative integers using scalar valued orthogonal polynomials. For a fuller account of the material below see [9, 12, 13].

Consider, with M. G. Krein, [20, 21], the set of polynomials of the real variable x with matrix coefficients of a fixed size d. All the matrices that appear below have this common size d and this is the appropriate choice when the state space is the cartesian product of the set of non-negative integers with the set $1, 2, 3, \ldots, d$.

Given a positive definite matrix valued measure $dM(x)$ with finite moments $\int_{\mathbb{R}} x^n dM(x)$, $n = 0, 1, 2, \ldots,$ consider the skew symmetric bilinear form defined for any pair of matrix valued polynomial functions $P(x)$ and $Q(x)$ by the numerical matrix

$$(P, Q) = (P, Q)_M = \int_{\mathbb{R}} P(x)dM(x)Q(x)^{\dagger},$$

where $Q(x)^{\dagger}$ denotes the conjugate transpose of $Q(x)$.

By the usual Gram–Schmidt construction this leads to the existence of a sequence of matrix valued orthogonal polynomials $P_n(x) = K_{n,n}x^n + K_{n,n-1}x^{n-1} + \cdots$ with non-singular leading coefficient $K_{n,n}$. We make no special assumption on $K_{n,n}$.

Given an orthogonal sequence $\{P_n(x)\}_{n\geq 0}$ of matrix valued orthogonal polynomials one gets by the usual argument a three term recursion relation

$$xP_n(x) = A_n P_{n-1}(x) + B_n P_n(x) + C_n P_{n+1}(x), \tag{3}$$

where A_n, B_n and C_n are matrices and the last one is non-singular. If we had insisted on orthonormal polynomials then we would get some relations among these coefficients.

It is convenient to introduce the block tridiagonal matrix $\mathbf{P}$

$$\mathbf{P} = \begin{pmatrix} B_0 & C_0 & & \\ A_1 & B_1 & C_1 & \\ & \ddots & \ddots & \ddots \end{pmatrix}.$$

If $\mathbf{P}_{i,j}$ denotes the i, j block of $\mathbf{P}$ we can generate a sequence of $d \times d$ matrix valued polynomials $Q_i(x)$ by imposing the three term recursion given above. By using the notation of the scalar case, we would have

$$\mathbf{P}Q(x) = xQ(x)$$

where the entries of the column vector $Q(x)$ are now $d \times d$ matrices.

Proceeding as in the scalar case, this relation can be iterated to give

$$\mathbf{P}^n Q(x) = x^n Q(x)$$

and if we assume the existence of a positive definite matrix valued measure $dM(x)$ as in Krein's theory, with the property

$$(Q_j, Q_j)\delta_{i,j} = \int_{\mathbb{R}} Q_i(x) dM(x) Q_j(x)^\dagger,$$

it is then clear that one can get an expression for the i, j entry of the block matrix $\mathbf{P}^n$ that would look exactly as in the scalar case, namely

$$(\mathbf{P}^n)_{i,j}(Q_j, Q_j) = \int_{\mathbb{R}} x^n Q_i(x) dM(x) Q_j(x)^\dagger.$$

The expression above, allowing one to compute the entries of $\mathbf{P}^n$ is usually called the Karlin-McGregor formula, see [16].

It may be worth noticing that the integrals above are different from the ones that appear when one uses the Fourier method. The same will be true in the quantum case.

Just as in the scalar case, the expression above becomes useful when we can get our hands on the matrix valued polynomials $Q_i(x)$ and the orthogonality measure $dM(x)$. When this is the case this formula allows us to compute the transition probabilities between any pair of states $i \leq j$ **in any number of steps** by using only the top j rows of the matrix $\mathbf{P}$. The "time dependence" has now been isolated to the term x^n and the study of its behaviour for large values of n can be handled with traditional methods. The same remark will apply in the quantum case and this will be used in Section 12.

We are now ready to tackle the example of random walk on the integers, when the probabilities of going right or left are p and q respectively. This is the most general translation invariant random walk on the integers with nearest neighbours transitions. We present it here to compare this analysis with its quantum counterpart, i.e., the quantum random walks with a constant coin on the integers analyzed in Sections 8 and 10.

If we "fold" the integers by relabelling the natural sequence

$$\cdots - 3, -2, -1, 0, 1, 2, 3 \ldots$$

in the fashion

$$\ldots 5, 3, 1, 0, 2, 4, 6 \ldots$$

then the transition probability matrix goes from being a scalar tridiagonal doubly infinite one with p in the $i, i+1$ diagonal and q in the

$i+1, i$ diagonal to the following semi-infinite block tridiagonal matrix (with 2×2 blocks)

$$\mathbf{P} = \begin{pmatrix} 0 & q & p & 0 & 0 & 0 & 0 & 0 & \dots \\ p & 0 & 0 & q & 0 & 0 & 0 & 0 & \dots \\ q & 0 & 0 & 0 & p & 0 & 0 & 0 & \dots \\ 0 & p & 0 & 0 & 0 & q & 0 & 0 & \dots \\ 0 & 0 & q & 0 & 0 & 0 & p & 0 & \dots \\ 0 & 0 & 0 & p & 0 & 0 & 0 & q & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}, \qquad p+q=1.$$

For this first example the appropriate matrix measure is already found in the original paper by S. Karlin and J. McGregor. It is given by

$$dM(x) = \frac{1}{\sqrt{4pq - x^2}} \begin{pmatrix} 1 & x/2q \\ x/2q & p/q \end{pmatrix} dx, \qquad |x| \le \sqrt{4pq}.$$

One does not find in the paper mentioned above the corresponding matrix valued orthogonal polynomials or the block tridiagonal matrix, but they can be easily given, see [12] and below.

In this example we have

$$B_0 = \begin{pmatrix} 0 & q \\ p & 0 \end{pmatrix}, \qquad B_k = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad k \ge 1,$$

$$A_k = \begin{pmatrix} q & 0 \\ 0 & p \end{pmatrix}, \quad k \ge 1, \qquad C_k = \begin{pmatrix} p & 0 \\ 0 & q \end{pmatrix}, \quad k \ge 0.$$

The orthogonal polynomials given by

$$A_k P_{k-1}(x) + B_k P_k(x) + C_k P_{k+1}(x) = x P_k(x),$$
$$P_{-1}(x) = \mathbf{0}, \quad P_0(x) = \mathbf{1},$$

where $\mathbf{0}$ and $\mathbf{1}$ are the null and identity matrix, can be easily expressed in terms of Chebyshev polynomials.

Let us denote by $U_n(x)$ the Chebyshev polynomials of the second kind, which satisfy

$$U_{n+1}(x) + U_{n-1}(x) = 2xU_n(x), \qquad U_{-1}(x) = 0 \qquad U_0(x) = 1. \tag{4}$$

The relation with the Chebyshev polynomials $U_n(x)$, is given by

$$P_k(x) = \begin{pmatrix} (q/p)^{\frac{k}{2}} & 0 \\ 0 & (p/q)^{\frac{k}{2}} \end{pmatrix} \left\{ \mathbf{1} U_k(x^*) - \begin{pmatrix} 0 & (q/p)^{\frac{1}{2}} \\ (p/q)^{\frac{1}{2}} & 0 \end{pmatrix} U_{k-1}(x^*) \right\},$$

where $x^* = x/2\sqrt{pq}$. This expression can be compared to the one in Section 10.

These ideas have been used recently to analyze more elaborate examples of classical random walks. The reader may consult [9, 12, 13, 14, 15].

3. Szegő polynomials and CMV matrices

All the information about a QRW is encoded in the unitary operator U governing the evolution of the system. Therefore, it is not strange that the theory of canonical matrix representations of unitary operators on Hilbert spaces should play an important role in the study of QRWs. Surprisingly, such a theory has been developed only recently (see [5, 6, 32]) giving rise to the so called CMV matrices, related to the Szegő polynomials.

Due to their relevance for the rest of the paper, we will summarize in this section the main facts about CMV matrices.

The basic idea is that, as a consequence of the spectral theorem, any unitary operator is unitarily equivalent to a direct sum of unitary multiplication operators, i.e., operators of the type

$$\begin{aligned} U_\mu\colon\ L^2_\mu(\mathbb{T}) &\to L^2_\mu(\mathbb{T}) \\ f(z) &\longrightarrow zf(z) \end{aligned} \tag{5}$$

μ being a probability measure on the unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$, and $L^2_\mu(\mathbb{T})$ the Hilbert space of μ-square-integrable functions with inner product

$$(f, g) = \int_{\mathbb{T}} \overline{f(z)}\, g(z)\, d\mu(z).$$

Thus, it is enough to discuss the canonical representations of unitary multiplication operators. Moreover, we can suppose that μ has an infinite support, otherwise $L^2_\mu(\mathbb{T})$ is finite-dimensional, so U_μ is unitarily diagonalizable.

Since the Laurent polynomials are dense in $L^2_\mu(\mathbb{T})$, a natural basis to obtain a matrix representation of U_μ is given by the Laurent polynomials $(\chi_j)_{j=0}^\infty$ obtained from the Gram-Schmidt orthonormalization of $\{1, z, z^{-1}, z^2, z^{-2}, \dots\}$ in $L^2_\mu(\mathbb{T})$.

The matrix $\mathcal{C} = (\chi_j, z\chi_k)_{j,k=0}^{\infty}$ of U_μ with respect to $(\chi_j)_{j=0}^{\infty}$ has the form

$$
\mathcal{C} = \begin{pmatrix}
\overline{\alpha}_0 & \rho_0\overline{\alpha}_1 & \rho_0\rho_1 & 0 & 0 & 0 & 0 & \dots \\
\rho_0 & -\alpha_0\overline{\alpha}_1 & -\alpha_0\rho_1 & 0 & 0 & 0 & 0 & \dots \\
0 & \rho_1\overline{\alpha}_2 & -\alpha_1\overline{\alpha}_2 & \rho_2\overline{\alpha}_3 & \rho_2\rho_3 & 0 & 0 & \dots \\
0 & \rho_1\rho_2 & -\alpha_1\rho_2 & -\alpha_2\overline{\alpha}_3 & -\alpha_2\rho_3 & 0 & 0 & \dots \\
0 & 0 & 0 & \rho_3\overline{\alpha}_4 & -\alpha_3\overline{\alpha}_4 & \rho_4\overline{\alpha}_5 & \rho_4\rho_5 & \dots \\
0 & 0 & 0 & \rho_3\rho_4 & -\alpha_3\rho_4 & -\alpha_4\overline{\alpha}_5 & -\alpha_4\rho_5 & \dots \\
\dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots
\end{pmatrix}, \tag{6}
$$

where $\rho_j = \sqrt{1 - |\alpha_j|^2}$ and $(\alpha_j)_{j=0}^{\infty}$ is a sequence of complex numbers such that $|\alpha_j| < 1$. The coefficients α_j are known as the Verblunsky parameters of the measure μ, and establish a bijection between the probability measures supported on an infinite set of the unit circle and the sequences in the open unit disk.

Another equally natural basis would be the Laurent polynomials $(x_j)_{j=0}^{\infty}$ obtained from the orthonormalization of $\{1, z^{-1}, z, z^{-2}, z^2, \dots\}$. They are given by

$$x_j(z) = \overline{\chi_j(1/\overline{z})}$$

and, consequently, the matrix of U_μ with respect to $(x_j)_{j=0}^{\infty}$ is the transpose $\mathcal{C}^T$ of $\mathcal{C}$.

As a consequence, we have the identities

$$
\begin{aligned}
&\chi(z)\mathcal{C} = z\chi(z), \qquad &&\chi = (\chi_0, \chi_1, \chi_2, \dots), \qquad &&\chi_0 = 1, \\
&\mathcal{C}x(z) = zx(z), \qquad &&x = (x_0, x_1, x_2, \dots)^T, \qquad &&x_0 = 1,
\end{aligned} \tag{7}
$$

which can be viewed as recurrences which determine the orthonormal Laurent polynomials.

The unitary matrices with the form (6) or its transpose are called CMV matrices, but we will reserve this name for the matrix in (6). Also, when talking about orthonormal Laurent polynomials, we will refer to $(x_j)_{j=0}^{\infty}$, which are the ones that we will normally use.

The canonical representations of the unitaries are the narrowest banded representations that can be obtained for all such operators. The previous results state that every unitary operator has a matrix representation which is a direct sum of CMV matrices, so the canonical representations of the unitaries are at least five-diagonal. That they are exactly five-diagonal has been proved in [6], where it was shown that not every unitary operator admits a four-diagonal representation.

The CMV matrices have also a tridiagonal factorization $\mathcal{C} = \mathcal{L}\mathcal{M}$, with two unitary 2×2-block diagonal symmetric factors given by

$$\begin{aligned} \mathcal{L} &= \operatorname{diag}(\Theta_0, \Theta_2, \Theta_4, \dots), \\ \mathcal{M} &= \operatorname{diag}(1, \Theta_1, \Theta_3, \dots), \end{aligned} \qquad \Theta_j = \begin{pmatrix} \overline{\alpha}_j & \rho_j \\ \rho_j & -\alpha_j \end{pmatrix}. \tag{8}$$

The Verblunsky parameters have a special meaning in terms of the Szegő polynomials $(\varphi_j)_{j=0}^{\infty}$, which come from orthonormalizing $\{z^j\}_{j=0}^{\infty}$, see [31, 11].

These polynomials are not so useful as a basis because the polynomials are not always dense in $L^2_\mu(\mathbb{T})$. Nevertheless, they are related to the orthonormal Laurent polynomials by

$$\begin{aligned} \chi_{2j}(z) &= z^{-j}\varphi^*_{2j}(z), \qquad & \chi_{2j+1}(z) &= z^{-j}\varphi_{2j+1}(z), \\ x_{2j}(z) &= z^{-j}\varphi_{2j}(z), \qquad & x_{2j+1}(z) &= z^{-j-1}\varphi^*_{2j+1}(z), \end{aligned} \tag{9}$$

where $\varphi^*_j(z) = z^j\overline{\varphi_j(1/\overline{z})}$.

The key result is that the Szegő polynomials are determined by the recurrence relation

$$\rho_j\varphi_{j+1}(z) = z\varphi_j(z) - \overline{\alpha}_j\varphi^*_j(z), \qquad \varphi_0 = 1, \tag{10}$$

so the recurrence for the monic orthogonal polynomials $(\phi_j)_{j=0}^{\infty}$ is

$$\phi_{j+1}(z) = z\phi_j(z) - \overline{\alpha}_j\phi^*_j(z), \qquad \phi_0 = 1, \tag{11}$$

which shows that $\alpha_j = -\overline{\phi_{j+1}(0)}$.

For some measures on the unit circle the Szegő polynomials, and therefore the Verblunsky parameters and the CMV matrix, are known explicitly, see [28]. Other cases can be analyzed following different methods.

For instance, given a sequence of Verblunsky parameters, the spectral analysis of the corresponding CMV matrix can be used to obtain information about the orthogonality measure because it is related to the spectral measure of the CMV matrix. Indeed, the support of the measure coincides with the spectrum of the CMV matrix, the mass points z_0 being the eigenvalues, which are simple and have eigenvectors given by $x(z_0)$. Bearing in mind (7), this means that $x(z_0) \in L^2(\mathbb{Z} \geq 0)$ exactly when z_0 is a mass point. Actually, $\mu(\{z_0\}) = 1/\|x(z_0)\|^2$.

These results will be of interest later on, see Section 12.

Perturbative results are useful to study new examples taking as a starting point known ones. The simplest example of this is a rotation of the measure by an angle ϑ, i.e.

$$d\mu(z) \to d\mu(e^{-i\vartheta}z).$$

The change of the monic orthogonal polynomials $\phi_j(z) \to e^{ij\vartheta}\phi_j(e^{-i\vartheta}z)$ shows that the effect of the rotation on the Verblunsky parameters is

$$\alpha_j \to e^{-i(j+1)\vartheta}\alpha_j \tag{12}$$

while (9) implies that the orthonormal Laurent polynomials transform as

$$x_{2j-1}(z) \to e^{-ij\vartheta}x_{2j-1}(e^{-i\vartheta}z), \qquad x_{2j}(z) \to e^{ij\vartheta}x_{2j}(e^{-i\vartheta}z). \tag{13}$$

The transformation above will play an important role in later sections.

Another tool for the study of Szegő polynomials is the Carathéodory function F of the orthogonality measure μ, defined by

$$F(z) = \int_{\mathbb{T}} \frac{t+z}{t-z}\, d\mu(t), \qquad |z|<1. \tag{14}$$

F is analytic on the open unit disc with McLaurin series

$$F(z) = 1 + 2\sum_{j=1}^{\infty} \overline{\mu}_j z^j, \qquad \mu_j = \int_{\mathbb{T}} z^j d\mu(z), \tag{15}$$

whose coefficients provide the moments μ_j of the measure μ.

F can be obtained as

$$F(z) = \lim_{j\to\infty} \frac{\tilde{\varphi}_j^*(z)}{\varphi_j^*(z)}, \qquad |z|<1, \tag{16}$$

where $\tilde{\varphi}_j$ are the Szegő polynomials whose Verblunsky parameters are given by $-\alpha_j$ if the original ones were α_j.

The Carathéodory function is a shortcut that allows one to recover the measure from the Szegő polynomials. If

$$d\mu(e^{i\theta}) = w(\theta)\frac{d\theta}{2\pi} + d\mu_s(e^{i\theta}), \qquad \theta \in (-\pi,\pi], \qquad \mu_s \text{ singular}, \tag{17}$$

the weight $w(\theta)$ is given by

$$w(\theta) = \lim_{r\uparrow 1} \mathrm{Re} F(re^{i\theta}), \tag{18}$$

and the support of μ_s lies on $\{e^{i\theta} : \lim_{r\uparrow 1} F(re^{i\theta}) = \infty\}$. In particular, $e^{i\theta_0}$ is a mass point of μ with mass $\mu(\{e^{i\theta_0}\})$ if and only if

$$\mu(\{e^{i\theta_0}\}) = \lim_{r\uparrow 1} \frac{1-r}{2} F(re^{i\theta_0}) \neq 0. \tag{19}$$

Two natural extensions of CMV matrices are of interest to us: doubly infinite CMV matrices and block CMV matrices.

Given a two-sided sequence $(\alpha_j)_{j\in\mathbb{Z}}$ we can define the doubly infinite CMV matrix $\mathcal{C} = \mathcal{L}\mathcal{M}$, where

$$\begin{aligned} \mathcal{L} &= \operatorname{diag}(\dots, \Theta_{-4}, \Theta_{-2}, \Theta_0, \Theta_2, \Theta_4, \dots), \\ \mathcal{M} &= \operatorname{diag}(\dots, \Theta_{-3}, \Theta_{-1}, \Theta_1, \Theta_3, \dots), \end{aligned}$$

and Θ_j, given in (8), acts on the indices j and $j+1$. We will use the same notations as for semi-infinite CMV matrices.

$\mathcal{C}$ is a five-diagonal doubly infinite unitary matrix with the form

$$\begin{array}{cccc|cccc} \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \rho_{-3}\overline{\alpha}_{-2} & -\alpha_{-3}\overline{\alpha}_{-2} & \rho_{-2}\overline{\alpha}_{-1} & \rho_{-2}\rho_{-1} & 0 & 0 & \dots \\ \dots & \rho_{-3}\rho_{-2} & -\overline{\alpha}_{-3}\rho_{-2} & -\alpha_{-2}\overline{\alpha}_{-1} & -\alpha_{-2}\rho_{-1} & 0 & 0 & \dots \\ \hline \dots & 0 & 0 & \rho_{-1}\overline{\alpha}_0 & -\alpha_{-1}\overline{\alpha}_0 & \rho_0\overline{\alpha}_1 & \rho_0\rho_1 & \dots \\ \dots & 0 & 0 & \rho_{-1}\rho_0 & -\alpha_{-1}\rho_0 & -\alpha_0\overline{\alpha}_1 & -\alpha_0\rho_1 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{array}$$

Doubly infinite CMV matrices are also related to the other generalization of interest: block CMV matrices. They appear in connection with matrix valued Szegő polynomials, see [8, 28, 29].

Given a positive definite $d \times d$ matrix valued measure $\boldsymbol{\mu}$ on the unit circle we can define the right and left "inner products"

$$(\boldsymbol{f}, \boldsymbol{g})_L = \int_{\mathbb{T}} \boldsymbol{g}(z)\, d\boldsymbol{\mu}(z)\, \boldsymbol{f}(z)^\dagger, \qquad (\boldsymbol{f}, \boldsymbol{g})_R = \int_{\mathbb{T}} \boldsymbol{f}(z)^\dagger d\boldsymbol{\mu}(z)\, \boldsymbol{g}(z),$$

for $\boldsymbol{f}, \boldsymbol{g}$ with values in the set of $d \times d$ matrices. Notice that the symbol † which denotes the adjoint matrix includes the conjugation of z. In what follows we suppose that $\int_{\mathbb{T}} d\boldsymbol{\mu}(z) = \mathbf{1}$ is the $d \times d$ unit matrix.

Now we can consider right and left matrix valued Szegő polynomials, $(\boldsymbol{\varphi}_j^R)_{j=0}^\infty$ and $(\boldsymbol{\varphi}_j^L)_{j=0}^\infty$, arising from the standard orthonormalization of $\{\mathbf{1} z^j\}_{j=0}^\infty$ with respect to $(\,,)_R$ and $(\,,)_L$ respectively.

Analogously to the scalar case, the matrix valued Szegő polynomials satisfy a recurrence given in terms of a sequence $(\boldsymbol{\alpha}_j)_{j=0}^\infty$ of $d \times d$ matrices such that $\|\boldsymbol{\alpha}_j\| < 1$. However, this recurrence mixes the right and left polynomials in the following way

$$\begin{aligned} \boldsymbol{\rho}_j^L \boldsymbol{\varphi}_{j+1}^L(z) &= z\boldsymbol{\varphi}_j^L(z) - \boldsymbol{\alpha}_j^\dagger \boldsymbol{\varphi}_j^{R*}(z), \\ \boldsymbol{\varphi}_{j+1}^R(z) \boldsymbol{\rho}_j^R &= z\boldsymbol{\varphi}_j^R(z) - \boldsymbol{\varphi}_j^{L*}(z) \boldsymbol{\alpha}_j^\dagger, \end{aligned} \qquad \boldsymbol{\varphi}_0^L = \boldsymbol{\varphi}_0^R = \mathbf{1},$$

where $\boldsymbol{\varphi}_j^*(z) = z^j \boldsymbol{\varphi}_j(1/\overline{z})^\dagger$ and $\boldsymbol{\rho}_j^L, \boldsymbol{\rho}_j^R$ are the positive definite matrices

$$\boldsymbol{\rho}_j^L = (1 - \boldsymbol{\alpha}_j^\dagger \boldsymbol{\alpha}_j)^{1/2}, \qquad \boldsymbol{\rho}_j^R = (1 - \boldsymbol{\alpha}_j \boldsymbol{\alpha}_j^\dagger)^{1/2}.$$

This mixture between right and left polynomials also appears in the connection with the orthonormal Laurent polynomials $(\boldsymbol{\chi}_j)_{j=0}^\infty, (\boldsymbol{x}_j)_{j=0}^\infty$

given by

$$\begin{aligned} &\boldsymbol{\chi}_{2j}(z) = z^{-j}\boldsymbol{\varphi}_{2j}^{L*}(z), \qquad &\boldsymbol{\chi}_{2j+1}(z) = z^{-j}\boldsymbol{\varphi}_{2j+1}^{R}(z),\\ &\boldsymbol{x}_{2j}(z) = z^{-j}\boldsymbol{\varphi}_{2j}^{L}(z), \qquad &\boldsymbol{x}_{2j+1}(z) = z^{-j-1}\boldsymbol{\varphi}_{2j+1}^{R*}(z), \end{aligned} \tag{20}$$

and related by $\boldsymbol{x}_j(z) = \boldsymbol{\chi}_j(1/\overline{z})^\dagger$. $(\boldsymbol{\chi}_j)_{j=0}^\infty$ comes from the orthonormalization of $\{\mathbf{1}, \mathbf{1}z, \mathbf{1}z^{-1}, \mathbf{1}z^2, \mathbf{1}z^{-2}, \dots\}$ with respect to $(\boldsymbol{,})_R$, and $(\boldsymbol{x}_j)_{j=0}^\infty$ from the orthonormalization of $\{\mathbf{1}, \mathbf{1}z^{-1}, \mathbf{1}z, \mathbf{1}z^{-2}, \mathbf{1}z^2, \dots\}$ with respect to $(\boldsymbol{,})_L$ (notice a slight difference with respect to [8], where the two kinds of Laurent polynomials discussed are both orthonormal with respect to $(\boldsymbol{,})_R$).

The matrix $\boldsymbol{\mathcal{C}}$ which determines the orthonormal Laurent polynomials through the recurrences

$$\begin{aligned} &\boldsymbol{\chi}(z)\boldsymbol{\mathcal{C}} = z\boldsymbol{\chi}(z), \qquad &\boldsymbol{\chi} = (\boldsymbol{\chi}_0, \boldsymbol{\chi}_1, \boldsymbol{\chi}_2, \dots), \qquad &\boldsymbol{\chi}_0 = \mathbf{1},\\ &\boldsymbol{\mathcal{C}}\boldsymbol{x}(z) = z\boldsymbol{x}(z), \qquad &\boldsymbol{x} = (\boldsymbol{x}_0, \boldsymbol{x}_1, \boldsymbol{x}_2, \dots)^T, \qquad &\boldsymbol{x}_0 = \mathbf{1}, \end{aligned} \tag{21}$$

is given by $\boldsymbol{\mathcal{C}} = \boldsymbol{\mathcal{L}}\boldsymbol{\mathcal{M}}$ with

$$\begin{aligned} &\boldsymbol{\mathcal{L}} = \operatorname{diag}(\boldsymbol{\Theta}_0, \boldsymbol{\Theta}_2, \boldsymbol{\Theta}_4, \dots),\\ &\boldsymbol{\mathcal{M}} = \operatorname{diag}(\mathbf{1}, \boldsymbol{\Theta}_1, \boldsymbol{\Theta}_3, \dots), \end{aligned} \qquad \boldsymbol{\Theta}_j = \begin{pmatrix} \boldsymbol{\alpha}_j^\dagger & \boldsymbol{\rho}_j^L \\ \boldsymbol{\rho}_j^R & -\boldsymbol{\alpha}_j \end{pmatrix}. \tag{22}$$

The unitary matrix $\boldsymbol{\mathcal{C}}$ is called a block CMV matrix. Its explicit form is

$$\boldsymbol{\mathcal{C}} = \begin{pmatrix} \boldsymbol{\alpha}_0^\dagger & \boldsymbol{\rho}_0^L\boldsymbol{\alpha}_1^\dagger & \boldsymbol{\rho}_0^L\boldsymbol{\rho}_1^L & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots \\ \boldsymbol{\rho}_0^R & -\boldsymbol{\alpha}_0\boldsymbol{\alpha}_1^\dagger & -\boldsymbol{\alpha}_0\boldsymbol{\rho}_1^L & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{0} & \boldsymbol{\alpha}_2^\dagger\boldsymbol{\rho}_1^R & -\boldsymbol{\alpha}_2^\dagger\boldsymbol{\alpha}_1 & \boldsymbol{\rho}_2^L\boldsymbol{\alpha}_3^\dagger & \boldsymbol{\rho}_2^L\boldsymbol{\rho}_3^L & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{0} & \boldsymbol{\rho}_2^R\boldsymbol{\rho}_1^R & -\boldsymbol{\rho}_2^R\boldsymbol{\alpha}_1 & -\boldsymbol{\alpha}_2\boldsymbol{\alpha}_3^\dagger & -\boldsymbol{\alpha}_2\boldsymbol{\rho}_3^L & \mathbf{0} & \mathbf{0} & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\alpha}_4^\dagger\boldsymbol{\rho}_3^R & -\boldsymbol{\alpha}_4^\dagger\boldsymbol{\alpha}_3 & \boldsymbol{\rho}_4^L\boldsymbol{\alpha}_5^\dagger & \boldsymbol{\rho}_4^L\boldsymbol{\rho}_5^L & \dots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\rho}_4^R\boldsymbol{\rho}_3^R & -\boldsymbol{\rho}_4^R\boldsymbol{\alpha}_3 & -\boldsymbol{\alpha}_4\boldsymbol{\alpha}_5^\dagger & -\boldsymbol{\alpha}_4\boldsymbol{\rho}_5^L & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix},$$

where the symbol $\mathbf{0}$ stands for the $d \times d$ null matrix.

Particularly simple is the case of diagonal Verblunsky parameters $\boldsymbol{\alpha}_j = \operatorname{diag}(\alpha_j^1, \dots, \alpha_j^d)$. The corresponding matrix orthonormal polynomials and orthogonality matrix measure are diagonal too. In other words, the recurrences in (21) split into d ones associated with scalar CMV matrices with Verblunsky parameters $\alpha_j^1, \dots, \alpha_j^d$.

Finally, the matrix valued Carathéodory function

$$\boldsymbol{F}(z) = \int_{\mathbb{T}} \frac{t+z}{t-z}\, d\boldsymbol{\mu}(t), \qquad |z| < 1, \tag{23}$$

and its real part $\operatorname{Re}\boldsymbol{F}(z) = (\boldsymbol{F}(z) + \boldsymbol{F}(z)^\dagger)/2$ allows one to recover the matrix measure $\boldsymbol{\mu}$ just as in the scalar case. In particular, the matrix moments $\boldsymbol{\mu}_j$ of $\boldsymbol{\mu}$ come from the McLaurin series of $\boldsymbol{F}$, i.e.,

$$\boldsymbol{F}(z) = \mathbf{1} + 2\sum \boldsymbol{\mu}_j^\dagger z^j, \qquad \boldsymbol{\mu}_j = \int_{\mathbb{T}} z^j d\boldsymbol{\mu}(z). \tag{24}$$

4. Quantum random walks

We will consider a few one-dimensional quantum random walks with pure states $|i\rangle \otimes |\uparrow\rangle$ and $|i\rangle \otimes |\downarrow\rangle$, where i runs over the non-negative integers or over all the integers, and with a one step transition mechanism given by a unitary matrix U. Our goal here is to give an explicit expression for the entries of the matrix U^n for $n = 0, 1, 2, \dots$ describing the time evolution of our process. More precisely, we will find a Karlin-McGregor (KMcG) formula for such entries.

The relevance of the CMV matrices, as the canonical representations of the unitaries, is clear. However, the reduction of an arbitrary infinite unitary matrix to CMV form can be a difficult task. Nevertheless, the QRWs usually considered in the literature include only nearest neighbour transitions. In this case it is possible to prove that the CMV form is obtained after a simple change of phases in the basis, see [6, Theorem 3.2 and Lemma 3.7]. Then, the relation of the CMV matrices with the Szegő polynomials provides the functions and measures needed to obtain a KMcG formula.

5. A very elementary example

A simple QRW on the non-negative integers corresponds to the unitary operator

$$S_+ = \sum_{i=0}^{\infty} |i+1\rangle\langle i| \otimes |\uparrow\rangle\langle\uparrow| + \sum_{i=1}^{\infty} |i-1\rangle\langle i| \otimes |\downarrow\rangle\langle\downarrow| + |0\rangle\langle 0| \otimes |\uparrow\rangle\langle\downarrow|, \tag{25}$$

which means that the transition mechanism moves spins at positions $0, 1, 2, \dots$ according to the following (deterministic) prescription: spins up at any location move one step to the right, spins down at $1, 2, 3, \dots$ move to the left, and finally a spin down at location 0 reverses orientation and stays at location 0. In the next unit of time this spin will move to location 1.

If we choose to order the pure states of our system as follows

$$|0\rangle \otimes |\uparrow\rangle, |0\rangle \otimes |\downarrow\rangle, |1\rangle \otimes |\uparrow\rangle, |1\rangle \otimes |\downarrow\rangle, \dots \tag{26}$$

then the transition matrix is

$$U_+ = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & \dots \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \end{pmatrix}.$$

We refer to the pure states, ordered in this fashion, as the zeroth, the first, the second state, etc.

However, there is another way to look at the transition matrix. We could think of the functions $1, z^{-1}, z, z^{-2}, z^2, \dots$ defined on the unit circle and form a column vector $x(z)$ with these functions. Applying our matrix U_+ to this vector is the same as multiplying the vector by z, which is another way of saying that for each value of z we have found a formal eigenvector with eigenvalue z for our matrix.

If we denote the components of this column vector by $x_j(z)$, $j = 0, 1, 2, \dots$, we claim that the probability amplitude of going in n (positive or negative) units of time from a pure state j to a pure state k (the indices j, k run over all the zeroth, first, second, ... pure states introduced above) is given by the integral

$$\frac{1}{2\pi i} \int_{|z|=1} \overline{x_k(z)}\, x_j(z) z^n \frac{dz}{z}.$$

It is completely elementary to see that this integral is either 0 or 1 and that in fact we get the correct expression for the amplitudes.

The above relation is not an accident. In fact, this example is the prototype of everything that follows. The matrix given above is the simplest example of CMV matrix, corresponding to null Verblunsky parameters. The Laurent polynomials $(x_j)_{j=0}^{\infty}$ are orthonormal with respect to the Lebesgue measure $dz/2\pi iz = d\theta/2\pi$. Therefore, the identity $Ux(z) = zx(z)$ gives

$$\int_{\mathbb{T}} \overline{x_k(z)}\, z^n x_j(z) \frac{dz}{2\pi iz} = \sum_{l=0}^{\infty} \int_{\mathbb{T}} \overline{x_k(z)}\, (U^n)_{j,l}\, x_l(z) \frac{dz}{2\pi iz} = (U^n)_{j,k}.$$

6. Another example

The natural extension of the previous example to the integers is the QRW associated with the unitary operator

$$S = \sum_{i \in \mathbb{Z}} |i+1\rangle\langle i| \otimes |\uparrow\rangle\langle\uparrow| + \sum_{i \in \mathbb{Z}} |i-1\rangle\langle i| \otimes |\downarrow\rangle\langle\downarrow|. \tag{27}$$

The evolution is now even simpler than the previous one: all spins up move to the right and all spins down move to the left.

Ordering the pure states as follows

$$\ldots, |-1\rangle \otimes |\uparrow\rangle, |-1\rangle \otimes |\downarrow\rangle, |0\rangle \otimes |\uparrow\rangle, |0\rangle \otimes |\downarrow\rangle, |1\rangle \otimes |\uparrow\rangle, |1\rangle \otimes |\downarrow\rangle, \ldots$$

the transition matrix U is the doubly infinite matrix

$$\begin{array}{ccccccc|ccccccc}
\ddots & \ddots & \ddots & \ddots & \ddots & & & & & & & & & \\
 & 0 & 0 & 0 & 0 & 1 & & & & & & & & \\
 & & 1 & 0 & 0 & 0 & 0 & & & & & & & \\
 & & & 0 & 0 & 0 & 0 & 1 & & & & & & \\
 & & & & 1 & 0 & 0 & 0 & 0 & & & & & \\
\hline
 & & & & & 0 & 0 & 0 & 0 & 1 & & & & \\
 & & & & & & 1 & 0 & 0 & 0 & 0 & & & \\
 & & & & & & & 0 & 0 & 0 & 0 & 1 & & \\
 & & & & & & & & 1 & 0 & 0 & 0 & 0 & \\
 & & & & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots
\end{array}$$

Clearly the model is more complicated than it needs to be: we can separate it into two non-interacting evolutions corresponding to spins up and down. Consider for instance the set of spins pointing up which move in one unit of time one step to the right. The corresponding matrix $U_\uparrow$ is now the doubly infinite matrix

$$\begin{array}{cccc|ccccc}
\ddots & \ddots & & & & & & & \\
 & 0 & 1 & & & & & & \\
 & & 0 & 1 & & & & & \\
 & & & 0 & 1 & & & & \\
\hline
 & & & & 0 & 1 & & & \\
 & & & & & 0 & 1 & & \\
 & & & & & & 0 & 1 & \\
 & & & & & & & \ddots & \ddots
\end{array}$$

The doubly infinite column vector $v(z) = (\ldots, z^{-2}, z^{-1}, 1, z, z^2, \ldots)^T$ clearly satisfies

$$U_\uparrow v(z) = zv(z).$$

Since the components $v_j(z) = z^j$, $j \in \mathbb{Z}$, of $v(z)$ are orthonormal with respect to the Lebesgue measure, arguments entirely similar to those of the last paragraph of the previous example show that

$$\int_{\mathbb{T}} \overline{v_k(z)}\, z^n v_j(z) \frac{dz}{2\pi i z} = (U_\uparrow^n)_{j,k},$$

an identity which can be trivially checked by a direct computation.

There is another approach to the problem that reduce this example to the previous one. Since all spins are pointing up we can ignore their orientation and concentrate on their locations $\dots, -2, -1, 0, 1, 2, \dots$ as a way of describing the pure states. There is now a useful trick (used in a previous example in Section 2) that consists in "folding" the set of all integers in the way

$$0, -1, 1, -2, 2, -3, 3, \dots$$

or equivalently relabelling them as follows

$$\dots, 5, 3, 1, 0, 2, 4, 6, \dots$$

With this relabelling the doubly infinite matrix $U_{\uparrow}$ becomes the semi-infinite matrix U_+ and we are back in the situation discussed in the previous example.

The evolution of the states with spins pointing down is also described by the matrix U_+ of the previous example, but the required "folding" in this case is

$$-1, 0, -2, 1, -3, 2, -4, \dots$$

Notice that the initial transition matrix U is the doubly infinite CMV matrix with null Verblunsky parameters. We will see that common QRWs on the integers, such as the Hadamard one, essentially correspond to other less trivial doubly infinite CMV matrices.

The elementary character of the previous examples is the reason to introduce them early on, since they show in an extremely simple way the typical features of the method that we will employ in more intrincate cases. For instance, the decoupling of a QRW on the integers into two QRWs on the non-negative integers will take place in the next examples too, a fact that simplifies considerably their analysis. Nevertheless, the decoupling in the following examples is not so easy to notice since it holds in a basis of mixed states instead of pure ones.

7. A more general case: QRWs with distinct coins

Here and in the rest of the paper "distinct coins" means not necessarily "constant coins".

The previous example on the integers can be generalized to more interesting QRWs with no decoupling between up and down states, by including possible transitions between such states. A simple way to do this is to consider the following dynamics: a spin up can move to the right and remain up or (finally we get away from deterministic models) move to the left and change orientation. A spin down can either go to the right and change orientation or go to the left and remain down.

In other words, only the nearest neighbour transitions such that the final spin (up/down) agrees with the direction of motion (right/left) are allowed. This dynamics bears a resemblance to the effect of a magnetic interaction on quantum system with spin: the spin decides the direction of motion.

Schematically, the allowed transitions are

$$
\begin{aligned}
|i\rangle \otimes |{\uparrow}\rangle &\longrightarrow \begin{cases} |i+1\rangle \otimes |{\uparrow}\rangle & \text{with probability amplitude } c^i_{11} \\ |i-1\rangle \otimes |{\downarrow}\rangle & \text{with probability amplitude } c^i_{21} \end{cases} \\
|i\rangle \otimes |{\downarrow}\rangle &\longrightarrow \begin{cases} |i+1\rangle \otimes |{\uparrow}\rangle & \text{with probability amplitude } c^i_{12} \\ |i-1\rangle \otimes |{\downarrow}\rangle & \text{with probability amplitude } c^i_{22} \end{cases}
\end{aligned}
$$

where, for each $i \in \mathbb{Z}$,

$$
C_i = \begin{pmatrix} c^i_{11} & c^i_{12} \\ c^i_{21} & c^i_{22} \end{pmatrix} \tag{28}
$$

is an arbitrary unitary matrix which we will call the i^{th} coin.

Notice that this is already more general than the Hadamard example usually discussed in the literature. We will analyze the general case of a constant quantum coin in more detail in the next section, and then the popular Hadamard special case in a later section.

The transition matrix U is the unitary doubly infinite matrix

$$
\left(\begin{array}{ccccccc|ccccccc}
\ddots & \ddots & \ddots & \ddots & \ddots & & & & & & & & & \\
 & 0 & c^{-2}_{21} & 0 & 0 & c^{-2}_{11} & & & & & & & & \\
 & & c^{-2}_{22} & 0 & 0 & c^{-2}_{12} & 0 & & & & & & & \\
 & & & 0 & c^{-1}_{21} & 0 & 0 & c^{-1}_{11} & & & & & & \\
 & & & & c^{-1}_{22} & 0 & 0 & c^{-1}_{12} & 0 & & & & & \\
\hline
 & & & & & 0 & c^{0}_{21} & 0 & 0 & c^{0}_{11} & & & & \\
 & & & & & & c^{0}_{22} & 0 & 0 & c^{0}_{12} & 0 & & & \\
 & & & & & & & 0 & c^{1}_{21} & 0 & 0 & c^{1}_{11} & & \\
 & & & & & & & & c^{1}_{22} & 0 & 0 & c^{1}_{12} & 0 & \\
 & & & & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots
\end{array}\right)
$$

which has the structure of a doubly infinite CMV matrix with null odd Verblunsky parameters

$$
\left(\begin{array}{ccccccc|ccccccc}
\ddots & \ddots & \ddots & \ddots & \ddots & & & & & & & & & \\
& 0 & \overline{\alpha}_{-4} & 0 & 0 & \rho_{-4} & & & & & & & & \\
& & \rho_{-4} & 0 & 0 & -\alpha_{-4} & 0 & & & & & & & \\
& & & 0 & \overline{\alpha}_{-2} & 0 & 0 & \rho_{-2} & & & & & & \\
& & & & \rho_{-2} & 0 & 0 & -\alpha_{-2} & 0 & & & & & \\
\hline
& & & & & 0 & \overline{\alpha}_{0} & 0 & 0 & \rho_{0} & & & & \\
& & & & & & \rho_{0} & 0 & 0 & -\alpha_{0} & 0 & & & \\
& & & & & & & 0 & \overline{\alpha}_{2} & 0 & 0 & \rho_{2} & & \\
& & & & & & & & \rho_{2} & 0 & 0 & -\alpha_{2} & 0 & \\
& & & & & & & & & \ddots & \ddots & \ddots & \ddots & \ddots
\end{array}\right)
$$

However, U is not exactly a CMV matrix unless the diagonal elements of every coin C_i are positive so that they can be identified with ρ_{2i}.

Notice that $|c^i_{11}| = |c^i_{22}|$ and $|c^i_{12}| = |c^i_{21}|$ due to the unitarity of C_i. The coin C_i will be called trivial when $c^i_{11} = c^i_{22} = 0$ and non trivial otherwise. If some coin is trivial then the transition matrix U becomes a direct sum of two unitary matrices. In what follows we will assume that every coin is non trivial, otherwise the QRW splits directly into independent simpler ones in the basis of pure states.

Now, a simple change of phases in the basis transforms U in a CMV matrix: if $e^{i\sigma^j_k}$ is the phase of c^j_{kk} then it is easy to check that $\mathcal{C} = \Lambda^\dagger U \Lambda$ is a doubly infinite CMV matrix where $\Lambda = \mathrm{diag}(\dots, \lambda_{-1}, \lambda_0, \lambda_1, \dots)$ is given by $\lambda_{2j+2} = e^{-i\sigma^j_1}\lambda_{2j}$ and $\lambda_{2j+1} = e^{i\sigma^j_2}\lambda_{2j-1}$ with $\lambda_{-1} = \lambda_0 = 1$. The corresponding Verblunsky parameters are

$$\alpha_{2j} = \overline{c}^j_{21}\frac{\lambda_{2j}}{\lambda_{2j-1}}, \qquad \alpha_{2j+1} = 0,$$

so that $\rho_{2j} = |c^j_{11}|$ are positive.

As in the previous example on all the integers, we can do a folding trick to transform the doubly infinite transition matrix in a semi-infinite one. The appropriate ordering of the pure states to obtain a banded semi-infinite matrix as narrow as possible is

$$
\begin{aligned}
&|0\rangle\otimes|\uparrow\rangle, |-1\rangle\otimes|\downarrow\rangle, |-1\rangle\otimes|\uparrow\rangle, |0\rangle\otimes|\downarrow\rangle, \\
&|1\rangle\otimes|\uparrow\rangle, |-2\rangle\otimes|\downarrow\rangle, |-2\rangle\otimes|\uparrow\rangle, |1\rangle\otimes|\downarrow\rangle, \qquad (29)\\
&\quad\dots \qquad\quad \dots \qquad\quad \dots \qquad\quad \dots
\end{aligned}
$$

which combines in a suitable way the orderings

$$|0\rangle\otimes|\uparrow\rangle, |-1\rangle\otimes|\uparrow\rangle, |1\rangle\otimes|\uparrow\rangle, |-2\rangle\otimes|\uparrow\rangle, \dots$$

and

$$|-1\rangle\otimes|\downarrow\rangle, |0\rangle\otimes|\downarrow\rangle, |-2\rangle\otimes|\downarrow\rangle, |1\rangle\otimes|\downarrow\rangle, \dots$$

used in the example discussed in Section 6. The reason for this choice is that, in contrast to that case, up and down states do not decouple now and we must interlace their orderings.

Let us denote by $\boldsymbol{U}, \boldsymbol{\mathcal{C}}, \boldsymbol{\Lambda}$ the result of performing such a reordering on $U, \mathcal{C}, \Lambda$. Then, $\boldsymbol{\mathcal{C}} = \boldsymbol{\Lambda}^\dagger \boldsymbol{U} \boldsymbol{\Lambda}$, with $\boldsymbol{\Lambda}$ diagonal unitary and $\boldsymbol{U}, \boldsymbol{\mathcal{C}}$ with a 2×2-block CMV structure. Moreover, $\boldsymbol{\mathcal{C}}$ is exactly such a block CMV matrix, and its matrix Verblunsky parameters $(\boldsymbol{\alpha}_j)_{j=0}^\infty$ are

$$\boldsymbol{\alpha}_{2j} = \begin{pmatrix} 0 & -\overline{\alpha}_{-2j-2} \\ \alpha_{2j} & 0 \end{pmatrix}, \qquad \boldsymbol{\alpha}_{2j+1} = \mathbf{0},$$

where $(\alpha_j)_{j\in\mathbb{Z}}$ are the Verblunsky parameters of $\mathcal{C}$. Explicitly,

$$\boldsymbol{\mathcal{C}} = \begin{pmatrix} \boldsymbol{\alpha}_0^\dagger & \mathbf{0} & \boldsymbol{\rho}_0^L & & & & & & \\ \boldsymbol{\rho}_0^R & \mathbf{0} & -\boldsymbol{\alpha}_0 & \mathbf{0} & & & & & \\ \mathbf{0} & \boldsymbol{\alpha}_2^\dagger & \mathbf{0} & \mathbf{0} & \boldsymbol{\rho}_2^L & & & & \\ & \boldsymbol{\rho}_2^R & \mathbf{0} & \mathbf{0} & -\boldsymbol{\alpha}_2 & \mathbf{0} & & & \\ & & \mathbf{0} & \boldsymbol{\alpha}_4^\dagger & \mathbf{0} & \mathbf{0} & \boldsymbol{\rho}_4^L & & \\ & & & \boldsymbol{\rho}_4^R & \mathbf{0} & \mathbf{0} & -\boldsymbol{\alpha}_4 & \mathbf{0} & \\ & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{30}$$

The positive definite matrices $\boldsymbol{\rho}_{2j}^R, \boldsymbol{\rho}_{2j}^L$ are given by

$$\boldsymbol{\rho}_{2j}^R = \begin{pmatrix} \rho_{2j-2} & 0 \\ 0 & \rho_{2j} \end{pmatrix}, \qquad \boldsymbol{\rho}_{2j}^L = \begin{pmatrix} \rho_{2j} & 0 \\ 0 & \rho_{2j-2} \end{pmatrix}$$

Summarizing, the class of QRWs on the integers with arbitrary non trivial quantum coins can be described either by using doubly infinite CMV matrices or 2×2-block CMV matrices, in both cases the odd Verblunsky parameters vanish. The interest of these results is that they allow us to obtain for some examples of these QRWs a KMcG formula in terms of matrix valued Szegő polynomials.

Such a KMcG formula comes from the fact that the block CMV matrix $\boldsymbol{\mathcal{C}}$ has an associated vector $\boldsymbol{x} = (\mathbf{1}, \boldsymbol{x}_1, \boldsymbol{x}_2, \dots)^T$ of left orthonormal Laurent polynomials satisfying $\boldsymbol{\mathcal{C}}\boldsymbol{x}(z) = z\boldsymbol{x}(z)$. Let Λ_j be the 2×2 diagonal blocks of $\boldsymbol{\Lambda} = \operatorname{diag}(\Lambda_0, \Lambda_1, \dots)$. Then, $\Lambda_0 = \mathbf{1}$ and $\boldsymbol{U}\boldsymbol{X}(z) = z\boldsymbol{X}(z)$ for $\boldsymbol{X} = (\mathbf{1}, \boldsymbol{X}_1, \boldsymbol{X}_2, \dots)^T$ defined by $\boldsymbol{X}_j = \Lambda_j \boldsymbol{x}_j$. Besides, $(\boldsymbol{X}_j)_{j=0}^\infty$ is left orthonormal with respect to the orthogonality measure $\boldsymbol{\mu}$ of $(\boldsymbol{x}_j)_{j=0}^\infty$ (i.e., $(\boldsymbol{X}_j)_{j=0}^\infty$ and $(\boldsymbol{x}_j)_{j=0}^\infty$ are left orthonormal

Laurent polynomials for the same measure with different normalizations). In consequence,

$$\int_{\mathbb{T}} z^n \boldsymbol{X}_j(z) d\boldsymbol{\mu}(z) \boldsymbol{X}_k(z)^\dagger = \sum_{l=0}^{\infty} \int_{\mathbb{T}} (\boldsymbol{U}^n)_{j,l} \boldsymbol{X}_l(z) d\boldsymbol{\mu}(z) \boldsymbol{X}_k(z)^\dagger = (\boldsymbol{U}^n)_{j,k},$$

which can be interpreted as a KMcG formula for the related QRW on the integers. Here $(\boldsymbol{U}^n)_{j,k}$ stands for the 2×2 blocks making up $\boldsymbol{U}^n = ((\boldsymbol{U}^n)_{j,k})_{j,k=0}^{\infty}$, i.e.,

$$\begin{aligned}
(\boldsymbol{U}^n)_{2j,2k} &= \begin{pmatrix} u^n_{j\uparrow,k\uparrow} & u^n_{j\uparrow,-(k+1)\downarrow} \\ u^n_{-(j+1)\downarrow,k\uparrow} & u^n_{-(j+1)\downarrow,-(k+1)\downarrow} \end{pmatrix}, \\
(\boldsymbol{U}^n)_{2j,2k+1} &= \begin{pmatrix} u^n_{j\uparrow,-(k+1)\uparrow} & u^n_{j\uparrow,k\downarrow} \\ u^n_{-(j+1)\downarrow,-(k+1)\uparrow} & u^n_{-(j+1)\downarrow,k\downarrow} \end{pmatrix}, \\
(\boldsymbol{U}^n)_{2j+1,2k} &= \begin{pmatrix} u^n_{-(j+1)\uparrow,k\uparrow} & u^n_{-(j+1)\uparrow,-(k+1)\downarrow} \\ u^n_{j\downarrow,k\uparrow} & u^n_{j\downarrow,-(k+1)\downarrow} \end{pmatrix}, \\
(\boldsymbol{U}^n)_{2j+1,2k+1} &= \begin{pmatrix} u^n_{-(j+1)\uparrow,-(k+1)\uparrow} & u^n_{-(j+1)\uparrow,k\downarrow} \\ u^n_{j\downarrow,-(k+1)\uparrow} & u^n_{j\downarrow,k\downarrow} \end{pmatrix},
\end{aligned} \tag{31}$$

$u^n_{j,k}$ being the probability amplitude to go from the pure state j to the pure state k in n steps.

The measure $\boldsymbol{\mu}$ and the orthonormal Laurent polynomials $(\boldsymbol{X}_j)_{j=0}^{\infty}$ in the above KMcG formula will be called the measure and orthonormal Laurent polynomials associated with the related QRW on the integers.

8. QRWs with a constant coin

The Hadamard QRW is an example of the QRWs described in the previous section. It corresponds to a constant coin $C_i = H$ given by

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{32}$$

The Hadamard QRW is an example of an unbiased QRW, i.e., a QRW with a constant coin such that all the allowed transitions are equiprobable.

We will consider in this section a more general class of QRWs on the integers: those which have an arbitrary constant (unitary) coin

$$C_i = C = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}. \tag{33}$$

Identifying C with the operator on the spin state space given by

$$C|\uparrow\rangle = c_{11}|\uparrow\rangle + c_{21}|\downarrow\rangle, \qquad C|\downarrow\rangle = c_{12}|\uparrow\rangle + c_{22}|\downarrow\rangle, \tag{34}$$

the QRW evolution operator can be written $S \otimes C$ with S as in (27).

Let $e^{i\sigma_k}$ be the phase of c_{kk}. According to the previous discussion, the doubly infinite transition matrix is $U = \Lambda\mathcal{C}\Lambda^\dagger$, where

$$\Lambda = \operatorname{diag}(\dots,\lambda_{-1},\lambda_0,\lambda_1,\dots), \qquad \lambda_{2j} = e^{-ij\sigma_1}, \qquad \lambda_{2j-1} = e^{ij\sigma_2},$$

and $\mathcal{C}$ is the doubly infinite CMV matrix with Verblunsky parameters

$$\alpha_{2j-1} = 0, \qquad \alpha_{2j} = \overline{c}_{21} e^{-i2j\vartheta}, \qquad \vartheta = \frac{1}{2}(\sigma_1+\sigma_2).$$

The semi-infinite form $\boldsymbol{U}$ of this transition matrix can be factorized as $\boldsymbol{U} = \boldsymbol{\Lambda}\boldsymbol{\mathcal{C}}\boldsymbol{\Lambda}^\dagger$ with $\boldsymbol{\Lambda} = \operatorname{diag}(\mathbf{1},\Lambda_1,\Lambda_2,\dots)$ given by

$$\Lambda_{2j-1} = \begin{pmatrix} e^{ij\sigma_1} & 0 \\ 0 & e^{ij\sigma_2} \end{pmatrix}, \qquad \Lambda_{2j} = \Lambda_{2j-1}^\dagger,$$

and $\boldsymbol{\mathcal{C}}$ the 2×2-block CMV matrix with Verblunsky parameters $\boldsymbol{\alpha}_j = A_j e^{-i(j+1)\vartheta}$, where

$$A_j = \begin{cases} \mathbf{0} & \text{odd } j, \\ A & \text{even } j, \end{cases} \qquad A = \begin{pmatrix} 0 & -\overline{a} \\ a & 0 \end{pmatrix}, \qquad a = \overline{c}_{21} e^{i\vartheta}.$$

The Verblunsky parameters $\boldsymbol{\alpha}_j$ are simultaneously unitarily diagonalizable because

$$P^\dagger A P = \begin{pmatrix} i|a| & 0 \\ 0 & -i|a| \end{pmatrix}, \qquad P = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i\frac{\overline{a}}{|a|} \\ -i\frac{a}{|a|} & 1 \end{pmatrix}.$$

Hence, we can use the infinite matrix $\boldsymbol{P} = \operatorname{diag}(P,P,P,\dots)$ to transform $\boldsymbol{\mathcal{C}}$ into a new block CMV matrix $\boldsymbol{\mathcal{C}}^{(0)} = \boldsymbol{P}^\dagger\boldsymbol{\mathcal{C}}\boldsymbol{P}$ with diagonal Verblunsky parameters $\boldsymbol{\alpha}_j^{(0)}$ given by

$$\boldsymbol{\alpha}_j^{(0)} = \begin{pmatrix} \alpha_j^{(0)} & 0 \\ 0 & -\alpha_j^{(0)} \end{pmatrix}, \qquad \alpha_j^{(0)} = a_j e^{-i(j+1)\vartheta},$$

where

$$a_j = \begin{cases} 0 & \text{odd } j, \\ i|a| & \text{even } j. \end{cases} \tag{35}$$

This means that, although the pure states do not decouple, there is a basis in which the QRW decouples in two independent ones corresponding to scalar CMV matrices with Verblunsky parameters $\pm\alpha_j^{(0)}$.

More precisely, let $x_j^\pm$ and $\mu_\pm$ be the orthonormal Laurent polynomials and measure associated with the Verblunsky parameters $\pm\alpha_j^{(0)}$.

Since $\boldsymbol{U} = \boldsymbol{Q}\boldsymbol{\mathcal{C}}^{(0)}\boldsymbol{Q}^\dagger$, $\boldsymbol{Q} = \boldsymbol{\Lambda}\boldsymbol{P}$, we find that $\boldsymbol{U}\boldsymbol{X}(z) = z\boldsymbol{X}(z)$ for $\boldsymbol{X} = (\mathbf{1}, \boldsymbol{X}_1, \boldsymbol{X}_2, \dots)^T$ defined by

$$\boldsymbol{X}_j = \Lambda_j \boldsymbol{x}_j, \qquad \boldsymbol{x}_j = P \begin{pmatrix} x_j^+ & 0 \\ 0 & x_j^- \end{pmatrix} P^\dagger,$$

and $\boldsymbol{X}_j$ are left orthonormal with respect to the same matrix measure $\boldsymbol{\mu}$ as $\boldsymbol{x}_j$, that is,

$$\boldsymbol{\mu} = P \begin{pmatrix} \mu_+ & 0 \\ 0 & \mu_- \end{pmatrix} P^\dagger.$$

Therefore,

$$\int_{\mathbb{T}} z^n \boldsymbol{X}_j(z)\, d\boldsymbol{\mu}(z)\, \boldsymbol{X}_k(z)^\dagger = (\boldsymbol{U}^n)_{j,k}, \tag{36}$$

which will yield a KMcG formula for the QRW with a constant coin on the integers once the measure $\boldsymbol{\mu}$ and the orthonormal Laurent polynomials $\boldsymbol{X}_j$ are obtained in Section 10.

So far, we have split a QRW on the integers with a constant coin into two QRWs on the non-negative integers. Now, to obtain a KMcG formula we just need to compute the scalar orthonormal Laurent polynomials $x_j^\pm$ and the corresponding scalar orthogonality measures $\mu_\pm$. Moreover, the corresponding Verblunsky coefficients are $\pm a_j e^{-i(j+1)\vartheta}$ with a_j given in (35), hence (12) shows that $\mu_\pm$ can be obtained rotating by an angle ϑ the measure with Verblunsky parameters

$$\pm\, i|a|,\ 0,\ \pm i|a|,\ 0,\ \pm i|a|,\ 0,\ \dots \qquad (|a| = |c_{21}|) \tag{37}$$

Explicitly, from (12) and (13) we find that

$$\begin{gathered} d\boldsymbol{\mu}(z) = d\hat{\boldsymbol{\mu}}(e^{-i\vartheta} z), \qquad \hat{\boldsymbol{\mu}} = P \begin{pmatrix} \hat{\mu}_+ & 0 \\ 0 & \hat{\mu}_- \end{pmatrix} P^\dagger, \\ \boldsymbol{X}_j(z) = \hat{\Lambda}_j \hat{\boldsymbol{x}}_j(e^{-i\vartheta} z), \qquad \hat{\boldsymbol{x}}_j = P \begin{pmatrix} \hat{x}_j^+ & 0 \\ 0 & \hat{x}_j^- \end{pmatrix} P^\dagger, \\ \hat{\Lambda}_{2j-1} = \begin{pmatrix} e^{ij(\sigma_1-\sigma_2)/2} & 0 \\ 0 & e^{ij(\sigma_2-\sigma_1)/2} \end{pmatrix}, \qquad \hat{\Lambda}_{2j} = \hat{\Lambda}_{2j-1}^\dagger, \end{gathered} \tag{38}$$

where $\hat{x}_j^\pm$ and $\hat{\mu}_\pm$ are the orthonormal Laurent polynomials and measures with Verblunsky parameters (37). Hence, the matrix Carathéodory function $\boldsymbol{F}$ of $\boldsymbol{\mu}$ is related to the Carathéodory functions $\hat{F}_\pm$ of $\hat{\mu}_\pm$ by

$$\boldsymbol{F}(z) = \hat{\boldsymbol{F}}(e^{-i\vartheta} z), \qquad \hat{\boldsymbol{F}} = P \begin{pmatrix} \hat{F}_+ & 0 \\ 0 & \hat{F}_- \end{pmatrix} P^\dagger. \tag{39}$$

A CMV matrix with the Verblunsky parameters (37) can be understood as the transition matrix of a QRW with a constant coin on the non-negative integers. Thus, a QRW with a constant coin on the integers always splits in two QRWs with constant coins on the non-negative integers. Such a splitting is not initially obvious since it takes place in a basis of mixed states.

It is worth to remark that the block CMV matrix related to a constant coin C on the integers depends only on the modulus of the entries of C (one of them determines the others by unitarity). This means that QRWs on the integers with a constant coin do not depend essentially on the phases of its entries. For an unbiased QRW all the entries of the coin C have equal modulus, so $|a| = |c_{21}| = 1/\sqrt{2}$ due to the unitarity of C. The Hadamard QRW is therefore just a canonical example of unbiased QRW on the integers.

Bearing in mind that we are reducing the problem on the integers to two problems on the non-negative integers, in the next section we will discuss completely the QRWs with a constant coin on the non-negative integers.

9. QRWs with a constant coin on the non-negative integers

QRWs with a constant coin on the non-negative integers are a preliminary step to complete the discussion of QRWs on the integers. Besides, these QRWs have their own interest because they present special features that do not appear for QRWs on the integers.

Let us suppose that we order the pure states on the non-negative integers as in (26). A unitary matrix like

$$U = \begin{pmatrix} c_{21}^0 & 0 & c_{11}^0 & & & & & & & \\ c_{22}^0 & 0 & c_{12}^0 & 0 & & & & & & \\ 0 & c_{21}^1 & 0 & 0 & c_{11}^1 & & & & & \\ & c_{22}^1 & 0 & 0 & c_{12}^1 & 0 & & & & \\ & & 0 & c_{21}^2 & 0 & 0 & c_{11}^2 & & & \\ & & & c_{22}^2 & 0 & 0 & c_{12}^2 & 0 & & \\ & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

can be understood as the transition matrix for a QRW on the non-negative integers with arbitrary (unitary) coins C_i as in (28) for $i = 0, 1, 2, \ldots$.

A constant coin C corresponds to the operator $S_+ \otimes C$ where S_+ is given in (25) and C is identified with the operator (34).

Exactly as in to Section 7, even in the case of (non trivial) distinct coins, a simple change of phases in the basis reduces U to a scalar CMV matrix with null odd Verblunsky coefficients: $\mathcal{C} = \Lambda^\dagger U \Lambda$ is CMV for

$\Lambda = \text{diag}(\lambda_0, \lambda_1, \dots)$ given by $\lambda_{2j+2} = e^{-i\sigma_1^j}\lambda_{2j}$, $\lambda_{2j+1} = e^{i\sigma_2^j}\lambda_{2j-1}$ with $\lambda_{-1} = \lambda_0 = 1$ and $e^{i\sigma_k^j}$ the phase of c_{kk}^j. Its Verblunsky parameters are given again by

$$\alpha_{2j} = \overline{c}_{21}^j \frac{\lambda_{2j}}{\lambda_{2j-1}}, \qquad \alpha_{2j+1} = 0,$$

so that $\rho_{2j} = |c_{11}^j|$ are positive.

If μ and x_j are the measure and orthonormal Laurent polynomials associated with $\mathcal{C}$, then $UX(z) = zX(z)$ with $X = (1, X_1, X_2, \dots)^T$ and $X_j = \lambda_j x_j$. Since μ makes the polynomials X_j orthonormal too,

$$\int_{\mathbb{T}} z^n X_j(z)\, \overline{X_k(z)}\, d\mu(z) = (U^n)_{j,k}, \tag{40}$$

which is a KMcG formula for a QRW with arbitrary distinct coins on the non-negative integers.

The above formula simply says that the transition matrix U has been identified as a matrix representation of the unitary multiplication operator U_μ on $L^2_\mu(\mathbb{T})$ given by (5).

The measure μ and the orthonormal Laurent polynomials X_j in (40) will be called the measure and orthonormal Laurent polynomials associated with the related QRW on the non-negative integers.

Following the arguments and notation of Section 8 we can see that a constant coin C leads to a rotation of the case associated with a CMV matrix with Verblunsky parameters

$$a,\ 0,\ a,\ 0,\ a,\ 0,\ \dots \qquad (a = \overline{c}_{21} e^{i\vartheta}) \tag{41}$$

In contrast to (37), the even Verblunsky parameters in (41) can have an arbitrary phase which comes from the phases of the coefficients of the coin. Hence, we should expect a stronger influence of the phases of the coin for constant coins on the non-negative integers compared to the same situation on the integers. This will bring in new possibilities when discussing the semi-infinite version of the Hadamard QRW, corresponding to $|a| = 1/\sqrt{2}$.

To be more precise, if $\Lambda = \text{diag}(\lambda_0, \lambda_1, \dots)$, $\lambda_{2j} = e^{-ij\sigma_1}$, $\lambda_{2j-1} = e^{ij\sigma_2}$, then $\mathcal{C} = \Lambda^\dagger U \Lambda$ is a CMV matrix whose measure μ is obtained by rotating by an angle ϑ the measure $\hat{\mu}$ with Verblunsky parameters (41). If x_j and $\hat{x}_j$ are the orthonormal Laurent polynomials associated with μ and $\hat{\mu}$ respectively, we know from (13) that $x_{2j-1}(z) = e^{-ij\vartheta}\hat{x}_{2j-1}(e^{-i\vartheta}z)$ and $x_{2j}(z) = e^{ij\vartheta}\hat{x}_{2j}(e^{-i\vartheta}z)$. So, according to the previous discussion, the Laurent polynomials

$$X_j(z) = \lambda_j x_j(z) = \hat{\lambda}_j\, \hat{x}_j(e^{-i\vartheta}z), \qquad \hat{\lambda}_{2j-1} = \hat{\lambda}_{2j} = e^{ij(\sigma_2-\sigma_1)/2}, \tag{42}$$

are orthonormal with respect to μ, satisfy $UX(z) = zX(z)$, $X = (1, X_1, X_2, \dots)^T$, and provide the KMcG formula (40), which can be rewritten as

$$(U^n)_{j,k} = e^{in\vartheta}\frac{\hat{\lambda}_j}{\hat{\lambda}_k}\int_{\mathbb{T}} z^n \hat{x}_j(z)\,\overline{\hat{x}_k(z)}\,d\hat{\mu}(z). \tag{43}$$

To get from (40) a KMcG formula for the QRWs with a constant coin on the non-negative integers we simply need $\hat{x}_j$ and $\hat{\mu}$, which are calculated in an appendix at the end of the paper. The main results from the appendix are summarized now:

An expression for the orthonormal Laurent polynomials is given by

$$\begin{aligned} \hat{x}_{2j-1}(z) &= U_j(y) - \rho^{-1}(z+a)U_{j-1}(y), \\ \hat{x}_{2j}(z) &= U_j(y) - \rho^{-1}(z^{-1}+\overline{a})U_{j-1}(y), \end{aligned} \qquad y = \frac{1}{2\rho}(z+z^{-1}),$$

with $\rho = \sqrt{1-|a|^2}$ and U_j the second kind Chebyshev polynomials given by (4). In particular, $\hat{x}_{2j}(z) = \overline{\hat{x}_{2j-1}(1/\overline{z})}$.

On the other hand, the measure is given by

$$\begin{aligned} d\hat{\mu}(e^{i\theta}) &= w(\theta)\frac{d\theta}{2\pi} + M\delta(\theta-\beta)d\theta, \\ w(\theta) &= \frac{\sqrt{\sin^2\theta - \sin^2\eta}}{|\sin\theta - \sin\beta|}, \qquad \theta \in [\eta, \pi-\eta] \cup [\eta-\pi, -\eta], \\ M &= \frac{|\mathrm{Re}a|}{\sqrt{1-|\mathrm{Im}a|^2}} = \frac{\sqrt{\sin^2\eta - \sin^2\beta}}{|\cos\beta|}, \end{aligned}$$

where the angles $\eta \in [0, \pi/2)$ and $\beta \in (-\pi, \pi]$ are defined by means of

$$\sin\eta = |a|, \qquad \sin\beta = -\mathrm{Im}a, \qquad \mathrm{sign}(\cos\beta) = \mathrm{sign}(\mathrm{Re}a).$$

The corresponding Carathéodory function is $F(z) = \hat{F}(e^{-i\vartheta}z)$ where

$$\hat{F}(z) = -\frac{\sqrt{(z-z^{-1})^2+4|a|^2}+2\mathrm{Re}a}{z-z^{-1}+2i\mathrm{Im}a} = -\frac{z-z^{-1}-2i\mathrm{Im}a}{\sqrt{(z-z^{-1})^2+4|a|^2}-2\mathrm{Re}a}.$$

Now that we have all the ingredients that enter in the integral in (43), notice that the only parameter that appears in it is the value of the complex number a. The parameter ϑ as well as the individual values of σ_1, σ_2 have an effect on $(U^n)_{j,k}$ but this appears only as a factor in front of the integral on the right hand side.

The measure $d\mu(z) = d\hat{\mu}(e^{-i\vartheta}z)$ appearing in (40) has in general a continuous weight plus a Dirac delta. The weight is supported on two symmetric arcs of angular amplitude 2η centered at $\pm ie^{i\vartheta}$. The mass point is located outside of the support of the weight and it is absent only when a is imaginary, which holds exactly when the coin is symmetric ($c_{12} = c_{21}$).

While the location of the weight only depends on $|a| = |c_{21}|$, its form and the location and mass of the Dirac delta also depend on the phase of $a = \overline{c}_{21} e^{i\vartheta}$. Therefore, the phases of the coin C have a remarkable influence in the semi-infinite QRWs with a constant coin, in marked contrast to the case of the integers.

10. QRWs with a constant coin on the integers

The results of the previous section permit us to complete the analysis of the QRWs with a constant coin on the integers. Let us remember the notation: $C = (c_{jk})_{j,k=1,2}$ is the constant coin, $e^{i\sigma_k}$ the phase of c_{kk}, $\vartheta = (\sigma_1 + \sigma_2)/2$ the angle of rotation, $a = \overline{c}_{21} e^{i\vartheta}$ and $\rho = \sqrt{1 - |a|^2}$.

The matrix ingredients $\boldsymbol{X}_j$, $\boldsymbol{\mu}$ of the KMcG formula (36) are given by (38) in terms of the scalar ones $\hat{x}_j^{\pm}$, $\hat{\mu}_{\pm}$ with Verblunsky parameters $\pm i|a|$, 0, $\pm i|a|$, 0, $\dots$, a specialization for a imaginary of the case a, 0, a, 0, $\dots$ analyzed in the appendix. This is precisely the case where the mass point disappears, so we can anticipate that the matrix measure for a constant coin on the integers is always given exclusively by a continuous matrix weight.

Combining the results of Section 8 and the appendix we get the following expressions for the scalar objects

$$\hat{F}_{\pm}(z) = -\frac{\sqrt{(z - z^{-1})^2 + 4|a|^2}}{z - z^{-1} \pm 2i|a|} = -\frac{z - z^{-1} \mp 2i|a|}{\sqrt{(z - z^{-1})^2 + 4|a|^2}},$$

$$d\hat{\mu}_{\pm}(e^{i\theta}) = w_{\pm}(\theta)\frac{d\theta}{2\pi}, \qquad w_{\pm}(\theta) = \sqrt{\frac{\sin\theta \mp \sin\eta}{\sin\theta \pm \sin\eta}},$$
$$\theta \in [\eta, \pi - \eta] \cup [\eta - \pi, -\eta], \qquad \sin\eta = |a|, \qquad \eta \in [0, \pi/2),$$

$$\begin{aligned} x_{2j-1}^{\pm}(z) &= U_j(y) - \rho^{-1}(z \pm i|a|)U_{j-1}(y), \\ x_{2j}^{\pm}(z) &= \overline{x_{2j-1}(1/\overline{z})}, \end{aligned} \qquad y = \frac{1}{2\rho}(z + z^{-1}),$$

so that the matrix objects in (38) and (39) are given by

$$\boldsymbol{F}(z) = \hat{\boldsymbol{F}}(e^{-i\vartheta} z),$$
$$\hat{\boldsymbol{F}}(z) = \frac{-1}{\sqrt{(z - z^{-1})^2 + 4|a|^2}} \begin{pmatrix} z - z^{-1} & 2\overline{a} \\ -2a & z - z^{-1} \end{pmatrix},$$

$$d\boldsymbol{\mu}(z) = d\hat{\boldsymbol{\mu}}(e^{-i\vartheta}z), \qquad d\hat{\boldsymbol{\mu}}(e^{i\theta}) = W(\theta)\frac{d\theta}{2\pi},$$
$$W(\theta) = \frac{1}{\sqrt{\sin^2\theta - \sin^2\eta}}\begin{pmatrix} |\sin\theta| & \mp i\overline{a} \\ \pm ia & |\sin\theta| \end{pmatrix} \quad \text{if } \begin{cases} \theta \in [\eta, \pi-\eta], \\ \theta \in [\eta-\pi, -\eta], \end{cases}$$

$$\boldsymbol{X}_j(z) = \hat{\Lambda}_j \hat{\boldsymbol{x}}_j(e^{-i\vartheta}z), \qquad \hat{\Lambda}_{2j-1} = \begin{pmatrix} e^{ij(\sigma_1-\sigma_2)/2} & 0 \\ 0 & e^{ij(\sigma_2-\sigma_1)/2} \end{pmatrix} = \hat{\Lambda}_{2j}^\dagger,$$
$$\hat{\boldsymbol{x}}_{2j-1}(z) = \mathbf{1}U_j(y) - \frac{1}{\rho}\begin{pmatrix} z & -\overline{a} \\ a & z \end{pmatrix} U_{j-1}(y), \qquad \hat{\boldsymbol{x}}_{2j}(z) = \hat{\boldsymbol{x}}_{2j-1}(1/\overline{z})^\dagger.$$

The expression for the polynomials $\boldsymbol{X}_j$ can be compared to the one at the end of Section 2.

11. The Hadamard QRW versus other unbiased QRWs

The Hadamard QRW is the unbiased QRW on the integers with constant coin (32). Applying the results of the previous section to this case gives

$$\boldsymbol{F}(z) = \frac{1}{\sqrt{1+z^4}}\begin{pmatrix} 1+z^2 & \sqrt{2}z \\ \sqrt{2}z & 1+z^2 \end{pmatrix},$$
$$d\boldsymbol{\mu}(e^{i\theta}) = \frac{1}{\sqrt{\cos 2\theta}}\begin{pmatrix} \sqrt{1+\cos 2\theta} & \pm 1 \\ \pm 1 & \sqrt{1+\cos 2\theta} \end{pmatrix}\frac{d\theta}{2\pi} \quad \text{if } \begin{cases} \theta \in [-\frac{\pi}{4}, \frac{\pi}{4}], \\ \theta \in [\frac{3\pi}{4}, \frac{5\pi}{4}], \end{cases}$$
$$\boldsymbol{X}_{2j-1}(z) = \begin{pmatrix} (-i)^j & 0 \\ 0 & i^j \end{pmatrix}\left\{\mathbf{1}U_j(y^*) + i\begin{pmatrix} \sqrt{2}z & -1 \\ -1 & \sqrt{2}z \end{pmatrix}U_{j-1}(y^*)\right\},$$
$$\boldsymbol{X}_{2j}(z) = \boldsymbol{X}_{2j-1}(1/z),$$

where, here and below,

$$y^* = \frac{z - z^{-1}}{\sqrt{2}i},$$

and the square root $\sqrt{1+z^4}$ is the analytic branch with value 1 at the origin. Notice that the measure $\boldsymbol{\mu}$ is symmetric with respect to the real line and the matrix coefficients of the Laurent polynomials $\boldsymbol{X}_j$ are real.

We can compare this case with a semi-infinite version with the same constant coin (32). Taking into account Section 9, the coin (32) yields on the non-negative integers

$$\begin{aligned}
F(z) &= \frac{\sqrt{1+z^4}}{1-\sqrt{2}z+z^2} = \frac{1+\sqrt{2}z+z^2}{\sqrt{1+z^4}}, \\
d\mu(e^{i\theta}) &= \frac{\sqrt{1+\cos 2\theta}\pm 1}{\sqrt{\cos 2\theta}}\frac{d\theta}{2\pi} \quad \text{if } \begin{cases}\theta\in[-\frac{\pi}{4},\frac{\pi}{4}],\\ \theta\in[\frac{3\pi}{4},\frac{5\pi}{4}],\end{cases} \\
X_{2j-1}(z) &= i^j\{U_j(y^*)+i(\sqrt{2}z-1)U_{j-1}(y^*)\}, \\
X_{2j}(z) &= (-1)^j X_{2j-1}(1/z).
\end{aligned}$$

We can observe the similarity between the Hadamard QRW and its version on the non-negative integers. Again, the measure μ is given by a symmetric weight and the Laurent polynomials X_j have real coefficients.

However, this similarity goes away for other unbiased QRWs. Consider for instance the constant equiprobable coin

$$C = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & -i\\ i & -1\end{pmatrix}. \tag{44}$$

Section 10 gives for the corresponding QRW on the integers

$$\begin{aligned}
\boldsymbol{F}(z) &= \frac{1}{\sqrt{1+z^4}}\begin{pmatrix}1+z^2 & i\sqrt{2}z\\ -i\sqrt{2}z & 1+z^2\end{pmatrix}, \\
d\boldsymbol{\mu}(e^{i\theta}) &= \frac{1}{\sqrt{\cos 2\theta}}\begin{pmatrix}\sqrt{1+\cos 2\theta} & \pm i\\ \mp i & \sqrt{1+\cos 2\theta}\end{pmatrix}\frac{d\theta}{2\pi} \quad \text{if } \begin{cases}\theta\in[-\frac{\pi}{4},\frac{\pi}{4}],\\ \theta\in[\frac{3\pi}{4},\frac{5\pi}{4}],\end{cases} \\
\boldsymbol{X}_{2j-1}(z) &= \begin{pmatrix}(-i)^j & 0\\ 0 & i^j\end{pmatrix}\left\{\mathbf{1}U_j(y^*)+i\begin{pmatrix}\sqrt{2}z & -i\\ i & \sqrt{2}z\end{pmatrix}U_{j-1}(y^*)\right\}, \\
\boldsymbol{X}_{2j}(z) &= \boldsymbol{X}_{2j-1}(1/z).
\end{aligned}$$

As in the Hadamard QRW, the measure $\boldsymbol{\mu}$ is given by a weight which is symmetric with respect to the real line.

From Section 9, the same constant coin (44) yields for the non-negative integers

$$\begin{aligned}
F(z) &= \frac{\sqrt{1+z^4}-i\sqrt{2}z}{1+z^2} = \frac{1+z^2}{\sqrt{1+z^4}+i\sqrt{2}z}, \\
d\mu(e^{i\theta}) &= \sqrt{\frac{\cos 2\theta}{1+\cos 2\theta}}\frac{d\theta}{2\pi}+\frac{1}{\sqrt{2}}\delta(\theta-\tfrac{\pi}{2})d\theta, \quad \theta\in[-\tfrac{\pi}{4},\tfrac{\pi}{4}]\cup[\tfrac{3\pi}{4},\tfrac{5\pi}{4}], \\
X_{2j-1}(z) &= i^j\{U_j(y^*)+i(\sqrt{2}z+i)U_{j-1}(y^*)\}, \\
X_{2j}(z) &= (-1)^j\overline{X_{2j-1}(1/\overline{z})}.
\end{aligned}$$

The differences between the infinite and the semi-infinite versions of this unbiased QRW are evident. On the non-negative integers the weight is symmetric with respect to the real line, but there is also a mass point which destroys such a symmetry for the full measure.

The similarities and differences observed above regarding the ingredients of the KMcG formulas for different QRWs reveal how close or far their probabilistic behaviours are from each other. To make this more evident let us obtain the probability amplitudes $u^n_{j,k}$ for a n-step transition between certain states j,k in the different examples.

For the examples on the integers, according to (31),

$$(\boldsymbol{U}^n)_{0,0} = \begin{pmatrix} u^n_{0\uparrow,0\uparrow} & u^n_{0\uparrow,-1\downarrow} \\ u^n_{-1\downarrow,0\uparrow} & u^n_{-1\downarrow,-1\downarrow} \end{pmatrix}.$$

Due to the translation invariance of any QRW with a constant coin on the integers, $(\boldsymbol{U}^n)_{0,0}$ gives the probability amplitudes $u^n_{k\uparrow,k\uparrow}$, $u^n_{k\downarrow,k\downarrow}$, $u^n_{k\uparrow,(k-1)\downarrow}$ and $u^n_{k\downarrow,(k+1)\uparrow}$ for any k.

On the other hand, the KMcG formula (36) states that $(\boldsymbol{U}^n)_{0,0} = \int_{\mathbb{T}} z^n \, d\boldsymbol{\mu}(z) = \boldsymbol{\mu}_n$ are the moments of the related measure, which, following (24), are provided by the McLaurin series of the Carathéodory function $\boldsymbol{F}$.

For the Hadamard QRW on the integers the expression of $\boldsymbol{F}$ gives, apart from the trivial moment $\boldsymbol{\mu}_0 = \mathbf{1}$,

$$\boldsymbol{\mu}_{4m} = \boldsymbol{\mu}_{4m+2} = \frac{c_m}{2}\mathbf{1}, \qquad \boldsymbol{\mu}_{4m+1} = \frac{c_m}{\sqrt{2}}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \boldsymbol{\mu}_{4m+3} = \mathbf{0},$$

where

$$c_0 = 1, \qquad c_n = (-1)^n \prod_{k=1}^{n} \left(1 - \frac{1}{2k}\right), \quad n \geq 1, \tag{45}$$

are the coefficients of the series $1/\sqrt{1+z} = \sum_{n=0}^{\infty} c_n z^n$. Hence,

$$u^n_{k\uparrow,k\uparrow} = u^n_{k\downarrow,k\downarrow} = \begin{cases} \frac{c_m}{2} & n=4m,4m+2, \\ 0 & n=2m+1, \end{cases}$$

$$u^n_{k\uparrow,(k-1)\downarrow} = u^n_{k\downarrow,(k+1)\uparrow} = \begin{cases} \frac{c_m}{\sqrt{2}} & n=4m+1, \\ 0 & n=2m,4m+3, \end{cases}$$

The non-diagonal elements of

$$(\boldsymbol{U}^n)_{1,0} = \begin{pmatrix} u^n_{-1\uparrow,0\uparrow} & u^n_{-1\uparrow,-1\downarrow} \\ u^n_{0\downarrow,0\uparrow} & u^n_{0\downarrow,-1\downarrow} \end{pmatrix},$$

permit us to complete the description of the n-step transition amplitudes between the spin states at the same site. From (36) and the expression of the polynomials $\boldsymbol{X}_k$ for the Hadamard QRW we get

$$(\boldsymbol{U}^n)_{1,0} = \int_{\mathbb{T}} \boldsymbol{X}_1(z) z^n d\boldsymbol{\mu} = \int_{\mathbb{T}} \left\{ \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + \sqrt{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} z^{-1} \right\} z^n d\boldsymbol{\mu}$$
$$= \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \boldsymbol{\mu}_n + \sqrt{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \boldsymbol{\mu}_{n-1},$$

thus, the values of the Hadamard moments give

$$u^n_{k\uparrow,k\downarrow} = -u^n_{k\downarrow,k\uparrow} = \begin{cases} -\frac{c_m}{2} & n{=}4m, \\ \frac{c_m}{2} & n{=}4m{+}2, \\ 0 & n{=}2m{+}1, \end{cases}$$
$$u^n_{k\uparrow,(k+1)\uparrow} = -u^n_{k\downarrow,(k-1)\downarrow} = \begin{cases} 0 & n{=}2m,4m{+}1, \\ \frac{c_m}{\sqrt{2}} & n{=}4m{+}3, \end{cases}$$

except for $u^1_{k\uparrow,(k+1)\uparrow} = -u^1_{k\downarrow,(k-1)\downarrow} = 1/\sqrt{2}$.

In the Hadamard example, all the n-step transitions between pure spin states for the same site are forbidden for odd n (except for $n = 1$), while for even n we find probabilities $|c_m|^2/4$ if $n = 4m, 4m+2$. The same result holds for any other unbiased QRW on the integers due to the similarity between the corresponding Carathéodory functions and orthonormal Laurent polynomials.

Consider now the Hadamard coin on the non-negative integers. From the McLaurin series of the associated Carathéodory function and (15) we find that, apart from $\mu_0 = 1$, the related moments are

$$\mu_{4m} = \mu_{4m+2} = \frac{c_m}{2}, \qquad \mu_{4m+1} = \frac{c_m}{\sqrt{2}}, \qquad \mu_{4m+3} = 0.$$

The KMcG formula (40) and the expression $X_1(z) = 1 - \sqrt{2} z^{-1}$ for the first orthonormal Laurent polynomial yield

$$(U^n)_{0,0} = \mu_n, \qquad (U^n)_{1,1} = 3\mu_n - \sqrt{2}\mu_{n+1} - \sqrt{2}\mu_{n-1},$$
$$(U^n)_{1,0} = \mu_n - \sqrt{2}\mu_{n-1}, \qquad (U^n)_{0,1} = \mu_n - \sqrt{2}\mu_{n+1}.$$

Therefore,

$$u^n_{0\uparrow,0\uparrow} = \begin{cases} \frac{c_m}{2} & n{=}4m,4m{+}2, \\ \frac{c_m}{\sqrt{2}} & n{=}4m{+}1, \\ 0 & n{=}4m{+}3, \end{cases} \qquad u^n_{0\downarrow,0\downarrow} = \begin{cases} \frac{c_m}{2} & n{=}4m,4m{+}2, \\ \frac{c_m}{\sqrt{2}} & n{=}4m{+}1, \\ -\frac{c_m+c_{m+1}}{\sqrt{2}} & n{=}4m{+}3, \end{cases}$$

$$u^n_{0\uparrow,0\downarrow} = \begin{cases} -\frac{c_m}{2} & n{=}4m, \\ 0 & n{=}4m{+}1, \\ \frac{c_m}{2} & n{=}4m{+}2, \\ -\frac{c_{m+1}}{\sqrt{2}} & n{=}4m{+}3, \end{cases} \qquad u^n_{0\downarrow,0\uparrow} = \begin{cases} \frac{c_m}{2} & n{=}4m, \\ 0 & n{=}4m{+}1, \\ -\frac{c_m}{2} & n{=}4m{+}2, \\ -\frac{c_m}{\sqrt{2}} & n{=}4m{+}3, \end{cases}$$

except for $u^1_{0\downarrow,0\downarrow} = 0$ and $u^1_{0\downarrow,0\uparrow} = -1/\sqrt{2}$.

The above results show that, concerning the n-step transitions between pure spin states at site 0, the Hadamard coin on the non-negative integers has the same probability amplitudes as the Hadamard coin on the integers for even n, while for odd n some of the transitions remain forbidden.

On the other hand, the Carathéodory function for the unbiased QRW on the non-negative integers with coin (44) yields, apart from $\mu_0 = 1$, the moments

$$\mu_{4m} = \frac{d_m}{2}, \qquad \mu_{4m+1} = \frac{i}{\sqrt{2}}, \qquad \mu_{4m+2} = -\frac{d_m}{2}, \qquad \mu_{4m+3} = -\frac{i}{\sqrt{2}},$$

where d_n are the coefficients of $\sqrt{1+z}/(1-z) = \sum_{n=0}^{\infty} d_n z^n$, so that $\sqrt{1+z^2}/(1+z) = \sum_{n=0}^{\infty} d_n(z^{2n} - z^{2n+1})$. Explicitly,

$$\begin{aligned} & d_n = \hat{c}_0 + \hat{c}_1 + \cdots + \hat{c}_n, \qquad \sqrt{1+z} = \sum_{n=0}^{\infty} \hat{c}_n z^n, \\ & \hat{c}_0 = 1, \qquad \hat{c}_1 = \frac{1}{2}, \qquad \hat{c}_n = \frac{(-1)^{n-1}}{2} \prod_{k=2}^{n} \left(1 - \frac{3}{2k}\right), \quad n \geq 2. \end{aligned} \tag{46}$$

Introducing $X_1(z) = -(i + \sqrt{2}z^{-1})$ in the KMcG formula (40) gives

$$\begin{aligned} & (U^n)_{0,0} = \mu_n, \qquad (U^n)_{1,1} = 3\mu_n + i\sqrt{2}\mu_{n+1} - i\sqrt{2}\mu_{n-1}, \\ & (U^n)_{1,0} = -(i\mu_n + \sqrt{2}\mu_{n-1}), \qquad (U^n)_{0,1} = i\mu_n - \sqrt{2}\mu_{n+1}. \end{aligned}$$

Hence,

$$u^n_{0\uparrow,0\uparrow} = \begin{cases} \frac{d_m}{2} & n=4m, \\ \frac{i}{\sqrt{2}} & n=4m+1, \\ -\frac{d_m}{2} & n=4m+2, \\ -\frac{i}{\sqrt{2}} & n=4m+3, \end{cases} \qquad u^n_{0\downarrow,0\downarrow} = \begin{cases} \frac{3d_m-4}{2} & n=4m, \\ i\frac{3-2d_m}{\sqrt{2}} & n=4m+1, \\ -\frac{3d_m-4}{2} & n=4m+2, \\ -i\frac{3-d_m-d_{m+1}}{\sqrt{2}} & n=4m+3, \end{cases}$$

$$u^n_{0\uparrow,0\downarrow} = \begin{cases} -i\frac{2-d_m}{2} & n=4m, \\ \frac{d_m-1}{\sqrt{2}} & n=4m+1, \\ i\frac{2-d_m}{2} & n=4m+2, \\ -\frac{d_{m+1}-1}{\sqrt{2}} & n=4m+3, \end{cases} \qquad u^n_{0\downarrow,0\uparrow} = \begin{cases} i\frac{2-d_m}{2} & n=4m, \\ -\frac{d_m-1}{\sqrt{2}} & n=4m+1, \\ -i\frac{2-d_m}{2} & n=4m+2, \\ \frac{d_m-1}{\sqrt{2}} & n=4m+3, \end{cases}$$

except for $u^1_{0\downarrow,0\downarrow} = 0$ and $u^1_{0\downarrow,0\uparrow} = -1/\sqrt{2}$.

The probability amplitudes of this example are quite different from those of the Hadamard coin on the non-negative integers. They also show quite a different behaviour when compared to any unbiased QRW on the integers, including the case of the same coin (44). In particular, if $n \geq 2$, this example has no forbidden n-step transitions between the pure spin states at site 0. This is due to the inequality $d_2 < d_n < d_1$ for $n \geq 3$, which is a consequence of (46) and the fact that $|\hat{c}_n|$ is decreasing and $\hat{c}_n$ has alternating signs for $n \geq 1$.

12. Asymptotics of QRWs

In Sections 7 and 9 we have seen that the transition matrix of any QRW (on $\mathbb{Z} \geq 0$ or $\mathbb{Z}$) with non trivial distinct coins has an associated (scalar or 2×2-matrix valued) measure. As in the previous section, the corresponding Carathéodory function allows us to compute the moments of the measure which, with the aid of the related orthonormal Laurent polynomials, provide through the KMcG formula the amplitudes of the n-step transitions for any value of n. This opens the possibility of studying the asymptotic behaviour of such amplitudes when n goes to infinity.

Several different authors have obtained specific asymptotic results, mainly in the case of the Hadamard walk, by using different methods. For a very good account, see [19]. We have not attempted any comparison between our rather general results and the many detailed results in the literature. The results in this section are given to indicate how our method could be used for similar purposes.

For instance, in the case of the Hadamard coin on the non-negative integers, as well as for any unbiased QRW on the integers, the n^{th} moment has zero limit when n goes to infinity because the coefficients

c_n in (45) satisfy $\lim_{n\to\infty} c_n = 0$. Therefore, $\lim_{n\to\infty} u^n_{0\uparrow,0\uparrow} = 0$ in these cases.

On the other hand, the unbiased QRW on the non-negative integers with coin (44) gives moments μ_n satisfying $\lim_{n\to\infty} |\mu_n| = 1/\sqrt{2}$ because, from (46),

$$\lim_{n\to\infty} d_n = \sum_{k=0}^{\infty} \hat{c}_k = \sqrt{1+z}\big|_{z=1} = \sqrt{2}.$$

Hence, the probabilities for returning to the spin up 0-state, if the system was originally in such a state, converge to a non-zero limit, i.e., $\lim_{n\to\infty} |u^n_{0\uparrow,0\uparrow}|^2 = 1/2$. Indeed, although the probability amplitudes $u^n_{0\uparrow,0\uparrow} = \mu_n$ do not converge in this example, the quantities $i^{-n}\mu_n$ actually converge to $1/\sqrt{2}$ when n goes to infinity.

The moments are given by only a few of the coefficients of the powers of the transition matrix U: the coefficient $(0,0)$ of U^n is the scalar moment μ_n in the case of the non-negative integers, while the coefficients $(0,0)$, $(0,-1)$, $(-1,0)$ and $(-1,-1)$ of U^n provide the matrix moment $\boldsymbol{\mu}_n$ for a QRW on the integers. However, as we saw in the previous section, the rest of the transition amplitudes can be calculated in terms of the moments using the KMcG formulas. In fact, according to Sections 7 and 9, this should be possible, not only for QRWs with a constant coin, but for any QRW with non trivial distinct coins. As a consequence, for all these kinds of QRWs, the asymptotic behaviour of the moments controls the asymptotic behaviour of the powers of the transition matrix. This is the idea behind the result given in the following proposition.

To get a better understanding of what is coming, we start with some remarks. Looking at our examples, we have to deal with the situation where the n^{th} moment multiplied by some phase $e^{-i\theta_n}$ is convergent. As we will see, this condition is connected with the situation where $e^{-i\theta_n}(U^n)_{i,j}$ is convergent for any i,j. Since the sequence U^n is uniformly bounded because U^n is unitary for any n, the existence of $\lim_{n\to\infty} e^{-i\theta_n}(U^n)_{i,j}$ for any i,j is equivalent to saying that $\lim_{n\to\infty} \psi e^{-i\theta_n} U^n \eta^\dagger$ exists for any row vectors $\psi,\eta \in L^2(\mathcal{I}\times\mathcal{S})$, which defines the familiar weak convergence of operators, see [17, Chapter III].

The weak limit $U^\infty = (U^\infty_{i,j})$, $U^\infty_{i,j} = \lim_{n\to\infty} e^{-i\theta_n}(U^n)_{i,j}$, when it exists, defines an operator on $L^2(\mathcal{I}\times\mathcal{S})$ which provides the asymptotic behaviour for n going to infinity of the n-step transition amplitude between any two states ψ, η because

$$\lim_{n\to\infty} \left(\psi U^n \eta^\dagger - e^{i\theta_n}\psi U^\infty \eta^\dagger\right) = 0.$$

Although U^∞ does not inherit in general the unitarity of U^n, it has a norm not greater than one because U^n does so for any n.

Proposition 12.1. *Let U be the transition matrix of a QRW on the integers or the non-negative integers with arbitrary non trivial distinct coins. Concerning the asymptotic behaviour as n goes to infinity of U^n and the n^{th} moment of the related orthogonality measure, we have the following results:*

1. *U^n converges weakly to zero if and only if the n^{th} moment converges to zero.*
2. *For any sequence $e^{i\theta_n}$ of phases, $e^{-i\theta_n}U^n$ has a non null weak limit if and only if the n^{th} moment multiplied by $e^{-i\theta_n}$ converges to a non null limit and $\lim_{n\to\infty} e^{i(\theta_{n+1}-\theta_n)}$ exists.*

Proof. Consider a QRW on the integers. Let $\boldsymbol{U}$ be the 2×2-block five-diagonal matrix obtained by performing the folding (29) on U. Then, U^n converges weakly to zero if and only if $\boldsymbol{U}^n$ does so.

The KMcG formula obtained in Section 7 states that the 2×2-blocks of $\boldsymbol{U}^n$ are given by

$$(\boldsymbol{U}^n)_{i,j} = \int_{\mathbb{T}} z^n \boldsymbol{X}_i(z) d\boldsymbol{\mu}(z) \boldsymbol{X}_j(z)^\dagger,$$

where $\boldsymbol{X}_i$ are the corresponding orthonormal Laurent polynomials. If $\boldsymbol{X}_i(z) = \sum_{k=p_i}^{q_i} A_{i,k} z^k$ with 2×2 matrix coefficients $A_{i,k}$, then

$$(\boldsymbol{U}^n)_{i,j} = \sum_{k=p_i}^{q_i}\sum_{l=p_j}^{q_j} A_{i,k}\boldsymbol{\mu}_{n+k-l}A_{j,l}^\dagger.$$

This equality implies that $\lim_{n\to\infty}(\boldsymbol{U}^n)_{i,j} = \mathbf{0}$ for any i,j exactly when $\lim_{n\to\infty}\boldsymbol{\mu}_n = \lim_{n\to\infty}(\boldsymbol{U}^n)_{0,0} = \mathbf{0}$, which proves (1).

Concerning (2), notice that $e^{-i\theta_n}U^n$ and $e^{-i\theta_n}\boldsymbol{U}^n$ have a non null weak limit simultaneously. Suppose that both $\lim_{n\to\infty} e^{-i\theta_n}\boldsymbol{\mu}_n$ and $\lim_{n\to\infty} e^{i(\theta_{n+1}-\theta_n)}$ exist. The above equality gives

$$e^{-i\theta_n}(\boldsymbol{U}^n)_{i,j} = \sum_{k=p_i}^{q_i}\sum_{l=p_j}^{q_j} e^{i(\theta_{n+k-l}-\theta_n)} A_{i,k} e^{-i\theta_{n+k-l}}\boldsymbol{\mu}_{n+k-l}A_{j,l}^\dagger.$$

If $\lim_{n\to\infty} e^{i(\theta_{n+1}-\theta_n)} = z_0$, then $\lim_{n\to\infty} e^{i(\theta_{n+k}-\theta_n)} = z_0^k$. Thus, the previous identity shows that $\lim_{n\to\infty} e^{-i\theta_n}(\boldsymbol{U}^n)_{i,j}$ exists for any i,j. Moreover, if $\lim_{n\to\infty} e^{-i\theta_n}\boldsymbol{\mu}_n \neq \mathbf{0}$, then $\lim_{n\to\infty} e^{-i\theta_n}(\boldsymbol{U}^n)_{i,j} \neq \mathbf{0}$ at least for $i=j=0$.

Conversely, assume that $\lim_{n\to\infty} e^{-i\theta_n}(\boldsymbol{U}^n)_{i,j}$ exists for any i,j and is non null for some i,j. Then, $\lim_{n\to\infty} e^{-i\theta_n}\boldsymbol{\mu}_n = \lim_{n\to\infty} e^{-i\theta_n}(\boldsymbol{U}^n)_{0,0}$ exists and must be non null because otherwise $\lim_{n\to\infty} e^{-i\theta_n}(\boldsymbol{U}^n)_{i,j} = \mathbf{0}$ for any i,j due to (1). Denote by U^∞ the (non null) weak limit of $e^{-i\theta_n}U^n$. Taking weak limits in $Ue^{-i\theta_n}U^n = e^{i(\theta_{n+1}-\theta_n)}e^{-i\theta_{n+1}}U^{n+1}$ we obtain $UU^\infty = \lim_{n\to\infty} e^{i(\theta_{n+1}-\theta_n)}U^\infty$, thus $e^{i(\theta_{n+1}-\theta_n)}$ must converge because U^∞ is not null.

The proof for a QRW on the non-negative integers is completely analogous and even simpler because we do not need the folding. □

As a consequence of the previous results, the transition matrix of any unbiased QRW on the integers converges weakly to zero, which means that the amplitude of the n-step transition between any two (finite or infinite) superposition of pure states converges to zero as n goes to infinity. This is also true for the Hadamard coin on the non-negative integers. On the contrary, the transition matrix U for the unbiased QRW on the non-negative integers with coin (44) should be such that $i^{-n}U^n$ converges weakly to some non vanishing weak limit U^∞. Indeed, we can compute such a weak limit with the aid of the following result.

Proposition 12.2. *Let U be the transition matrix of a QRW on the non-negative integers with arbitrary non trivial distinct coins. If, for a sequence $e^{i\theta_n}$ of phases, $e^{-i\theta_n}U^n$ has a non null weak limit U^∞, the related orthogonality measure μ has a mass point z_0 to which $e^{i(\theta_{n+1}-\theta_n)}$ converges and*

$$U^\infty = \mu_\infty X(z_0)X(z_0)^\dagger, \qquad \mu_\infty = \lim_{n\to\infty} e^{-i\theta_n}\mu_n,$$

with $X = (1, X_1, X_2 \dots)^T$ the associated column vector of orthonormal Laurent polynomials and μ_n the moments of μ. Furthermore,

$$\lim_{n\to\infty} e^{-i\theta_n} z_0^n = \frac{\mu_\infty}{\mu(\{z_0\})},$$

so that $\lim_{n\to\infty} z_0^{-n}\mu_n = \mu(\{z_0\})$ and $z_0^{-n}U^n$ converges weakly to

$$\mu(\{z_0\})X(z_0)X(z_0)^\dagger = \frac{1}{\|X(z_0)\|^2}\, X(z_0)X(z_0)^\dagger,$$

which is the orthogonal projection onto the eigenspace of U associated with the eigenvalue z_0.

Proof. Suppose that $e^{-i\theta_n}U^n$ converges weakly to a non null limit U^∞. From Proposition 12.1 we know that $\lim_{n\to\infty} e^{-i\theta_n}\mu_n = \mu_\infty \neq 0$ and $\lim_{n\to\infty} e^{i(\theta_{n+1}-\theta_n)} = z_0 \in \mathbb{T}$. The arguments at the end of the proof of such proposition yield the identity $UU^\infty = z_0 U^\infty$. Thus, the non null columns of U^∞ must be eigenvectors of U with eigenvalue z_0.

Let $\mathcal{C}$ be the CMV matrix related to U, and let x be the corresponding column vector of orthonormal Laurent polynomials. Bearing in mind that $U = \Lambda\mathcal{C}\Lambda^\dagger$ and $X = \Lambda x$ with Λ unitary diagonal, the comments in Section 3 show that z_0 must be a mass point of μ with a mass given by $\mu(\{z_0\}) = 1/\|x(z_0)\|^2 = 1/\|X(z_0)\|^2$. Moreover, the eigenvectors of U with eigenvalue z_0 must be spanned by $X(z_0)$, so the columns of U^∞ should be proportional to $X(z_0)$, i.e.,

$$U^\infty = X(z_0)Y, \qquad Y = (Y_0, Y_1, \dots) \in L^2(\mathbb{Z} \geq 0).$$

Notice that $Y_0 = U^\infty_{0,0} = \lim_{n\to\infty} e^{-i\theta_n}(U^n)_{0,0} = \mu_\infty$.

On the other hand, $e^{-i\theta_n}(U^T)^n$ converges weakly to $(U^\infty)^T$. The unitarity of U implies that z_0 must be an eigenvalue of U^T too, and the corresponding eigenvectors must be spanned by $\overline{X(z_0)}$. Therefore, similar arguments to the previous ones show that

$$(U^\infty)^T = \overline{X(z_0)}Z, \qquad Z = (Z_0, Z_1, \dots) \in L^2(\mathbb{Z} \geq 0),$$

with $Z_0 = \mu_\infty$.

Therefore, the matrix $\overline{X(z_0)}Z$ must be equal to $Y^T X(z_0)^T$. Identifying the first column of both matrices gives $Y^T = Z_0\overline{X(z_0)} = \mu_\infty\overline{X(z_0)}$, hence $U^\infty = \mu_\infty X(z_0)X(z_0)^\dagger$.

From $U^\infty = \mu_\infty X(z_0)X(z_0)^\dagger$ we obtain

$$\begin{aligned}\mu_\infty\|X(z_0)\|^4 = X(z_0)^\dagger U^\infty X(z_0) &= \lim_{n\to\infty} X(z_0)^\dagger e^{-i\theta_n}U^n X(z_0) = \\ &= \lim_{n\to\infty} e^{-i\theta_n} z_0^n \|X(z_0)\|^2,\end{aligned}$$

which proves that $\lim_{n\to\infty} e^{-i\theta_n} z_0^n = \mu_\infty\|X(z_0)\|^2 = \mu_\infty/\mu(\{z_0\})$. The rest of the identities follow easily from this equality. □

The second part of Proposition 12.2 asserts that, when $e^{-i\theta_n}U^n$ has a non null weak limit, we can suppose without loss of generality that $e^{i\theta_n}$ is z_0^n, with z_0 the mass point of μ to which $e^{i(\theta_{n+1}-\theta_n)}$ must converge and, then, μ_∞ becomes $\mu(\{z_0\})$.

For instance, in the case of the unbiased QRW on the non-negative integers with coin (44), $\lim_{n\to\infty} i^{-n}\mu_n = 1/\sqrt{2}$ is the mass of the only mass point $z_0 = i$ of the corresponding measure. According to Proposition 12.2, the weak limit U^∞ of $i^{-n}U^n$ is

$$U^\infty = \frac{1}{\sqrt{2}} X(i)X(i)^\dagger, \qquad X = (1, X_1, X_2, \dots)^T,$$

where X_k are the associated orthonormal Laurent polynomials given in Section 11, so

$$X_{2j-1}(i) = i^j\{U_j(\sqrt{2}) - (\sqrt{2}+1)U_{j-1}(\sqrt{2})\},$$
$$X_{2j}(i) = (-1)^j\overline{X_{2j-1}(i)} = X_{2j-1}(i).$$

Recurrence (4) for the Chebyshev polynomials U_j implies that $U_j(\sqrt{2}) = 2\sqrt{2}U_{j-1}(\sqrt{2}) - U_{j-2}(\sqrt{2})$, hence

$$\begin{aligned} X_{2j}(i) &= i^j\{(\sqrt{2}-1)U_{j-1}(\sqrt{2}) - U_{j-2}(\sqrt{2})\} = \\ &= i^j(\sqrt{2}-1)\{U_{j-1}(\sqrt{2}) - (\sqrt{2}+1)U_{j-2}(\sqrt{2})\} = \\ &= i(\sqrt{2}-1)X_{2j-2}(i). \end{aligned}$$

Therefore, $X_{2j-1}(i) = X_{2j}(i) = (i(\sqrt{2}-1))^j$ and

$$U^{\infty}_{2j-1,2k-1} = U^{\infty}_{2j-1,2k} = U^{\infty}_{2j-1,2k} = U^{\infty}_{2j,2k} = \frac{i^{j-k}}{\sqrt{2}}(\sqrt{2}-1)^{j+k}.$$

This allows us to compute the asymptotic transition amplitude between any two states. In particular, denoting $\lim_{n\to\infty}(a_n/b_n) = 1$ by $a_n \sim_n b_n$,

$$u^n_{j\uparrow,k\uparrow} \sim_n \frac{i^{n+j-k}}{\sqrt{2}}(\sqrt{2}-1)^{j+k}, \qquad u^n_{j\downarrow,k\downarrow} \sim_n \frac{i^{n+j-k}}{\sqrt{2}}(\sqrt{2}-1)^{j+k+2},$$
$$u^n_{j\uparrow,k\downarrow} \sim_n \frac{i^{n+j-k-1}}{\sqrt{2}}(\sqrt{2}-1)^{j+k+1}, \qquad u^n_{j\downarrow,k\uparrow} \sim_n \frac{i^{n+j-k+1}}{\sqrt{2}}(\sqrt{2}-1)^{j+k+1}.$$

These asymptotic results give further indications of the different probabilistic behaviour of an unbiased QRW when considered on the non-negative integers or in all the integers.

13. Recurrence properties of QRWs

For a classical random walk there is an important notion that goes back at least to G. Polya, see [26]. We say that a state is recurrent if, having started there at the initial time, one returns to it with probability one. Otherwise we say that the state is transient. For a so-called irreducible chain either all states are recurrent or they are all transient. A recurrent state is called positive recurrent if the expected value for the time of (first) return to it is finite. When dealing with a birth-and-death process on the non-negative integers the corresponding orthogonality measure $dm(x)$ has support in the interval $[-1, 1]$ and plays an important role in studying these notions.

For instance, the process is recurrent exactly when

$$\int_{-1}^{1} \frac{dm(x)}{1-x} = \infty. \tag{47}$$

Notice that this integral is the sum of all moments of the measure $dm(x)$ and that the n^{th} moment is the probability of going from the state 0 to itself in n steps.

The process returns to the origin in a finite expected time when the measure has a mass at $x = 1$. The existence of

$$\lim_{n\to\infty}(P^n)_{i,j}$$

is equivalent to $dm(x)$ having no mass at $x = -1$. If this is the case this limit is positive exactly when $dm(x)$ has some mass at $x = 1$.

In the classical case one gets a lot of milage out of the generating function $S(z)$ of the moments of $dm(x)$ given by

$$S(z) = \int_{-1}^{1} \frac{dm(x)}{1 - xz}.$$

In particular the generating function $G(z)$ of the sequence g_n giving the probability of a first return to the origin in n steps

$$G(z) = \sum_{n=0}^{\infty} z^n g_n$$

is related to $S(z)$ by

$$G(z) = 1 - \frac{1}{S(z)}.$$

Therefore we have that $G(1) = 1$ (indicating that one returns to state 0 with probability one) exactly when $S(1)$ is infinite as noticed above. This relation allows us to compute the expected time to return to state 0. This expected value is given by $G'(1)$.

We are confident that these ideas and results should have a natural translation to the quantum case using the tools provided by the orthonormal Laurent polynomials on the unit circle. Indeed, an approach to the asymptotics of the powers of the transition matrix using such a machinery has been presented in the previous section.

We will see now that the notion of quantum recurrence can be described nicely in terms of the Carathéodory function introduced earlier, which will play in the quantum case a similar role to the generating function $S(z)$ of the moments for a classical random walk. Nevertheless, the condition for the characterization of quantum recurrence will be somewhat different from (47).

The study of the recurrence properties in the quantum case raises special issues because a quantum measurement destroys the initial evolution since the system collapses into a pure state when a measurement is performed. Therefore, the notion of a return to a given state **for the**

first time in a certain number of steps has to be interpreted with care in the quantum case. Such an analysis in terms of a specific measurement scheme, involving an ensemble of identically prepared QRWs, has been proposed recently, see [30].

The bottom line of this analysis is that, in the quantum case, the recurrence of a state is characterized by the divergence of the series of probabilities to return to such a state in n steps. After the modifications which are necessary to make sense of the notion of recurrence in the quantum case, this result is completely analogous to the classical one. Its importance lies on the fact that the notion of a return to a state in a certain number of steps is completely meaningful in the quantum case and its probability can be computed using the transition matrix of the QRW.

More precisely, following the interpretation of the quantum recurrence given in [30], a state ψ of a QRW with transition matrix U is recurrent exactly when

$$\sum_{n=1}^{\infty} p_n(\psi) = \infty, \qquad p_n(\psi) = |\psi U^n \psi^\dagger|^2, \tag{48}$$

where $p_n(\psi)$ stands for the probability to return to the state ψ in n steps.

Consider a QRW on the non-negative integers with non trivial distinct coins. The recurrence of the state numbered as 0, i.e., the spin up at site 0, is characterized by the divergence of $\sum_{n=1}^{\infty} |(U^n)_{0,0}|^2 = \sum_{n=1}^{\infty} |\mu_n|^2$. From the McLaurin series (15) of the related Carathéodory function $F(z)$ we obtain

$$\int_0^{2\pi} |F(e^{i\theta})|^2 \frac{d\theta}{2\pi} = 1 + 2\sum_{n=1}^{\infty} |\mu_n|^2,$$

where $F(e^{i\theta}) = \lim_{r\uparrow 1} F(re^{i\theta})$, which exists for Lebesgue almost every $\theta \in [0, 2\pi)$, see [27, Chapter 17]. Therefore, $|0\rangle \otimes |\uparrow\rangle$ is recurrent exactly when the radial limit of $F(z)$ does not lie on $L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$.

The generalization of this result to an arbitrary state, as well as to QRWs on the integers, is the purpose of the proposition below. In what follows we write $F(z) = F(z, d\mu)$ when we need to make explicit the measure corresponding to a Carathéodory function, and similarly for matrix valued Carathéodory functions. Besides, we will assume that any scalar or matrix valued Carathéodory function is radially extended Lebesgue almost everywhere on the unit circle (see [8] for the matrix case).

Proposition 13.1. *Consider a QRW with non trivial distinct coins on* $\mathcal{I} = \mathbb{Z}$ *or* $\mathbb{Z} \geq 0$*.*

(1) *If* $\mathcal{I} = \mathbb{Z} \geq 0$*, let* μ *be the related orthogonality measure and let us number the states* $|0\rangle \otimes |\uparrow\rangle, |0\rangle \otimes |\downarrow\rangle, |1\rangle \otimes |\uparrow\rangle, |1\rangle \otimes |\downarrow\rangle, \dots$ *as* $|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, \dots$*. A state* $|\Psi\rangle = \sum_{k=0}^{\infty} \psi_k |k\rangle$ *is transient if and only if*

$$F(z, |f|^2 d\mu) \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T}), \qquad f = \sum_{k=0}^{\infty} \psi_k X_k,$$

where X_k *are the corresponding orthonormal Laurent polynomials.*

(2) *If* $\mathcal{I} = \mathbb{Z}$*, let* $\boldsymbol{\mu}$ *be the related orthogonality matrix measure and let us number the states* $|0\rangle \otimes |\uparrow\rangle, |{-1}\rangle \otimes |\downarrow\rangle, |{-1}\rangle \otimes |\uparrow\rangle, |0\rangle \otimes |\downarrow\rangle, \dots$ *as* $|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, \dots$*. A state* $|\Psi\rangle = \sum_{k=0}^{\infty} \psi_k |k\rangle$ *is transient if and only if*

$$F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger) \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T}), \qquad \boldsymbol{f} = \sum_{k=0}^{\infty} (\psi_{2k}, \psi_{2k+1}) \boldsymbol{X}_k,$$

where $\boldsymbol{X}_k$ *are the corresponding matrix orthonormal Laurent polynomials.*

Proof. We will only prove (2) since the proof of (1) is similar and simpler. Consider a QRW on the integers with non trivial distinct coins. Let $\boldsymbol{U}$ be the semi-infinite transition matrix obtained performing the folding (29) on the doubly infinite transition matrix U. The recurrence of the state $|\Psi\rangle$ is equivalent to the divergence of $\sum_{n=0}^{\infty} p_n(\psi)$, where $p_n(\psi) = |\psi \boldsymbol{U}^n \psi^\dagger|^2$ and $\psi = (\psi_0, \psi_1, \dots)$ is the wave function of $|\Psi\rangle$ corresponding to the same folding.

Denoting $\boldsymbol{\psi}_k = (\psi_{2k}, \psi_{2k+1})$, the KMcG formula permits us to write

$$\psi \boldsymbol{U}^n \psi^\dagger = \sum_{j,k=0}^{\infty} \boldsymbol{\psi}_j (\boldsymbol{U}^n)_{j,k} \boldsymbol{\psi}_k^\dagger = \sum_{j,k=0}^{\infty} \int_{\mathbb{T}} z^n \boldsymbol{\psi}_j \boldsymbol{X}_j(z) d\boldsymbol{\mu}(z) \boldsymbol{X}_k(z) \boldsymbol{\psi}_k^\dagger =$$

$$= \int_{\mathbb{T}} z^n \boldsymbol{f}(z) d\boldsymbol{\mu}(z) \boldsymbol{f}(z)^\dagger, \qquad \boldsymbol{f} = \sum_{k=0}^{\infty} \boldsymbol{\psi}_k \boldsymbol{X}_k.$$

The above equality identifies $\psi \boldsymbol{U}^n \psi^\dagger$ as the n^{th} moment of the scalar measure $\boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger$. Therefore, the same arguments given before the proposition show that the divergence of $\sum_{n=0}^{\infty} |\psi \boldsymbol{U}^n \psi^\dagger|^2$ is equivalent to $F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger) \notin L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$. □

Notice that this proposition associates with any state a scalar function $f \in L^2_\mu(\mathbb{T})$ or a 2-dimensional vector valued function $\boldsymbol{f} \in L^2_{\boldsymbol{\mu}}(\mathbb{T})$, depending on whether the QRW is on $\mathbb{Z} \geq 0$ or $\mathbb{Z}$, so that $F(z, |f|^2 d\mu)$ and $F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger)$ are both scalar Carathéodory functions. We will refer to f and $\boldsymbol{f}$ as the functions associated with the corresponding state.

The condition (47) for the classical recurrence at the origin depends only on the behaviour of generating function $S(z)$ of the moments at $z = 1$. In contrast, the characterization of the quantum recurrence in terms of Carathéodory functions has to do with their global behaviour on the whole unit circle.

Proposition 13.1 has the drawback that it is not given in terms of the Carathéodory function of the original measure associated with the QRW, which is the one that we directly know, but in terms of the Carathéodory function of a modification of such a measure. The following result shows that this problem can be overcome, at least when analyzing the recurrence of a local state, i.e., a state which is a superposition of a finite number of pure states.

Notice that the function associated with any local state is a scalar Laurent polynomial f in the case $\mathbb{Z} \geq 0$, or a 2-dimensional vector valued Laurent polynomial $\boldsymbol{f}$ in the case $\mathbb{Z}$.

Proposition 13.2. *For any positive definite $d \times d$ matrix valued measure $\boldsymbol{\mu}$ and any d-dimensional vector valued Laurent polynomial $\boldsymbol{f}$*

$$F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger) \in L^2_{\frac{d\theta}{2\pi}} \Leftrightarrow \boldsymbol{f}(z)\boldsymbol{F}(z, d\boldsymbol{\mu})\boldsymbol{f}(z)^\dagger \in L^2_{\frac{d\theta}{2\pi}}.$$

Proof. If $\boldsymbol{f} = \sum_{k=p}^{q} \boldsymbol{a}_k z^k$, $\boldsymbol{a}_k \in \mathbb{C}^d$, then

$$F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger) = \sum_{j,k=p}^{q} \boldsymbol{a}_j \boldsymbol{F}_{j-k}(z) \boldsymbol{a}_k^\dagger, \qquad \boldsymbol{F}_k(z) = \int_{\mathbb{T}} \frac{t+z}{t-z}\, t^k d\boldsymbol{\mu}(t).$$

Writing

$$\frac{t+z}{t-z}\, t^k = (t+z)t^{k-1} + z\,\frac{t+z}{t-z}\, t^{k-1}$$

we find that

$$\boldsymbol{F}_k(z) = \boldsymbol{\mu}_k + \boldsymbol{\mu}_{k-1} z + z \boldsymbol{F}_{k-1}(z).$$

Bearing in mind that $\boldsymbol{F}_0(z) = \boldsymbol{F}(z, d\boldsymbol{\mu})$, the iteration of the above equality yields $\boldsymbol{F}_k(z) = \boldsymbol{L}_k(z) + z^k \boldsymbol{F}(z, d\boldsymbol{\mu})$ for some matrix valued Laurent polynomial $\boldsymbol{L}_k$.

In consequence, $F(z, \boldsymbol{f} d\boldsymbol{\mu} \boldsymbol{f}^\dagger) = L(z) + \boldsymbol{f}(z)\boldsymbol{F}(z, d\boldsymbol{\mu})\boldsymbol{f}(z)^\dagger$ for some scalar Laurent polynomial L. This relation proves the proposition. □

Although this proposition holds for matrix measures of arbitrary dimension d, we will use it only for $d = 1, 2$, which are the cases related to QRWs on $\mathbb{Z} \geq 0$ and $\mathbb{Z}$. Combining this result and Proposition

13.1 we see that the local transient states can be characterized by $|f|^2 F(z,d\mu) \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$ in $\mathbb{Z} \geq 0$ and $\boldsymbol{f}(z)\boldsymbol{F}(z,d\boldsymbol{\mu})\boldsymbol{f}(z)^\dagger \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$ in $\mathbb{Z}$.

These alternative conditions provide a very practical way to determine the local transient states: they must have as an associated function a Laurent polynomial which cancels the singularities of the Carathéodory function which are responsible for the non integrability.

Remember that the state $|0\rangle \otimes |\uparrow\rangle$ of a QRW on $\mathbb{Z} \geq 0$ is transient exactly when $F(z,d\mu) \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$. Then, $|f(z)|^2 F(z,d\mu) \in L^2_{\frac{d\theta}{2\pi}}(\mathbb{T})$ for any Laurent polynomial f, so we find the following direct consequence of the previous results.

Corollary 13.1. *The local states of a QRW on the non-negative integers with non trivial distinct coins are all transient if and only if the state $|0\rangle \otimes |\uparrow\rangle$ is transient.*

Let us apply the previous results to the analysis of the recurrence for the examples of QRWs given in Section 11.

Consider first the Hadamard coin on the non-negative integers. The corresponding Carathéodory function can be written as

$$F(z) = \sqrt{\frac{(z+z_0)(z+\overline{z}_0)}{(z-z_0)(z-\overline{z}_0)}}, \qquad z_0 = \frac{1}{\sqrt{2}}(1+i),$$

for some choice of the square root. $|F|^2$ has two singularities on $\mathbb{T}$: z_0 and $\overline{z}_0$. Neither is Lebesgue integrable, so the state given by a spin up at the origin is recurrent.

Local transient states are characterized by an associated Laurent polynomial f such that $|f|^4|F|^2$ is Lebesgue integrable on $\mathbb{T}$. Therefore, the local transient states are those with an associated Laurent polynomial vanishing at z_0 and $\overline{z}_0$.

Any superposition of up and down states at site 0 has an associated function lying in $\operatorname{span}\{X_0, X_1\} = \operatorname{span}\{1, z^{-1}\} = z^{-1}\operatorname{span}\{1, z\}$. Such a function can not cancel both singularities of F, thus any mixed spin state at the origin is recurrent.

However, transient states can appear if we consider a mixing of spin states at sites 0 and 1. The Laurent polynomial associated with a state $a\,|0\rangle \otimes |\uparrow\rangle + b\,|0\rangle \otimes |\downarrow\rangle + c\,|1\rangle \otimes |\uparrow\rangle$ is in $\operatorname{span}\{X_0, X_1, X_2\} = \operatorname{span}\{1, z^{-1}, z^2\} = z^{-1}\operatorname{span}\{1, z, z^2\}$, so it can vanish at both, z_0 and $\overline{z}_0$. The Laurent polynomial related to such a state is $a + bX_1 + cX_2$, so it is transient exactly when

$$a + bX_1(z_0) + cX_2(z_0) = 0, \qquad a + bX_1(\overline{z}_0) + cX_2(\overline{z}_0) = 0.$$

Since $X_1(z) = 1 - \sqrt{2}z^{-1}$ and $X_2(z) = -X_1(1/z)$ we find that the solutions of the above equations are $a = 0$ and $c = -b$. This means that the transient states with the referred form are spanned by

$$|0\rangle \otimes |{\downarrow}\rangle - |1\rangle \otimes |{\uparrow}\rangle.$$

Following a similar reasoning, and using the form of the third orthonormal Laurent polynomial $X_3(z) = 1 + \sqrt{2}(z - z^{-1})(1 - \sqrt{2}z^{-1})$, it is easy to obtain the transient states mixing all the up and down states at sites 0 and 1. The result is that such transient states are those lying in the span of

$$|0\rangle \otimes |{\downarrow}\rangle - |1\rangle \otimes |{\uparrow}\rangle, \qquad |0\rangle \otimes |{\uparrow}\rangle + |1\rangle \otimes |{\downarrow}\rangle.$$

Let us see what happens if we change the Hadamard coin by another equiprobable coin like (44). Then, the Carathéodory function

$$F(z) = \frac{\sqrt{1+z^4} - i\sqrt{2}z}{z^2+1}$$

has a single non integrable singularity at i because $-i$ is a removable one. Thus the spin up at the origin is recurrent once again.

However, in contrast with the Hadamard coin, this QRW has transient states at the origin. Such transient states $a\,|0\rangle \otimes |{\uparrow}\rangle + b\,|0\rangle \otimes |{\downarrow}\rangle$ have an associated Laurent polynomial $a + bX_1$ which must vanish at i. Since $X_1(z) = -(\sqrt{2}z^{-1} + i)$ we find that $a + bX_1(i) = 0$ is solved by $b = i(1+\sqrt{2})a$, which shows that the states spanned by

$$|0\rangle \otimes |{\uparrow}\rangle + i(1+\sqrt{2})\,|0\rangle \otimes |{\downarrow}\rangle$$

are transient.

We can also look for the transient states mixing the spin states at sites 0 and 1. Using the fact that $X_2(z) = -\overline{X_1(1/\overline{z})}$ and $X_3(z) = 1 + i\sqrt{2}(z - z^{-1})(i\sqrt{2}z^{-1} - 1)$ we obtain a 3-dimensional subspace of transient states $a\,|0\rangle \otimes |{\uparrow}\rangle + b\,|0\rangle \otimes |{\downarrow}\rangle + c\,|1\rangle \otimes |{\uparrow}\rangle + d\,|1\rangle \otimes |{\downarrow}\rangle$ given by the equation

$$a + i(\sqrt{2}-1)(b+c) + (i(\sqrt{2}-1))^2 d = 0.$$

The QRWs analyzed above are archetypical examples of QRWs on the non-negative integers with a non trivial constant coin. They show the two possible recurrence behaviours, if one leaves aside the singular case of a diagonal coin, which is related to null Verblunsky parameters.

If the coin is symmetric the QRW is associated with an imaginary parameter $a = \overline{c}_{21}e^{i\vartheta}$. Then, the expression of the Carathéodory function F given in Section 9 shows that $|F|^2$ has two non integrable singularities on the unit circle. Indeed, like in the Hadamard case, F^2 is a quotient of two coprime polynomials of degree 2 with their roots on $\mathbb{T}$.

Hence, the recurrence properties for a (non trivial and non diagonal) symmetric coin on the non-negative integers are qualitatively similar to those obtained for the Hadamard one. In particular, any state at site 0 is recurrent for such a coin.

On the contrary, a non symmetric coin is related to a parameter $a = \overline{c}_{21} e^{i\vartheta}$ with a non null real part. The corresponding Carathéodory function F has only one non removable singularity z_0 on the unit circle. More precisely, $F(z) = F_0(z)/(z - z_0)$ with $|F_0|^2$ integrable on $\mathbb{T}$ and $F_0(z_0) \neq 0$, exactly as for the coin (44). Therefore, the recurrence properties for the coin (44) are qualitatively the same as for any other (non trivial and non diagonal) non symmetric coin on the non-negative integers. For instance, these coins always have a 1-dimensional transient subspace at site 0.

Finally, consider the Hadamard coin on the integers. Just as in the case of the Hadamard coin on the non-negative integers, the Carathéodory function

$$\boldsymbol{F}(z) = \frac{1}{\sqrt{1+z^4}} \boldsymbol{F}_0(z), \qquad \boldsymbol{F}_0(z) = \begin{pmatrix} 1+z^2 & \sqrt{2}z \\ \sqrt{2}z & 1+z^2 \end{pmatrix},$$

has singularities at $z_0 = (1+i)/\sqrt{2}$ and $\overline{z}_0$, but also at $-z_0$ and $-\overline{z}_0$. Any of them can cause the non integrability of $|\boldsymbol{f}\boldsymbol{F}\boldsymbol{f}^\dagger|^2$ for a 2-dimensional vector valued Laurent polynomial $\boldsymbol{f}$.

The local transient states are those whose associated vector Laurent polynomial $\boldsymbol{f}$ is such that the scalar Laurent polynomial $\boldsymbol{f}\boldsymbol{F}_0\boldsymbol{f}^\dagger$ vanishes at $\pm z_0$ and $\pm\overline{z}_0$. On these singularities $\boldsymbol{F}_0$ is proportional to a semidefinite matrix,

$$\boldsymbol{F}_0(\pm z_0) = (1+i) \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix}, \qquad \boldsymbol{F}_0(\pm \overline{z}_0) = (1-i) \begin{pmatrix} 1 & \pm 1 \\ \pm 1 & 1 \end{pmatrix},$$

hence $\boldsymbol{f}\boldsymbol{F}_0\boldsymbol{f}^\dagger$ vanishes on such points if and only if $\boldsymbol{f}\boldsymbol{F}_0$ does so.

Any vector Laurent polynomial $\boldsymbol{f} = (a_1, a_2)\boldsymbol{X}_0 + (b_1, b_2)\boldsymbol{X}_1$ has the form $\boldsymbol{f}(z) = z^{-1}\boldsymbol{p}(z)$ where $\boldsymbol{p}$ is a vector polynomial with $\deg \boldsymbol{p} \leq 1$. Therefore, $\deg \boldsymbol{p}\boldsymbol{F}_0 \leq 3$ and $\boldsymbol{f}\boldsymbol{F}_0$ can not vanish on four different points. This means that any superposition of spin states at sites -1 and 0 is recurrent. Taking into account the translation invariance of the QRW, we find that any superposition of spin states which mixes only two contiguous sites is recurrent.

Thus, a transient state must involve sites which are not contiguous. The simplest way to do that is to consider a vector Laurent polynomial $\boldsymbol{f} = (a_1, a_2)\boldsymbol{X}_0 + (b_1, b_2)\boldsymbol{X}_1 + (c_1, c_2)\boldsymbol{X}_2$ which corresponds to a state $c_2 |{-2}\rangle \otimes |{\downarrow}\rangle + b_1 |{-1}\rangle \otimes |{\uparrow}\rangle + a_2 |{-1}\rangle \otimes |{\downarrow}\rangle + a_1 |0\rangle \otimes |{\uparrow}\rangle + b_2 |0\rangle \otimes |{\downarrow}\rangle + c_1 |1\rangle \otimes |{\uparrow}\rangle$.

Using the expressions

$$\boldsymbol{X}_1(z) = \begin{pmatrix} \sqrt{2}z^{-1} & -1 \\ 1 & -\sqrt{2}z^{-1} \end{pmatrix}, \qquad \boldsymbol{X}_2(z) = \boldsymbol{X}_1(1/z),$$

the conditions $\boldsymbol{f}(\pm z_0)\boldsymbol{F}_0(\pm z_0) = \boldsymbol{f}(\pm \overline{z}_0)\boldsymbol{F}_0(\pm \overline{z}_0) = 0$ become

$$(a_1, a_2)\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} + i(b_1, b_2)\begin{pmatrix} \mp 1 \\ 1 \end{pmatrix} + i(c_1, c_2)\begin{pmatrix} \pm 1 \\ -1 \end{pmatrix} = 0,$$

$$(a_1, a_2)\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} + i(b_1, b_2)\begin{pmatrix} \pm 1 \\ -1 \end{pmatrix} + i(c_1, c_2)\begin{pmatrix} \mp 1 \\ 1 \end{pmatrix} = 0,$$

which have the solutions $a_1 = a_2 = 0$, $b_1 = c_1$ and $b_2 = c_2$. That is, the transient states obtained are spanned by

$$|-2\rangle \otimes |{\downarrow}\rangle + |0\rangle \otimes |{\downarrow}\rangle, \qquad |-1\rangle \otimes |{\uparrow}\rangle + |1\rangle \otimes |{\uparrow}\rangle.$$

Then, the translation invariance permits us to identify as transient subspaces all those spanned by states with the form

$$|k\rangle \otimes |{\downarrow}\rangle + |k+2\rangle \otimes |{\downarrow}\rangle, \qquad |k+1\rangle \otimes |{\uparrow}\rangle + |k+3\rangle \otimes |{\uparrow}\rangle.$$

These kinds of results are not specific of the Hadamard QRW, but similar recurrence properties hold for any non trivial and non diagonal constant coin on the integers. Such recurrence properties are a consequence of the general expression for the Carathéodory function $\boldsymbol{F}$ obtained in Section 10, which shows that $\boldsymbol{F}$ has four singularities on the unit circle, with the only exception being the case of null Verblunsky parameters, which corresponds to a diagonal coin. More precisely, for an arbitrary non trivial and non diagonal coin, $\boldsymbol{F} = (1/\sqrt{q})\boldsymbol{F}_0$ with q a scalar polynomial of degree 4 with 4 different roots on $\mathbb{T}$ and $\boldsymbol{F}_0$ a matrix polynomial of degree 2 which is proportional to a semidefinite non null matrix on the roots of q. These general results are the only ingredients necessary to deduce recurrence properties qualitatively similar to those ones obtained above for the Hadamard QRW on the integers.

The fact that any state at a given site is recurrent for an unbiased QRW on the integers was proved in [30]. However, the fact that the states mixing only two consecutive sites are recurrent too, as well as the existence of transient states involving non-contiguous sites is new. Moreover, the comments of the previous paragraph show that these recurrence properties also hold for any QRW with a non trivial and non diagonal constant coin. These general results, together with the analysis of the recurrence for QRWs on the non-negative integers, constitute a novelty which illustrates some of the possibilities of this new approach to QRWs.

14. Conclusions

Classical random walks have been traditionally studied using three different methods. Two of these have already been used in the quantum case. In this paper we propose an approach to the study of QRWs that is inspired by the third of these methods.

Our approach reproduces known results, but also provides new ones and new methods of analysis, like the use of the orthonormal Laurent polynomials to study the asymptotics or the analysis of quantum recurrence using Carathéodory functions.

This approach can handle non translation invariant QRWs, as well as situations where the structure of the one step transitions is richer than the ones considered so far. We intend to study some of these cases in the future by using CMV matrices where all the Verblunsky parameters are allowed to be non-zero; the examples discussed here have a simpler structure. This approach can also be adapted in a natural way to deal with cases when the walk can go to infinity in rather complicated networks as well as in the case of regular networks in various dimensions.

Whereas in the classical case when dealing with an irreducible random walk we have a simple dicotomy: either all states are recurrent or all states are transient, we have seen here examples where the situation in the quantum case is much more involved. This remains as an important area for further investigation.

It is also important to note that this approach can be easily adapted to the case when the number of degrees of freedom in our spins is arbitrary. One should consider some of the examples in [30], such as the Grover or the Fourier ones.

Since the effective use of this approach rests on one's ability to give concrete expressions for the orthogonal polynomials and the orthogonality measure going along with a given CMV matrix there are two natural ways to proceed: start with some of the examples where all the spectral data is known, such as those in [28], and explore the nature of the corresponding QRW, or conversely start with some QRW of interest and try to compute its associated orthogonality measure and polynomials. This is what we have done in this paper.

It would be nice to look into the QRW that goes along with the analog of the Gaussian in the circle, namely the Rogers-Szegő case. It would also be of interest to study examples where the measure is purely discrete.

These, as well as many other questions, remain as an interesting challenge.

15. Appendix

Let us calculate the measure $\hat{\mu}$ and the orthonormal Laurent polynomials $\hat{x}_n$ with Verblunsky parameters $a, 0, a, 0, a, 0, \ldots$ for an arbitrary complex number a with $|a| < 1$. For convenience we will omit the "hats" in what follows.

Setting $\rho = \sqrt{1-|a|^2}$, the related CMV matrix is

$$\mathcal{C} = \left(\begin{array}{c|cc|cc|cc|c}
\overline{a} & 0 & \rho & & & & & \\
\rho & 0 & -a & & & & & \\
\hline
 & \overline{a} & 0 & 0 & \rho & & & \\
 & \rho & 0 & 0 & -a & & & \\
\hline
 & & & \overline{a} & 0 & 0 & \rho & \\
 & & & \rho & 0 & 0 & -a & \\
\hline
 & & & & & & \ddots & \ddots
\end{array}\right).$$

The second recurrence of (7), which determines the sequence x_j, states that $(\mathcal{C} - z)x = 0$, $x_0 = 1$, which can be written as

$$\begin{pmatrix} \overline{a} & -z \\ \rho & 0 \end{pmatrix} \begin{pmatrix} x_{2n-1} \\ x_{2n} \end{pmatrix} + \begin{pmatrix} 0 & \rho \\ -z & -a \end{pmatrix} \begin{pmatrix} x_{2n+1} \\ x_{2n+2} \end{pmatrix} = \mathbf{0}, \qquad x_0 = x_{-1} = 1,$$

or equivalently

$$\begin{pmatrix} x_{2n+1} \\ x_{2n+2} \end{pmatrix} = T \begin{pmatrix} x_{2n-1} \\ x_{2n} \end{pmatrix}, \qquad T = \frac{1}{\rho} \begin{pmatrix} z^{-1} & -a \\ -\overline{a} & z \end{pmatrix}, \qquad \begin{pmatrix} x_{-1} \\ x_0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

From this identity we see by induction that $x_{2n}(z) = \overline{x_{2n-1}(1/\overline{z})}$. Using (9) and (10), this is simply a consequence of the vanishing of the odd Verblunsky parameters. Thus we only need to calculate x_{2n-1}. We also have

$$\begin{pmatrix} x_{2n-1} \\ x_{2n} \end{pmatrix} = T^n \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

Consequently, if $\lambda_\pm$ are the eigenvalues of T, there exist coefficients $B_\pm$ independent of n such that

$$x_{2n-1} = B_+ \lambda_+^n + B_- \lambda_-^n. \tag{49}$$

The eigenvalues $\lambda_\pm$ of T are the solutions λ of

$$\lambda^2 - \rho^{-1}(z + z^{-1})\lambda + 1 = 0. \tag{50}$$

Therefore, $x_{2n-1}(z)$ are solutions Y_n of the second order difference equation

$$Y_{n+1} + Y_{n-1} = 2yY_n, \qquad y = \frac{1}{2\rho}(z + z^{-1}),$$

which is solved by $U_n(y)$, U_n being the Chebysev polynomials of second kind, given by (4). Indeed, the sequences $U_n(y)$ and $U_{n-1}(y)$ are independent solutions of this difference equation, thus, there exist coefficients γ, δ independent of n such that

$$x_{2n-1} = \gamma\, U_n(y) + \delta\, U_{n-1}(y),$$

Evaluating this identity for $x_{-1}(z) = 1$ and $x_1(z) = \rho^{-1}(z^{-1} - a)$ yields

$$\gamma(z) = 1, \qquad \delta(z) = -\rho^{-1}(z + a),$$

giving finally

$$\begin{aligned} x_{2n-1}(z) &= U_n(y) - \rho^{-1}(z+a)U_{n-1}(y), \\ x_{2n}(z) &= U_n(y) - \rho^{-1}(z^{-1}+\overline{a})U_{n-1}(y), \end{aligned} \qquad y = \frac{1}{2\rho}(z + z^{-1}). \tag{51}$$

This gives the orthonormal Laurent polynomials $(x_j)_{j=0}^{\infty}$.

To find the corresponding orthogonality measure μ we proceed with the calculation of the Carathéodory function $F(z)$, $|z| < 1$, using (16). Bearing in mind (9) we can write

$$F(z) = \lim_{n\to\infty} \frac{\tilde{x}_{2n-1}(z)}{x_{2n-1}(z)}, \qquad |z| < 1, \tag{52}$$

where $\tilde{x}_j$ are the orthonormal Laurent polynomials with Verblunsky parameters

$$-a,\ 0,\ -a,\ 0,\ -a,\ 0,\ \ldots$$

To take the limit (52) we will use the expression (49) for x_j, and a similar one changing $a \to -a$ for $\tilde{x}_j$. The eigenvalues $\lambda_\pm$ of T are

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

where we choose the square root so that $|\lambda_+| > |\lambda_-|$ for $0 < |z| < 1$ (using $\lambda_+\lambda_- = 1$ and $\lambda_+ + \lambda_- = \rho^{-1}(z + z^{-1})$ it is not difficult to see that $|\lambda_+| \neq |\lambda_-|$ for $0 < |z| < 1$). Then, (52) gives

$$F = \frac{\tilde{B}_+}{B_+},$$

where $\tilde{B}_+$ is obtained from B_+ changing $a \to -a$.

Using (49) for $n = 0, 1$ we obtain

$$B_+ = \frac{\rho^{-1}(z^{-1} - a) - \lambda_-}{\lambda_+ - \lambda_-}.$$

Thus, the invariance of $\lambda_\pm$ under $a \to -a$ yields

$$F(z) = \frac{z^{-1}+a-\rho\lambda_-}{z^{-1}-a-\rho\lambda_-} = \frac{z-z^{-1}-\sqrt{(z-z^{-1})^2+4|a|^2}-2a}{z-z^{-1}-\sqrt{(z-z^{-1})^2+4|a|^2}+2a} =$$

$$= -\frac{\sqrt{(z-z^{-1})^2+4|a|^2}+2\mathrm{Re}a}{z-z^{-1}+2i\mathrm{Im}a} = -\frac{z-z^{-1}-2i\mathrm{Im}a}{\sqrt{(z-z^{-1})^2+4|a|^2}-2\mathrm{Re}a}.$$

We can obtain the weight $w(\theta)$ of the decomposition (17) for μ using (18) by taking the limit $r \uparrow 1$ of $\mathrm{Re}F(z)$, $z = re^{i\theta}$. Taking into account the choice we have made for the square root, when $|\sin\theta| \leq |a|$,

$$\lim_{r\uparrow 1} \sqrt{(z-z^{-1})^2+4|a|^2} = \pm 2\sqrt{|a|^2-\sin^2\theta} \quad \text{ if } \begin{cases} \cos\theta \geq 0, \\ \cos\theta \leq 0, \end{cases}$$

while, for $|\sin\theta| \geq |a|$,

$$\lim_{r\uparrow 1} \sqrt{(z-z^{-1})^2+4|a|^2} = \mp 2i\sqrt{\sin^2\theta-|a|^2} \quad \text{ if } \begin{cases} \sin\theta \geq 0, \\ \sin\theta \leq 0. \end{cases}$$

This allows one to obtain $w(\theta) = \lim_{r\uparrow 1} \mathrm{Re}F(re^{i\theta})$ which is given by

$$w(\theta) = \frac{\sqrt{\sin^2\theta-|a|^2}}{|\sin\theta+\mathrm{Im}a|}, \qquad |\sin\theta| \geq |a|,$$

and zero otherwise. Equivalently,

$$w(\theta) = \frac{\sqrt{\sin^2\theta-\sin^2\eta}}{|\sin\theta-\sin\beta|}, \qquad \theta \in [\eta, \pi-\eta] \cup [\eta-\pi, -\eta],$$

where the angles $\eta \in [0, \pi/2)$ and $\beta \in (-\pi, \pi]$ are defined by

$$\sin\eta = |a|, \qquad \sin\beta = -\mathrm{Im}a, \qquad \mathrm{sign}(\cos\beta) = \mathrm{sign}(\mathrm{Re}a).$$

The choice of the sign of $\cos\beta$ does not affect for the weight, but will be important for the discussion of the mass points.

Thus the weight is supported on two symmetric arcs of angular amplitude 2η centered at $\pm i$.

Concerning the singular part of the measure, its support must lie in $\{e^{i\theta} : \lim_{r\uparrow 1} F(re^{i\theta}) = \infty\}$. From the expression of $F(z)$ given previously we see that there is only one possible point in this support: $e^{i\beta}$. Thus it can only be a mass point with a mass given by (19), which yields

$$\mu(\{e^{i\beta}\}) = \frac{|\mathrm{Re}a|}{\sqrt{1-|\mathrm{Im}a|^2}} = \frac{\sqrt{\sin^2\eta-\sin^2\beta}}{|\cos\beta|}.$$

The mass point is located outside the support of the weight because $|\sin\beta| \leq \sin\eta$. Indeed, β lies on $(-\eta,\eta)$ or in its symmetric arc depending whether Re$a > 0$ or Re$a < 0$. In the limit case Re$a = 0$ the mass point dissapears.

References

[1] A. Ambainis, *Quantum walks and their algorithmic applications*, International Journal of Quantum Information **1** (2003) 507–518.

[2] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, J. Watrous, *One dimensional quantum walks*, Proc. of the ACM Symposium on Theory and Computation (STOC'01), July 2001, ACM, NY, 2001, pp. 37–49.

[3] A. Bressler, R. Pemantle, *Quantum random walks in one dimension via generating functions*, DMTCS proc. AH, 2007, pp. 403–414.

[4] O. Bourget, J. S. Howland, A. Joye, *Spectral Analysis of Unitary Band Matrices*, Commun. Math. Phys. **234** (2003) 191–227.

[5] M. J. Cantero, L. Moral, L. Velázquez, *Five-diagonal matrices and zeros of orthogonal polynomials on the unit circle*, Linear Algebra Appl. **362** (2003) 29–56.

[6] M.J. Cantero, L. Moral, L. Velázquez, *Minimal representations of unitary operators and orthogonal polynomials on the unit circle*, Linear Algebra Appl. **405** (2005) 40–65.

[7] H. Carteret, M. Ismail, B. Richmond, *Three routes to the exact aymptotics for the one dimensional random quantum walk*, J. Physics A **36** (2003) 8775–8795.

[8] D. Damanik, A. Pushnitski, B. Simon, *The analytic theory of matrix orthogonal polynomials*, Surveys in Approximation Theory **4** (2008) 1–85.

[9] H. Dette, B. Reuther, W. Studden, M. Zygmunt, *Matrix measures and random walks with a block tridiagonal transition matrix*, SIAM J. Matrix Anal. Appl. **29**, No. 1 (2006) 117–142.

[10] W. Feller, *On second order differential operators*, Ann. of Math. **61**, No. 1 (1955) 90–105.

[11] Ya. L. Geronimus, *Orthogonal Polynomials*, Consultants Bureau, New York, 1961.

[12] F. A. Grünbaum, *Random walks and orthogonal polynomials: some challenges*, in Probability, Geometry and Integrable systems, Mark Pinsky and Bjorn Birnir editors, MSRI publication vol 55, 2007, pp. 241–260, see also arXiv math PR/0703375.

[13] F. A. Grünbaum, *QBD processes and matrix valued orthogonal polynomials: some new explicit examples*, Dagstuhl Seminar Proceedings 07461, Numerical Methods in structured Markov Chains, 2007, D. Bini editor.

[14] F. A. Grünbaum, *Block tridiagonal matrices and a beefed-up version of the Ehrenfest urn model*, in M. G. Krein 100's anniversary volume, Odessa, Ukraine, 2008.

[15] F. A. Grünbaum, M. D. de la Iglesia, *Matrix valued orthogonal polynomials arising from group representation theory and a family of quasi-birth-and-death processes*, SIAM J. Matrix Anal. Appl. **30**, No. 2 (2008) 741–761.

[16] S. Karlin, J. McGregor, *Random walks*, Illinois J. Math. **3** (1959) 66–81.

[17] T. Kato, *Perturbation theory for linear operators*, second edition, Springer-Verlag, Berlin-New York, 1976.
[18] J. Kempe, *Quantum random walks-an introductory overview*, Contemporary Physics **44**, No. 4 (2003) 307–327.
[19] N. Konno, *Quantum walks*, in Quantum Potential Theory, U. Franz, M. Schürmann, editors, Lecture notes in Mathematics 1954, Springer Verlag, Berlin Heidelberg, 2008.
[20] M. G. Krein, *Fundamental aspects of the representation theory of hermitian operators with deficiency index* (m, m), AMS Translations, Series 2, vol. 97, Providence, Rhode Island (1971), pp. 75–143.
[21] M. G. Krein, *Infinite* J*-matrices and a matrix moment problem*, Dokl. Akad. Nauk SSSR **69**, No. 2 (1949) 125–128.
[22] W. Ledermann, G. E. Reuter, *Spectral theory for the differential equations of simple birth and death processes*, Philos. Trans. Roy. Soc. London, Ser. A **246** (1954) 321–369.
[23] H. P. McKean, jr., *Elementary solutions for certain parabolic partial differential equations*, Trans. Amer. Math. Soc. **82** (1956) 519–548.
[24] D. Meyer, *From quantum cellular automata to quantum lattice gases*, J. Stat. Physics **85** (1996) 551–574, quant-ph/9604003.
[25] A. Nayak, A. Vishwanath, *Quantum walk on the line*, Center for Discrete Mathematics & Theoretical Computer Science, 2000, quant-ph/0010117.
[26] G. Polya, *Über eine Aufgabe der Wahrscheinlichkeitsrechnung betreffend die Irrfahrt im Strassennetz*, Mathematische Annalen **84** (1921) 149–160.
[27] W. Rudin, *Real and Complex Analysis*, second edition, McGraw-Hill Book Co., New York-Düsseldorf-Johannesburg, 1974.
[28] B. Simon, *Orthogonal Polynomials on the Unit Circle, Part 1: Classical Theory*, AMS Colloq. Publ., vol. 54.1, AMS, Providence, RI, 2005.
[29] B. Simon, *CMV matrices: Five years after*, J. Comput. Appl. Math. **208** (2007) 120–154.
[30] M. Stefanak, T. Kiss, I. Jex, *Recurrence properties of unbiased coined quantum walks on infinite d dimensional lattices*, arXiv: 0805.1322v2 [quant-ph] 4 Sep 2008.
[31] G. Szegő, *Orthogonal Polynomials*, 4th ed., AMS Colloq. Publ., vol. 23, AMS, Providence, RI, 1975.
[32] D. S. Watkins, *Some perspectives on the eigenvalue problem*, SIAM Rev. **35** (1993) 430–471.

(F. A. Grünbaum) Department of Mathematics, University of California, Berkeley, CA, 94720

(M. J. Cantero, L. Moral, L. Velázquez) Departamento de Matemática Aplicada, Universidad de Zaragoza, Zaragoza, Spain