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INSTITUTO DE MATEMÁTICA E ESTATÍSTICA
PROGRAMA DE PÓS-GRADUAÇÃO EM MATEMÁTICA

STATISTICS OF QUANTUM MARKOV CHAINS IN TERMS OF
MATRIX-VALUED ORTHOGONAL POLYNOMIALS

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PORTO ALEGRE, JUNHO DE 2022

Tese submetida por Newton Loebens¹ como requisito parcial para a obtenção do grau de Doutor em Matemática pelo Programa de Pós-Graduação em Matemática do Instituto de Matemática e Estatística da Universidade Federal do Rio Grande do Sul.

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Data de Defesa: 14/06/2022.

¹Bolsista da Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) no período 2018-2022.

Resumo. Neste trabalho estudamos propriedades espectrais e estatísticas de passeios quânticos abertos em termos de polinômios ortogonais com coeficientes matriciais. Relembramos o problema de existência de medidas matriciais em conjunto com cálculos concretos de conceitos estatísticos básicos dos passeios, tais como probabilidades de transição e recorrência de vértices. Concentramos a discussão no modelo de cadeias de Markov quânticas introduzido por S. Gudder, na classe particular de passeios quânticos abertos(OQWs), introduzidos por S. Attal et al., e numa versão contínua de OQWs (denotada por CTOQWs) introduzida por Bardet et. al. Por fim, generalizamos a equivalência entre recorrência de cadeias de Markov a tempo-contínuo e sua cadeia de saltos através de um CTOQW especial.

Palavras-chave: mecânica quântica; passeios quânticos; operadores positivos; polinômios ortogonais matriciais; recorrência.

Abstract. In this work we study spectral and statistical properties of open quantum walks in terms of matrix-valued orthogonal polynomials. We recall the problem of the existence of matrix-valued measures together with concrete calculations of basic statistics of the walk, such as probability transitions and site recurrence. The discussion concentrates on the models of quantum Markov chains, due to S. Gudder, on the particular class of open quantum walks (OQWs), due to S. Attal et al., and on a continuous-time version of OQWs introduced by Bardet et. al. To finish, we generalize the equivalence between the recurrence of continuous-time Markov chains with its jump chain through a special CTOQW.

Keywords: quantum mechanics; quantum walks; positive operators; matrix-valued orthogonal polynomials; recurrence.

AGRADECIMENTOS

Sou muito grato pelo auxílio financeiro da Capes que tornou possível a realização deste doutorado e ao CNPq pelas bolsas do PIC, PICME e mestrado, todas elas em sequência após minhas conquistas na OBMEP.

Agradeço ao Colégio Estadual Cônego Afonso Scherer, à Unisinos e à UFRGS, que foram as instituições onde estudei para chegar ao tão sonhado título de doutor.

Obrigado à banca por aceitar o convite de avaliar minha tese e pelas diversas contribuições que fortaleceram meus resultados. Estendo o agradecimento a todos meus professores, do colégio até o doutorado.

Os resultados que obtive são versões quânticas de processos denominados “birth-death chains”, que são generalizações de um tipo especial de cadeias de Markov. Antes de implementar o caso quântico, estudei a versão clássica pelo livro do professor Manuel [19], que foi disponibilizado a mim pelo autor antes mesmo de sua publicação. Ainda, Manuel é co-autor de um dos trabalhos que deu origem à minha tese, em conjunto com o professor Carlos e eu. Por tudo isso e pelas diversas lições envolvendo polinômios ortogonais, agradeço ao professor Manuel.

Pelas orientações no mestrado e doutorado, pelos diversos conselhos e sugestões, pela grande ajuda nas minhas buscas por bolsas e colaborações de pesquisa e pela disponibilidade em sempre responder minhas diversas dúvidas sobre meu futuro profissional e até pessoal, agradeço ao meu orientador Carlos.

Agradeço aos diversos amigos que a UFRGS me deu. Em especial, o Daniel, o Leonardo e o Félix, que foram meus vizinhos durante grande parte do doutorado e que, apesar da distância, permaneceram perto de mim através de vídeo chamadas e mensagens por redes sociais.

Além dos citados acima, a UFRGS e a mecânica quântica me deram dois amigos que são colegas de pesquisa e que estarão perto de mim para sempre: Thomas e Luiz.

Algumas pessoas contribuíram com meu doutorado das maneiras mais variadas. Em especial, agradeço à Maria Helena e ao Rogério pela amizade e diversas sugestões desde os tempos de Unisinos; à Josiane pelos passeios e disponibilidade em ajudar nas minhas diversas inscrições de processos seletivos; ao Renato e à Rosângela por disponibilizarem seu apartamento, carinho e preocupação que ajudaram a resolver meus diversos problemas durante aquela estadia.

Lembro aqui das diversas caronas que recebi através da secretaria da saúde de Santa Maria do Herval que permitiram que eu tivesse a chance de permanecer perto da minha família ao longo do curso e sou muito grato por isso.

Infelizmente meu pai não pôde ver minhas conquistas, porém, no pouco tempo que tivemos juntos, ele ajudou muito na definição do meu caráter e a entender a importância dos meus estudos. Agradeço ao meu pai por sua contribuição eterna no meu desenvolvimento e até mesmo pela escolha do meu nome, que facilitou minhas relações pessoais no mundo acadêmico da física-matemática e afins. A mecânica quântica não permite tal afirmação, caso contrário diria que meu pai teve uma visão profético na escolha desse nome.

Agradeço imensamente aos meus irmãos Solange e Neumar, que me apoiaram durante toda minha vida e que fizeram muitas vezes o papel de pais na minha criação.

Pelas diversas respostas rápidas aos diversos problemas que encontrei em minha jornada e por terem estado sempre me gratulando pelas minhas conquistas, agradeço aos meus sobrinhos Yago e Bruna e cunhada Caroline.

Ao Roberto, agradeço por ter contribuído de maneira direta em solucionar muitos dos percalços que tive para chegar até aqui, por sua amizade única e pela sua infinita empatia.

Por fim, gostaria de agradecer a minha mãe Petronila. Todas as minhas conquistas serão sempre divididas contigo, serão inspiradas por ti e serão dedicadas a ti. Eu poderia tentar escrever um número ou procurar uma fórmula que representasse o quão importante tu és para mim, mas é muito óbvio que não há (e nunca haverá) matemática suficiente para descrever tal expressão.

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Introduction

In the classical theory, discrete-time birth-death chains on $\mathbb{Z}_{\geq 0}$ are described by a transition probability matrix of the form

$$P = \begin{bmatrix} r_0 & p_0 & 0 & 0 & \cdots \\ q_1 & r_1 & p_1 & 0 & \cdots \\ 0 & q_2 & r_2 & p_2 & \cdots \\ \vdots & \vdots & \vdots & \ddots & \ddots \end{bmatrix}, \quad r_0 + p_0 \leq 1, \quad p_n + r_n + q_n = 1, \quad n \geq 1.$$

The case $p_0 + r_0 < 1$ can be identified as having an extra vertex v (say vertex $v = -1$), then v is an absorbing barrier for the chain, thus the walk never leaves v after it was hit for the first time.

Let $\{Q_n(x)\}_{n \geq 0}$ be the sequence of polynomials defined by the three-term recurrence relation

$$\begin{aligned} Q_0(x) &= 1, & Q_{-1}(x) &= 0, \\ xQ_n(x) &= p_n Q_{n+1}(x) + r_n Q_n(x) + q_n Q_{n-1}(x), & n &\geq 0, \end{aligned}$$

that is, $xQ(x) = PQ(x)$, where $Q(x) = (Q_0(x), Q_1(x), \dots)^T$. Then we have $x^n Q = P^n Q$, i.e.

$$x^n Q_i(x) = \sum_{k=0}^{\infty} P_{ik}^n Q_k(x), \quad i \geq 0. \tag{0.0.1}$$

For a birth-death chain with transition probabilities $p_n, r_n, q_{n+1}, n \geq 0$, Favard's Theorem [15] (see also [29]) assures the existence of a probability measure ψ supported on $[-1, 1]$ such that the polynomials $\{Q_n(x)\}_{n \geq 0}$ are orthogonal with respect to ψ . Multiplying both sides of the equation (0.0.1) by $Q_j(x)$ and integrating with respect to ψ , we obtain the Karlin-McGregor formula [29], which gives the probability of reaching vertex j in n steps, given that the process started at vertex i . This formula is given by

$$P_{ij}^n = \frac{\int_{-1}^1 x^n Q_i(x) Q_j(x) d\psi(x)}{\int_{-1}^1 Q_j^2(x) d\psi(x)}.$$

From a theoretical point of view, it is interesting to ask whether such classical constructions can be adapted so that one can also study quantum systems [8, 16] as well. This has been studied in the case of unitary quantum walks, where the relevant orthogonal polynomials are described in terms of the theory of CMV matrices [10, 11]. Regarding the setting of open quantum dynamics, the problem of studying orthogonal polynomials and associated measures is an interesting one as well, although we would have to consider operators which are no longer unitary.

The main purpose of this thesis is to explore the basic theory of matrix-valued orthogonal polynomials applied to an open quantum setting by providing results on weight matrices and describing several examples², hopefully encouraging the communities of quantum dynamics and orthogonal polynomials to attempt further developments on this line of research. A first step in this direction has been discussed in [28], where a procedure for obtaining weight matrices associated with open quantum walks (OQWs) [4] on the half-line was described, this being in terms of a well-known result due to Durán [21].

The setting we will consider in the first chapter concerns the class of quantum Markov chains (QMCs) on the line, as defined by S. Gudder [25]. This model is revised in detail in Section 1.1. The main difference with OQWs

²Those examples were computed with the software Maple 15.

is that the transition maps are not only given by conjugations of the form $X \mapsto VXV^*$, but, instead, the effect transitions can be chosen to be any completely positive map. This larger class of examples expands the potential applicability of the theory and also makes it easier to find evolutions which are distinct from classical dynamics. With an improved understanding of weight matrices, one is now able to present basic results on recurrence and positive recurrence of QMCs, as we will see in Sections 1.2 and 1.3. The use of the Stieltjes transform allows us to further extend recent results on homogeneous OQWs on the line regarding criteria for site-recurrence [27]. Sections 1.4 and 1.5 illustrate the theory with examples on finite segments and on the half-line, while Section 1.6 explains how to consider QMCs acting on the integer line, further extending the applicability of the theory. Finally, by a proper variation of the Karlin-McGregor formula for weight matrices, we are able to discuss weight matrices which are not necessarily symmetric. This has been examined by Zygmunt [37, 38], and such theory leads to interesting examples of QMCs, as described in Section 1.7.

The setting of the second chapter concerns the class of continuous-time open quantum walks (CTOQWs) on the line. This model is revised in detail in Section 2.2. Analogous to the discrete-time model, an improved understanding of weight matrices allows us to present basic results on recurrence and positive recurrence of CTOQWs, as we will see in Section 2.3. Section 2.4 illustrates the theory with examples on finite segments, on the half-line and on the real line. Section 2.5 illustrates some rates of CTOQWs concerning its quantum trajectories, allowing us to describe the quantum jump chain of a class of CTOQWs and recurrence properties in Section 2.6.

Chapter 1

Quantum Markov chains

In this chapter we present the notion of quantum Markov chains [25] and open quantum walks [4]. We remark that part of the exposition presented here consist of joint collaboration with M. D. de la Iglesia and can be seen in the preprint [20].

1.1 Preliminaries

Let \mathcal{H} be a separable Hilbert space with inner product $\langle \cdot | \cdot \rangle$, whose closed subspaces will be referred to as subspaces for short. The superscript $*$ will denote the adjoint operator. The Banach algebra $\mathcal{B}(\mathcal{H})$ of bounded linear operators on \mathcal{H} is the topological dual of its ideal $\mathcal{I}(\mathcal{H})$ of trace-class operators with trace norm

$$\|\rho\|_1 = \text{Tr}(|\rho|), \quad |\rho| = \sqrt{\rho^* \rho},$$

through the duality [2, Lec. 6]

$$\langle \rho, X \rangle = \text{Tr}(\rho X), \quad \rho \in \mathcal{I}(\mathcal{H}), \quad X \in \mathcal{B}(\mathcal{H}). \quad (1.1.1)$$

If $\dim \mathcal{H} = k < \infty$, then $\mathcal{B}(\mathcal{H}) = \mathcal{I}(\mathcal{H})$ is identified with the set of square matrices of order k , denoted by $M_k(\mathbb{C})$. The duality (1.1.1) yields a useful characterization of the positivity of an operator $\rho \in \mathcal{I}(\mathcal{H})$:

$$\rho \in \mathcal{I}(\mathcal{H}) : \quad \rho \geq 0 \Leftrightarrow \text{Tr}(\rho X) \geq 0, \quad \forall X \in \mathcal{B}(\mathcal{H}), \quad X \geq 0,$$

and similarly for the positivity of $X \in \mathcal{B}(\mathcal{H})$.

In this work, we assume that we have a quantum particle acting either on the integer line, the integer half-line, or on a finite segment, that is, we have that the set of vertices V is labeled by \mathbb{Z} , $\mathbb{Z}_{\geq 0}$ or a finite set $\{0, 1, \dots, N\}$, respectively. In this work, vertices are also called sites. The state of the system is described by a column vector

$$\rho = \begin{bmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \vdots \end{bmatrix}, \quad \rho_i \in \mathcal{I}(\mathcal{H}), \quad \rho_i \geq 0, \quad \sum_{i \in V} \text{Tr}(\rho_i) = 1. \quad (1.1.2)$$

After one time step, the system evolves to the state $\Phi(\rho)$ given by $\Phi(\rho)_i = \sum_{j \in V} \Phi_{ij}(\rho_j)$, where

$$\Phi = \begin{bmatrix} \Phi_{00} & \Phi_{01} & \Phi_{02} & \dots \\ \Phi_{10} & \Phi_{11} & \Phi_{12} & \dots \\ \Phi_{20} & \Phi_{21} & \Phi_{22} & \dots \\ \dots & \dots & \dots & \dots \end{bmatrix}$$

is called a **Quantum Markov Chain** (QMC) [25]: this means that the Φ_{ij} are completely positive (CP) maps on $\mathcal{I}(\mathcal{H})$ and the column sums $\sum_{i \in V} \Phi_{ij}$ are trace-preserving (TP) (the summations are assumed to converge in the strong operator topology), see Figure 1. A density ρ of the form (1.1.2) will be called a **QMC density**. The set of density operators acting on a subspace \mathcal{K} of \mathcal{H} will be denoted by $\mathcal{D}(\mathcal{K})$.

An important particular class of CP maps is given by the ones of the form

$$\Phi_{ij}(\rho) = B_{ij}\rho B_{ij}^*, \quad B_{ij} \in \mathcal{B}(\mathcal{H}), \quad \sum_{k \in V} B_{kj}^* B_{kj} = I, \quad \forall i, j \in V. \quad (1.1.3)$$

The summation above must be understood in the strong sense, and the corresponding identity is the trace-preserving condition for the columns of the QMC Φ . We will say that B_{ij} is the effect matrix of transitioning from vertex j to vertex i . QMCs for which Φ_{ij} can be written in the form (1.1.3) are called **Open Quantum Random Walks** (OQWs), following the terminology established by S. Attal et al. [4]. Explicitly, OQWs are QMCs of the form

$$\Phi(\rho) = \sum_{i \in V} \left(\sum_{j \in V} B_{ij} \rho_j B_{ij}^* \right) \otimes |i\rangle\langle i|, \quad (1.1.4)$$

and, as any QMC, they may be alternatively seen as CP-TP maps on $\mathcal{I}(\mathcal{H} \otimes V)$.

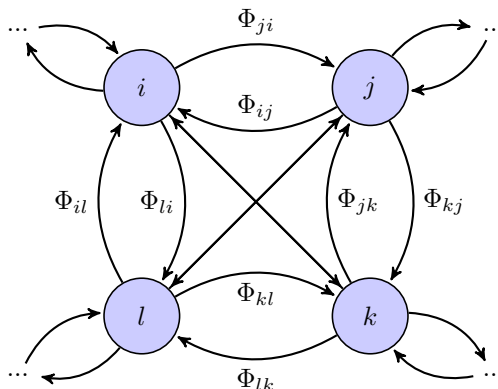


Figure 1.1: Schematic illustration of QMCs. The walk is realized on a graph with a set of vertices denoted by i, j, k, l, \dots and each operator Φ_{ij} is a completely positive map describing a transformation in the internal degree of freedom of the particle during the transition from vertex j to vertex i . For simplicity of illustration some edges are not labeled. In the particular case that all maps are conjugations, i.e., for every i, j , $\Phi_{ij} = B_{ij} \cdot B_{ij}^*$ for certain matrices B_{ij} the QMC is called an open quantum walk. In this work, the graphs considered will be either a line segment, the half-line, or the integer line.

The vector representation $vec(A)$ of $A \in M_k(\mathbb{C})$, given by stacking together its rows, will be a useful tool. For instance,

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \Rightarrow vec(A) := \begin{bmatrix} a_{11} \\ a_{12} \\ a_{21} \\ a_{22} \end{bmatrix}.$$

The vec mapping satisfies $vec(AXB^T) = (A \otimes B) vec(X)$ [26] for any square matrices A, B, X , with \otimes denoting the Kronecker product. In particular, $vec(BXB^*) = vec(BX\bar{B}^T) = (B \otimes \bar{B}) vec(X)$, from which we can obtain the matrix representation $\hat{\Phi}$ for a CP map $\sum_i B_i \cdot B_i^*$ when the underlying Hilbert space \mathcal{H} is finite-dimensional:

$$\hat{\Phi} = \sum_i [B_i], \quad [B] := B \otimes \bar{B}.$$

Here the operators B_i are identified with some matrix representation. We have that $[B]^* = [B^*]$, where B^* denotes the Hermitian transpose of a matrix B . Then, the vector and matrix representation of states and CP maps may be easily adapted to QMCs. In fact, since any element of $\mathcal{I}_V(\mathcal{H})$ is block diagonal, when $\dim \mathcal{H} < \infty$, it may be represented by combining the vector representations of the finite diagonal blocks,

$$\rho = \sum_{i \in V} \rho_i \otimes |i\rangle\langle i| \Rightarrow \vec{\rho} := \begin{bmatrix} vec(\rho_1) \\ vec(\rho_2) \\ \vdots \end{bmatrix}.$$

Then, the OQW (1.1.4) admits the block matrix representation

$$\overrightarrow{\Phi(\rho)} = \widehat{\Phi} \overrightarrow{\rho}, \quad \widehat{\Phi} = \begin{bmatrix} [B_{00}] & [B_{01}] & \cdots \\ [B_{10}] & [B_{11}] & \cdots \\ \vdots & \vdots & \ddots \end{bmatrix},$$

and analogously for QMCs. We will often identify Φ with its block matrix representation and omit the hat, as the usage of such object will be clear from the context. Also, we will sometimes write X instead of $[X]$ in contexts where no confusion arises.

Although the above definitions concern QMCs on general graphs, we remark that in this work we will deal exclusively with the one-dimensional situation, more specifically, with the nearest neighbor QMC or quantum birth-death chain, e.g.,

$$\Phi = \begin{bmatrix} B_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (1.1.5)$$

for certain operators A_i, B_i, C_i , and the remaining ones being equal to zero.

1.1.1 The calculation of probabilities for QMCs

By letting $\rho \otimes |i\rangle\langle i|$ be an initial density matrix concentrated at site $|i\rangle$, we can describe n iterations of the QMC (1.1.5). By setting $\rho^{(0)} = \rho \otimes |i\rangle\langle i|$, $\text{Tr}(\rho) = 1$, we write (assume $C_0 = 0$)

$$\Phi^n(\rho \otimes |i\rangle\langle i|) = \sum_{k \geq 0} \rho_k^{(n)} \otimes |k\rangle\langle k|, \quad \rho_k^{(n)} = C_k \rho_{k+1}^{(n-1)} C_k^* + B_k \rho_k^{(n-1)} B_k^* + A_k \rho_{k-1}^{(n-1)} A_k^*, \quad n = 1, 2, \dots$$

Then, the probability of reaching site $|j\rangle$ at the n -th step, given that we started at site $|i\rangle$ with initial density ρ concentrated at i is given by

$$p_{ji;\rho}(n) = p_n(\rho \otimes |i\rangle \rightarrow |j\rangle) := \text{Tr}(\rho_j^{(n)}) = \text{Tr} \left(\text{vec}^{-1} \left[(\widehat{\Phi}^n)_{ji} \text{vec}(\rho) \right] \right),$$

where $(\widehat{\Phi}^n)_{ji}$ is the (j, i) -th block of the block matrix $\widehat{\Phi}^n$, the n -th power of the block representation $\widehat{\Phi}$.

Following [5, 14], we say that vertex i is **recurrent** with respect to ρ , or simply **ρ -recurrent**, if

$$\sum_{n=0}^{\infty} p_{ii;\rho}(n) = \infty. \quad (1.1.6)$$

Otherwise, we say that vertex i is **transient** with respect to ρ , or **ρ -transient**. We say that, with respect to a fixed QMC, vertex i is **recurrent** if it is ρ -recurrent with respect to every density ρ concentrated in i , and **transient** if it is ρ -transient with respect to every density in i . Finally, we say that a QMC Φ is recurrent if every site is recurrent, and we define transient QMCs analogously.

The series appearing in equation (1.1.6) denotes the mean number of returns to vertex i , given that the walk started with initial density operator ρ , thus, when this number is infinite, the mean number of returns to vertex i is infinite.

Remark 1.1. *We note that in the setting of QMCs, one can also consider the notion of monitored recurrence, see e.g. [5, 23, 27]. For simplicity, we will not consider such definition in this work, and we refer the reader to the references for a detailed discussion on such matter.*

Finally, we will be able to discuss expected return times to sites of QMCs in terms of the following notion. Let T denote a positive map (that is, such that if $X \geq 0$ then $T(X) \geq 0$) acting on the space $\mathcal{I}(\mathcal{H})$ of trace-class operators of a Hilbert space \mathcal{H} . We say that T is irreducible if the only orthogonal projections P such that $T(P\mathcal{I}(\mathcal{H})P) \subset P\mathcal{I}(\mathcal{H})P$, are $P = 0$ and $P = I$, see [12, 13] for more on this. Then, we say that a QMC Φ is **positive recurrent** if it is irreducible and if it admits an invariant distribution. We note that by [[5], Thm. 4.3 and 4.5] for positive recurrent OQWs, we have finite expected return times for every density and site, and the same reasoning provides the analogous result in the case of QMCs.

1.1.2 Auxilliary notation: compact form

In some of the examples we study in this work we will use the following algebraic simplification. We know that the matrix representation of the conjugation map induced by an order 2 matrix $M = (m_{ij})$ is given by

$$[M] = M \otimes \overline{M} = \begin{bmatrix} |m_{11}|^2 & m_{11}\overline{m}_{12} & \overline{m}_{11}m_{12} & |m_{12}|^2 \\ m_{11}\overline{m}_{21} & m_{11}\overline{m}_{22} & m_{12}\overline{m}_{21} & m_{12}\overline{m}_{22} \\ \overline{m}_{11}m_{21} & \overline{m}_{12}m_{21} & \overline{m}_{11}m_{22} & \overline{m}_{12}m_{22} \\ |m_{21}|^2 & m_{21}\overline{m}_{22} & \overline{m}_{21}m_{22} & |m_{22}|^2 \end{bmatrix} = \begin{bmatrix} a & b & \bar{b} & c \\ d & e & f & g \\ \bar{d} & \bar{f} & \bar{e} & \bar{g} \\ h & j & \bar{j} & k \end{bmatrix}, \quad m_{ij} \in \mathbb{C}.$$

Let us consider the setting for which all of the above coefficients are real, and acting on positive semidefinite matrices with real entries. Then

$$[M]vec(\rho) = \begin{bmatrix} a & b & b & c \\ d & e & f & g \\ d & f & e & g \\ h & j & j & k \end{bmatrix} \begin{bmatrix} x \\ y \\ y \\ z \end{bmatrix} = \begin{bmatrix} ax + 2by + cz \\ dx + (e + f)y + gz \\ dx + (e + f)y + gz \\ hx + 2jy + kz \end{bmatrix}, \quad \rho = \begin{bmatrix} x & y \\ y & z \end{bmatrix}.$$

In this particular setting we note that the above computation can be codified in a more economic way, namely, via the correspondence

$$[M]vec(\rho) \leftrightarrow \check{M}\check{\rho} := \begin{bmatrix} a & 2b & c \\ d & e + f & g \\ h & 2j & k \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} a + 2by + cz \\ dx + (e + f)y + gz \\ hx + 2jy + kz \end{bmatrix}. \quad (1.1.7)$$

We call the map \check{M} the **compact form** of the conjugation induced by M , or simply the compact form of M . It is clear that many calculations coming from quantum mechanical models can be written in terms of real numbers only and, even though the real coefficient assumption often precludes us from complete generality, we are still able to learn useful information about 1-qubit quantum channels.

The following properties of the compact form are proven by a routine calculation:

1. $\check{M}\check{R} = \check{M}\check{R}$ for any matrices, resembling the matrix representation property $[MR] = [M][R]$.
2. The compact form preserves the computation of product of conjugations acting on positive definite matrices. That is, if M and R are matrices then $[M][R]vec(\rho)$ corresponds to $\check{M}\check{R}\check{\rho}$.

1.2 Weight matrices

Let W be a weight matrix, i.e. a $N \times N$ matrix of measures supported in the real line such that $dW(y) - dW(x) \geq 0$ (positive semidefinite) for $x < y$. We also allow the case of discrete measures, those appearing naturally in the case of walks acting on a finite number of vertices. Define the matrix-valued inner product given by

$$(P, Q) := \int_{\mathbb{R}} P^*(x) dW(x) Q(x). \quad (1.2.1)$$

Also regarding positive semidefiniteness, we recall that $(P, P) \geq 0$, $(P, P) > 0$ whenever $\det(P) \neq 0$ and $(P, P) = 0$ if and only if $P \equiv 0$. Let $\{Q_n(x)\}_{n \geq 0}$ denote a sequence of matrix-valued orthogonal polynomials with respect to such product, with nonsingular leading coefficients. Then

$$\int_{\mathbb{R}} Q_n^*(x) dW(x) Q_m(x) = \|Q_n\|^2 \delta_{nm}.$$

The set of polynomials will be called orthonormal if $\|Q_n\|^2 = (Q_n, Q_n) = I$, $n \geq 0$. It is well-known that any family of matrix-valued orthogonal polynomials satisfies a three-term recurrence relation of the form

$$xQ_n(x) = Q_{n+1}(x)A_n + Q_n(x)B_n + Q_{n-1}(x)C_n, \quad n \geq 0, \quad Q_0(x) = I, \quad Q_{-1}(x) = 0, \quad (1.2.2)$$

for certain A_n, B_n, C_{n+1} , $n \geq 0$, square matrices. This gives rise to a block tridiagonal Jacobi matrix of the form

$$P = \begin{bmatrix} B_0 & C_1 & & 0 \\ A_0 & B_1 & C_2 & \\ & A_1 & B_2 & C_3 \\ 0 & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (1.2.3)$$

so that (1.2.2) can be written as $xQ(x) = Q(x)P$, where $Q(x) = (Q_0(x), Q_1(x), \dots)$. Let us now see the inverse problem, i.e. under what conditions we can guarantee the existence of a weight matrix given a block tridiagonal matrix of the form (1.2.3). As discussed previously, namely, whenever the weight matrix exists, the (i, j) -th block of the block matrix P^n can be written as

$$(P^n)_{ij} = (Q_i(x), Q_i(x))^{-1} \left(\int_{\mathbb{R}} x^n Q_i^*(x) dW(x) Q_j(x) \right).$$

However, unlike the one-dimensional case, a system of matrix-valued polynomials $\{Q_n(x)\}_{n \geq 0}$ satisfying such recurrence relation is not necessarily orthogonal with respect to an inner product induced by a weight matrix. In view of this, Dette et al. describe an existence criterion.

Let Σ be a $d^2 \times d^2$ weight matrix and denote by

$$S_k = \int x^k d\Sigma(x), \quad k = 0, 1, \dots$$

the corresponding moments. The block Hankel matrices are defined by

$$\underline{H}_{2m} = \begin{bmatrix} S_0 & \cdots & S_m \\ \vdots & & \vdots \\ S_m & \cdots & S_{2m} \end{bmatrix}, \quad m \geq 0.$$

Theorem 1.2. ([18, Theorem 2.1]) *Assume that the matrices $A_n, C_{n+1}, n \geq 0$, in the one-step block tridiagonal transition matrix (1.2.3) are nonsingular. There exists a weight matrix W supported on the real line with positive definite Hankel matrices $\underline{H}_{2m} (m \in \mathbb{Z}_{\geq 0})$ such that the polynomials defined by (1.2.2) are orthogonal with respect to the measure $dW(x)$ if and only if there exists a sequence of nonsingular matrices $\{R_n\}_{n \geq 0}$ such that*

1. $R_n B_n R_n^{-1}$ is Hermitian, $\forall n = 0, 1, 2, \dots$
2. $R_n^* R_n = (A_0^* \cdots A_{n-1}^*)^{-1} (R_0^* R_0) C_1 \cdots C_n$, $\forall n = 1, 2, \dots$

Following the idea of [28], a nearest neighbour QMC has a block tridiagonal matrix of the form

$$\hat{\Phi} = \begin{bmatrix} B_0 & C_1 & & 0 \\ A_0 & B_1 & C_2 & \\ & A_1 & B_2 & C_3 \\ 0 & & \ddots & \ddots & \ddots \end{bmatrix}. \quad (1.2.4)$$

In order to find the corresponding weight matrix associated to $\hat{\Phi}$, we need to find nonsingular matrices $\{R_n\}_{n \geq 0}$ such that

$$\Pi_n := R_n^* R_n = (A_0^* \cdots A_{n-1}^*)^{-1} \Pi_0 C_1 \cdots C_n \quad \text{and} \quad \Pi_n B_n = B_n^* \Pi_n, \quad n = 1, 2, \dots$$

Finally, we note that we have a version of the Karlin-McGregor formula for QMCs, in close analogy with the result seen in [28, Theorem 1.2]:

Theorem 1.3. (Karlin-McGregor formula for QMCs). *Let $\hat{\Phi}$ in (1.2.4) be the matrix representation of a QMC Φ . Assume that there exists a weight matrix W associated with $\hat{\Phi}$. Then we have*

$$p_{ji;\rho}(n) = \text{Tr} \left(\text{vec}^{-1} \left[(Q_j(x), Q_j(x))^{-1} \left(\int_{\mathbb{R}} x^n Q_j^*(x) dW(x) Q_i(x) \right) \text{vec}(\rho) \right] \right),$$

where $\rho = \rho_i \otimes |i\rangle\langle i|$ is a density matrix concentrated on vertex i and $\{Q_n(x)\}_{n \geq 0}$ are the matrix-valued orthogonal polynomials defined by (1.2.2).

Remark 1.4. *The inner product introduced in (1.2.1) is different from the one used in many papers on this subject (see for instance [18, 21, 22, 28, 38, 37] and references therein). The standard inner product used is called **left** inner product*

$$(P, Q)_L := \int_{\mathbb{R}} P(x) dW(x) Q^*(x),$$

which is different from the one defined by (1.2.1), which sometimes is called **right** inner product (see [35]). We obviously have $(P, Q) = (P^*, Q^*)_L$.

1.3 Recurrence and first passage

Consider the Stieltjes transform of a weight matrix W with support on the real line given by

$$B(z; W) := \int_{\mathbb{R}} \frac{dW(x)}{z - x}, \quad z \in \mathbb{C} \setminus \mathbb{R}. \quad (1.3.1)$$

Let $N \in \{1, 2, \dots\}$ and Φ be a QMC described by

$$\Phi = \begin{bmatrix} B_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (1.3.2)$$

where $A_n, B_n, C_{n+1} \in M_{N^2}(\mathbb{C})$, $n \geq 0$. Assume there exists a weight matrix W such that

$$\Phi_{ij}^{(n)} = \Pi_i \left(\int_{\mathbb{R}} x^n Q_i^*(x) dW(x) Q_j(x) \right), \quad (1.3.3)$$

where $\Pi_i = \left(\int_{\mathbb{R}} Q_i^*(x) dW(x) Q_i(x) \right)^{-1}$. Now let us define a generating function associated with hitting probabilities from j to i with respect to the QMC Φ , i.e.

$$\Phi_{ij}(s) := \sum_{n=0}^{\infty} \Phi_{ij}^{(n)} s^n, \quad \Phi_{ij}^{(n)} = \mathbb{P}_i \Phi^n \mathbb{P}_j, \quad (1.3.4)$$

where \mathbb{P}_k is the projection map onto the space generated by the state $|k\rangle$ on $\mathbb{Z}_{\geq 0}$. We will start with the following result concerning ρ -recurrence.

Theorem 1.5. *Let ρ be some density. A vertex $i \in V$ is ρ -recurrent if and only if*

$$\lim_{s \uparrow 1} \text{Tr} \left[\text{vec}^{-1} \left(\Pi_i \int_{\mathbb{R}} \frac{1}{1 - sx} Q_i^*(x) dW(x) Q_i(x) \text{vec}(\rho) \right) \right] = \infty.$$

As a consequence, vertex $|0\rangle$ is ρ -recurrent if and only if

$$\lim_{z \downarrow 1} \text{Tr} \left[\text{vec}^{-1} (B(z; W) \text{vec}(\rho)) \right] = \infty, \quad (1.3.5)$$

where $B(z; W)$ is defined by (1.3.1).

Proof. By Fubini's Theorem and for $|sx| < \infty$ we have

$$\begin{aligned} \Phi_{ji}(s) &= \sum_{n=0}^{\infty} s^n \Phi_{ji}^{(n)} = \sum_{n=0}^{\infty} \Pi_j \int_{\mathbb{R}} (sx)^n Q_j^*(x) dW(x) Q_i(x) \\ &= \Pi_j \int_{\mathbb{R}} \sum_{n=0}^{\infty} (sx)^n Q_j^*(x) dW(x) Q_i(x) = \Pi_j \int_{\mathbb{R}} \frac{1}{1 - sx} Q_j^*(x) dW(x) Q_i(x). \end{aligned} \quad (1.3.6)$$

Then

$$\lim_{s \uparrow 1} \text{Tr} (\text{vec}^{-1} (\Phi_{ji}(s) \text{vec}(\rho))) = \lim_{s \uparrow 1} \sum_{n=0}^{\infty} \text{Tr} \left(\text{vec}^{-1} \left(s^n \Phi_{ji}^{(n)} \text{vec}(\rho) \right) \right) = \sum_{n=0}^{\infty} p_{ji; \rho}(n).$$

By taking $s = 1/z$, we obtain (1.3.5). □

In a similar way we can prove that an irreducible OQW Φ with associated weight matrix W is recurrent with respect to some density ρ if and only if

$$\lim_{s \uparrow 1} \text{Tr} \left(\int \frac{dW(x)}{1 - xs} \rho \right) = \infty.$$

Regarding positive recurrence in terms of the spectral matrix W , we have the following:

Proposition 1.6. *For an irreducible OQW Φ (1.3.2) admitting a weight matrix W , the walk is positive recurrent if and only if the weight matrix W has a finite jump at $x = 1$.*

Proof. An irreducible, positive recurrent OQW always admits a faithful (strictly positive), invariant distribution by [30, Theorem 5.8]. Therefore, we conclude, by [13, Corollary 5.4], that

$$\lim_{n \rightarrow \infty} \text{Tr}(\mathbb{P}_0 \Phi^{2n} \mathbb{P}_0 \rho) > 0.$$

Since $x^{2n} \rightarrow 0$ monotonically in $x \in (-1, 1)$, from Theorem 1.3 we see that the limit is positive if the spectral measure has positive jumps at $x = 1$ or at $x = -1$. However, there cannot be a jump at $x = -1$ since, otherwise, the size of the jump would be

$$-\lim_{n \rightarrow \infty} \text{Tr} \left(\text{vec}^{-1} \left[\int_{-1}^1 x^{2n+1} dW(x) \text{vec}(\rho) \right] \right) = -\lim_{n \rightarrow \infty} \text{Tr}(\mathbb{P}_0 \Phi^{2n+1} \mathbb{P}_0 \rho) \leq 0.$$

But this quantity must be positive, so there is no jump at $x = -1$, for any choice of density ρ . Therefore, the OQW is positive recurrent if and only if there is a jump at $x = 1$. □

Let us now derive an expression for first passage probabilities of QMCs in terms of matrix-valued polynomials only. The following discussion is inspired by the classical reasoning presented in [19], with the main result being formula (1.3.13) presented below, which allows us to obtain first visit probabilities in terms of matrix polynomials in a simple manner. For $k \geq 0$, consider the QMC Φ with matrix representation

$$\Phi = \left[\begin{array}{cccc|ccc} B_0 & C_1 & & & & & \\ A_0 & B_1 & C_2 & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & A_{k-1} & B_k & C_{k+1} & & \\ \hline & & & A_k & B_{k+1} & C_{k+2} & \\ & & & & A_{k+1} & B_{k+2} & C_{k+3} \\ & & & & & \ddots & \ddots & \ddots \end{array} \right],$$

where $B_n, A_n, C_{n+1} \in M_N(\mathbb{C})$, $n \geq 0$. As usual, we recursively define the following matrix-valued polynomials,

$$\begin{aligned} Q_0(x) &= I_N, & Q_{-1}(x) &= 0 \\ xQ_n(x) &= Q_{n+1}(x)A_n + Q_n(x)B_n + Q_{n-1}(x)C_n, \end{aligned} \tag{1.3.7}$$

that is, $xQ(x) = Q(x)\Phi$, where $Q(x) = (Q_0(x), Q_1(x), \dots)$. Suppose that Φ satisfies the conditions of Theorem 1.2, so the polynomials defined by (1.3.7) are orthogonal with respect to a weight matrix W and $\Pi\Phi = \Phi^*\Pi$, where $\Pi = \text{diag}(\Pi_0, \Pi_1, \dots)$ and $\Pi_j = R_j^* R_j$, $j \geq 0$. Analogously to the classical case, we define the **k -th associated polynomials**

$$xQ_n^{(k)}(x) = \delta_{nk} + Q_{n+1}^{(k)}(x)A_n + Q_n^{(k)}(x)B_n + Q_{n-1}^{(k)}(x)C_n.$$

Note that $Q_n^{(k)}(x) = 0$ if $0 \leq n \leq k$ and $\deg(Q_n^{(k)}(x)) = n - k - 1$ if $n > k$. Consider the generating function $\Phi(s)$ associated with Φ defined by (1.3.4). Assuming $\|s\Phi\| < 1$, $\Phi_{ji}(s)$ converges for every i, j , thus

$$\sum_{n=0}^{\infty} (s\Phi)^n (I - s\Phi) = I \Rightarrow \Phi(s) - \Phi(s)(s\Phi) = I.$$

Therefore, we have the equation

$$\Phi(s) = I + \Phi(s)(s\Phi),$$

which can be rewritten by blocks as

$$\begin{aligned} \Phi_{j0}(s) &= \delta_{j0} + \Phi_{j0}(s)B_0 + \Phi_{j1}(s)A_0, & j \geq 0 \\ \Phi_{ji}(s) &= \delta_{ji} + \Phi_{j,i-1}(s)C_i + \Phi_{j,i}(s)B_i + \Phi_{j,i+1}(s)A_i, & i \geq 1, j \geq 0. \end{aligned} \tag{1.3.8}$$

A particular solution of (1.3.8) is given by

$$\Phi_{ji}(s) = s^{-1}Q_i^{(j)}(s^{-1}).$$

On the other hand, the general solution of $\Phi(s) = \Phi(s)(s\Phi)$, which is

$$\Phi_{ji}(s) = g_j(s)Q_i(s^{-1})$$

gives

$$\Phi_{ji}(s) = \Phi_{j,i-1}(s)C_i + \Phi_{j,i}(s)B_i + \Phi_{j,i+1}(s)A_i,$$

and consequently, the general solution of (1.3.8) is

$$\Phi_{ji}(s) = s^{-1}Q_i^{(j)}(s^{-1}) + g_j(s)Q_i(s^{-1}).$$

Since $Q_0^{(j)} = 0$ and $Q_0 = 1$, one has $\Phi_{j0}(s) = g_j(s)Q_0(s^{-1}) = g_j(s)$. Moreover, since $\Phi_{ji}^{(n)} = \Pi_j^{-1}\Phi_{ij}^{(n)*}\Pi_i$, we have

$$\Phi_{j0}(s) = \sum_{n=0}^{\infty} s^n \Pi_j^{-1} \Phi_{0j}^{(n)*} \Pi_0 = \Pi_j^{-1} \Phi_{0j}(s) \Pi_0,$$

so we obtain the general solution for $g_j(s)$:

$$\begin{aligned} g_j(s) &= \Phi_{j0}(s) = \Pi_j^{-1} \Phi_{j0}(s) \Pi_0 \\ &= \Pi_j^{-1} \left(s^{-1}Q_j^{(0)}(s^{-1}) + g_0(s)Q_j(s^{-1}) \right) \Pi_0 = \Pi_j^{-1} \left(s^{-1}Q_j^{(0)}(s^{-1}) + \Phi_{00}(s)Q_j(s^{-1}) \right) \Pi_0. \end{aligned}$$

Therefore the general solution for $\Phi_{ij}(s)$ is given by

$$\Phi_{ji}(s) = s^{-1}Q_i^{(j)}(s^{-1}) + \Pi_j^{-1} \left(s^{-1}Q_j^{(0)}(s^{-1}) + \Phi_{00}(s)Q_j(s^{-1}) \right) \Pi_0 Q_i(s^{-1}). \quad (1.3.9)$$

If we assume $i < j$, then $Q_i^{(j)} = 0$ and (1.3.9) becomes

$$\Phi_{ji}(s) = \Pi_j^{-1} \left(s^{-1}Q_j^{(0)}(s^{-1}) + \Phi_{00}(s)Q_j(s^{-1}) \right) \Pi_0 Q_i(s^{-1}). \quad (1.3.10)$$

Now consider the first passage time operator $F(s)$ satisfying

$$\begin{aligned} F(s) &= [F_{ji}(s)]_{j,i=0,1,2,\dots} \\ F_{ji}(s) &= \Phi_{jj}(s)^{-1}(\Phi_{ji}(s) - \delta_{ji}I), \end{aligned} \quad (1.3.11)$$

that is, with definition given by

$$F(z) = z\mathbb{P}\Phi(I - z\mathbb{Q}\Phi)^{-1}, \quad (1.3.12)$$

where \mathbb{P} and $\mathbb{Q} = I - \mathbb{P}$ are bounded projections from \mathcal{H} onto supplementary closed subspaces of \mathcal{H} . Further, we denote by \mathbb{P}_k the projection map onto the space generated by the state $|k\rangle$ on $\mathbb{Z}_{\geq 0}$ and $\mathbb{Q}_k := I - \mathbb{P}_k$. In this way, we are able to calculate the probability of every reaching vertex j , given that we have started at vertex i and density ρ , by writing

$$p(\rho \otimes |i\rangle \rightarrow |j\rangle) = \lim_{z \uparrow 1} \text{Tr}(F_{ji}(z)\rho) = \lim_{z \uparrow 1} \text{Tr}(z\mathbb{P}_j\Phi(I - z\mathbb{Q}_j\Phi)^{-1}\rho),$$

where \mathbb{P}_j is the j -th block entry of \mathbb{P} and \mathbb{Q}_j is the j -th block entry of \mathbb{Q} .

By [24], $F(s)$ defined as above indeed satisfies equation (1.3.11). So, let $i < j$ and $\rho \in M_N(\mathbb{C})$, then by equation (1.3.10)

$$\begin{aligned} F_{ji}(s) &= \Phi_{jj}(s)^{-1}\Phi_{ji}(s) \\ &= Q_j(s^{-1})^{-1}\Pi_0^{-1} \left[\left(s^{-1}Q_j^{(0)}(s^{-1}) + \Phi_{00}(s)Q_j(s^{-1}) \right) \right]^{-1} \Pi_j \\ &\quad \times \Pi_j^{-1} \left(s^{-1}Q_j^{(0)}(s^{-1}) + \Phi_{00}(s)Q_j(s^{-1}) \right) \Pi_0 Q_i(s^{-1}) = Q_j(s^{-1})^{-1}Q_i(s^{-1}). \end{aligned}$$

Therefore, by (1.3.11), we obtain

$$F_{ji}(s) = Q_j(s^{-1})^{-1}Q_i(s^{-1}), \quad i < j. \quad (1.3.13)$$

In particular, the condition $Q_0 = I$ gives

$$F_{10}(s) = Q_1(s^{-1})^{-1} = \left[\left(\frac{1}{s}I - B_0 \right) A_0^{-1} \right]^{-1} = sA_0(I - sB_0)^{-1}. \quad (1.3.14)$$

Example 1.7. Let Φ be the representation matrix of an OQW on $V = \{0, 1, 2\}$ of the form

$$\Phi = \begin{bmatrix} 0 & [C] \\ [A] & \begin{bmatrix} 0 & [C] \\ [A] & 0 \end{bmatrix} \end{bmatrix}, \quad A = \frac{1}{2} \begin{bmatrix} -1 & 0 \\ 1 & \sqrt{2} \end{bmatrix}, \quad C = \frac{1}{2} \begin{bmatrix} 1 & -\sqrt{2} \\ -1 & 0 \end{bmatrix}.$$

Since $A^*A < I$, the walk has an absorbing barrier in the frontier. Also, we have

$$(I - sQ_1\Phi) = \begin{bmatrix} I_4 & X & 0 \\ 0 & I_4 & 0 \\ 0 & Y & I_4 \end{bmatrix}, \quad X = \frac{s}{4} \begin{bmatrix} -1 & \sqrt{2} & \sqrt{2} & -2 \\ 1 & 0 & -\sqrt{2} & 0 \\ 1 & -\sqrt{2} & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}, \quad Y = \frac{s}{4} \begin{bmatrix} -1 & 0 & 0 & 0 \\ 1 & \sqrt{2} & 0 & 0 \\ 1 & 0 & \sqrt{2} & 0 \\ -1 & -\sqrt{2} & -\sqrt{2} & -2 \end{bmatrix}.$$

and

$$F_{10}(s) = sP_1\Phi(I - sQ_1\Phi)^{-1}P_0 = \frac{s}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1 & -\sqrt{2} & 0 & 0 \\ -1 & 0 & -\sqrt{2} & 0 \\ 1 & \sqrt{2} & \sqrt{2} & 2 \end{bmatrix}.$$

The first two associated polynomials are given by

$$Q_0(x) = I_4, \quad Q_1(x) := 2x \begin{bmatrix} 2 & 0 & 0 & 0 \\ -\sqrt{2} & -\sqrt{2} & 0 & 0 \\ -\sqrt{2} & 0 & -\sqrt{2} & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix},$$

from which we can calculate the product $Q_1(s^{-1})^{-1}Q_0(s^{-1})$, which equals $F_{10}(s)$ as expected. Then, for $\rho =$

$$\begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}, \quad \text{we obtain}$$

$$p(\rho \otimes |0\rangle \rightarrow |1\rangle) = \lim_{s \uparrow 1} \text{Tr}(F_{10}(s)\rho) = \frac{1 + \sqrt{2}\text{Re}(b)}{2} \in \left[\frac{2 - \sqrt{2}}{4}, \frac{2 + \sqrt{2}}{4} \right],$$

since $\text{Re}(b) \in [-1/2, 1/2]$.

◇

Example 1.8. Let $\gamma \in \mathbb{R}$ and $k_\gamma = 2 + 2\gamma^2$ and Φ be the representation matrix of an OQW of the form

$$\Phi = \begin{bmatrix} [B_0] & [C_1] \\ [A_0] & \begin{bmatrix} [B_1] & [C_2] \\ [A_1] & [B_2] & [C_3] \\ \ddots & \ddots & \ddots \end{bmatrix} \end{bmatrix}, \quad B_0 = \frac{1}{\sqrt{k_\gamma}} \begin{bmatrix} -1 & \sqrt{2}\gamma \\ 0 & 1 \end{bmatrix}, \quad A_0 = \frac{1}{\sqrt{k_\gamma}} \begin{bmatrix} \sqrt{2}\gamma & 1 \\ 1 & 0 \end{bmatrix}.$$

We notice that $F_{10}(s)$ does not depend on the blocks A_k, B_k, C_k for $k = 1, 2, 3, \dots$, thus such blocks can be chosen arbitrarily so that $A_k^*A_k + B_k^*B_k + C_k^*C_k = I$ for $k \geq 1$. Then, equation (1.3.12) gives

$$F_{10}(s) = \frac{s}{2 + 2\gamma^2 - s} \begin{bmatrix} 2\gamma^2 & \frac{\sqrt{2}\gamma(2\gamma^2s + 2 - 2\gamma^2 - s)}{2 + s + 2\gamma^2} & \frac{\sqrt{2}\gamma(2\gamma^2s + 2 - 2\gamma^2 - s)}{2 + s + 2\gamma^2} & \frac{s + 4\gamma^2s + 4\gamma^4s + 2 + 2\gamma^2}{2 + s + 2\gamma^2} \\ \sqrt{2}\gamma & -\frac{2\gamma^2s}{2 + s + 2\gamma^2} & \frac{2\gamma^2 + 2 - 2\gamma^2s - s}{2 + s + 2\gamma^2} & \frac{\sqrt{2}\gamma(1 + 2\gamma^2)}{2 + s + 2\gamma^2} \\ \sqrt{2}\gamma & \frac{2\gamma^2 + 2 - 2\gamma^2s - s}{2 + s + 2\gamma^2} & -\frac{2\gamma^2s}{2 + s + 2\gamma^2} & \frac{\sqrt{2}\gamma(1 + 2\gamma^2)}{2 + s + 2\gamma^2} \\ 1 & -\frac{\sqrt{2}\gamma s}{2 + s + 2\gamma^2} & -\frac{\sqrt{2}\gamma s}{2 + s + 2\gamma^2} & \frac{2\gamma^2s}{2 + s + 2\gamma^2} \end{bmatrix},$$

and, as expected, this is the same matrix obtained by formula (1.3.14). For $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$, we obtain, for every ρ , that

$$\begin{aligned} p(\rho \otimes |0\rangle \rightarrow |1\rangle) &= \lim_{s \uparrow 1} \text{Tr}(F_{10}(s)\rho) \\ &= \lim_{s \uparrow 1} \frac{4\gamma^4(as - a - s) + 4\gamma\sqrt{2}(s-1)\text{Re}(b)(\gamma^2 + 1) + 2\gamma^2(2as - 3s - 2a - 1) - 2 - s}{(2 + s + 2\gamma^2)(-2 + s - 2\gamma^2)} = 1. \end{aligned}$$

We note that, in principle, we are able to obtain probabilities regarding vertices which are arbitrarily distant from one another but, as the distance between them increases, the task of performing explicit calculations may become unpractical. In such cases, it may be preferable to use the generating function (1.3.12).

◇

1.4 A QMC on a finite number of vertices

Let us first consider a walk induced by the block matrix on the $N + 1$ nodes indexed as $\{0, 1, \dots, N\}$,

$$\Phi = \begin{bmatrix} B & rI & & & \\ tI & B & rI & & \\ & tI & B & rI & \\ & \ddots & \ddots & \ddots & \\ & & & tI & B & rI \\ & & & & tI & B \end{bmatrix}, \quad 0 < r, t < 1,$$

where if $B = [\Phi_B]$, $\Phi_B = V_1^* \cdot V_1 + V_2^* \cdot V_2$, with

$$V_1 = \sqrt{s} \begin{bmatrix} a & b \\ b & -a \end{bmatrix}, \quad V_2 = \sqrt{s(1 - a^2 - b^2)} I_2.$$

We can write

$$B = s \begin{bmatrix} 1 - b^2 & ab & ab & b^2 \\ ab & 1 - 2a^2 - b^2 & b^2 & -ab \\ ab & b^2 & 1 - 2a^2 - b^2 & -ab \\ b^2 & -ab & -ab & 1 - b^2 \end{bmatrix}.$$

For simplicity we assume $0 < a, b, s < 1$, $a^2 + b^2 < 1$. In this way we have that $\text{Tr}(\Phi(X)) = s\text{Tr}(X)$, so we suppose that $r + s + t = 1$ in order to have that Φ is trace-preserving, with the exception of the first and last nodes (we remark that another restriction on r, s, t will be needed, see below).

By the classical symmetrization

$$\mathcal{R} = \text{diag}(R_0, R_1, \dots, R_N), \quad R_i = \left(\sqrt{\frac{r}{t}} \right)^{i-1} I_4, \quad i = 1, \dots, N, \quad R_0 = I_4,$$

we obtain

$$J = \mathcal{R}\Phi\mathcal{R}^{-1} = \begin{bmatrix} B & kI & & & \\ kI & B & kI & & \\ & kI & B & kI & \\ & \ddots & \ddots & \ddots & \\ & & & kI & B & kI \\ & & & & kI & B \end{bmatrix}, \quad k = \sqrt{rt}.$$

The matrix-valued polynomials $\{Q_n\}_{n \geq 0}$ defined by

$$\begin{aligned} Q_0(x) &= I, \quad Q_{-1}(x) = 0, \\ xQ_0(x) &= Q_0(x)B + kQ_1(x), \\ xQ_i(x) &= kQ_{i-1}(x) + Q_i(x)B + kQ_{i+1}(x), \quad i = 1, \dots, N-1, \end{aligned}$$

can be identified with the Chebyshev polynomials of the second kind $\{U_n\}_{n \geq 0}$. Indeed, it is possible to see that $Q_n(x) = U_n((x-B)/2k)$, $n \geq 0$. Now, if we define

$$R_{N+1}(x) := Q_N(x)(x-B) - kQ_{N-1}(x),$$

we have that the zeros of $\det(R_{N+1}(x))$ coincide with the eigenvalues of $J = \mathcal{R}\Phi\mathcal{R}^{-1}$. A simple calculation shows that

$$R_{N+1}(x) = kU_{N+1}\left(\frac{x-B}{2k}\right).$$

We would like to solve the equation $\det(R_{N+1}(x)) = 0$. Recalling the representation

$$U_n\left(\frac{z}{2}\right) = \prod_{j=1}^n \left(z - 2 \cos\left(\frac{j\pi}{n+1}\right)\right),$$

we obtain, for the matrix-valued case at hand,

$$\begin{aligned} \det(R_{N+1}(x)) &= k^4 \det\left(U_{N+1}\left(\frac{x-B}{2k}\right)\right) = k^4 \det\left[\prod_{j=1}^{N+1} \left(\frac{xI_4 - B}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) I_4\right)\right] \\ &= k^4 \prod_{j=1}^{N+1} \det\left[\left(\frac{xI_4 - B}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) I_4\right)\right]. \end{aligned}$$

Noting that the eigenvalues of B are s and $s(1-2a^2-2b^2)$ (both with multiplicity 2) we have

$$\begin{aligned} &\det\left[\left(\frac{xI_4 - B}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) I_4\right)\right] \\ &= \det \begin{bmatrix} \frac{x-s}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) & & & \\ & 0 & \frac{x-s}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) & \\ & & & \frac{x-s(1-2a^2-2b^2)}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) \\ & & & & \frac{x-s(1-2a^2-2b^2)}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right) \end{bmatrix} \\ &= \left[\frac{x-s}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right)\right]^2 \left[\frac{x-s(1-2a^2-2b^2)}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right)\right]^2. \end{aligned}$$

Hence,

$$\det(R_{N+1}(x)) = k^4 \prod_{j=1}^{N+1} \left[\frac{x-s}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right)\right]^2 \left[\frac{x-s(1-2a^2-2b^2)}{k} - 2 \cos\left(\frac{j\pi}{N+2}\right)\right]^2, \quad k = \sqrt{rt},$$

which is a polynomial of degree $4(N+1)$ having $2(N+1)$ distinct roots (all of multiplicity 2). Therefore, the roots are of the form

$$x_j = s + 2k \cos\left(\pi \frac{j+1}{N+2}\right), \quad j = 0, \dots, N,$$

$$y_j = s(1-2a^2-2b^2) + 2k \cos\left(\pi \frac{j+1}{N+2}\right), \quad j = 0, \dots, N,$$

all being of multiplicity 2, except in the case where the collection of zeros x_N and y_N overlap, so the multiplicity changes accordingly (see the example below). The expressions on the roots also make clear that we must have further restrictions on the values of r , s and t (recall $k = \sqrt{rt}$) so that $x_j, y_j \in [-1, 1]$, for all $j = 0, \dots, N$. For instance, by imposing $0 < k < 1/4$ we obtain a corresponding restriction on s (we omit the details).

The above root calculation should be compared with the classical case with a translation of s units, for which the roots of R_{N+1} are

$$x_j = s + 2\sqrt{rt} \cos\left(\pi \frac{j+1}{N+1}\right), \quad j = 0, \dots, N,$$

once again regarding a random walk with a proper restriction on r, s, t so that $x_j \in [-1, 1]$, for all j .

Now we compute the matrix weights on the zeros above. Such calculation needs to take in consideration the fact that each root is double (we omit the discussion for the case of larger multiplicities). In this case the residue calculation gives us that

$$W_j = g'_j(\lambda_j), \quad g_j(\lambda) := -(\lambda_j - \lambda)^2 (J - \lambda I)_{00}^{-1}, \quad \lambda_j = x_j, y_j, \quad j = 0, \dots, N, \quad (1.4.1)$$

an expression which can be deduced from (see [22])

$$(J - \lambda I)_{ij}^{-1} = \sum_{k=0}^N \frac{P_i^*(\lambda_k) W_k P_j(\lambda_k)}{\lambda_k - \lambda},$$

and noting that this corresponds to the Laurent sum of the operator on the left-hand side except for the sign change $\lambda_k - \lambda = -(\lambda - \lambda_k)$. With formula (1.4.1), a calculation shows that for every N we have a corresponding set of multiples of the matrices given by

$$W_{a,b;1} := \frac{1}{2(a^2 + b^2)} \begin{bmatrix} 2a^2 + b^2 & ab & ab & b^2 \\ ab & b^2 & b^2 & -ab \\ ab & b^2 & b^2 & -ab \\ b^2 & -ab & -ab & 2a^2 + b^2 \end{bmatrix}, \quad W_{a,b;2} := \frac{1}{2(a^2 + b^2)} \begin{bmatrix} b^2 & -ab & -ab & -b^2 \\ -ab & b^2 + 2a^2 & -b^2 & ab \\ -ab & -b^2 & b^2 + 2a^2 & ab \\ -b^2 & ab & ab & b^2 \end{bmatrix}.$$

More precisely, we have a collection of $4(N + 1)$ roots with weights

$$\begin{aligned} \psi(x_j) &= \frac{2}{N+2} \sin^2 \left(\pi \frac{j+1}{N+2} \right) W_{a,b;1}, \quad j = 0, \dots, N, \\ \psi(y_j) &= \frac{2}{N+2} \sin^2 \left(\pi \frac{j+1}{N+2} \right) W_{a,b;2}, \quad j = 0, \dots, N. \end{aligned}$$

This should be compared with the classical setting, recalling that in such case,

$$\psi(x_j) = \frac{2}{N+2} \sin^2 \left(\pi \frac{j+1}{N+2} \right) = \frac{1}{2pq(N+2)} (4pq - x_j^2), \quad j = 0, \dots, N. \quad (1.4.2)$$

We note a few basic properties of $W_{a,b;1}$ and $W_{a,b;2}$. First, both are positive semidefinite matrices with eigenvalues 0 and 1 (multiplicity 2). Moreover, seen as linear maps, $W_{a,b;1}$ is trace-preserving, whereas $W_{a,b;2}$ transforms densities into traceless matrices. Also $W_{a,b;1}$ admits the following Kraus representation

$$W_{a,b;1} = \sum_{i=1}^3 W_i^1 \otimes \overline{W_i^1}, \quad W_1^1 = \frac{1}{2(a^2 + b^2)} \begin{bmatrix} a & b \\ b & -a \end{bmatrix}, \quad W_2^1 = \frac{a}{2(a^2 + b^2)} I_2, \quad W_3^1 = \frac{b}{2(a^2 + b^2)} I_2,$$

from which we conclude that such weight represents a completely positive map. However, $W_{a,b;2}$ does not represent a positive map in general, as illustrated by an inspection with certain density examples.

For a specific instance of the above take $N = 4$ (5 sites), so we have 20 roots, with weights

$$\frac{1}{3} W_{a,b;1}, \quad \frac{1}{3} W_{a,b;2},$$

associated with zeros s and $s(1 - 2a^2 - 2b^2)$ respectively; weights

$$\frac{1}{4} W_{a,b;1}, \quad \frac{1}{4} W_{a,b;2},$$

associated with zeros $s \pm k$, $s(1 - 2a^2 - 2b^2) \pm k$ respectively; and weights

$$\frac{1}{12} W_{a,b;1}, \quad \frac{1}{12} W_{a,b;2},$$

associated with zeros $s \pm \sqrt{3}k$, and $s(1 - 2a^2 - 2b^2) \pm \sqrt{3}k$ respectively. If, moreover, $s = a = b = k = 1/2$, we have

$$\{x_j\}_{j=0\dots 4} = \left\{ -\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0, \frac{1}{2}, \frac{\sqrt{3}}{2} \right\}, \quad \{y_j\}_{j=0\dots 4} = \left\{ \frac{-\sqrt{3}+1}{2}, 0, \frac{1}{2}, 1, \frac{\sqrt{3}+1}{2} \right\},$$

each with multiplicity 2 except for 0 and $1/2$ with multiplicity 4 (noting that in this case, $1 - 2a^2 - 2b^2 = 0$). This should be compared with the classical setting, see (1.4.2).

1.5 An example of a QMC on $\mathbb{Z}_{\geq 0}$

Consider the walk induced by the block matrix on $\mathbb{Z}_{\geq 0}$ given by

$$\Phi = \begin{bmatrix} 0 & C & & 0 \\ A & 0 & C & \\ & A & 0 & C \\ 0 & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (1.5.1)$$

where A and C are the compact forms (see (1.1.7)) of $R_1 \otimes \overline{R_1} + R_2 \otimes \overline{R_2}$ and $L_1 \otimes \overline{L_1} + L_2 \otimes \overline{L_2}$, respectively, and

$$L_1 = \sqrt{p/2}I_2, \quad L_2 = \sqrt{(1-p)/2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad R_1 = \sqrt{q/2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad R_2 = \sqrt{(1-q)/2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}.$$

Observe that $R_1^*R_1 + R_2^*R_2 + L_1^*L_1 + L_2^*L_2 = I_2$. Therefore,

$$A = \frac{1}{2} \begin{bmatrix} q & 0 & 1-q \\ 0 & 1-2q & 0 \\ 1-q & 0 & q \end{bmatrix}, \quad C = \frac{1}{2} \begin{bmatrix} p & 0 & 1-p \\ 0 & 1 & 0 \\ 1-p & 0 & p \end{bmatrix}.$$

The matrices A and B are simultaneously diagonalizable, i.e.,

$$A = \mathcal{U} \begin{bmatrix} 1/2 & & \\ & 1/2 - q & \\ & & q - 1/2 \end{bmatrix} \mathcal{U}^*, \quad C = \mathcal{U} \begin{bmatrix} 1/2 & & \\ & 1/2 & \\ & & p - 1/2 \end{bmatrix} \mathcal{U}^*, \quad \mathcal{U} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & -1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{bmatrix}. \quad (1.5.2)$$

Choosing

$$\Pi_n = \begin{bmatrix} 1 & & \\ & (1-2q)^n & \\ & & \left(\frac{1-2q}{1-2p}\right)^n \end{bmatrix},$$

we can symmetrize the operator (1.5.1), getting that each of the nonzero blocks are given by

$$\frac{1}{2}\mathcal{U} \begin{bmatrix} 1 & & \\ & \sqrt{1-2q} & \\ & & \sqrt{(1-2p)(1-2q)} \end{bmatrix} \mathcal{U}^*.$$

The Stieltjes transform associated with (1.5.1) is given by

$$B(z; W) = 2\mathcal{U} \begin{bmatrix} z - \sqrt{z^2 - 1} & & \\ & \frac{z - \sqrt{z^2 - (1-2q)}}{1-2q} & \\ & & \frac{z - \sqrt{z^2 - (1-2p)(1-2q)}}{(1-2p)(1-2q)} \end{bmatrix} \mathcal{U}^*. \quad (1.5.3)$$

Therefore, we get an absolutely continuous weight matrix given by

$$dW(x) = \frac{2}{\pi} \mathcal{U} D(x) \mathcal{U}^* dx,$$

where

$$D(x) = \begin{bmatrix} [\omega_1(x)]_+ & & \\ & [\omega_2(x)]_+ & \\ & & [\omega_3(x)]_+ \end{bmatrix},$$

where

$$\omega_1(x) = \sqrt{1-x^2}, \quad \omega_2(x) = \frac{\sqrt{1-2q-x^2}}{1-2q}, \quad \omega_3(x) = \frac{\sqrt{(1-2p)(1-2q)-x^2}}{(1-2p)(1-2q)}. \quad (1.5.4)$$

Here we are using the notation $[f(x)]_+ = f(x)$ if $f(x) \geq 0$ and 0 otherwise. Similar results can be obtained if we do not consider the compact form.

Now consider the same walk as before in (1.5.1), but adding a matrix B at the upper-left corner, i.e.

$$\tilde{\Phi} = \begin{bmatrix} B & C & & 0 \\ A & 0 & C & \\ & A & 0 & C \\ 0 & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (1.5.5)$$

where B is a matrix which we assume it can be written as

$$B = \frac{1}{2}\mathcal{U} \begin{bmatrix} b_1 & & \\ & b_2 & \\ & & b_3 \end{bmatrix} \mathcal{U}^*, \quad (1.5.6)$$

with \mathcal{U} defined by (1.5.2). According to Theorem 2.6 of [18], the Stieltjes transform $B(z; \tilde{W})$ associated with (1.5.5) can be written as $B(z; \tilde{W}) = (B(z; W)^{-1} - B)^{-1}$. Since we are assuming (1.5.6) and taking in mind (1.5.3), we obtain

$$B(z; \tilde{W}) = 2\mathcal{U} \begin{bmatrix} \frac{1}{z - \sqrt{z^2 - 1}} - b_1 & & \\ & \frac{1 - 2q}{z - \sqrt{z^2 - (1 - 2q)}} - b_2 & \\ & & \frac{(1 - 2p)(1 - 2q)}{z - \sqrt{z^2 - (1 - 2p)(1 - 2q)}} - b_3 \end{bmatrix}^{-1} \mathcal{U}^*.$$

After rationalization and some computations we obtain

$$B(z; \tilde{W}) = 2\mathcal{U} \begin{bmatrix} \frac{-z + b_1 + \sqrt{z^2 - 1}}{2b_1z - 1 - b_1^2} & & \\ & \frac{-z + b_2 - \sqrt{z^2 - (1 - 2q)}}{2b_2z - 1 + 2q - b_2^2} & \\ & & \frac{-z + b_3 + \sqrt{z^2 - (1 - 2p)(1 - 2q)}}{2b_3z - (1 - 2p)(1 - 2q) - b_3^2} \end{bmatrix} \mathcal{U}^*. \quad (1.5.7)$$

Therefore the weight matrix is given by $\tilde{W} = \tilde{W}_{ac} + \tilde{W}_d$, where the absolutely continuous part is given by

$$d\tilde{W}_{ac}(x) = \frac{2}{\pi} \mathcal{U} \begin{bmatrix} \frac{[\sqrt{1 - x^2}]_+}{1 + b_1^2 - 2b_1x} & & \\ & \frac{[\sqrt{1 - 2q - x^2}]_+}{1 - 2q + b_2^2 - 2b_2x} & \\ & & \frac{[\sqrt{(1 - 2p)(1 - 2q) - x^2}]_+}{(1 - 2p)(1 - 2q) + b_3^2 - 2b_3x} \end{bmatrix} \mathcal{U}^* dx.$$

Observe that the denominators are always nonnegative in the range of the definition of each square root. The discrete part \tilde{W}_d is given by three Dirac deltas located at the poles of the Stieltjes transform (1.5.7), i.e.

$$\tilde{W}_d(x) = \mathcal{U} \begin{bmatrix} \tilde{W}(\{z_1\}) \delta_{z_1}(x) & & \\ & \tilde{W}(\{z_2\}) \delta_{z_2}(x) & \\ & & \tilde{W}(\{z_3\}) \delta_{z_3}(x) \end{bmatrix} \mathcal{U}^*,$$

where

$$z_1 = \frac{1 + b_1^2}{2b_1}, \quad z_2 = \frac{1 - 2q + b_2^2}{2b_2}, \quad z_3 = \frac{(1 - 2p)(1 - 2q) + b_3^2}{2b_3},$$

and

$$\begin{aligned}\widetilde{W}(\{z_1\}) &= \frac{b_1^2 - 1}{b_1^2} \mathbf{1}_{\{b_1^2 > 1\}}, \\ \widetilde{W}(\{z_2\}) &= \frac{b_2^2 - (1 - 2q)}{b_2^2} \mathbf{1}_{\{b_2^2 > 1 - 2q\}}, \\ \widetilde{W}(\{z_3\}) &= \frac{b_3^2 - (1 - 2p)(1 - 2q)}{b_3^2} \mathbf{1}_{\{b_3^2 > (1 - 2p)(1 - 2q)\}}.\end{aligned}$$

Observe that in principle b_1, b_2 and b_3 can be taken as any real numbers, but we are interested in finding under what conditions the points z_1, z_2 and z_3 are located inside the interval $[-1, 1]$ (so that all the support of \widetilde{W} is inside the interval $[-1, 1]$). By the definition it is possible to see that $|z_1| \leq 1, |z_2| \leq 1, |z_3| \leq 1$, if and only if $b_1 = 1$, and

$$\begin{aligned}b_2 &\in [-1 - \sqrt{2q}, -1 + \sqrt{2q}] \cup [1 - \sqrt{2q}, 1 + \sqrt{2q}], \\ b_3 &\in [-1 - \sqrt{2(p+q-2pq)}, -1 + \sqrt{2(p+q-2pq)}] \cup [1 - \sqrt{2(p+q-2pq)}, 1 + \sqrt{2(p+q-2pq)}].\end{aligned}$$

Joining this with the conditions under we have positive jumps, we have that $\widetilde{W}(\{z_1\}) = 0$ and $\widetilde{W}(\{z_2\}), \widetilde{W}(\{z_3\})$ are positive if

$$\begin{aligned}b_2 &\in [-1 - \sqrt{2q}, -\sqrt{1-2q}] \cup (\sqrt{1-2q}, 1 + \sqrt{2q}], \\ b_3 &\in [-1 - \sqrt{2(p+q-2pq)}, -\sqrt{(1-2p)(1-2q)}] \cup (\sqrt{(1-2p)(1-2q)}, 1 + \sqrt{2(p+q-2pq)}].\end{aligned}$$

The particular case where $B \equiv A$ is given by $b_1 = 1, b_2 = 1 - 2q, b_3 = 2q - 1$. Therefore $z_1 = 1, z_2 = 1 - q, z_3 = p + q - 1, \widetilde{W}(\{z_1\}) = \widetilde{W}(\{z_2\}) = 0$ and

$$\widetilde{W}(\{z_3\}) = \frac{2(p-q)}{1-2q} \mathbf{1}_{\{p > q\}}.$$

The weight matrix is then given by $\widetilde{W} = \widetilde{W}_{ac} + \widetilde{W}_d$, where

$$d\widetilde{W}_{ac}(x) = \frac{1}{\pi} \mathcal{U} \left[\begin{array}{c} \left[\sqrt{\frac{1+x}{1-x}} \right]_+ \\ \frac{\left[\sqrt{1-2q-x^2} \right]_+}{(1-2q)(1-q-x)} \\ \frac{\left[\sqrt{(1-2p)(1-2q)-x^2} \right]_+}{(1-2q)(1-p-q+x)} \end{array} \right] \mathcal{U}^* dx. \quad (1.5.8)$$

and

$$\widetilde{W}_d(x) = \frac{p-q}{1-2q} \mathbf{1}_{\{p > q\}} \begin{bmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{bmatrix} \delta_{p+q-1}(x). \quad (1.5.9)$$

Observe that in this situation, as expected, the support of \widetilde{W} is inside the interval $[-1, 1]$.

Let us now study recurrence of this QMC in terms of the corresponding weight matrices. Note that the QMC determined by (1.5.1) is such that vertex 0 admits a transition to an absorbing state, so we have the transience of this walk with respect to such site. Let us prove this in terms of the associated measure. First, recall that the trace is invariant by the change of coordinates \mathcal{U} which, on its turn, does not depend on x . Therefore, we need only to examine the behavior of ω_1 and ω_3 in (1.5.4). Regarding ω_1 , a calculation gives that

$$\lim_{z \uparrow 1} \int_{-1}^1 \frac{\sqrt{1-x^2}}{1-zx} dx = \lim_{z \uparrow 1} \frac{\pi(z^2 - 1 + \sqrt{1-z^2})}{z^2 \sqrt{1-z^2}} = \pi,$$

so the above limit is finite. Regarding ω_3 , note that since $0 < p, q < 1$, we have $a := (1-2p)(1-2q) > 0$ if and only if both p and q are greater than $1/2$ or both are less than $1/2$. If this is the case, we have that $\omega_3(x) \geq 0$ if $x \in (-\sqrt{a}, \sqrt{a})$. If we write $q = p + \epsilon$ (with $\epsilon \in (\frac{1}{2} - p, 1 - p)$ if $\frac{1}{2} < p < 1$), we obtain

$$\lim_{z \uparrow 1} \int_{-\sqrt{a}}^{\sqrt{a}} \frac{\sqrt{a-x^2}}{1-zx} dx = \pi(1 - \sqrt{4p(1-p)} + 2\epsilon(1-2p)), \quad (1.5.10)$$

which is also a finite number (as expected, the term inside the root is always positive under the above restrictions). A similar reasoning holds in the case $0 < p < \frac{1}{2}$, where we write $q = p + \epsilon$, with $\epsilon \in (-p, \frac{1}{2} - p)$. In the case that ω_3 does not have a positive part, the trace computation is determined by ω_1 . Since $\mathcal{U}^*\rho$ is also a density matrix we conclude that, in every case, site 0 is transient with respect to any initial density.

Now considering (1.5.5) with $B = A$ (see (1.5.8) and (1.5.9)), we have, regarding $\tilde{\omega}_1$, that

$$\lim_{z \uparrow 1} \int_{-1}^1 \frac{1}{1-zx} \sqrt{\frac{1+x}{1-x}} dx = \lim_{z \uparrow 1} \frac{\pi(1+z-\sqrt{1-z^2})}{z\sqrt{1-z^2}} = \infty.$$

Regarding $\tilde{\omega}_3$, we note that the denominator is positive if $x \in (-\sqrt{a}, \sqrt{a})$, which can be seen as in the transient walk above (i.e., consider the cases for which $p, q \in (0, \frac{1}{2})$ or $p, q \in (\frac{1}{2}, 1)$). But then the limit to be examined is the same as for the transient walk, namely, eq. (1.5.10), which is finite. We have concluded that recurrence of site 0 depends on the initial choice of density matrix. For instance, the densities

$$\rho_\alpha = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \otimes |0\rangle\langle 0|, \quad \rho_\beta = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \otimes |0\rangle\langle 0|,$$

are such that site 0 is recurrent with respect to ρ_α but transient with respect to ρ_β . More generally, site 0 will be recurrent with respect to any density matrix $\rho \otimes |0\rangle\langle 0|$ for which $\rho_{11} > 0$. It would be interesting to find examples of matrices B at the block position $(0, 0)$ for which the resulting walks are irreducible (if this is in fact possible, a guess would be to obtain a change of coordinates \mathcal{V} distinct from \mathcal{U}).

Remark 1.9. *If B in (1.5.6) is not simultaneously diagonalizable with A and C , it is possible to derive again the weight matrix assuming that $B = \frac{1}{2}\mathcal{V}\text{diag}\{b_1, b_2, b_3\}\mathcal{V}^*$, where \mathcal{V} is unitary. The corresponding weight matrix will be also unitarily diagonalizable.*

1.6 Spectral analysis of QMCs on \mathbb{Z}

In this section, we treat the case of tridiagonal QMCs on the real line, that is, the set of vertices V will consist of the integers, thus the walk will have one-step transition probabilities from $|i\rangle$ to $|i-1\rangle, |i\rangle$ or $|i+1\rangle$ and there are no barriers. Starting from a tridiagonal QMC Φ on \mathbb{Z} , where each of the blocks of the matrix representation is of order $N^2 \times N^2$, we will construct a new tridiagonal QMC on $\mathbb{Z}_{\geq 0} \times \{1, 2\}$, where each of the blocks of the matrix representation is of dimension $2N^2 \times 2N^2$ with a possible barrier on site $|0\rangle$. This is what we call the **folding trick** and was introduced for the first time in [6]. Finally, recurrence of this type of walks will be discussed via an application of the Stieltjes transform.

Consider then the matrix representation for a tridiagonal QMC on \mathbb{Z} , given by

$$\Phi = \left[\begin{array}{ccc|ccc} \ddots & & \ddots & & & \\ & \ddots & & B_{-2} & C_{-1} & \\ & & & A_{-2} & B_{-1} & C_0 \\ \hline & & & & A_{-1} & B_0 & C_1 \\ & & & & & A_0 & B_1 & C_2 \\ & & & & & & A_1 & B_2 & C_3 \\ & & & & & & & \ddots & \ddots & \ddots \end{array} \right], \quad (1.6.1)$$

where each block A_k, B_k, C_k is an $N^2 \times N^2$ matrix given by a summation

$$X_k = \sum_{r=1}^{t_k} [Y_r], \quad Y_r \in M_N(\mathbb{C}), \quad [Y_r] = Y_r \otimes \bar{Y}_r,$$

and we assume that there exists a sequence of Hermitian matrices $(E_n)_{n \in \mathbb{Z}} \in M_{N^2}(\mathbb{C})$ and non-singular matrices $(R_n)_{n \in \mathbb{Z}} \in M_{N^2}(\mathbb{C})$ such that

$$\begin{aligned} A_n^* R_{n+1}^* R_{n+1} &= R_n^* R_n C_{n+1}, \quad n \geq 0 \\ R_{-n-1}^* R_{-n-1} C_{-n} &= A_{-n-1}^* R_{-n}^* R_{-n}, \quad n \geq 0, \end{aligned} \quad R_n B_n = E_n R_n, \quad n \in \mathbb{Z}. \quad (1.6.2)$$

The previous conditions coincide with those of Theorem 1.2 when we consider the first line with the walk restricted to $\mathbb{Z}_{\geq 0}$ and the second line with the walk restricted to $\mathbb{Z}_{< 0}$. Let us define

$$\Pi_j := R_j^* R_j \in M_{N^2}(\mathbb{C}), \quad j \in \mathbb{Z}.$$

Consider the two independent families of matrix-valued polynomials defined recursively from (1.6.1) as

$$\begin{aligned} Q_0^1(x) &= I_{N^2}, & Q_0^2(x) &= 0, \\ Q_{-1}^1(x) &= 0, & Q_{-1}^2(x) &= I_{N^2}, \\ xQ_n^\alpha(x) &= Q_{n+1}^\alpha(x)A_n + Q_n^\alpha(x)B_n + Q_{n-1}^\alpha(x)C_n, & \alpha &= 1, 2, \quad n \in \mathbb{Z}. \end{aligned} \tag{1.6.3}$$

and the block vectors $Q^\alpha(x) = (\dots, Q_{-2}^\alpha(x), Q_{-1}^\alpha(x), Q_0^\alpha(x), Q_1^\alpha(x), Q_2^\alpha(x), \dots)$, $\alpha = 1, 2$, are linearly independent solutions, depending on the initial values at $n = 0$, of the eigenvalue equation $xQ^\alpha(x) = Q^\alpha(x)\Phi$.

As in the classical case, we introduce the block tridiagonal matrix

$$\check{\Phi} = \begin{bmatrix} G_0 & N_1 & & & \\ M_0 & G_1 & N_2 & & \\ & M_1 & G_2 & N_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

where each block entry is a $2N^2 \times 2N^2$ matrix, given by

$$\begin{aligned} G_0 &= \begin{bmatrix} B_0 & A_{-1} \\ C_0 & B_{-1} \end{bmatrix}, & M_n &= \begin{bmatrix} A_n & 0 \\ 0 & C_{-n-1} \end{bmatrix}, & n &\geq 0, \\ G_n &= \begin{bmatrix} B_n & 0 \\ 0 & B_{-n-1} \end{bmatrix}, & N_n &= \begin{bmatrix} C_n & 0 \\ 0 & A_{-n-1} \end{bmatrix}, & n &\geq 1. \end{aligned}$$

The term *folding trick* comes from the transformation of the original walk Φ , whose graph is represented in Figure 1.2, to the QMC described by $\check{\Phi}$, which is represented by the folded walk in Figure 1.3.

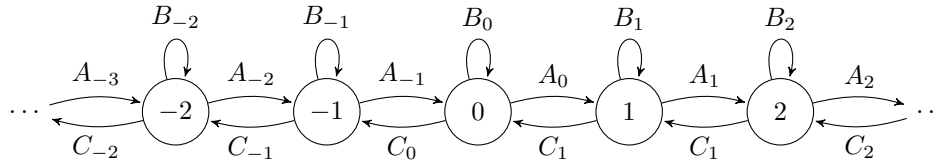


Figure 1.2: QMC Φ on \mathbb{Z} .

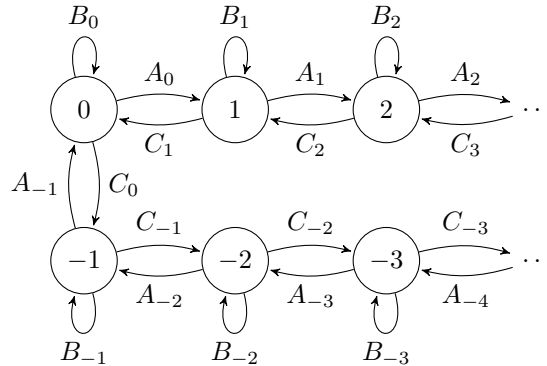


Figure 1.3: Folded walk of Φ on $\mathbb{Z}_{\geq 0} \times \{1, 2\}$ given by $\check{\Phi}$.

Note that $\check{\Phi}$ is a block tridiagonal matrix on $\mathbb{Z}_{\geq 0}$, thereby we can apply all the properties we have seen in previous sections. The following polynomials are defined in terms of (1.6.3),

$$Q_n(x) = \begin{bmatrix} Q_n^1(x) & Q_{-n-1}^1(x) \\ Q_n^2(x) & Q_{-n-1}^2(x) \end{bmatrix} \in M_{2N^2}(\mathbb{C}), \quad n \geq 0, \tag{1.6.4}$$

and these satisfy

$$\begin{aligned} x\mathcal{Q}_0(x) &= \mathcal{Q}_1(x)M_0 + \mathcal{Q}_0(x)G_0, \quad \mathcal{Q}_0(x) = I_{2N^2}, \\ x\mathcal{Q}_n(x) &= \mathcal{Q}_{n+1}(x)M_n + \mathcal{Q}_n(x)G_n + \mathcal{Q}_{n-1}(x)N_n, \quad n = 1, 2, \dots \end{aligned}$$

The leading coefficient of $\mathcal{Q}_n(x)$ is always a nonsingular matrix. Moreover, for

$$\check{R}_n := \begin{bmatrix} R_n & 0_{N^2} \\ 0_{N^2} & R_{-n-1} \end{bmatrix}, \quad n \geq 0, \quad \check{E}_0 := \begin{bmatrix} E_0 & R_0 A_{-1} R_{-1}^{-1} \\ R_{-1} C_0 R_0^{-1} & E_{-1} \end{bmatrix}, \quad \check{E}_n := \begin{bmatrix} E_n & 0_{N^2} \\ 0_{N^2} & E_{-n-1} \end{bmatrix}, \quad n \geq 1,$$

we see that the block matrices of $\check{\Phi}$ satisfy the conditions (1.6.2) for $n \geq 0$:

$$M_n^* \check{R}_{n+1}^* \check{R}_{n+1} = \check{R}_n^* \check{R}_n N_{n+1}, \quad \check{R}_n G_n = \check{E}_n \check{R}_n,$$

where matrices \check{R}_n are non-singular and \check{E}_n are Hermitian for all $n \geq 0$. Defining

$$\check{\Pi}_j := \check{R}_j^* \check{R}_j \in M_{2N^2}(\mathbb{C}), \quad j = 0, 1, 2, \dots,$$

the correspondence between $\check{\Pi}_j$ and Π_j is

$$\check{\Pi}_j := \begin{bmatrix} \Pi_j & 0_{N^2} \\ 0_{N^2} & \Pi_{-j-1} \end{bmatrix}.$$

By [18] (see also (1.3.3)), there exists a weight matrix W leading to the Karlin-McGregor formula for $\check{\Phi}$:

$$\check{\Phi}_{ji}^{(n)} = \check{\Pi}_j \int_{\mathbb{R}} x^n \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x). \quad (1.6.5)$$

Once we have found the weight matrix appearing on (1.6.5), we can also obtain the blocks $\Phi_{ji}^{(n)}$ of the original walk Φ . The key for this operation is the following proposition:

Proposition 1.10. *Assume that Φ is a QMC of the form (1.6.1). The relation between $\check{\Phi}_{ij}^{(n)}$ and $\Phi_{ij}^{(n)}$ is*

$$\check{\Phi}_{ji}^{(n)} = \begin{bmatrix} \Phi_{ji}^{(n)} & \Phi_{j,-i-1}^{(n)} \\ \Phi_{-j-1,i}^{(n)} & \Phi_{-j-1,-i-1}^{(n)} \end{bmatrix}, \quad i, j \in \mathbb{Z}_{\geq 0}. \quad (1.6.6)$$

Proof. Since $\check{\Phi}_{ji} = 0_{2d^2}$ for $|i-j| > 1$, it is easy to see that (1.6.6) holds for $n = 1$. So, suppose that (1.6.6) is valid for some n , then

$$\begin{aligned} \check{\Phi}_{ji}^{(n+1)} &= [\check{\Phi}\check{\Phi}^n]_{ji} = \sum_{k=0}^{\infty} \check{\Phi}_{jk} \check{\Phi}_{ki}^{(n)} = \check{\Phi}_{j,j-1} \check{\Phi}_{j-1,i}^{(n)} + \check{\Phi}_{jj} \check{\Phi}_{ji}^{(n)} + \check{\Phi}_{j,j+1} \check{\Phi}_{j+1,i}^{(n)} \\ &= M_{j-1} \check{\Phi}_{j-1,i}^{(n)} + G_j \check{\Phi}_{ji}^{(n)} + N_{j+1} \check{\Phi}_{j+1,i}^{(n)}. \end{aligned}$$

By the induction hypothesis and the result above,

$$\begin{aligned} \check{\Phi}_{ji}^{(n+1)} &= \\ & \begin{bmatrix} A_{j-1} & 0 \\ 0 & C_{-j} \end{bmatrix} \begin{bmatrix} \Phi_{j-1,i}^{(n)} & \Phi_{j-1,-i-1}^{(n)} \\ \Phi_{-j,i}^{(n)} & \Phi_{-j,-i-1}^{(n)} \end{bmatrix} + \begin{bmatrix} B_j & 0 \\ 0 & B_{-j-1} \end{bmatrix} \begin{bmatrix} \Phi_{j,i}^{(n)} & \Phi_{j,-i-1}^{(n)} \\ \Phi_{-j-1,i}^{(n)} & \Phi_{-j-1,-i-1}^{(n)} \end{bmatrix} \\ & + \begin{bmatrix} C_{j+1} & 0 \\ 0 & A_{-j-2} \end{bmatrix} \begin{bmatrix} \Phi_{j+1,i}^{(n)} & \Phi_{j+1,-i-1}^{(n)} \\ \Phi_{-j-2,i}^{(n)} & \Phi_{-j-2,-i-1}^{(n)} \end{bmatrix} \\ & = \begin{bmatrix} A_{j-1} \Phi_{j-1,i}^{(n)} + B_j \Phi_{j,i}^{(n)} + C_{j+1} \Phi_{j+1,i}^{(n)} & A_{j-1} \Phi_{j-1,-i-1}^{(n)} + B_j \Phi_{j,-i-1}^{(n)} + C_{j+1} \Phi_{j+1,-i-1}^{(n)} \\ C_{-j} \Phi_{-j,i}^{(n)} + B_{-j-1} \Phi_{-j-1,i}^{(n)} + A_{-j-2} \Phi_{-j-2,i}^{(n)} & C_{-j} \Phi_{-j,-i-1}^{(n)} + B_{-j-1} \Phi_{-j-1,-i-1}^{(n)} + A_{-j-2} \Phi_{-j-2,-i-1}^{(n)} \end{bmatrix} \\ & = \begin{bmatrix} \Phi_{ji}^{(n+1)} & \Phi_{j,-i-1}^{(n+1)} \\ \Phi_{-j-1,i}^{(n+1)} & \Phi_{-j-1,-i-1}^{(n+1)} \end{bmatrix}. \end{aligned}$$

□

Note that we can evaluate $\check{\Phi}_{ji}^{(n)}$ by (1.6.5) and then extract the block $\Phi_{ji}^{(n)}$ as in (1.6.6). Further, for a density operator $\rho \in M_N(\mathbb{C})$, we have

$$p_{ji;\rho}(n) = \text{Tr} \left(\Phi_{ji}^{(n)} \rho \right) = \text{Tr} \left(\begin{bmatrix} \Phi_{ji}^{(n)} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right) = \text{Tr} \left(\begin{bmatrix} I_{N^2} & 0 \\ 0 & 0 \end{bmatrix} \check{\Phi}_{ji}^{(n)} \begin{bmatrix} I_{N^2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right).$$

However, we would like to obtain the probability above avoiding the evaluation of $\check{\Phi}_{ji}^{(n)}$. This can be done via a generalization of the Karlin-McGregor formula on $\mathbb{Z}_{\geq 0}$. We proceed as follows: first, write the decomposition

$$dW(x) = \begin{bmatrix} dW_{11}(x) & dW_{12}(x) \\ dW_{21}(x) & dW_{22}(x) \end{bmatrix},$$

where $dW_{21}(x) = dW_{12}^*(x)$, since $dW(x)$ is positive definite. Then one has for $i, j \in \mathbb{Z}_{\geq 0}$,

$$\begin{aligned} \check{\Phi}_{ji}^{(n)} &= \check{\Pi}_j \int_{\mathbb{R}} x^n \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x) \\ &\stackrel{(1.6.4)}{=} \begin{bmatrix} \Pi_j & 0 \\ 0 & \Pi_{-j-1} \end{bmatrix} \int_{\mathbb{R}} x^n \begin{bmatrix} Q_j^1(x) & Q_{-j-1}^1(x) \\ Q_j^2(x) & Q_{-j-1}^2(x) \end{bmatrix}^* \begin{bmatrix} dW_{11}(x) & dW_{12}(x) \\ dW_{12}^*(x) & dW_{22}(x) \end{bmatrix} \begin{bmatrix} Q_i^1(x) & Q_{-i-1}^1(x) \\ Q_i^2(x) & Q_{-i-1}^2(x) \end{bmatrix} \\ &= \sum_{\alpha, \beta=1}^2 \begin{bmatrix} \Pi_j \int_{\mathbb{R}} x^n Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^\beta(x) & \Pi_j \int_{\mathbb{R}} x^n Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_{-i-1}^\beta(x) \\ \Pi_{-j-1} \int_{\mathbb{R}} x^n Q_{-j-1}^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^\beta(x) & \Pi_{-j-1} \int_{\mathbb{R}} x^n Q_{-j-1}^{\alpha*}(x) dW_{\alpha\beta}(x) Q_{-i-1}^\beta(x) \end{bmatrix}. \end{aligned}$$

Joining equation above and Proposition 1.10, we obtain the Karlin-McGregor formula for a QMC on \mathbb{Z} , given by

$$\Phi_{ji}^{(n)} = \sum_{\alpha, \beta=1}^2 \Pi_j \int_{\mathbb{R}} x^n Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^\beta(x), \quad \text{for any } i, j \in \mathbb{Z}, n \geq 0. \quad (1.6.7)$$

Conversely, if there exist weight matrices $dW_{11}(x), dW_{12}(x), dW_{22}(x)$ such that $\Phi_{ji}^{(n)}$ is of the form (1.6.7), then $\check{\Phi}_{ji}^{(n)}$ is of the form

$$\check{\Phi}_{ji}^{(n)} = \check{\Pi}_j \int_{\mathbb{R}} x^n \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x).$$

The weight matrix

$$W(x) = \begin{bmatrix} W_{11}(x) & W_{12}(x) \\ W_{12}^*(x) & W_{22}(x) \end{bmatrix},$$

is called the spectral block matrix of Φ .

Remark 1.11. Extending Theorem 1.5 to the QMC on \mathbb{Z} , we observe that, since $Q_0^1 = Q_{-1}^2 = I_N$ and $Q_0^2 = Q_{-1}^1 = 0_N$, we have

$$\begin{aligned} \sum_{n=0}^{\infty} p_{00;\rho}(n) &= \sum_{n=0}^{\infty} \text{Tr} \left[\Phi_{00}^{(n)} \text{vec}(\rho) \right] = \lim_{z \rightarrow 1} \sum_{n=0}^{\infty} z^n \text{Tr} \left[\Pi_0 \int_{\mathbb{R}} x^n Q_0^{1*}(x) dW_{11} Q_0^1(x) \text{vec}(\rho) \right] \\ &= \lim_{z \rightarrow 1} \sum_{n=0}^{\infty} \text{Tr} \left[\Pi_0 \int_{\mathbb{R}} (zx)^n(x) dW_{11}(x) \text{vec}(\rho) \right] = \lim_{z \rightarrow 1} \text{Tr} \left[\Pi_0 \frac{dW_{11}(x)}{1-zx} \text{vec}(\rho) \right] \\ &= \lim_{z \rightarrow 1} z \text{Tr} \left[\Pi_0 B(z^{-1}; W_{11}) \text{vec}(\rho) \right] = \lim_{z \rightarrow 1} \text{Tr} \left[\Pi_0 B(z; W_{11}) \text{vec}(\rho) \right], \end{aligned}$$

where $B(z; W)$ is the Stieltjes transform of a weight matrix W defined by (1.3.1). Analogously,

$$\sum_{n=0}^{\infty} p_{-1,-1;\rho}(n) = \lim_{z \rightarrow 1} \text{Tr} \left[\Pi_{-1} B(z; W_{22}) \text{vec}(\rho) \right].$$

Since we are assuming that Π_0 and Π_{-1} are positive definite matrices, vertex $|0\rangle$ is ρ -recurrent if and only if

$$\lim_{z \downarrow 1} \text{Tr} (B(z; W_{11}) \text{vec}(\rho)) = \infty,$$

and vertex $|-1\rangle$ is ρ -recurrent if and only if

$$\lim_{z \downarrow 1} \text{Tr} (B(z; W_{22}) \text{vec}(\rho)) = \infty.$$

Let us write the matrix Φ in the form

$$\Phi = \begin{bmatrix} \Phi^- & C \\ A & \Phi^+ \end{bmatrix}, \quad C = \begin{bmatrix} \vdots & \vdots & \vdots & \dots \\ 0 & 0 & 0 & \dots \\ C_0 & 0 & 0 & \dots \end{bmatrix}, \quad A = \begin{bmatrix} \dots & 0 & 0 & A_{-1} \\ \dots & 0 & 0 & 0 \\ \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix}, \quad (1.6.8)$$

$$\Phi^+ = \begin{bmatrix} B_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \quad \Phi^- = \begin{bmatrix} \ddots & & & & \\ & A_{-4} & B_{-3} & C_{-2} & \\ & & A_{-3} & B_{-2} & C_{-1} \\ & & & A_{-2} & B_{-1} \end{bmatrix}.$$

Our goal now is to write the Stieltjes transforms associated with the weight matrices $W_{\alpha\beta}$, $\alpha, \beta = 1, 2$, in terms of the Stieltjes transforms associated with W_{\pm} , the weight matrices associated with Φ^{\pm} . For that we will need the following lemma.

Lemma 1.12. [24] *Let \mathcal{B} be a Banach space and $T_1 : \text{Dom}(T_1) \rightarrow \mathcal{B}$ and $T_2 : \text{Dom}(T_2) \rightarrow \mathcal{B}$ be linear operators with block representations*

$$T_1 = \begin{bmatrix} A & 0 \\ C & D \end{bmatrix} \quad \text{and} \quad T_2 = \begin{bmatrix} A & C \\ 0 & D \end{bmatrix},$$

respectively. If A and D are invertible, then T_1 and T_2 have inverses, given by

$$T_1^{-1} = \begin{bmatrix} A^{-1} & 0 \\ -D^{-1}CA^{-1} & D^{-1} \end{bmatrix} \quad \text{and} \quad T_2^{-1} = \begin{bmatrix} A^{-1} & -A^{-1}CD^{-1} \\ 0 & D^{-1} \end{bmatrix}.$$

Denote by \mathbb{P}_k , \mathbb{P}_k^- and \mathbb{P}_k^+ the projection maps onto the space generated by site $|k\rangle$ on \mathbb{Z} , $\mathbb{Z}_{<0}$ and $\mathbb{Z}_{\geq 0}$, respectively, and $\mathbb{Q}_k = I_{\mathbb{Z}} - \mathbb{P}_k$, $\mathbb{Q}_k^- = I_{\mathbb{Z}_{<0}} - \mathbb{P}_k^-$, $\mathbb{Q}_k^+ = I_{\mathbb{Z}_{\geq 0}} - \mathbb{P}_k^+$. Then, applying Lemma 1.12, we obtain

$$\begin{aligned} \Phi(I - z\mathbb{Q}_0\Phi)^{-1} &= \begin{bmatrix} \Phi^- & C \\ A & \Phi^+ \end{bmatrix} \begin{bmatrix} I - z\Phi^- & -zC \\ 0 & I - z\mathbb{Q}_0^+\Phi^+ \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \Phi^- & C \\ A & \Phi^+ \end{bmatrix} \begin{bmatrix} (I - z\Phi^-)^{-1} & z(I - z\Phi^-)^{-1}C(I - z\mathbb{Q}_0^+\Phi^+)^{-1} \\ 0 & (I - z\mathbb{Q}_0^+\Phi^+)^{-1} \end{bmatrix} \\ &= \begin{bmatrix} \Phi^-(I - z\Phi^-)^{-1} & [z\Phi^-(I - z\Phi^-)^{-1} + I]C(I - z\mathbb{Q}_0^+\Phi^+)^{-1} \\ A(I - z\Phi^-)^{-1} & [zA(I - z\Phi^-)^{-1}C + \Phi^+](I - z\mathbb{Q}_0^+\Phi^+)^{-1} \end{bmatrix}. \end{aligned} \quad (1.6.9)$$

By the same arguments,

$$\begin{aligned} \Phi(I - z\mathbb{Q}_{-1}\Phi)^{-1} &= \begin{bmatrix} \Phi^- & C \\ A & \Phi^+ \end{bmatrix} \begin{bmatrix} I - z\mathbb{Q}_{-1}^-\Phi^- & 0 \\ -zA & I - z\Phi^+ \end{bmatrix}^{-1} \\ &= \begin{bmatrix} \Phi^- & C \\ A & \Phi^+ \end{bmatrix} \begin{bmatrix} (I - z\mathbb{Q}_{-1}^-\Phi^-)^{-1} & 0 \\ z(I - z\Phi^+)^{-1}A(I - z\mathbb{Q}_{-1}^-\Phi^-)^{-1} & (I - z\Phi^+)^{-1} \end{bmatrix} \\ &= \begin{bmatrix} (\Phi^- + zC(I - z\Phi^+)^{-1}A)(I - z\mathbb{Q}_{-1}^-\Phi^-)^{-1} & C(I - z\Phi^+)^{-1} \\ (I + z\Phi^+(I - z\Phi^+)^{-1})A(I - z\mathbb{Q}_{-1}^-\Phi^-)^{-1} & \Phi^+(I - z\Phi^+)^{-1} \end{bmatrix}, \end{aligned}$$

and

$$C(I - z\mathbb{Q}_0\Phi^+)^{-1} = \begin{bmatrix} \vdots & \vdots & \vdots & \dots \\ 0 & 0 & 0 & \dots \\ C_0 & 0 & 0 & \dots \end{bmatrix} \begin{bmatrix} I & 0 \\ * & * \end{bmatrix}^{-1} = \begin{bmatrix} \vdots & \vdots & \dots \\ 0 & 0 & \dots \\ C_0 & 0 & \dots \end{bmatrix}.$$

Denoting

$$\Phi^-(z) := \sum_{n=0}^{\infty} z^n (\Phi^-)^n = (I - z\Phi^-)^{-1}, \quad \Phi^+(z) := \sum_{n=0}^{\infty} z^n (\Phi^+)^n = (I - z\Phi^+)^{-1},$$

we obtain

$$\begin{aligned} F_{00}(z) &= z\mathbb{P}_0\Phi(I - z\mathbb{Q}_0\Phi)^{-1}\mathbb{P}_0 \\ &= \begin{bmatrix} 0 & & & \\ 0 & z\mathbb{P}_0^+ [zA(I - z\Phi^-)^{-1}C(I - z\mathbb{Q}_0\Phi^+)^{-1} + \Phi^+(I - z\mathbb{Q}_0^+\Phi^+)^{-1}] \mathbb{P}_0^+ & & \end{bmatrix}, \end{aligned}$$

where the only non-null block equals

$$\begin{aligned} &= z^2 \mathbb{P}_0^+ \left[\begin{array}{ccc} \cdots & A_{-1} \Phi_{-1,-2}^-(z) & A_{-1} \Phi_{-1,-1}^-(z) \\ \cdots & 0 & 0 \\ \cdots & 0 & 0 \\ & \vdots & \vdots \end{array} \right] \left[\begin{array}{cccc} \vdots & \vdots & \vdots & \\ 0 & 0 & 0 & \cdots \\ C_0 & 0 & 0 & \cdots \end{array} \right] \mathbb{P}_0^+ + F_{00}^+(z) \\ &= z^2 \mathbb{P}_0^+ \begin{bmatrix} A_{-1} \Phi_{-1,-1}^-(z) C_0 & 0 \\ 0 & 0 \end{bmatrix} \mathbb{P}_0^+ + F_{00}^+(z) = z^2 \begin{bmatrix} A_{-1} \Phi_{-1,-1}^-(z) C_0 & 0 \\ 0 & 0 \end{bmatrix} + F_{00}^+(z). \end{aligned}$$

Note that $F_{00}(z)$ has only one non-null $N^2 \times N^2$ block, due to the projections multiplying on the left and on the right-hand side. Without loss of generality, we will rewrite this kind of blocks as its only non-null block. For instance, we have

$$F_{00}(z) = z^2 A_{-1} \Phi_{-1,-1}^-(z) C_0 + F_{00}^+(z).$$

Applying twice the equation

$$F_{ji}(s) = \Phi_{jj}(s)^{-1} (\Phi_{ji}(s) - \delta_{ji} I), \quad (1.6.10)$$

for $F_{00}(z)$ and $F_{00}^+(z)$, we obtain

$$I - \Phi_{00}(z)^{-1} = z^2 A_{-1} \Phi_{-1,-1}^-(z) C_0 + I - \Phi_{00}^+(z)^{-1},$$

and after some algebra, we get

$$\Phi_{00}(z) = \Phi_{00}^+(z) (I - z^2 A_{-1} \Phi_{-1,-1}^-(z) C_0 \Phi_{00}^+(z))^{-1}. \quad (1.6.11)$$

Analogously,

$$\begin{aligned} F_{-1,-1}(z) &= z \mathbb{P}_{-1}^- [\Phi^- (I - z \mathbb{Q}_{-1} \Phi^-)^{-1} + z C (I - z \Phi^+)^{-1} A (I - z \mathbb{Q}_0 \Phi^-)^{-1}] \mathbb{P}_{-1}^- \\ &= F_{-1,-1}^-(z) + z^2 C \Phi_{00}^+(z) A_{-1}, \end{aligned}$$

thus

$$\begin{aligned} \Phi_{-1,-1}(z) &= (I - F_{-1,-1}(z))^{-1} = (I - F_{-1,-1}^-(z) - z^2 C \Phi_{00}^+(z) A_{-1})^{-1} \\ &= \Phi_{-1,-1}^-(z) (I - z^2 C_0 \Phi_{00}^+(z) A_{-1} \Phi_{-1,-1}^-(z))^{-1}, \end{aligned}$$

that is,

$$\Phi_{-1,-1}(z) = \Phi_{-1,-1}^-(z) (I - z^2 C_0 \Phi_{00}^+(z) A_{-1} \Phi_{-1,-1}^-(z))^{-1}. \quad (1.6.12)$$

Now we use equation (1.6.9) to obtain

$$F_{0,-1}(z) = z \mathbb{P}_0 A (I - z \Phi^-)^{-1} \mathbb{P}_{-1} = z A_{-1} \Phi_{-1,-1}^-(z),$$

which, together with equations (1.6.10) and (1.6.11), gives

$$\Phi_{0,-1}(z) = \Phi_{00}(z) F_{0,-1}(z) = z \Phi_{00}^+(z) (I - z^2 A_{-1} \Phi_{-1,-1}^-(z) C_0 \Phi_{00}^+(z))^{-1} A_{-1} \Phi_{-1,-1}^-(z). \quad (1.6.13)$$

In the same way,

$$F_{-1,0}(z) = z C_0 \Phi_{00}^+(z),$$

gives

$$\Phi_{-1,0}(z) = \Phi_{-1,-1}(z) F_{-1,0}(z) = z \Phi_{-1,-1}^-(z) (I - z^2 C_0 \Phi_{00}^+(z) A_{-1} \Phi_{-1,-1}^-(z))^{-1} C_0 \Phi_{00}^+(z). \quad (1.6.14)$$

We notice that the block matrices of both Φ^+ and Φ^- satisfy the conditions of equation (1.6.2), thus there are positive weight matrices W_{\pm} associated with Φ^{\pm} for which the associated polynomials are orthogonal. Then, we can write

$$\Pi_0^+ := \int_{\mathbb{R}} dW_+ \quad \text{and} \quad \Pi_{-1}^- := \int_{\mathbb{R}} dW_- .$$

Recalling that (see (1.3.4))

$$\Phi_{ji}(s) = \Pi_j \int_{\mathbb{R}} \frac{1}{1 - sx} Q_j^*(x) dW(x) Q_i(x),$$

and $Q_0^1 = Q_{-1}^2 = I_{N^2}$, $Q_0^2 = Q_{-1}^1 = 0_{N^2}$, we obtain the following Stieltjes transforms relations

$$\begin{aligned} B(z^{-1}; W_{11}) &= z\Pi_0^{-1}\Phi_{00}(z), & B(z^{-1}; W_{22}) &= z\Pi_{-1}^{-1}\Phi_{-1,-1}(z), & B(z^{-1}; W_{12}) &= z\Pi_{-1}^{-1}\Phi_{0,-1}(z), \\ B(z^{-1}; W_{21}) &= z\Pi_{-1}^{-1}\Phi_{-1,0}(z), & B(z^{-1}; W_+) &= z(\Pi_0^+)^{-1}\Phi_{00}^+(z), & B(z^{-1}; W_-) &= z(\Pi_{-1}^-)^{-1}\Phi_{-1,-1}^-(z). \end{aligned}$$

Joining with the identities (1.6.11),(1.6.12),(1.6.13),(1.6.14), the new Stieltjes transform identities are obtained:

$$\begin{aligned} \Pi_0 B(z; W_{11}) &= \Pi_0^+ B(z; W_+) (I - A_{-1} \Pi_{-1}^- B(z; W_-) C_0 \Pi_0^+ B(z; W_+))^{-1}, \\ \Pi_{-1} B(z; W_{22}) &= \Pi_{-1}^- B(z; W_-) (I - C_0 \Pi_0^+ B(z; W_+) A_{-1} \Pi_{-1}^- B(z; W_-))^{-1}, \\ \Pi_0 B(z; W_{12}) &= \Pi_0^+ B(z; W_+) (I - A_{-1} \Pi_{-1}^- B(z; W_-) C_0 \Pi_0^+ B(z; W_+))^{-1} A_{-1} \Pi_{-1}^- B(z; W_-), \\ \Pi_{-1} B(z; W_{21}) &= \Pi_{-1}^- B(z; W_-) (I - C_0 \Pi_0^+ B(z; W_+) A_{-1} \Pi_{-1}^- B(z; W_-))^{-1} C_0 \Pi_0^+ B(z; W_+). \end{aligned} \tag{1.6.15}$$

Sometimes the operators Π_i^+ and Π_i^- are equal to the identity operator. In this case, (1.6.15) are reduced to

$$\begin{aligned} \Pi_0 B(z; W_{11}) &= B(z; W_+) (I - A_{-1} B(z; W_-) C_0 B(z; W_+))^{-1}, \\ \Pi_{-1} B(z; W_{22}) &= B(z; W_-) (I - C_0 B(z; W_+) A_{-1} B(z; W_-))^{-1}, \\ \Pi_0 B(z; W_{12}) &= B(z; W_+) (I - A_{-1} B(z; W_-) C_0 B(z; W_+))^{-1} A_{-1} B(z; W_-), \\ \Pi_{-1} B(z; W_{21}) &= B(z; W_-) (I - C_0 B(z; W_+) A_{-1} B(z; W_-))^{-1} C_0 B(z; W_+). \end{aligned} \tag{1.6.16}$$

The above results will be applied in the following examples so that one is able to conclude recurrence properties of the walk.

Example 1.13. Let Φ be a homogeneous OQW on $\mathcal{S} = \mathbb{Z}$ with matrix representation

$$\Phi = \left[\begin{array}{cc|ccc} \ddots & \ddots & & & \\ \ddots & 0 & [L] & & \\ & [R] & 0 & & \\ \hline & & [R] & [L] & \\ & & & 0 & [L] \\ & & & [R] & 0 & [L] \\ & & & & & \ddots & \ddots & \ddots \end{array} \right], \quad R = \begin{bmatrix} \frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}, \quad L = \begin{bmatrix} \frac{\sqrt{2}}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix}.$$

In order to study recurrence or transience of the walk for each density operator on \mathbb{C}^2 , we will apply the Stieltjes transformation discussed above. The polynomials associated with Φ are

$$\begin{aligned} Q_0^1(x) &= I_4, & Q_0^2(x) &= 0_4 \\ Q_{-1}^1(x) &= 0_4, & Q_{-1}^2(x) &= I_4 \\ xQ_n^\alpha(x) &= Q_{n+1}^\alpha(x)[R] + Q_{n-1}^\alpha(x)[L], & \alpha, \beta &= 1, 2, \quad n \in \mathbb{Z}. \end{aligned}$$

The weight matrix associated with Φ^+ is

$$W_+(x) = \left[\begin{array}{ccc} \frac{3\sqrt{2}}{4\pi} \left[\sqrt{\left(4 - \frac{9x^2}{2}\right)} \right]_+ & & \\ & \frac{2^{1/4}\sqrt{3}}{2\pi} \left[\sqrt{(\sqrt{2}(2\sqrt{2} - 3x^2))} \right]_+ & \\ & & \frac{2^{1/4}\sqrt{3}}{2\pi} \left[\sqrt{(\sqrt{2}(2\sqrt{2} - 3x^2))} \right]_+ & \\ & & & \frac{2(x^2 - 1 + \sqrt{1-x^2})}{x^2(1-x^2)} \end{array} \right]$$

and since the matrices are diagonal, it is easy to see that $W_+(x) = W_-(x)$. The weight matrix $W_{11}(x)$ is obtained by an application of the first formula of (1.6.15),

$$B(z; W_{11}) = B(z; W_+) (I - A_{-1} B(z; W_+) C_0 B(z; W_+))^{-1},$$

and then we apply the Perron-Stieltjes inversion formula to obtain the referred measure. After some calculus, we have, for a density matrix $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$ on \mathbb{C}^2 ,

$$\begin{aligned} \sum_{n=0}^{\infty} p_{00;\rho}(n) &= \sum_{n=0}^{\infty} \text{Tr} \left(\Phi_{00}^{(n)} \text{vec}(\rho) \right) = \lim_{z \rightarrow 1} \text{Tr} \left(\Phi_{00}(z) \text{vec}(\rho) \right) = \lim_{z \rightarrow 1} \text{Tr} \left(B(W_{11}, z) \text{vec}(\rho) \right) \\ &\stackrel{(1.6.11)}{=} \lim_{z \rightarrow 1} \frac{1-a}{\sqrt{1-z^2}} + \frac{6a(8\sqrt{2}z^2 + 3\sqrt{18-16z^2} - 9\sqrt{2})}{(3\sqrt{2} + \sqrt{18-16z^2})(18-16z^2)} = \begin{cases} \infty, & \text{if } a < 1 \\ 3/2, & \text{if } a = 1 \end{cases}. \end{aligned}$$

Therefore site $|0\rangle$ is ρ -transient for $\rho = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ and ρ -recurrent otherwise.

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It is worth recalling that the weight matrix of the example above is a particular case of Proposition 1.3 of [28].

Example 1.14. Consider a QMC $\hat{\Phi}$ induced by the block matrix on $V = \{0, 1, 2, \dots\}$ given by

$$\Phi = \begin{bmatrix} B & rI & & & \\ tI & B & rI & & \\ & tI & B & rI & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad 0 < r, t < 1,$$

where $B = [\sigma_B]$, $\sigma_B = V_1^* \cdot V_1 + V_2^* \cdot V_2$, where V_1 and V_2 are the same as in the example appearing in Section 1.4. For simplicity we assume $0 < a, b, s < 1$, $a^2 + b^2 < 1$. In this way we have that $\text{Tr}(\sigma(X)) = s \text{Tr}(X)$, so we suppose that $r + s + t = 1$ in order to have that $\hat{\Phi}$ is trace-preserving. The matrices $R_n = \left(\sqrt{\frac{r}{t}}\right)^n$ satisfy the conditions of Equation (1.6.2), thus we denote

$$\Pi_n = R_n^* R_n = \left(\frac{r}{t}\right)^n.$$

By the classical symmetrization

$$\mathcal{Y} = \text{diag}(Y_0, Y_1, \dots), \quad Y_i = \left(\sqrt{\frac{r}{t}}\right)^{i-1} I_4, \quad i = 0, 1, \dots,$$

we obtain

$$J = \mathcal{Y} \Phi \mathcal{Y}^{-1} = \begin{bmatrix} B & kI & & & \\ kI & B & kI & & \\ & kI & B & kI & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad k = \sqrt{rt}.$$

The matrix B is symmetric, thus we can apply the spectral theorem to get

$$B = UDU^*, \quad D = s \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 - 2a^2 - 2b^2 & 0 \\ 0 & 0 & 0 & 1 - 2a^2 - 2b^2 \end{bmatrix},$$

where

$$U = \frac{\sqrt{2}}{2} \begin{bmatrix} 1 & \frac{a}{\sqrt{a^2+b^2}} & -\frac{b}{\sqrt{2a^2+b^2}} & -\frac{ab}{\sqrt{2a^2+b^2}\sqrt{a^2+b^2}} \\ 0 & \frac{b}{\sqrt{a^2+b^2}} & \frac{2a}{\sqrt{2a^2+b^2}} & -\frac{b^2}{\sqrt{2a^2+b^2}\sqrt{a^2+b^2}} \\ 0 & \frac{b}{\sqrt{a^2+b^2}} & 0 & \frac{\sqrt{2a^2+b^2}}{\sqrt{a^2+b^2}} \\ 1 & -\frac{a}{\sqrt{a^2+b^2}} & \frac{b}{\sqrt{2a^2+b^2}} & \frac{ab}{\sqrt{2a^2+b^2}\sqrt{a^2+b^2}} \end{bmatrix},$$

which gives

$$H(x) := U \begin{bmatrix} \frac{(s-x)^2}{k^2} - 4 & 0 & 0 & 0 \\ 0 & \frac{(s-x)^2}{k^2} - 4 & 0 & 0 \\ 0 & 0 & \frac{(s(1-2a^2-2b^2)-x)^2}{k^2} - 4 & 0 \\ 0 & 0 & 0 & \frac{(s(1-2a^2-2b^2)-x)^2}{k^2} - 4 \end{bmatrix} U^*,$$

and then the associated weight matrix is ([21])

$$dW(x) = \frac{1}{4\pi k(a^2 + b^2)} \times \left([w_1(x)]_+ \begin{bmatrix} 2a^2 + b^2 & ab & ab & b^2 \\ ab & b^2 & b^2 & -ab \\ ab & b^2 & b^2 & -ab \\ b^2 & -ab & -ab & 2a^2 + b^2 \end{bmatrix} + [w_2(x)]_+ \begin{bmatrix} b^2 & -ab & -ab & -b^2 \\ -ab & 2a^2 + b^2 & -b^2 & ab \\ -ab & -b^2 & 2a^2 + b^2 & ab \\ -b^2 & ab & ab & b^2 \end{bmatrix} \right) dx,$$

where

$$w_1(x) = \sqrt{4 - \frac{(s-x)^2}{k^2}}, \quad w_2(x) = \sqrt{4 - \frac{(s(1-2a^2-2b^2)-x)^2}{k^2}}.$$

Note that we can rewrite the weight matrix in terms of $w_1(x), w_2(x)$ and B by

$$\begin{aligned} dW(x) &= \frac{w_1(x)}{4\pi k(a^2 + b^2)} ((2a^2 + 2b^2 - 1)I_4 + \frac{1}{s}B) + \frac{w_2(x)}{4\pi k(a^2 + b^2)} (I_4 - \frac{1}{s}B) \\ &= \frac{1}{2k\pi} U \begin{bmatrix} [w_1(x)]_+ & & & \\ & [w_1(x)]_+ & & \\ & & [w_2(x)]_+ & \\ & & & [w_2(x)]_+ \end{bmatrix} U^*, \end{aligned} \quad (1.6.17)$$

whose support is given by

$$\begin{aligned} R := \text{supp}(dW) &= \{y \in \mathbb{R} : \frac{1}{k}(yI_4 - B) \text{ has an eigenvalue in } [-2, 2]\} \\ &= [-2k + s(1 - 2a^2 - 2b^2), s + 2k]. \end{aligned} \quad (1.6.18)$$

The Stieltjes transform of W is

$$B(z; W) = \int_R \frac{1}{2k\pi} U \begin{bmatrix} \frac{w_1(x)}{z-x} & & & \\ & \frac{w_1(x)}{z-x} & & \\ & & \frac{w_2(x)}{z-x} & \\ & & & \frac{w_2(x)}{z-x} \end{bmatrix} U^* dx, \quad (1.6.19)$$

where the integrals of the elements on the diagonal are

$$\begin{aligned} \int_R \frac{w_1(x)dx}{z-x} &= \frac{\pi}{k}(z - s - i\sqrt{4k^2 - (s-z)^2}) := 2k\pi h_1(z), \\ \int_R \frac{w_2(x)dx}{z-x} &= \frac{\pi}{k}(z - s(1 - 2a^2 - 2b^2) - i\sqrt{4k^2 - (s(1 - 2a^2 - 2b^2) - z)^2}) := 2k\pi h_2(z). \end{aligned} \quad (1.6.20)$$

The transience of this walk can be computed by using Theorem 1.5:

$$\begin{aligned} \lim_{z \downarrow 1} \text{Tr} \left[z \text{vec}^{-1} \left(B(z; W) \text{vec} \left(\begin{bmatrix} u & v \\ v^* & 1-u \end{bmatrix} \right) \right) \right] &= \frac{1 - s + \sqrt{s^2 - 2s + 1 - 4k}}{2k^2} \\ &= \frac{r + t + \sqrt{r^2 - 2rt + t^2}}{2rt} \\ &= \begin{cases} 1/r, & \text{if } t \geq r \\ 1/t, & \text{otherwise.} \end{cases} \end{aligned}$$

Now, for any density operator on \mathbb{C}^2 , we have by Remark 1.11 that

$$\sum_{n=0}^{\infty} p_{00;\rho}(n) = \lim_{z \rightarrow 1} \text{Tr}(\Pi_0^{-1} B(z; W_{11}) \text{vec}(\rho)) = \lim_{z \rightarrow 1} \frac{1}{\sqrt{z(z-4k)}} = \begin{cases} \frac{1}{\sqrt{1-4k}}, & \text{if } k < 1/4, \\ \infty, & \text{if } k = 1/4. \end{cases}$$

That is, the walk Φ (for $s = 2k$) is recurrent only when $k = 1/4$ and this happens for $t = r = 1/4$. For the general case we can follow the same steps to obtain

$$\sum_{n=0}^{\infty} p_{00;\rho}(n) = \lim_{z \rightarrow 1} \frac{1}{\sqrt{z^2 - 2sz + s^2 - 4k^2}} = \begin{cases} \frac{1}{\sqrt{1-2s+s^2-4k^2}}, & \text{if } s \neq 1-2k, \\ \infty, & \text{if } s = 1-2k. \end{cases}$$

Since we are assuming $r + s + t = 1$ and $k = \sqrt{rt}$, recurrence occurs when $0 = r - 2\sqrt{rt} + t = (\sqrt{r} - \sqrt{t})^2$, that is, when $t = r$.

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Remark 1.15. The example in Section 1.4 is such that $\sigma_B + t^2 I < I$, thus $\sum_{j=0}^{\infty} p_{0j;\rho}(n) < 1$ for some initial density operator ρ . This case is interpreted as a walk with a vertex named $|-1\rangle$, which is an absorbing vertex of the QMC, giving the correction $\sum_{j=-1}^{\infty} p_{0j;\rho}(n) = 1$. Now we point out the difference that an absorbing vertex on the QMC can take: the QMC Φ acting on $\mathbb{Z}_{\geq 0}$ has an absorbing vertex on site $|0\rangle$, and it is transient for any choice of t, r, s, a, b . On the other hand, for a, b, s fixed and $t = r = 1 - s$, the extended QMC on the integer line is always recurrent.

1.7 Non-symmetric weight matrices

As discussed previously, Theorem 1.2 describes the fundamental conditions regarding the existence of a positive weight matrix associated with a given QMC. Then, a natural question arises: is there anything that can be done in the case of QMC that do not satisfy such conditions, perhaps involving a non symmetric matrix of measures? Based on [37], we are in fact able to discuss a non-general Karlin-McGregor formula for Φ by using a different kind of polynomial orthogonality, where the term *non-general* means that we obtain the (i, j) -th block entry of Φ^n only for $i = 0$, which will allow us to obtain certain developments for the recurrence problems we are interested in.

We will be mostly interested in homogeneous QMCs, that is, operators Φ of the form (1.3.2), such that $A_n = A, B_n = B, C_{n+1} = C, \forall n = 0, 1, 2, \dots$ for some $A, B, C \in M_{N^2}(\mathbb{C})$. For instance, if we have a homogeneous QQW with

$$A = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, \quad C = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad B = 0_2,$$

then $A_0 C_1$ is not Hermitian, consequently it is not possible to obtain a proper positive definite weight matrix W that makes the corresponding matrix-valued polynomials orthogonal with respect to W . However, we may consider another kind of orthogonality for the associated polynomials in terms of a reasoning seen in [37]. For a homogeneous QMC, Theorem 3.4 of [37] assures the existence of a weight matrix W supported on some subspace Δ of \mathbb{C} such that the polynomials $Q_n(x)$, defined recursively by

$$\begin{aligned} Q_0(x) &= I_{N^2}, & Q_{-1}(x) &= 0_{N^2}, \\ xQ_n(x) &= Q_{n+1}(x)A_n + Q_n(x)B_n + Q_{n-1}(x)C_n, \end{aligned} \tag{1.7.1}$$

satisfy

$$\int_{\Delta} x^k dW(x) Q_n(x) = 0, \tag{1.7.2}$$

for all integers $n > k \geq 0$. Polynomials $\{Q_n(x)\}_{n \geq 0}$ for which there exists a weight matrix W satisfying (1.7.2) are called **semi-orthogonal polynomials** with respect to W . Since this concept of orthogonality is weaker, the Karlin-McGregor formula for non-symmetric QMCs will be weaker as well. Nevertheless, we will be able to obtain an application of such construction for the problem of recurrence.

For completeness, let us derive the Karlin-McGregor formula for non-symmetric weight matrices with the necessary adaptations with respect to semi-orthogonality. We have $x^n Q(x) = Q(x)\Phi^n$, where $Q(x) = (Q_0(x), Q_1(x), \dots)$. Component-wise,

$$x^n Q_r(x) = \sum_{k=0}^{\infty} Q_k(x)\Phi_{kr}^{(n)}. \quad (1.7.3)$$

Fix $i, j \in \mathbb{Z}_{\geq 0}$ vertices. Fix a time parameter n with the extra condition $n \geq i$, then multiply $Q_j^*(x)$ on the left-hand side of (1.7.3) with $r = j + i$ and integrate on Δ to obtain

$$\int_{\Delta} x^n Q_j^*(x) dW(x) Q_{j+i}(x) = \sum_{k=0}^{\infty} \int_{\Delta} Q_j^*(x) dW(x) Q_k(x) \Phi_{k, j+i}^{(n)} \stackrel{(1.7.2)}{=} \sum_{k=0}^j \int_{\Delta} Q_j^*(x) dW(x) Q_k(x) \Phi_{k, j+i}^{(n)}. \quad (1.7.4)$$

Hypothesis $n < i$ in this situation would make the integral on the left-hand side of (1.7.4) to vanish, by an application of (1.7.2). The same idea is applied to the right-hand side of (1.7.4), where we want the sum of integrals to become only one term, which happens for the particular case $j = 0$:

$$\int_{\Delta} x^n Q_0^*(x) dW(x) Q_i(x) = \int_{\Delta} Q_0^*(x) dW(x) Q_0(x) \Phi_{0,i}^{(n)}.$$

Hence, we obtain the Karlin McGregor Formula for non-symmetric QMCs:

$$\Phi_{0,i}^{(n)} = \left(\int_{\Delta} dW(x) \right)^{-1} \int_{\Delta} x^n dW(x) Q_i(x), \quad i \in \mathbb{Z}_{\geq 0}, \quad n = 0, 1, 2, \dots \quad (1.7.5)$$

This equation gives, for a fixed vertex $i \in \mathbb{Z}_{\geq 0}$, the $(0, i)$ -th block entry of Φ^n for any time $n \geq 0$. The case $n \geq i$ follows from the construction above and, for $n < i$, $\Phi_{0,i}^{(n)} = 0_{d^2}$ since Φ is block tridiagonal and the right-hand side of equation (1.7.5) vanishes by equation (1.7.2). Therefore, we can obtain the probability for the walker to reach site $|0\rangle$, given that it started on site $|i\rangle$ with initial state $\rho \in M_N(\mathbb{C})$, by

$$p_{0i;\rho}(n) = \text{Tr} \left(\Phi_{0,i}^{(n)} \rho \right) = \text{Tr} \left(\left(\int_{\Delta} dW(x) \right)^{-1} \int_{\Delta} x^n dW(x) Q_i(x) \rho \right), \quad i \in \mathbb{Z}_{\geq 0}, \quad n = 0, 1, 2, \dots$$

Regarding the case of a finite number of vertices $V = \{0, 1, 2, \dots, N\}$, we proceed as expected: the eigenvalues of Φ are the roots of the determinant of

$$R_{N+1}(x) = Q_N(x)(xI - B_N) - Q_{N-1}(x)C_N,$$

where $\{Q_n(x)\}_{n=0}^N$ are the polynomials associated with Φ . Suppose that Φ describes a homogeneous QMC, then $\{Q_n(x)\}_{n=0}^N$ are semi-orthogonal with respect to the measure

$$W_k = \lim_{z \rightarrow \lambda_k} (\lambda_k - z) ([\Phi] - zI)_{00}^{-1},$$

that is,

$$\sum_{k=1}^{\tau} \lambda_k^i W_k Q_j(\lambda_k) = 0,$$

for $j > i$, where τ is the number of eigenvalues of Φ counting multiplicities. The Karlin-McGregor formula for this kind of QMC is then

$$\Phi_{0j}^{(n)} = \sum_{k=1}^{\tau} \lambda_k^n W_k Q_j(\lambda_k).$$

Example 1.16. Let Φ be the homogeneous OQW with 3 vertices defined by

$$\Phi = \begin{bmatrix} 0 & [C] & 0 \\ [A] & 0 & [C] \\ 0 & [A] & 0 \end{bmatrix}, \quad A = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} \quad C = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}. \quad (1.7.6)$$

The polynomials associated with Φ are

$$Q_0(x) = I_4, \quad Q_1(x) = x[A]^{-1}, \quad Q_2(x) = xQ_1(x)[A]^{-1} - [C][A]^{-1}.$$

Hence the eigenvalues of Φ are precisely the roots of

$$R_3(x) = xQ_2(x) - Q_1(x)[C],$$

which are

$$\begin{aligned} \lambda_1 &= 0, & \lambda_2 &= -\frac{\sqrt{2}}{3}, & \lambda_3 &= \frac{\sqrt{2}}{3}, & \lambda_4 &= -\frac{\sqrt{3}}{3}, & \lambda_5 &= \frac{\sqrt{3}}{3}, \\ \lambda_6 &= -\frac{\sqrt{2\sqrt{6}-3}}{6} + i\frac{\sqrt{2\sqrt{6}+3}}{6}, & \lambda_7 &= \frac{\sqrt{2\sqrt{6}-3}}{6} - i\frac{\sqrt{2\sqrt{6}+3}}{6}, \\ \lambda_8 &= -\frac{\sqrt{2\sqrt{6}-3}}{6} - i\frac{\sqrt{2\sqrt{6}+3}}{6}, & \lambda_9 &= \frac{\sqrt{2\sqrt{6}-3}}{6} + i\frac{\sqrt{2\sqrt{6}+3}}{6}, \end{aligned}$$

λ_1 has multiplicity 4. Joining the results of [22] and [37], we obtain

$$\sum_{k=1}^9 Q_i^*(\lambda_k)W_kQ_j(\lambda_k) = \begin{cases} 0_4, & \text{if } i > j \\ F_{ij} \in M_4(\mathbb{C}), \text{ not necessarily null} & \text{if } i \leq j \end{cases},$$

where

$$\begin{aligned} W_k &= \lim_{z \rightarrow \lambda_k} (\lambda_k - z)([\Phi] - zI_{12})_{00}^{-1} \\ &= \lim_{z \rightarrow \lambda_k} \left((\lambda_k - z) \frac{1}{81z^6 - 3z^2 - 2} \times \right. \\ &\quad \left. \begin{bmatrix} -\frac{81z^6 + 9z^4 - 2z^2 - 2}{z} & -\frac{27z^4 + 6z^2 - 1}{3z} & -\frac{27z^4 + 6z^2 - 1}{3z} & -z(9z^2 + 5) \\ \frac{27z^4 + 6z^2 - 1}{3z} & -\frac{729z^8 - 162z^6 - 54z^4 - z^2 + 2}{z(9z^2 - 2)} & \frac{z(81z^4 + 27z^2 - 14)}{9z^2 - 2} & \frac{21z^2 + 1}{3z} \\ \frac{27z^4 + 6z^2 - 1}{3z} & \frac{z(81z^4 + 27z^2 - 14)}{9z^2 - 2} & -\frac{729z^8 - 162z^6 - 54z^4 - z^2 + 2}{z(9z^2 - 2)} & \frac{21z^2 + 1}{3z} \\ -z(9z^2 + 5) & -\frac{21z^2 + 1}{3z} & -\frac{21z^2 + 1}{3z} & -z(81z^4 + 7) \end{bmatrix} \right). \end{aligned}$$

Those values are

$$W_1 = \frac{1}{6} \begin{bmatrix} 6 & 1 & 1 & 0 \\ -1 & 3 & 0 & 1 \\ -1 & 0 & 3 & 1 \\ 0 & -1 & -1 & 0 \end{bmatrix}, \quad W_2 = W_3 = \frac{1}{8} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad W_4 = W_5 = \frac{1}{12} \begin{bmatrix} 1 & 1 & 1 & 2 \\ -1 & -1 & -1 & -2 \\ -1 & -1 & -1 & -2 \\ 2 & 2 & 2 & 4 \end{bmatrix},$$

$$W_6 = W_7 = \begin{bmatrix} \frac{3-i\sqrt{5}}{-90+6i\sqrt{15}} & -\frac{1}{12} & -\frac{1}{12} & \frac{7-i\sqrt{15}}{-30+18i\sqrt{15}} \\ -\frac{1}{12} & \frac{5}{30-6i\sqrt{15}} & \frac{5}{30-6i\sqrt{15}} & \frac{-15-7i\sqrt{15}}{-180+12i\sqrt{15}} \\ -\frac{1}{12} & \frac{5}{30-6i\sqrt{15}} & \frac{5}{30-6i\sqrt{15}} & \frac{-15-7i\sqrt{15}}{-180+12i\sqrt{15}} \\ \frac{7-i\sqrt{15}}{-30+18i\sqrt{15}} & \frac{15+7i\sqrt{15}}{-180+12i\sqrt{15}} & \frac{15+7i\sqrt{15}}{-180+12i\sqrt{15}} & \frac{11+3i\sqrt{15}}{-30+18i\sqrt{15}} \end{bmatrix},$$

$$W_8 = W_9 = \begin{bmatrix} \frac{-3-i\sqrt{5}}{-90+6i\sqrt{15}} & -\frac{1}{12} & -\frac{1}{12} & \frac{-7-i\sqrt{15}}{-30+18i\sqrt{15}} \\ -\frac{1}{12} & -\frac{5}{30-6i\sqrt{15}} & -\frac{5}{30-6i\sqrt{15}} & \frac{15-7i\sqrt{15}}{-180+12i\sqrt{15}} \\ -\frac{1}{12} & -\frac{5}{30-6i\sqrt{15}} & -\frac{5}{30-6i\sqrt{15}} & \frac{15-7i\sqrt{15}}{-180+12i\sqrt{15}} \\ \frac{-7-i\sqrt{15}}{-30+18i\sqrt{15}} & \frac{-15+7i\sqrt{15}}{-180+12i\sqrt{15}} & \frac{-15+7i\sqrt{15}}{-180+12i\sqrt{15}} & \frac{-11+3i\sqrt{15}}{30+18i\sqrt{15}} \end{bmatrix}.$$

A simple calculation shows that

$$dW(x) = \sum_{k=1}^9 W_k = I_4.$$

Therefore the Karlin-McGregor formula for this OQW is

$$\Phi_{0,i}^{(n)} = \left(\int_{\Delta} dW(x) \right)^{-1} \int_{\Delta} x^n dW(x) Q_i(x) = \sum_{k=1}^9 \lambda_k^n W_k Q_i(\lambda_k), \quad i = 0, 1, 2, \quad n \geq i.$$

For instance, we have

$$\Phi_{0,2}^{(10)} = \sum_{k=1}^9 \lambda_k^n W_k Q_2(\lambda_k) = \frac{1}{59049} \begin{bmatrix} 63 & -45 & -45 & 54 \\ -27 & 26 & 10 & -45 \\ -27 & 10 & 26 & -45 \\ 90 & -27 & -27 & 63 \end{bmatrix},$$

which agrees with the corresponding block of Φ^{10} . The probability of the walker to be on site $|0\rangle$ after 10 steps, given that it started on site $|2\rangle$ with initial density operator $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$ is

$$p_{02;\rho}(10) = \text{Tr} \left[\text{vec}^{-1} \left(\frac{1}{59049} \begin{bmatrix} 63 & -45 & -45 & 54 \\ -27 & 26 & 10 & -45 \\ -27 & 10 & 26 & -45 \\ 90 & -27 & -27 & 63 \end{bmatrix} \begin{bmatrix} a \\ b \\ b^* \\ 1-a \end{bmatrix} \right) \right] = \frac{13 + 4a - 16\text{Re}(b)}{6561}.$$

Analogously,

$$p_{02;\rho}(2) = \frac{1 + 4a - 4\text{Re}(b)}{9}, \quad p_{02;\rho}(3) = 0, \quad p_{02;\rho}(4) = \frac{1}{27}.$$

However, the general Karlin-McGregor formula does not apply for this OQW. Indeed, we have

$$\Phi_{2,2}^{(2)} = \frac{1}{9} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 1 \\ 0 & -1 & 0 & 1 \\ 1 & -1 & -1 & 1 \end{bmatrix},$$

and

$$\frac{1}{18} \begin{bmatrix} 15 & 37 & 37 & 82 \\ 24 & 32 & 30 & 18 \\ 24 & 30 & 32 & 18 \\ 25 & 29 & 29 & 6 \end{bmatrix} = \left(\sum_{k=1}^9 Q_2^*(\lambda_k) W_k Q_2(\lambda_k) \right)^{-1} \left(\sum_{k=1}^9 \lambda_k^2 Q_2^*(\lambda_k) W_k Q_2(\lambda_k) \right) \neq \Phi_{2,2}^{(2)}.$$

The reason why this is happening is that Q_2 and Q_0 are not orthogonal, since

$$\sum_{k=1}^9 Q_0^*(\lambda_k) W_k Q_2(\lambda_k) = \frac{1}{4} \begin{bmatrix} -2 & 4 & 4 & 28 \\ -8 & -21 & -21 & -62 \\ -8 & -21 & -21 & -62 \\ 4 & 18 & 18 & 68 \end{bmatrix}.$$

Let us study now the case of a larger number of sites n . Consider

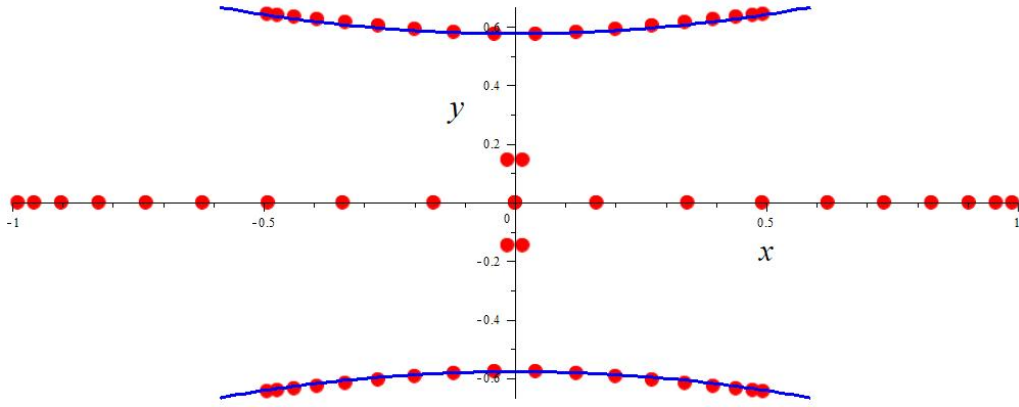
$$\Phi = \begin{bmatrix} 0 & [C] & & & \\ [A] & 0 & [C] & & \\ & & \ddots & \ddots & \ddots \\ & & & [A] & 0 & [C] \\ & & & & [A] & 0 \end{bmatrix} \in M_{4n}(\mathbb{C}),$$

where A, C are defined by (1.7.6). The compact form of Φ is given by

$$\check{\Phi} = \begin{bmatrix} 0 & C & & & \\ A & 0 & C & & \\ & \ddots & \ddots & \ddots & \\ & & A & 0 & C \\ & & & A & 0 \end{bmatrix} \in M_{3n}(\mathbb{C}), \quad A = \frac{1}{3} \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 1 & -2 & 1 \end{bmatrix}, \quad C = \frac{1}{3} \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix}.$$

If we evaluate the eigenvalues $\lambda_1, \dots, \lambda_{3n}$ of $\check{\Phi}$ and put them on the complex plane, the outcome is a graph of the form represented in Figure 1.4. Each dot represents an eigenvalue of $\check{\Phi}$.

◇

Figure 1.4: Eigenvalues of $\check{\Phi}$ with 20 vertices.

Example 1.17. Let Φ be a homogeneous QMC with 5 vertices defined by

$$\Phi = \begin{bmatrix} [B_0] & [C_1] + [C_2] & 0 & 0 & 0 \\ [A_1] + [A_2] & [B_0] & [C_1] + [C_2] & 0 & 0 \\ & [A_1] + [A_2] & [B_0] & [C_1] + [C_2] & 0 \\ & & [A_1] + [A_2] & [B_0] & [C_1] + [C_2] \\ & & & [A_1] + [A_2] & [B_0] \end{bmatrix},$$

where

$$B_0 = \frac{\sqrt{5}}{5} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, C_1 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, C_2 = \frac{\sqrt{5}}{5} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, A_1 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, A_2 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}.$$

In compact form, Φ becomes

$$\check{\Phi} = \begin{bmatrix} B & C & 0 & 0 & 0 \\ A & B & C & 0 & 0 \\ 0 & A & B & C & 0 \\ 0 & 0 & A & B & C \\ 0 & 0 & 0 & A & B \end{bmatrix}, B = \frac{1}{5} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, A = \frac{1}{5} \begin{bmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 2 & 0 & 2 \end{bmatrix}, C = \frac{1}{5} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}.$$

The eigenvalues of $\check{\Phi}$ are given by

$$\lambda_1 = 0, \lambda_2 = -\frac{1}{5}, \lambda_3 = \frac{1}{5}, \lambda_4 = \frac{3}{5}, \lambda_5 = -\frac{\sqrt{2}}{5}, \lambda_6 = \frac{\sqrt{2}}{5},$$

$$\lambda_7 = -\frac{\sqrt{6}}{5}, \lambda_8 = \frac{\sqrt{6}}{5}, \lambda_9 = \frac{1}{5} - \frac{2\sqrt{3}}{5}, \lambda_{10} = \frac{1}{5} + \frac{2\sqrt{3}}{5},$$

where $\lambda_1, \lambda_5, \lambda_6, \lambda_7$ and λ_8 have multiplicity 2. The weight matrix is given by

$$W_1 = \begin{bmatrix} 1/3 & 0 & 0 \\ 0 & 1/3 & 0 \\ 2/11 & 0 & 0 \end{bmatrix}, W_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -1/2 & 0 & 1/4 \end{bmatrix}, W_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -8/15 & 0 & 1/3 \end{bmatrix}, W_4 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1/6 & 0 & 1/4 \end{bmatrix}$$

$$W_5 = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/4 & 0 \\ \frac{104+\sqrt{2}}{292} & 0 & 0 \end{bmatrix}, W_6 = \begin{bmatrix} 1/4 & 0 & 0 \\ 0 & 1/4 & 0 \\ \frac{104-\sqrt{2}}{292} & 0 & 0 \end{bmatrix}, W_7 = \begin{bmatrix} 1/12 & 0 & 0 \\ 0 & 1/12 & 0 \\ -\frac{17\sqrt{6}}{20} - \frac{67}{30} & 0 & 0 \end{bmatrix},$$

$$W_8 = \begin{bmatrix} 1/12 & 0 & 0 \\ 0 & 1/12 & 0 \\ \frac{17\sqrt{6}}{20} - \frac{67}{30} & 0 & 0 \end{bmatrix}, W_9 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{10529}{4818} + \frac{3016\sqrt{3}}{2409} & 0 & 1/12 \end{bmatrix}, W_{10} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \frac{10529}{4818} - \frac{3016\sqrt{3}}{2409} & 0 & 1/12 \end{bmatrix}.$$

The polynomials $Q_n(x)$ associated with $\check{\Phi}$ (see (1.7.1)) satisfy (1.7.2), that is,

$$\sum_{j=1}^{10} \lambda_j^n W(j) Q_k(\lambda_j) = 0,$$

for all integers $n > k \geq 0$. As an example, formula (1.7.5) gives, for $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$, that

$$\check{\Phi}_{0,3}^{(7)} = \sum_{k=1}^{10} \lambda_k^7 W(k) Q_3(\lambda_k) = \frac{8}{78125} \begin{bmatrix} 52 & 0 & 0 \\ 0 & 52 & 0 \\ 907 & 0 & 579 \end{bmatrix} \implies p_{03,\rho}(7) = \frac{4632 + 608a}{15625}.$$

◇

Let us now consider the case of infinite vertices. For that we recall that the Stieltjes transform $B(z; W)$ associated with a homogeneous QMC Φ with matrix representation

$$\Phi = \begin{bmatrix} B & C & & & \\ A & B & C & & \\ & A & B & C & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

where $A, C \in M_{N^2}(\mathbb{C})$ are non-singular, is given by

$$B(z; W) = (z - B - CB(z; W)A)^{-1}. \quad (1.7.7)$$

Similarly, the Stieltjes transform $B(z; \widetilde{W})$ associated with a QMC $\widetilde{\Phi}$ with matrix representation

$$\widetilde{\Phi} = \begin{bmatrix} B_0 & C & & & \\ A_0 & B & C & & \\ & A & B & C & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

where $A_0, A, C \in M_{N^2}(\mathbb{C})$ are non-singular, is given by

$$B(z; \widetilde{W}) = (z - B_0 - CB(z; W)A_0)^{-1}. \quad (1.7.8)$$

Example 1.18. Take $V = \mathbb{Z}_{\geq 0}$ and matrices $R = L = \frac{1}{\sqrt{2}}I_2$,

$$B_1 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad B_2 = \frac{\sqrt{5}}{5} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_1 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, \quad R_2 = \frac{\sqrt{5}}{5} \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}.$$

We define a QMC on V whose compact form is

$$\check{\Phi} = \begin{bmatrix} B_0 & C & & & \\ A_0 & 0 & C & & \\ & A & 0 & C & \\ & & A & 0 & C \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \quad B_0 = \check{B}_1 + \check{B}_2, \quad A_0 = \check{R}_1 + \check{R}_2, \quad C = \check{L}, \quad A = \check{R}.$$

Denote by $\check{\Phi}_0$ the matrix

$$\check{\Phi}_0 = \begin{bmatrix} 0 & C & & & \\ A & 0 & C & & \\ & A & 0 & C & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

and W, W_0 the weight matrices associated with $\check{\Phi}$ and $\check{\Phi}_0$, respectively. Using (1.7.7) and (1.7.8) we obtain

$$B(z; W_0)(z) = (2z + 2\sqrt{z^2 - 1})I_3.$$

and

$$B(z; W) = \frac{5}{5z^2 - 6z + 5} \begin{bmatrix} 2\sqrt{z^2 - 1} + 3z - 1 & 0 & 0 \\ 0 & 2\sqrt{z^2 - 1} + 3z - 1 & 0 \\ \frac{2((25z^2 - 20z - 1)\sqrt{z^2 - 1} + 25z^3 - 20z^2 - 13z + 8)}{5z^2 - 18z + 13} & 0 & 2\sqrt{z^2 - 1} + 3z - 3 \end{bmatrix}.$$

With the Stieltjes transform, we may obtain the associated weight matrix for $\check{\Phi}$ by applying the Perron-Stieltjes inversion formula. A simple calculation shows that the weight matrix W is given by

$$W(x) = \frac{5}{\pi(5x^2 - 6x + 5)} \begin{bmatrix} 2\sqrt{1 - x^2} & 0 & 0 \\ 0 & 2\sqrt{1 - x^2} & 0 \\ \frac{2(25x^2 - 20x - 1)\sqrt{1 - x^2}}{5x^2 - 18x + 13} & 0 & 2\sqrt{1 - x^2} \end{bmatrix}, \quad x \in [-1, 1].$$

We now have

$$\int_{-1}^1 Q_i^*(x) dW(x) Q_j(x) = 0, \quad i > j,$$

thus formula (1.7.5) holds.

Let us now analyze recurrence of the first vertex of both QMCs $\check{\Phi}$ and $\check{\Phi}_0$. By (1.3.5), we are able to conclude whether the walk is recurrent just by considering the Stieltjes transform associated with the QMC, that is, we do not need to obtain the explicit weight matrix associated with the referred QMC. Above, we determined the weight matrix for completeness, and in order to write the transitions probabilities of the walk described by $\check{\Phi}$ using the Karlin-McGregor formula.

Applying limits to the Stieltjes transform $B(z; W_0)$ and $B(z; W)$ associated with $\check{\Phi}_0$ and $\check{\Phi}$, respectively, we obtain

$$\lim_{z \rightarrow 1} \text{Tr}(B(z, W_0)\rho) = \lim_{z \rightarrow 1} 2z + 2\sqrt{z^2 - 1} = 2,$$

and using l'Hospital's rule we get

$$\lim_{z \rightarrow 1} \text{Tr}(B(z, W)\rho) = \infty,$$

for any density operator $\rho \in M_2(\mathbb{C})$. Therefore, by (1.3.5), the first vertex $|0\rangle$ is transient for $\check{\Phi}_0$ and recurrent for $\check{\Phi}$.

◇

Example 1.19. Take $V = \mathbb{Z}_{\geq 0}$ and matrices

$$R_1 = \frac{1}{\sqrt{7}} \begin{bmatrix} 1 & 0 \\ -1 & \sqrt{3} \end{bmatrix}, \quad R_2 = \frac{1}{\sqrt{7}} \begin{bmatrix} 1 & 0 \\ 1 & \sqrt{3} \end{bmatrix}, \quad L_1 = \frac{1}{\sqrt{7}} \begin{bmatrix} \sqrt{3} & 0 \\ 0 & 1 \end{bmatrix}. \quad (1.7.9)$$

We define a QMC on V whose compact form is

$$\check{\Phi} = \begin{bmatrix} 0 & C & & & \\ A & 0 & C & & \\ & A & 0 & C & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad A = \check{R}_1 + \check{R}_2, \quad C = \check{L}_1.$$

The Stieltjes transform associated with $\check{\Phi}$ satisfies

$$B(z; W)(zI_3 - CB(z; W)A) = I_3,$$

for which a solution is

$$B(z; W) = \frac{7}{12} \begin{bmatrix} 7z - i\sqrt{-49z^2 + 24} & 0 & 0 \\ 0 & 7z - i\sqrt{-49z^2 + 24} & 0 \\ \frac{-343z^3 + 140z + (49z^2 - 8)\sqrt{49z^2 - 24}}{49z^2 - 32} & 0 & 7z - i\sqrt{-49z^2 + 24} \end{bmatrix}. \quad (1.7.10)$$

The weight matrix associated with $\check{\Phi}$ is then

$$W(x) = \frac{7}{12} \begin{bmatrix} \sqrt{24-49x^2} & 0 & 0 \\ 0 & \sqrt{24-49x^2} & 0 \\ -\frac{(49x^2+8)\sqrt{24-49x^2}}{49x^2-32} & 0 & \sqrt{24-49x^2} \end{bmatrix}, \quad x \in \left[-\frac{2\sqrt{6}}{7}, \frac{2\sqrt{6}}{7} \right].$$

The polynomials associated with $\check{\Phi}$, $Q_k(x)$, satisfy

$$\int_{-\frac{2\sqrt{6}}{7}}^{\frac{2\sqrt{6}}{7}} x^i dW(x) Q_j(x) = 0, \quad i > j,$$

thus formula (1.7.5) holds. Finally, we conclude that vertex $|0\rangle$ is transient, since

$$\begin{aligned} \sum_{n=0}^{\infty} p_{00;\rho}(n) &= \lim_{z \rightarrow 1} \text{Tr}(B(z, W)\rho) \\ &= \frac{49z - 7\sqrt{49z^2 - 24}}{12} + \frac{7a - 343z^3 + 140z + (49z^2 - 8)\sqrt{49z^2 - 24}}{12(49z^2 - 32)} = \frac{119 + 7a}{102} < \infty. \end{aligned}$$

◇

Example 1.20. Let us consider the QMC on $V = \mathbb{Z}_{\geq 0}$ whose compact form is

$$\check{\Phi} = \begin{bmatrix} C & C & & & \\ A & 0 & C & & \\ & A & 0 & C & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad A = \check{R}_1 + \check{R}_2, \quad C = \check{L}_1,$$

where

$$R_1 = \frac{1}{\sqrt{7}} \begin{bmatrix} 1 & 0 \\ -1 & \sqrt{3} \end{bmatrix}, \quad R_2 = \frac{1}{\sqrt{7}} \begin{bmatrix} 1 & 0 \\ 1 & \sqrt{3} \end{bmatrix}, \quad L_1 = \frac{1}{\sqrt{7}} \begin{bmatrix} \sqrt{3} & 0 \\ 0 & 1 \end{bmatrix}.$$

This QMC is similar to the one on Example 1.19 with the difference that the first block is replaced by C . Now $\check{\Phi}$ is trace preserving and the associated Stieltjes transform to $\check{\Phi}$, $B(z; W)$, satisfies

$$B(z; W)(zI_3 - C - CB(z; \check{W})A) = I_3,$$

where $B(z; \check{W})$ is the associated Stieltjes transform to the QMC on Example 1.19. Thus, we obtain

$$B(z; W) = \begin{bmatrix} \frac{7}{6} \frac{7z-6+\sqrt{49z^2-24}}{5-7z} & 0 & 0 \\ 0 & \frac{7}{2} \frac{-7z+2\sqrt{3}-\sqrt{49z^2-24}}{7\sqrt{3z-9}} & 0 \\ \frac{343z^3-196z^2-126z+64+(49z^2-28z-4)\sqrt{49z^2-24}}{160-384z-21z^2+588z^3-343z^4} & 0 & \frac{1}{2} \frac{7z-2+\sqrt{49z^2-24}}{1-z} \end{bmatrix}.$$

Therefore,

$$\begin{aligned} \sum_{n=0}^{\infty} p_{00;\rho}(n) &= \lim_{z \rightarrow 1} \text{Tr}(B(z; W)\rho) \\ &= \frac{7}{3} \frac{(343z^3 + (49z^2 - 20)\sqrt{49z^2 - 24} - 182z)a}{343z^3 - 245z^2 - 224z + 160} + \frac{1}{2} \frac{7z - 2 + \sqrt{49z^2 - 24}}{1 - z} = \infty, \end{aligned}$$

for any density operator $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$. Hence, this QMC is recurrent.

◇

Applying the folding trick to a nonpositive measure. It is worth noting that the folding trick can also be applied to QMCs whose matrix representations are not symmetrizable, allowing us to examine the associated recurrence problem. In fact, let us recall equation (1.6.11):

$$\Phi_{00}(z) = \Phi_{00}^+(z)(I - z^2 A_{-1} \Phi_{-1,-1}^-(z) C_0 \Phi_{00}^+(z))^{-1}.$$

In order to analyze recurrence of site $|0\rangle$ of a given QMC on \mathbb{Z} , we have to calculate $\sum_{n=0}^{\infty} p_{00;\rho}(n) = \sum_{n=0}^{\infty} \text{Tr}(\Phi_{00}^{(n)} \rho)$ for each density operator ρ . This can be done by using equation (1.6.11) in the following way:

$$\sum_{n=0}^{\infty} \Phi_{00}^{(n)} = \lim_{z \uparrow 1} \Phi_{00}(z) = \lim_{z \uparrow 1} \Pi_0^+ B(z; W_+) (I - A_{-1} \Pi_{-1}^- B(z; W_-) C_0 \Pi_0^+ B(z; W_+))^{-1}, \quad (1.7.11)$$

where the Stieltjes transform appearing on the right-hand side are obtained by applying (1.3.6).

Chapter 2

Continuous-time open quantum walks

2.1 General setting

In this work, we assume that we have a quantum particle acting either on the integer line, the integer half-line, or on a finite segment, that is, we have that the set of vertices V is labeled by $\mathbb{Z}, \mathbb{Z}_{\geq 0}$ or a finite set $\{0, 1, \dots, N\}$, respectively. We will also call vertices as **sites**. The state of the system is described by a column vector

$$\rho = \begin{bmatrix} \rho_0 \\ \rho_1 \\ \rho_2 \\ \vdots \end{bmatrix}, \quad \rho_i \in \mathcal{I}(\mathcal{H}), \quad \rho_i \geq 0, \quad \sum_{i \in V} \text{Tr}(\rho_i) = 1. \quad (2.1.1)$$

An operator **semigroup** \mathcal{T} on a Hilbert space \mathcal{H} is a family of bounded linear operators (T_t) acting on \mathcal{H} , $t \geq 0$, such that

$$T_t T_s = T_{t+s}, \quad s, t \in \mathbb{R}^+, \quad T_0 = I_{\mathcal{H}}.$$

If $t \mapsto T_t$ is continuous for the operator norm of \mathcal{H} , then \mathcal{T} is said to be **uniformly continuous**. This class of semigroups is characterized by the following result:

Theorem 2.1. [7], page 161] *The following assertions are equivalent for a semigroup \mathcal{T} on \mathcal{H} :*

1. \mathcal{T} is uniformly continuous;
2. There exists a bounded operator L on \mathcal{H} such that

$$T_t = e^{tL}, \quad t \in \mathbb{R}^+.$$

Further, if the conditions are satisfied, then

$$L = \lim_{t \rightarrow 0^+} \frac{T_t - I_{\mathcal{H}}}{t}.$$

The operator L is called the **generator** of \mathcal{T} .

2.2 CTOQWs

A semigroup $\mathcal{T} := (\mathcal{T}_t)_{t \geq 0}$ of CPTP maps acting on $\mathcal{I}_1(\mathcal{H})$, set of trace-class operators on \mathcal{H} , is called a **Quantum Markov Semigroup** (QMS) on $\mathcal{I}_1(\mathcal{H})$. When $\lim_{t \rightarrow 0} \|\mathcal{T}_t - Id\| = 0$, then \mathcal{T} has a generator $\mathcal{L} = \lim_{t \rightarrow 0^+} (\mathcal{T}_t - Id)/t$ (see [31]), which is a bounded operator on $\mathcal{I}_1(\mathcal{H})$, also known as **Lindblad operator**.

We consider a finite or countable set of vertices V and then take the composite system

$$\mathcal{H} = \bigoplus_{i \in V} \mathfrak{h}_i,$$

where each \mathfrak{h}_i denotes a separable Hilbert space. The label $i \in V$ is interpreted as being the position of the walker and, when the walker is located at the vertex $i \in V$, its internal state is encoded in the space \mathfrak{h}_i , describing the internal degrees of freedom of the particle when it is sitting at site $i \in V$. Since we will be considering only examples with $\mathfrak{h}_i = \mathfrak{h}_j$ for all $i, j \in V$, we let $\mathfrak{h}_i = \mathfrak{h}$ for every $i \in V$.

The set of diagonal density operator acting on \mathcal{H} will be denoted by

$$\mathcal{D} = \left\{ \sum_{i \in V} \rho(i) |i\rangle \langle i| : \rho(i) = \rho(i)^*, \quad \rho(i) \geq 0, \quad \sum_{i \in V} \text{Tr}(\rho(i)) = 1 \right\}.$$

Definition 2.2. A *Continuous-time Open Quantum Walk (CTOQW)* is an uniformly continuous QMS on $\mathcal{I}_1(\mathcal{H})$ with Lindblad operator of the form

$$\begin{aligned} \mathcal{L} : \mathcal{I}_1(\mathcal{H}) &\rightarrow \mathcal{I}_1(\mathcal{H}) \\ \rho &\mapsto -i[H, \rho] + \sum_{i, j \in V} \left(S_i^j \rho S_i^{j*} - \frac{1}{2} \{S_i^{j*} S_i^j, \rho\} \right), \end{aligned} \quad (2.2.1)$$

where, consistently with the notation, we write $S_i^j = R_i^j \otimes |j\rangle \langle i|$ for bounded operators $R_i^j \in \mathcal{B}(\mathfrak{h}_i, \mathfrak{h}_j)$. Moreover, H and S_i^j are bounded operators on \mathcal{H} of the form $H = \sum_{i \in V} H_i \otimes |i\rangle \langle i|$, H_i is self-adjoint on \mathfrak{h}_i , S_i^j is a bounded operator on \mathcal{H} with $\sum_{i, j \in V} S_i^{j*} S_i^j$ converging in the strong sense. Also, $[A, B] \equiv AB - BA$ is the commutator between A and B and $\{A, B\} \equiv AB + BA$ is the anti-commutator between A and B .

Then, we have $\rho = \sum_{i \in V} \rho(i) \otimes |i\rangle \langle i| \in \mathcal{D}$, $e^{t\mathcal{L}}(\rho) = \mathcal{T}_t(\rho) = \sum_{i \in V} \rho_t(i) \otimes |i\rangle \langle i|$, $\forall t \geq 0$, with

$$\frac{d}{dt} \rho_t(i) = -i[H_i, \rho_t(i)] + \sum_{j \in V} \left(R_j^i \rho_t(j) R_j^{i*} - \frac{1}{2} \{R_i^{j*} R_i^j, \rho_t(i)\} \right).$$

An alternative way to rewrite (2.2.1) is given by equation (18.7) in [5]:

$$\mathcal{L}(\rho) = \sum_{i \in V} \left(G_i \rho(i) + \rho(i) G_i^* + \sum_{j \in V} R_j^i \rho(j) R_j^{i*} \right) \otimes |i\rangle \langle i|, \quad (2.2.2)$$

where

$$G_i = -iH_i - \frac{1}{2} \sum_{j \in V} R_i^{j*} R_i^j.$$

Note that we then have $G_i + G_i^* = -\sum_{j \in V} R_i^{j*} R_i^j$.

Starting the walk on site $|i\rangle$ with initial density operator $\rho \in \mathcal{S}(\mathfrak{h}_i) = \sum_{i \in V} \rho(i) |i\rangle \langle i|$, the quantum measurement of the position gives rise to a probability distribution p_0 on V , such that

$$p_0(i) = \mathbb{P}(\text{the quantum particle is in site } |i\rangle) = \text{Tr}(\rho(i))$$

and for evolution on time $t \geq 0$,

$$p_t(i) = \mathbb{P}(\text{the quantum particle, at time } t, \text{ is in site } |i\rangle) = \text{Tr}(\rho_t(i)),$$

where

$$e^{t\mathcal{L}}(\rho) = \sum_{i \in V} \rho_t(i) \otimes |i\rangle \langle i|.$$

The vector and matrix representation of states and CP maps may be easily adapted to CTOQWs. In fact, since any element of $\mathcal{I}_V(\mathcal{H})$ is block diagonal, when $\dim \mathcal{H} < \infty$, it may be represented by combining the vector representations of the finite diagonal blocks,

$$\rho = \sum_{i \in V} \rho_i \otimes |i\rangle \langle i| \quad \Rightarrow \quad \vec{\rho} := \begin{bmatrix} \text{vec}(\rho_1) \\ \text{vec}(\rho_2) \\ \vdots \end{bmatrix}.$$

Then, the CTOQW (2.2.2) admits a **block matrix representation**

$$\overrightarrow{e^{t\mathcal{L}}(\rho)} = e^{t\hat{\mathcal{L}}} \overrightarrow{\rho}, \quad \hat{\mathcal{L}} = \begin{bmatrix} G_0^\alpha & [R_1^0] & [R_2^0] & \cdots \\ [R_0^1] & G_1^\alpha & [R_2^1] & \cdots \\ [R_0^2] & [R_1^2] & G_2^\alpha & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix},$$

where

$$G_i^\alpha = -iH_i \otimes I + iI \otimes \overline{H_i} - \frac{1}{2} \sum_{j=0}^{\infty} \left(R_i^{j*} R_i^j \otimes I + I \otimes \overline{R_i^{j*} R_i^j} \right), \quad i = 0, 1, 2, \dots$$

We will often identify \mathcal{L} with its block matrix representation and omit the hat, as the usage of such object will be clear from context. Also, we will sometimes write X instead of $[X]$ in contexts where no confusion arises.

It is worth noting that although the above definitions concern CTOQWs on general graphs, in this work we will deal exclusively with the one-dimensional situation which we may also call quantum birth-death process, and represented by

$$\mathbf{L} = \begin{bmatrix} B_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (2.2.3)$$

for certain operators A_i, B_i, C_i , and the remaining operators being equal to zero. The above representation is for a quantum particle acting on the integer half-line $\mathbb{Z}_{\geq 0}$, but we will also study examples acting on a finite set $\{0, 1, \dots, N\}$ or the integer line \mathbb{Z} .

The blocks of \mathcal{L} in (2.2.3) are then

$$\begin{aligned} G_0^\alpha &= -iH_0 \otimes I + iI \otimes \overline{H_0} - \frac{1}{2} \sum_{j=0}^1 \left(R_0^{j*} R_0^j \otimes I + I \otimes \overline{R_0^{j*} R_0^j} \right) \\ G_i^\alpha &= -iH_i \otimes I + iI \otimes \overline{H_i} - \frac{1}{2} \sum_{j=i-1}^{i+1} \left(R_i^{j*} R_i^j \otimes I + I \otimes \overline{R_i^{j*} R_i^j} \right), \quad i = 1, 2, \dots \\ A_i &= [R_i^{i+1}], \quad B_i = [R_i^i], \quad C_{i+1} = [R_{i+1}^i], \quad i = 0, 1, 2, \dots \end{aligned}$$

For simplicity, we will write

$$[A_i] = A_i \otimes \overline{A_i}, \quad [B_i] = B_i \otimes \overline{B_i}, \quad [C_i] = C_i \otimes \overline{C_i},$$

and

$$G_i^\alpha = -iH_i \otimes I + iI \otimes \overline{H_i} - \frac{1}{2} [(A_i^* A_i + B_i^* B_i + C_i^* C_i) \otimes I + I \otimes \overline{(A_i^* A_i + B_i^* B_i + C_i^* C_i)}].$$

When G_i^α is the same for all i , then we will write $G^\alpha = G_i^\alpha$.

2.2.1 Recurrence and transience for CTOQWs

Let us denote by X_t the process that indicates the position of the walker and by ρ_t the density operator at time t , then, by [33], the process $\mu_t = (X_t, \rho_t)$ is a Markov process. Analogous to the classical walk, let us discretize a CTOQW by a process $\{X(n\delta), n \geq 0\}$, where $\delta > 0$, having one-step transition probabilities $p_{ji;\rho}(\delta)$ (thus it has n step transition probabilities $p_{ji;\rho}(n\delta)$). This process is called δ -**skeleton** of $\{X(t), t \geq 0\}$.

Let Λ be a CTOQW, $i \in V, \rho \in \mathcal{S}(\mathfrak{h}_i)$ and $\delta > 0$. We say that a vertex i is

- **ρ -recurrent**¹ if

$$\int_0^\infty p_{ii;\rho}(t) dt = \infty.$$

Otherwise, i is said to be **ρ -transient**;

¹In the continuous-time version, the mean number of returns to some site is given by an integral. This integral should be compared with the series (1.1.6).

- **ρ -SJK-recurrent**² on the δ -skeleton if

$$\sum_{n=0}^{\infty} p_{ii;\rho}(n\delta) = \infty.$$

Otherwise, i is said to be **ρ -SJK-transient** on the δ -skeleton;

- **recurrent** if i is ρ -recurrent for all $\rho \in S_{\mathfrak{h}_i}$;
- **transient** if i is ρ -transient for some $\rho \in S_{\mathfrak{h}_i}$;
- **SJK-recurrent** if i is ρ -SJK-recurrent on the δ -skeleton for all $\rho \in S_{\mathfrak{h}_i}$;
- **SJK-transient** if i is ρ -SJK-transient on the δ -skeleton for some $\rho \in S_{\mathfrak{h}_i}$.

Remark 2.3. *Further, in this section, we shall show that for a semi-finite CTOQW which are of our interest, that a vertex is ρ -recurrent on the δ -skeleton if and only if it is ρ -recurrent on the δ' -skeleton for any $\delta' > 0$. So, the definitions of SJK-recurrence and SJK-transience are consistent.*

Definition 2.4. *A CTOQW is said to be:*

- **recurrent** if every vertex is recurrent;
- **transient** if every vertex is transient;
- **SJK-recurrent** if every vertex is SJK-recurrent;
- **SJK-transient** if every vertex is SJK-transient.

Example 2.5. *Let $V = \{1, 2, 3, 4\}$, $\mathcal{L} = \Phi - I$ a generator of a CTOQW, Φ a quantum channel with Kraus operators*

$$\begin{aligned} B_{11} &:= \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix}, B_{21} := \begin{bmatrix} 0 & i \\ 0 & 0 \end{bmatrix}, B_{12} := \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \\ B_{32} &:= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, B_{23} := \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, B_{24} := \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \end{aligned}$$

$B_{ji} = 0$ for the remain blocks.

We take a density operator $\tau = \sum_{i=1}^4 \tau(i) \otimes |i\rangle \langle i|$ to write the explicit form of the generator \mathcal{L} by

$$\begin{aligned} \mathcal{L}(\tau) &= (-\tau(1) + B_{11}\rho(1)B_{11}^* + B_{21}\rho(2)B_{21}^*) \otimes |1\rangle \langle 1| \\ &+ (-\tau(2) + B_{12}\rho(1)B_{12}^* + B_{32}\rho(3)B_{32}^*) \otimes |2\rangle \langle 2| + (-\tau(3) + B_{23}\rho(2)B_{23}^*) \otimes |3\rangle \langle 3| \\ &+ (-\tau(4) + B_{24}\rho(2)B_{24}^*) \otimes |4\rangle \langle 4|. \end{aligned}$$

The graph in Figure 2.1 represents this CTOQW. This CTOQW has two recurrent and two transient vertices.

Indeed, for $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$, one has

$$\int_0^{\infty} p_{33;\rho}(t) dt = \int_0^{\infty} \left[a \left(\frac{1}{2} + \frac{e^{-2t}}{2} - e^{-t} \right) + e^{-t} \right] dt = \begin{cases} 1, & \text{if } a = 0 \\ \infty, & \text{if } a \in (0, 1] \end{cases},$$

meaning that $|3\rangle$ is ρ -transient for $\rho = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ and ρ' -recurrent for any $\rho' \neq \rho$, that is, vertex $|3\rangle$ is transient. Similarly, we can also obtain that vertices $|1\rangle$ and $|2\rangle$ are recurrent and $|4\rangle$ is transient.

◇

²The notion of SJK-recurrence in the discrete time unitary setting is described on [36]. SJK-recurrence is named after the initials of the authors of the that work.

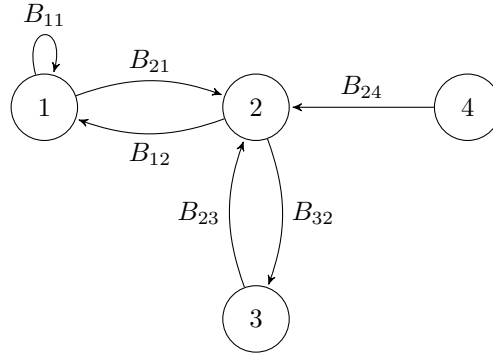


Figure 2.1: CTOQW with two recurrent and two transient vertices.

2.2.2 Further properties on the transition probabilities

The following results gives some properties of the transition function which have a fundamental importance on the next definitions and results, since it gives sufficient conditions to the transition functions be strictly positive for t sufficient large.

Proposition 2.6. *For any vertex of a CTOQW,*

$$p_{ji;\rho}(\alpha + \beta) = \sum_k p_{jk;\rho'_{ki}(\beta)}(\alpha) p_{ki;\rho}(\beta), \quad (2.2.4)$$

where

$$\rho'_{ki}(\beta) := \frac{\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho}{\text{Tr}(\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho)}, \quad \forall \alpha, \beta \geq 0.$$

Since on the Markov process there is one only quantum state $\rho = 1 \in \mathbb{C}$, equation Chapman-Kolmogorov Identity is a particular case of (2.2.4).

Remark 2.7. *The classical Chapman-Kolmogorov does not apply for CTOQW. Indeed, consider the CTOQW on example 2.5. For $\rho = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$,*

$$\sum_{k=1}^4 p_{0k;\rho} \left(\frac{\pi}{\sqrt{3}} \right) p_{k0;\rho} \left(\frac{\pi}{\sqrt{3}} \right) = \frac{1}{9} \left(\sqrt{3} e^{-\frac{\sqrt{3}\pi}{2}} - 2 \right)^2,$$

however

$$p_{00;\rho} \left(\frac{2\pi}{\sqrt{3}} \right) = \frac{2 - e^{-\sqrt{3}\pi}}{3},$$

therefore we can not consider $\rho = \rho'_{ki}(\beta)$ on equation (2.2.4) because

$$\sum_{k=1}^4 p_{0k;\rho} \left(\frac{\pi}{\sqrt{3}} \right) p_{k0;\rho} \left(\frac{\pi}{\sqrt{3}} \right) \neq p_{00;\rho} \left(\frac{2\pi}{\sqrt{3}} \right).$$

To get around this situation, in order to show equivalence between recurrence and SJK-recurrence, we show that the function $g(\rho, s) = p_{ji;\rho}(s)$ is jointly continuous under the variables $s \in [0, \infty)$ and $\rho \in \mathcal{S}_{\mathfrak{h}_i}$.

Proposition 2.8. *Let Λ_t a CTOQW and $i, j \in V$. Denote $W_i := \mathcal{S}_{\mathfrak{h}_i} \times [0, +\infty)$, then the function $g : W_i \rightarrow [0, 1]$ defined by $g(\rho, s) = p_{ji;\rho}(s)$ is jointly continuous on W_i .*

Proposition 2.9. *Let \mathcal{L} be the generator of a CTOQW and $i \in V$. Then*

1. For all $\rho \in \mathcal{S}_{\mathfrak{h}_i}$ and $t \geq 0$, $p_{ii;\rho}(t) > 0$;
2. If $p_{ij;\rho}(t) > 0$ for some $t > 0$, then $p_{ij;\rho}(s) > 0, \forall s \geq t$;

3. If $p_{ii;\rho}(t) = 1$ for some $t > 0$, then $p_{ii;\rho}(s) = 1, \forall s \in [0, t]$;
4. If $\delta > 0$, $\dim(\mathfrak{h}_i) < \infty$ and there exists $0 \leq t_0 \leq \delta$ such that $p_{ji;\rho}(t_0) > 0$, then the minimum $N_{ji} := \min\{p_{ji;\rho}(s) : \rho \in \mathcal{S}_{\mathfrak{h}_i} \text{ and } s \in [t_0, \delta]\}$ is attained on $(0, 1]$. When $j = i$, we denote $N_{ii} = N_i$.

A generalization from the classical case to the quantum model is presented below. As on the classical model, the proof is based on the Mean Value Theorem for Integrals, with the addition in which convergence and divergence of the integrals and the series are looked on the tail of the series. This is necessary because we do not have the Levy Dichotomy³ on the quantum model, only the results on Proposition 2.9.

Theorem 2.10. *Let $\delta > 0$ and $i, j \in V$ vertices of the graph on which a CTOQW is defined. If $\dim(\mathfrak{h}_j) < \infty$, then*

$$\sum_{n=0}^{\infty} p_{ji;\rho}(n\delta) = +\infty \Leftrightarrow \int_0^{\infty} p_{ji;\rho}(t) = +\infty.$$

Consequently, i is ρ -recurrent if, and only if, i is ρ -SJK-recurrent in the δ -skeleton.

Now we have an equivalence among the CTOQW and its discretized random walk with n -step transition probabilities on the δ -skeleton. The next results associates the ρ -recurrence among faithful (ρ is non-singular and therefore it is positive definite) and non-faithful (ρ is singular and therefore it is positive semidefinite) densities for a vertex with finite internal degrees.

Proposition 2.11. *Let Λ a CTOQW, $i \in V$, $\dim(\mathfrak{h}_i) = n < \infty$ and $\tilde{\rho} \in \mathcal{S}(\mathfrak{h}_i)$ and suppose that i is $\tilde{\rho}$ -recurrent.*

1. For any faithful $\rho \in \mathcal{S}(\mathfrak{h}_i)$, i is ρ -recurrent;
2. If $\rho \in \mathcal{S}(\mathfrak{h}_i)$ and there exists $\delta \geq 0$ such that $\rho'_{ii}(\delta)$ is faithful, then i is ρ -recurrent;
3. If $n \geq 2$, there is a non-faithful density ρ on $\mathcal{S}_{\mathfrak{h}_i}$ in which i is ρ -recurrent;
4. If $n = 2$, then the non-faithful density ρ on item (3) is pure.

Remark 2.12. *By contraposition, we get by the first item of the Proposition 2.11 that if $i \in V$, $\dim(\mathfrak{h}_i) = n < \infty$ and $\rho \in \mathcal{S}(\mathfrak{h}_i)$ faithful with i being ρ -transient, then i is ρ' -transient for any ρ' .*

2.3 Weight Matrices

In this section we introduce the Karlin-McGregor Formula for CTOQW with set of vertices of the forms $V = \{0, 1, 2, \dots, N\}$ and $V = \mathbb{Z}_+ = \{0, 1, 2, \dots\}$. Then we will be able to give a recurrence criterion for vertex $|0\rangle$ based on the Stieltjes transform of the associated measure.

Following [17], we pick $d \in \{1, 2, 3, \dots\}$, $(A_n)_{n \geq 0}$, $(B_n)_{n \geq 0}$, and $(C_n)_{n \geq 1}$, such that the block tridiagonal matrix

$$\hat{\mathcal{L}} = \begin{bmatrix} B_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad (2.3.1)$$

represents a generator of a CTOQW Λ .

Define recursively the associated matrix-valued polynomials from the matrix $\hat{\mathcal{L}}$ on (2.3.1) by

$$\begin{aligned} Q_0(x) &= I_d, & Q_{-1}(x) &= 0_d \\ -xQ_n(x) &= Q_{n+1}(x)A_n + Q_n(x)B_n + Q_{n-1}(x)C_n, & n &= 0, 1, 2, \dots, \end{aligned} \quad (2.3.2)$$

that is, $Q(x) = (Q_0(x), Q_1(x), \dots)$ are solutions of the equation $-xQ(x) = Q(x)\hat{\mathcal{L}}$. Here we denote I_d and 0_d the identity and the null matrix of dimension $d \times d$.

We recall property $\Lambda'_t = \hat{\mathcal{L}}\Lambda_t$, where $\Lambda_t = e^{t\hat{\mathcal{L}}}$ and define the two-variable function

$$f(x, t) = Q(x)\Lambda_t, \quad x \in \mathbb{C}, \quad t \in [0, \infty).$$

³The Levy Dichotomy asserts that, for a continuous Markov chain, for vertices $i \neq j$, we have $p_{ij}(t) > 0$ for every $t > 0$ or $p_{ij}(t) = 0$ for every $t > 0$.

One has

$$\frac{\partial f(x, t)}{\partial t} = Q(x)\Lambda'_t = Q(x)\hat{\mathcal{L}}\Lambda_t = -xQ(x)\Lambda_t = -xf(x, t), \quad f(x, 0) = Q(x),$$

whose solution is $f(x, t) = e^{-xt}Q(x)$. Hence $e^{-xt}Q(x) = Q(x)\Lambda_t$. Componentwise,

$$e^{-xt}Q_i(x) = \sum_{k=0}^{\infty} Q_k(x)\Lambda_{ki}(t), \quad (2.3.3)$$

where $\Lambda_{ki}(t)$ is the (k, i) -th block of $\Lambda(t)$.

If there exists a weight matrix Σ such that the matrix-valued polynomials $\{Q_n(x)\}_{n \geq 0}$ are orthogonal with respect to Σ , in the following sense

$$\int Q_j^*(x)d\Sigma(x)Q_i(x) = \delta_{ji}F_i, \quad \det(F_i) \neq 0,$$

then multiplying on the left side of (2.3.3) by $Q_j^*(x)$ and integrating with respect to Σ we obtain

$$\int_{\mathbb{R}} e^{-xt}Q_j^*(x)d\Sigma(x)Q_i(x) = \int_{\mathbb{R}} Q_j^*(x)d\Sigma(x)Q_j(x)\Lambda_{ji}(t),$$

therefore for any $i, j \in V$, we have the **Karlin-McGregor Formula for CTOQW**:

$$\Lambda_{ji}(t) = \left(\int Q_j^*(x)d\Sigma(x)Q_j(x) \right)^{-1} \left(\int e^{-xt}Q_j^*(x)d\Sigma(x)Q_i(x) \right), \quad (2.3.4)$$

$\Lambda(t) = (\Lambda_{ji}(t))_{j,i=0,1,\dots}$. For more details about how to construct this formula see [17].

Sometimes we will write (2.3.4) as

$$\Lambda_{ji}(t) = \Pi_j \left(\int e^{-xt}Q_j^*(x)d\Sigma(x)Q_i(x) \right),$$

where

$$\Pi_j = \left(\int Q_j^*(x)d\Sigma(x)Q_j(x) \right)^{-1}.$$

Therefore, the transition probabilities may be obtained by

$$p_{ji;\rho}(t) = \text{Tr} \left[\Pi_j \int e^{-xt}Q_j^*(x)d\Sigma(x)Q_i(x)\rho \right].$$

Theorem 2.13. *Let Λ be a tridiagonal CTOQW on $\mathbb{Z}_{\geq 0} = \{0, 1, 2, \dots\}$ and Σ its associated weight matrix. Vertex $|j\rangle$ is ρ -recurrent if and only if*

$$\lim_{\lambda \rightarrow 0} \text{Tr} \left[\Pi_j \int_{\mathbb{C}} \frac{Q_j^*(x)d\Sigma(x)Q_i(x)}{\lambda + x} \rho \right] = \infty.$$

Proof. For each pair $i, j \in V$ we have

$$\begin{aligned} \int_0^{\infty} p_{ji;\rho}(t)dt &= \lim_{\lambda \rightarrow 0} \int_0^{\infty} e^{-\lambda t} p_{ji;\rho}(t)dt \\ &= \lim_{\lambda \rightarrow 0} \int_0^{\infty} e^{-\lambda t} \text{Tr} \left[\Pi_j \int_{\mathbb{C}} e^{-xt}Q_j^*(x)d\Sigma(x)Q_i(x)\rho \right] dt \\ &= \lim_{\lambda \rightarrow 0} \text{Tr} \left[\Pi_j \int_{\mathbb{C}} \left(\int_0^{\infty} e^{-(\lambda+x)t} dt \right) Q_j^*(x)d\Sigma(x)Q_i(x)\rho \right] \\ &= \lim_{\lambda \rightarrow 0} \text{Tr} \left[\Pi_j \int_{\mathbb{C}} \frac{Q_j^*(x)d\Sigma(x)Q_i(x)}{\lambda + x} \rho \right]. \end{aligned}$$

□

We recall the **Stieltjes transform** associated to Σ :

$$B(z, \Sigma) = \int_{\mathbb{C}} \frac{d\Sigma(x)}{z - x},$$

thus we obtain the straightforward consequence of Theorem 2.13:

Corollary 2.14. *Let Λ be a tridiagonal CTOQW on $\mathbb{Z}_{\geq 0} = \{0, 1, 2, \dots\}$ and Σ its associated weight matrix. Vertex $|0\rangle$ is ρ -recurrent if and only if*

$$-\lim_{z \rightarrow 0} \text{Tr}[\Pi_0 B(z, \Sigma)\rho] = \infty.$$

2.3.1 Some basic results

The following are basic results from the setting of matrix-valued orthogonal polynomials, which will be used in this work.

1. Let Σ be a $d^2 \times d^2$ weight matrix and denote by

$$S_k = \int x^k d\Sigma(x), \quad k = 0, 1, \dots$$

the corresponding moments. The block Hankel matrices are defined by

$$\underline{H}_{2m} = \begin{bmatrix} S_0 & \cdots & S_m \\ \vdots & & \vdots \\ S_m & \cdots & S_{2m} \end{bmatrix}, \quad m \geq 0.$$

Theorem 2.15 (Theorem 2.1 of [17]). *Consider the block matrix $\hat{\mathcal{L}}$ given by Equation (2.3.1), assume that A_n, C_{n+1} , $n \geq 0$ are nonsingular matrices and $B_n \geq 0$ for all n . Now let $\{Q_n(x)\}_{n \geq 0}$ be the sequence of matrix-valued polynomials defined by (2.3.2). Then there exists a weight matrix Σ with positive definite block Hankel matrices \underline{H}_{2m} , $m \geq 0$, such that the sequence of polynomials $\{Q_n(x)\}_{n \geq 0}$ is orthogonal with respect to Σ if and only if there is a sequence of nonsingular matrices $(R_n)_{n \geq 0}$ such that*

$$\begin{aligned} R_n B_n R_n^{-1} & \text{ is symmetric, } \quad n \geq 0, \\ R_n^* R_n & = (A_0^* \cdots A_{n-1}^*)^{-1} R_0^* R_0 C_1 \cdots C_n, \quad n \geq 0. \end{aligned} \tag{2.3.5}$$

Moreover, $S_0 = (R_0^* R_0)^{-1}$.

2. Perturbation of Stieltjes transform:

Theorem 2.16 (Theorem 2.3 of [17]). *Consider the block matrix $\hat{\mathcal{L}}$ given by Equation (2.3.1) and the matrix $\tilde{\mathcal{L}}$ which is the same as $\hat{\mathcal{L}}$ but with a perturbation on the first block, that is,*

$$\tilde{\mathcal{L}} = \begin{bmatrix} \tilde{B}_0 & C_1 & & & \\ A_0 & B_1 & C_2 & & \\ & A_1 & B_2 & C_3 & \\ & & & \ddots & \ddots & \ddots \end{bmatrix}.$$

If Σ is the weight matrix associated to $\hat{\mathcal{L}}$ with positive definite block Hankel matrices such that $R_0 \tilde{B}_0 R_0^{-1}$ is symmetric and such that $(R_n)_{n \geq 0}$ is a sequence of matrices which satisfies condition (2.3.5), then there exists a weight matrix $\tilde{\Sigma}$ corresponding to $\tilde{\mathcal{L}}$. If the weight matrix Σ and $\tilde{\Sigma}$ are determined by their moments, then the Stieltjes transforms of the measures satisfy

$$B(z, \Sigma) = \left\{ B(z, \tilde{\Sigma})^{-1} - S_0^{-1} (\tilde{B}_0 - B_0) \right\}^{-1}.$$

where each block entry is a $2d^2 \times 2d^2$ matrix, given by

$$D_0 = \begin{bmatrix} G_0^\alpha + [B_0] & [A_{-1}] \\ [C_0] & G_{-1}^\alpha + [B_{-1}] \end{bmatrix}, \quad M_n = \begin{bmatrix} [A_n] & 0 \\ 0 & [C_{-n-1}] \end{bmatrix}, \quad n \geq 0, \\ D_n = \begin{bmatrix} G_n^\alpha + [B_n] & 0 \\ 0 & G_{-n-1}^\alpha + [B_{-n-1}] \end{bmatrix}, \quad N_n = \begin{bmatrix} [C_n] & 0 \\ 0 & [A_{-n-1}] \end{bmatrix}, \quad n \geq 1.$$

The term *folding trick* comes from the transformation of the original generator $\hat{\mathcal{L}}$, whose graph is represented in Figure 2.2, to the generator described by $\check{\mathcal{L}}$, which is represented by the folded walk in Figure 2.3.

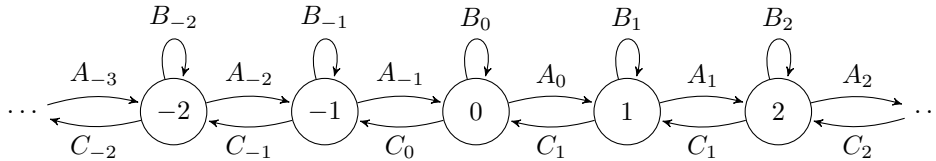


Figure 2.2: Generator $\hat{\mathcal{L}}$ of a CTOQW on \mathbb{Z} .

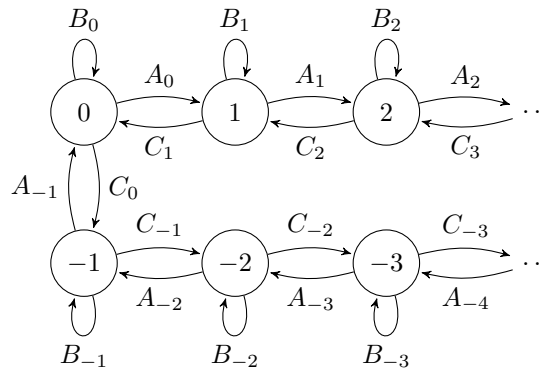


Figure 2.3: Folded walk of $\hat{\mathcal{L}}$ on $\mathbb{Z}_{\geq 0} \times \{1, 2\}$ given by $\check{\mathcal{L}}$.

Note that $\check{\mathcal{L}}$ is a block tridiagonal matrix on $\mathbb{Z}_{\geq 0}$, thereby we can apply all the properties we have seen in previous sections. The following $2d^2 \times 2d^2$ matrix polynomials are defined in terms of (2.3.8),

$$\mathcal{Q}_n(x) = \begin{bmatrix} Q_n^1(x) & Q_{-n-1}^1(x) \\ Q_n^2(x) & Q_{-n-1}^2(x) \end{bmatrix}, \quad n \geq 0, \quad (2.3.9)$$

and these satisfy

$$x\mathcal{Q}_0(x) = \mathcal{Q}_1(x)M_0 + \mathcal{Q}_0(x)D_0, \quad \mathcal{Q}_0(x) = I_{2d^2}, \\ x\mathcal{Q}_n(x) = \mathcal{Q}_{n+1}(x)M_n + \mathcal{Q}_n(x)D_n + \mathcal{Q}_{n-1}(x)N_n, \quad n = 1, 2, \dots$$

The leading coefficient of $\mathcal{Q}_n(x)$ is always a nonsingular matrix. Moreover, for

$$\check{R}_n := \begin{bmatrix} R_n & 0_{d^2} \\ 0_{d^2} & R_{-n-1} \end{bmatrix}, \quad n \geq 0, \quad \check{E}_0 := \begin{bmatrix} E_0 & R_0[A_{-1}]R_{-1}^{-1} \\ R_{-1}[C_0]R_0^{-1} & E_{-1} \end{bmatrix}, \quad \check{E}_n := \begin{bmatrix} E_n & 0_{d^2} \\ 0_{d^2} & E_{-n-1} \end{bmatrix}, \quad n \geq 1,$$

we see that the block matrices of $\check{\mathcal{L}}$ satisfy the conditions (2.3.7) for $n \geq 0$:

$$M_n^* \check{R}_{n+1}^* \check{R}_{n+1} = \check{R}_n^* \check{R}_n N_{n+1}, \quad \check{R}_n D_n = \check{E}_n \check{R}_n,$$

where matrices \check{R}_n are non-singular and \check{E}_n are Hermitian for all $n \geq 0$. Defining

$$\check{\Pi}_j := \check{R}_j^* \check{R}_j \in M_{2d^2}(\mathbb{C}), \quad j = 0, 1, 2, \dots,$$

the correspondence between $\check{\Pi}_j$ and Π_j is

$$\check{\Pi}_j := \begin{bmatrix} \Pi_j & 0_{d^2} \\ 0_{d^2} & \Pi_{-j-1} \end{bmatrix}.$$

By [18], there exists a weight matrix W leading to the Karlin-McGregor formula for $\check{\Lambda} = e^{t\check{\mathcal{L}}}$:

$$\check{\Lambda}_{ji}(t) = \check{\Pi}_j \int_{\mathbb{R}} e^{-xt} \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x). \quad (2.3.10)$$

Once we have found the weight matrix appearing on (2.3.10), we can also obtain the blocks $\Lambda_{ji}(t)$ of the original walk generated by $\hat{\mathcal{L}}$. The key for this operation is the following proposition:

Proposition 2.18. *Assume that $\hat{\mathcal{L}}$ is the generator of a CTOQW of the form (2.3.6). The relation between $\check{\Lambda}_{ji}(t)$ and $\Lambda_{ji}(t)$ is*

$$\check{\Lambda}_{ji}(t) = \begin{bmatrix} \Lambda_{ji}(t) & \Lambda_{j,-i-1}(t) \\ \Lambda_{-j-1,i}(t) & \Lambda_{-j-1,-i-1}(t) \end{bmatrix}, \quad i, j \in \mathbb{Z}_{\geq 0}. \quad (2.3.11)$$

Proof. First we use Proposition 2.18 (replace $\check{\Phi}_{ji}^{(n)}$ and $\hat{\Phi}_{ji}^{(n)}$ by $\check{\mathcal{L}}_{ji}^n$ and $\hat{\mathcal{L}}_{ji}^n$ respectively) to obtain that

$$\check{\mathcal{L}}_{ji}^n = \begin{bmatrix} \hat{\mathcal{L}}_{ji}^n & \hat{\mathcal{L}}_{j,-i-1}^n \\ \hat{\mathcal{L}}_{-j-1,i}^n & \hat{\mathcal{L}}_{-j-1,-i-1}^n \end{bmatrix}, \quad i, j \in \mathbb{Z}_{\geq 0}, \quad \text{for all } n = 0, 1, 2, \dots,$$

hence we obtain for every $i, j \in \mathbb{Z}_{\geq 0}$ the expression

$$\check{\Lambda}_{ji}(t) = (e^{t\check{\mathcal{L}}})_{ji} = \sum_{n=0}^{\infty} \frac{t^n}{n!} \check{\mathcal{L}}_{ji}^n = \sum_{n=0}^{\infty} \frac{t^n}{n!} \begin{bmatrix} \hat{\mathcal{L}}_{ji}^n & t^n \hat{\mathcal{L}}_{j,-i-1}^n \\ \hat{\mathcal{L}}_{-j-1,i}^n & \hat{\mathcal{L}}_{-j-1,-i-1}^n \end{bmatrix} = \begin{bmatrix} \Lambda_{ji}(t) & \Lambda_{j,-i-1}(t) \\ \Lambda_{-j-1,i}(t) & \Lambda_{-j-1,-i-1}(t) \end{bmatrix}.$$

□

Note that we can evaluate $\check{\Lambda}_{ji}(t)$ by (2.3.10) and then extract the block $\Lambda_{ji}(t)$ as in (2.3.11). Further, for a density operator ρ we have

$$p_{ji;\rho}(n) = \text{Tr}(\Lambda_{ji}(t)\rho) = \text{Tr} \left(\begin{bmatrix} \Lambda_{ji}(t) & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right) = \text{Tr} \left(\begin{bmatrix} I_{d^2} & 0 \\ 0 & 0 \end{bmatrix} \check{\Lambda}_{ji}(t) \begin{bmatrix} I_{d^2} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \rho \\ 0 \end{bmatrix} \right).$$

However, we would like to obtain the probability above avoiding the evaluation of $\check{\Lambda}_{ji}(t)$. This can be done via a generalization of the Karlin-McGregor formula on $\mathbb{Z}_{\geq 0}$. We proceed as follows: first, write the decomposition

$$dW(x) = \begin{bmatrix} dW_{11}(x) & dW_{12}(x) \\ dW_{21}(x) & dW_{22}(x) \end{bmatrix},$$

where $dW_{21}(x) = dW_{12}^*(x)$, since $dW(x)$ is positive definite. Then one has for $i, j \in \mathbb{Z}_{\geq 0}$,

$$\begin{aligned} \check{\Lambda}_{ji}(t) &= \check{\Pi}_j \int_{\mathbb{R}} e^{-xt} \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x) \\ &\stackrel{(2.3.9)}{=} \begin{bmatrix} \Pi_j & 0_{d^2} \\ 0_{d^2} & \Pi_{-j-1} \end{bmatrix} \int_{\mathbb{R}} e^{-xt} \begin{bmatrix} Q_j^1(x) & Q_{-j-1}^1(x) \\ Q_j^2(x) & Q_{-j-1}^2(x) \end{bmatrix}^* \begin{bmatrix} dW_{11}(x) & dW_{12}(x) \\ dW_{12}^*(x) & dW_{22}(x) \end{bmatrix} \begin{bmatrix} Q_i^1(x) & Q_{-i-1}^1(x) \\ Q_i^2(x) & Q_{-i-1}^2(x) \end{bmatrix} \\ &= \sum_{\alpha, \beta=1}^2 \begin{bmatrix} \Pi_j \int_{\mathbb{R}} e^{-xt} Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^{\beta}(x) & \Pi_j \int_{\mathbb{R}} e^{-xt} Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_{-i-1}^{\beta}(x) \\ \Pi_{-j-1} \int_{\mathbb{R}} e^{-xt} Q_{-j-1}^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^{\beta}(x) & \Pi_{-j-1} \int_{\mathbb{R}} e^{-xt} Q_{-j-1}^{\alpha*}(x) dW_{\alpha\beta}(x) Q_{-i-1}^{\beta}(x) \end{bmatrix}. \end{aligned}$$

Joining equation above and Proposition 2.18, we obtain the Karlin-McGregor formula for a CTOQW on \mathbb{Z} , given by

$$\Lambda_{ji}(t) = \sum_{\alpha, \beta=1}^2 \Pi_j \int_{\mathbb{R}} e^{-xt} Q_j^{\alpha*}(x) dW_{\alpha\beta}(x) Q_i^{\beta}(x), \quad \text{for any } i, j \in \mathbb{Z}, \quad n \geq 0. \quad (2.3.12)$$

Conversely, if there exist weight matrices $dW_{11}(x), dW_{12}(x), dW_{22}(x)$ such that $\Lambda_{ji}(t)$ is of the form (2.3.12), then $\check{\Lambda}_{ji}(t)$ is of the form

$$\check{\Phi}_{ji}^{(n)} = \check{\Pi}_j \int_{\mathbb{R}} e^{-xt} \mathcal{Q}_j^*(x) dW(x) \mathcal{Q}_i(x).$$

The weight matrix

$$W(x) = \begin{bmatrix} W_{11}(x) & W_{12}(x) \\ W_{12}^*(x) & W_{22}(x) \end{bmatrix},$$

is called the spectral block matrix of \mathcal{L} .

Remark 2.19. Extending Theorem 2.14 to the CTOQW on \mathbb{Z} , we observe that, since $Q_0^1 = Q_{-1}^2 = I_d$ and $Q_0^2 = Q_{-1}^1 = 0_d$, we obtain

$$\int_0^\infty p_{00;\rho}(t) dt = \lim_{z \uparrow 0} \text{Tr} [\Pi_0 B(z; W_{11}) \text{vec}(\rho)].$$

where $B(z; W)$ is the Stieltjes transform of a weight matrix W . Analogously,

$$\int_0^\infty p_{-1,-1;\rho}(t) dt = \lim_{z \uparrow 0} \text{Tr} [\Pi_{-1} B(z; W_{22}) \text{vec}(\rho)].$$

Since we are assuming that Π_0 and Π_{-1} are positive definite matrices, we apply Corollary 2.14 to verify that vertex $|0\rangle$ is ρ -recurrent if and only if

$$\lim_{z \uparrow 0} \text{Tr} (B(z; W_{11}) \text{vec}(\rho)) = \infty,$$

and vertex $|-1\rangle$ is ρ -recurrent if and only if

$$\lim_{z \uparrow 0} \text{Tr} (B(z; W_{22}) \text{vec}(\rho)) = \infty.$$

Let us write the matrix $\hat{\mathcal{L}}$ in the form

$$\check{\mathcal{L}} = \begin{bmatrix} \hat{\mathcal{L}}^- & C \\ A & \hat{\mathcal{L}}^+ \end{bmatrix}, \quad C = \begin{bmatrix} \vdots & \vdots & \vdots & \dots \\ 0 & 0 & 0 & \dots \\ [C_0] & 0 & 0 & \dots \end{bmatrix}, \quad A = \begin{bmatrix} \dots & 0 & 0 & [A_{-1}] \\ \dots & 0 & 0 & 0 \\ \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \end{bmatrix},$$

$$\hat{\mathcal{L}}^+ = \begin{bmatrix} [G_0^\alpha + [B_0]] & [C_1] & & & \\ [A_0] & G_1^\alpha + [B_1] & [C_2] & & \\ & [A_1] & G_2^\alpha + [B_2] & [C_3] & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

$$\hat{\mathcal{L}}^- = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ & [A_{-4}] & G_{-3}^\alpha + [B_{-3}] & [C_{-2}] & \\ & & [A_{-3}] & G_{-2}^\alpha + [B_{-2}] & [C_{-1}] \\ & & & [A_{-2}] & G_{-1}^\alpha + [B_{-1}] \end{bmatrix}.$$

Our goal now is to write the Stieltjes transforms associated with the weight matrices $W_{\alpha\beta}$, $\alpha, \beta = 1, 2$, in terms of the Stieltjes transforms associated with W_{\pm} , the weight matrices associated with $\hat{\mathcal{L}}^{\pm}$.

We introduce the generating function of \mathcal{L}

$$\Phi(s) := \sum_{n=0}^{\infty} s^n \hat{\mathcal{L}}^n$$

to obtain an explicit form for the Laplace Transform of $\Lambda(t)$ on the following way:

$$\hat{\Lambda}_{ji}(t) = \int_0^\infty e^{-xt} \Lambda_{ji}(x) dx = \sum_{n=0}^{\infty} \int_0^\infty e^{-xt} \frac{x^n}{n!} \hat{\mathcal{L}}_{ji}^n dx = \sum_{n=0}^{\infty} \frac{t^n}{n!} \hat{\mathcal{L}}_{ji}^n = \sum_{n=0}^{\infty} \frac{\hat{\mathcal{L}}_{ji}^n}{t^{n+1}} = \frac{\Phi_{ji}(t^{-1})}{t}.$$

Using equations (1.6.11),(1.6.12),(1.6.13) and (1.6.14) applied to $\Phi_{ji}(s^{-1}) = s\hat{\Lambda}_{ji}(s)$, we obtain

$$\hat{\Lambda}_{00}(z) = \hat{\Lambda}_{00}^+(z)(I - [A_{-1}]\hat{\Lambda}_{-1,-1}^-(z)[C_0]\hat{\Lambda}_{00}^+(z))^{-1}. \quad (2.3.13)$$

$$\hat{\Lambda}_{-1,-1}(z) = \hat{\Lambda}_{-1,-1}^-(z)(I - [C_0]\hat{\Lambda}_{00}^+(z)[A_{-1}]\hat{\Lambda}_{-1,-1}^-(z))^{-1}. \quad (2.3.14)$$

$$\hat{\Lambda}_{0,-1}(z) = z^{-1}\hat{\Lambda}_{00}^+(z)(I - [A_{-1}]\hat{\Lambda}_{-1,-1}^-(z)[C_0]\hat{\Lambda}_{00}^+(z))^{-1}[A_{-1}]\hat{\Lambda}_{-1,-1}^-(z). \quad (2.3.15)$$

$$\hat{\Lambda}_{-1,0}(z) = z^{-1}\hat{\Lambda}_{-1,-1}^-(z)(I - [C_0]\hat{\Lambda}_{00}^+(z)[A_{-1}]\hat{\Lambda}_{-1,-1}^-(z))^{-1}[C_0]\hat{\Lambda}_{00}^+(z). \quad (2.3.16)$$

We notice that the block matrices of both $\check{\mathcal{L}}^+$ and $\check{\mathcal{L}}^-$ satisfy the conditions of equation (2.3.7), thus there are positive weight matrices W_{\pm} associated with $\check{\mathcal{L}}^{\pm}$ for which the associated polynomials are orthogonal. Then, we can write

$$\Pi_0^+ := \int_{\mathbb{R}} dW_+ \quad \text{and} \quad \Pi_{-1}^- := \int_{\mathbb{R}} dW_- .$$

The Laplace Transform of $\Lambda_{ji}(t)$ can be associated to the Stieltjes transform using that

$$\hat{\Lambda}_{ji}(s) = \int_0^{\infty} e^{-ts} \Lambda_{ji}(t) dt = \int_0^{\infty} e^{-ts} \left(\Pi_j \int_{\mathbb{R}} e^{-xt} Q_j^*(x) dW(x) Q_i(x) dt \right) = \Pi_j \int_{\mathbb{R}} \frac{Q_j^*(x) dW(x) Q_i(x)}{s+x},$$

$s > 0$, that is,

$$\hat{\Lambda}_{ji}(-s) = \Pi_j \int_{\mathbb{R}} \frac{Q_j^*(x) dW(x) Q_i(x)}{x-s}, \quad s < 0,$$

thereby we recall that $Q_0^1 = Q_{-1}^2 = I_{d^2}$, $Q_0^2 = Q_{-1}^1 = 0_{d^2}$ in order to obtain the relations

$$\begin{aligned} B(z; W_{11}) &= \Pi_0^{-1} \hat{\Lambda}_{00}(-z), & B(z; W_{22}) &= \Pi_{-1}^{-1} \hat{\Lambda}_{-1,-1}(-z), & B(z^{-1}; W_{12}) &= \Pi_{-1}^{-1} \hat{\Lambda}_{0,-1}(-z), \\ B(z; W_{21}) &= \Pi_{-1}^{-1} \hat{\Lambda}_{-1,0}(-z), & B(z; W_+) &= (\Pi_0^+)^{-1} \hat{\Lambda}_{00}^+(-z), & B(z^{-1}; W_-) &= (\Pi_{-1}^-)^{-1} \hat{\Lambda}_{-1,-1}^-(-z). \end{aligned}$$

Joining with the identities (2.3.13),(2.3.14),(2.3.15),(2.3.16), the new Stieltjes transform identities are obtained:

$$\begin{aligned} \Pi_0 B(z; W_{11}) &= \Pi_0^+ B(z; W_+) (I - [A_{-1}] \Pi_{-1}^- B(z; W_-) [C_0] \Pi_0^+ B(z; W_+))^{-1}, \\ \Pi_{-1} B(z; W_{22}) &= \Pi_{-1}^- B(z; W_-) (I - [C_0] \Pi_0^+ B(z; W_+) [A_{-1}] \Pi_{-1}^- B(z; W_-))^{-1}, \\ \Pi_0 B(z; W_{12}) &= \Pi_0^+ B(z; W_+) (I - [A_{-1}] \Pi_{-1}^- B(z; W_-) [C_0] \Pi_0^+ B(z; W_+))^{-1} [A_{-1}] \Pi_{-1}^- B(z; W_-), \\ \Pi_{-1} B(z; W_{21}) &= \Pi_{-1}^- B(z; W_-) (I - [C_0] \Pi_0^+ B(z; W_+) [A_{-1}] \Pi_{-1}^- B(z; W_-))^{-1} [C_0] \Pi_0^+ B(z; W_+). \end{aligned} \quad (2.3.17)$$

Sometimes the operators Π_i^+ and Π_i^- are equal to the identity operator. In this case, (2.3.17) are reduced to

$$\begin{aligned} B(z; W_{11}) &= B(z; W_+) (I - [A_{-1}] B(z; W_-) [C_0] B(z; W_+))^{-1}, \\ B(z; W_{22}) &= B(z; W_-) (I - [C_0] B(z; W_+) [A_{-1}] B(z; W_-))^{-1}, \\ B(z; W_{12}) &= B(z; W_+) (I - [A_{-1}] B(z; W_-) [C_0] B(z; W_+))^{-1} [A_{-1}] B(z; W_-), \\ B(z; W_{21}) &= B(z; W_-) (I - [C_0] B(z; W_+) [A_{-1}] B(z; W_-))^{-1} [C_0] B(z; W_+). \end{aligned} \quad (2.3.18)$$

Equations (2.3.17) and (2.3.18) allow us to obtain the Stieltjes transform of the CTOQW with $V = \mathbb{Z}$ when we know the Stieltjes transform associated to the walks on $\mathbb{Z}_{\geq 0}$ and $\mathbb{Z}_{\leq 0}$. Since we are interested on the recurrence and transience of the CTOQWs, those equations are enough to obtain this information as it will be seen on the next section.

Remark 2.20. A sufficient condition for $\Pi_i^+ = \Pi_i^- = I$ is to have $A_n = C_{n+1}^*$ and $B_n = B_n^*$ for every $n \in \mathbb{Z}$, since we will always have $G_n = G_n^*$ for all $n \in \mathbb{Z}$ in this case and therefore we can take $R_i = I$ for all $i \in \mathbb{Z}$ (see Equation (2.3.7)). On the other hand, those conditions are not necessary, since we can find examples with R_n being any unitary matrices for each n .

2.4 Examples

In this section we present examples of matrix weights associated to tridiagonal CTOQWs and then we evaluate statistics properties of the random walks with finite and infinite number of vertices.

where we have put $G = -\text{diag}(g_1, g_2, g_3, g_4)$ and $K = -\text{diag}(k_1, k_2, k_3, k_4)$. Since $g_2 = g_3$ and $k_2 = k_3$, $\det(R_{N+1}(x))$ is a polynomial of degree $4(N+1)$ having $3(N+1)$ distinct roots, which are of the form

$$\begin{aligned} x_j &= -g_1 - 2k_1 \cos\left(\pi \frac{j+1}{N+2}\right) = a_1^2 + c_1^2 - 2a_1c_1 \cos\left(\pi \frac{j+1}{N+2}\right), \\ y_j &= -g_2 - 2k_2 \cos\left(\pi \frac{j+1}{N+2}\right) = \sqrt{a_1c_1a_2c_2} - (a_1^2 + c_1^2 + a_2^2 + c_2^2) \cos\left(\pi \frac{j+1}{N+2}\right), \\ z_j &= -g_4 - 2k_4 \cos\left(\pi \frac{j+1}{N+2}\right) = a_2^2 + c_2^2 - 2a_2c_2 \cos\left(\pi \frac{j+1}{N+2}\right), \quad j = 0, \dots, N, \end{aligned}$$

each y_j being of multiplicity 2. There can be cases of eigenvalues with a greater multiplicity, which happens when the collection of zeros x_N, y_N and z_N overlap, so the multiplicity changes accordingly.

Let us compute the weight matrixs on the zeros above. We have

$$W_j = g'_j(\lambda_j), \quad g_j(\lambda) := -(\lambda_j - \lambda)^2(-J - \lambda I)_{00}^{-1}, \quad \lambda_j = x_j, y_j, z_j, \quad j = 0, \dots, N, \quad (2.4.1)$$

an expression which can be deduced from (see [22])

$$(-J - \lambda I)_{ij}^{-1} = \sum_{k=0}^N \frac{P_i^*(\lambda_k) W_k P_j(\lambda_k)}{\lambda_k - \lambda},$$

and noting that this corresponds to the Laurent sum of the operator on the left-hand side except for the sign change $\lambda_k - \lambda = -(\lambda - \lambda_k)$. With formula (2.4.1), a calculation shows that for every N we have a corresponding set of multiples of the matrices given by

$$W_{K;1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad W_{K;2} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad W_{K;3} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

More precisely, we have a collection of $3(N+1)$ roots with weights

$$\begin{aligned} \psi(x_j) &= \frac{2}{N+2} \sin^2\left(\pi \frac{j+1}{N+2}\right) W_{K;1}, \quad j = 0, \dots, N, \\ \psi(y_j) &= \frac{2}{N+2} \sin^2\left(\pi \frac{j+1}{N+2}\right) W_{K;2}, \quad j = 0, \dots, N. \\ \psi(z_j) &= \frac{2}{N+2} \sin^2\left(\pi \frac{j+1}{N+2}\right) W_{K;2}, \quad j = 0, \dots, N. \end{aligned}$$

For a specific instance of the above take $N = 2$ (3 sites), so we have 9 roots, with weights

$$\frac{1}{4}W_{K;1}, \quad \frac{1}{4}W_{K;2}, \quad \frac{1}{4}W_{K;3}$$

associated with zeros $a_1^2 + c_1^2 - 2a_1c_1$, $\sqrt{a_1c_1a_2c_2} - (a_1^2 + c_1^2 + a_2^2 + c_2^2)$ and $a_2^2 + c_2^2 - 2a_2c_2$ respectively; weights

$$\frac{1}{2}W_{K;1}, \quad \frac{1}{2}W_{K;2}, \quad \frac{1}{2}W_{K;3}$$

associated with zeros $a_1^2 + c_1^2 - \sqrt{2}a_1c_1$, $\sqrt{a_1c_1a_2c_2} - \sqrt{2}(a_1^2 + c_1^2 + a_2^2 + c_2^2)/2$ and $a_2^2 + c_2^2 - \sqrt{2}a_2c_2$ respectively; and weights

$$\frac{1}{4}W_{K;1}, \quad \frac{1}{4}W_{K;2}, \quad \frac{1}{4}W_{K;3}$$

associated with zeros $a_1^2 + c_1^2$, $\sqrt{a_1c_1a_2c_2}$ and $a_2^2 + c_2^2$ respectively.

Now, let us consider the walk on the half-line.

The matrix

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0^\alpha & [C] & & & \\ [A] & G^\alpha & [C] & & \\ & [A] & G^\alpha & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad \begin{aligned} G^\alpha &= -\frac{1}{2}((A^*A + C^*C) \otimes I_2 + I_2 \otimes (A^*A + C^*C)) \\ G_0^\alpha &= -\frac{1}{2}((A^*A) \otimes I_2 + I_2 \otimes (A^*A)) \end{aligned}$$

is a valid generator of a CTOQW. Also,

$$G^\alpha = - \begin{bmatrix} a_1^2 + c_1^2 & 0 & 0 & 0 \\ 0 & \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2} & 0 & 0 \\ 0 & 0 & \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2} & 0 \\ 0 & 0 & 0 & a_2^2 + c_2^2 \end{bmatrix},$$

$$G_0^\alpha = - \begin{bmatrix} a_1^2 & 0 & 0 & 0 \\ 0 & \frac{a_1^2 + a_2^2}{2} & 0 & 0 \\ 0 & 0 & \frac{a_1^2 + a_2^2}{2} & 0 \\ 0 & 0 & 0 & a_2^2 \end{bmatrix}.$$

If we take $K := [(AC)]^{1/2}$ then we obtain the symmetrization

$$J = \mathcal{R}(-\hat{\mathcal{L}})\mathcal{R}^{-1} = \begin{bmatrix} -G_0^\alpha & K & & & \\ K & -G^\alpha & K & & \\ & K & -G^\alpha & K & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

where K is positive definite,

$$\mathcal{R} = \text{diag}(R_0, R_1, \dots, R_N), \quad R_i = [A^{-1}C]^{i-1}, \quad i = 1, 2, 3, \dots, N, \quad R_0 = I_4.$$

Let us obtain the weight matrix associated to \tilde{J} ,

$$\tilde{J} := \begin{bmatrix} -G^\alpha & K & & & \\ K & -G^\alpha & K & & \\ & K & -G^\alpha & K & \\ & & \ddots & \ddots & \ddots \end{bmatrix},$$

using the results of A.J. Durán ([21]).

Since G^α and K commute it is easy to see that the matrix $H_{A,B}(x)$ given by [21] is

$$H(x) = (xI + G^\alpha)^2 K^{-2} - 4I_4 = (xI + G^\alpha)^2 [AC]^{-1} - 4I_4$$

$$= \begin{bmatrix} \frac{(x - a_1^2 - c_1^2)^2}{a_1^2 c_1^2} - 4 & 0 & 0 & 0 \\ 0 & \frac{(x - \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2})^2}{a_1 a_2 c_1 c_2} - 4 & 0 & 0 \\ 0 & 0 & \frac{(x - \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2})^2}{a_1 a_2 c_1 c_2} - 4 & 0 \\ 0 & 0 & 0 & \frac{(x - a_2^2 - c_2^2)^2}{a_2^2 c_2^2} - 4 \end{bmatrix}.$$

The associated weight matrix to \tilde{J} is

$$d\tilde{\Sigma}(x) = \frac{1}{2\pi} K^{-1} \sqrt{\text{diag}(h_1, h_2, h_3, h_4)} = \frac{1}{2\pi} \begin{bmatrix} d_1(x) & 0 & 0 & 0 \\ 0 & d_2(x) & 0 & 0 \\ 0 & 0 & d_3(x) & 0 \\ 0 & 0 & 0 & d_4(x) \end{bmatrix} dx, \quad (2.4.2)$$

where h_j represents the j -th diagonal entry of the diagonal appearing on the representation of $H(x)$ and

$$d_1(x) = \frac{\left[\sqrt{4a_1^2 c_1^2 - (x - a_1^2 - c_1^2)^2} \right]_+}{a_1^2 c_1^2}, \quad d_4(x) = \frac{\left[\sqrt{4a_2^2 c_2^2 - (x - a_2^2 - c_2^2)^2} \right]_+}{a_2^2 c_2^2}$$

$$d_2(x) = d_3(x) = \frac{\left[\sqrt{4a_1 a_2 c_1 c_2 - \left(x - \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2} \right)^2} \right]_+}{2a_1 a_2 c_1 c_2}.$$

Here we are using the notation $[f(x)]_+ = f(x)$ if $f(x) \geq 0$ and 0 otherwise.

We are interested on the transitions of the CTOQW, thus only $d_1(x)$ and $d_4(x)$ contribute for the calculus of the trace when we evaluate

$$\text{Tr} \left(\begin{bmatrix} d_1(x) & 0 & 0 & 0 \\ 0 & d_2(x) & 0 & 0 \\ 0 & 0 & d_3(x) & 0 \\ 0 & 0 & 0 & d_4(x) \end{bmatrix} \text{vec}(\rho) \right),$$

thereby we will avoid the massive calculations using terms as $d_2(x)$ and $d_3(x)$ appearing on the sequel of this section.

The Stieltjes transform is

$$B(z, \tilde{\Sigma}) = K^{-1} \sqrt{\text{diag}(h_1, h_2, h_3, h_4)} = \begin{bmatrix} w_1(z) & 0 & 0 & 0 \\ 0 & w_2(z) & 0 & 0 \\ 0 & 0 & w_3(z) & 0 \\ 0 & 0 & 0 & w_4(z) \end{bmatrix}, \quad (2.4.3)$$

where $w_2(z) = w_3(z)$ is a function that does not vanish and

$$w_1(z) = \frac{z - a_1^2 - c_1^2 - i\sqrt{4a_1^2 c_1^2 - (z - a_1^2 - c_1^2)^2}}{2a_1^2 c_1^2},$$

$$w_4(z) = \frac{z - a_2^2 - c_2^2 - i\sqrt{4a_2^2 c_2^2 - (z - a_2^2 - c_2^2)^2}}{2a_2^2 c_2^2}.$$

Since the measure is obtained on the terms of [21], we must have $\Pi_0 = I_4$, then we use equation (2.20) of [17] to obtain the Stieltjes transform of the weight matrix associated to J :

$$B(z, \Sigma) = \left(B(z, \tilde{\Sigma})^{-1} + (G_0^\alpha - G^\alpha) \right)^{-1} = \begin{bmatrix} \sigma_1(z) & 0 & 0 & 0 \\ 0 & * & 0 & 0 \\ 0 & 0 & * & 0 \\ 0 & 0 & 0 & \sigma_2(z) \end{bmatrix},$$

where

$$\sigma_j(z) = \frac{z - a_j^2 + c_j^2 + \sqrt{-4a_j^2 c_j^2 + (z + a_j^2 + c_j^2)^2}}{2c_j^2 z}, \quad j = 1, 2.$$

It is a simple calculation to verify that $\lim_{z \uparrow 0} \sigma_j(z) = \infty \Leftrightarrow a_j \leq c_j$, thus, given a density operator $\rho = \begin{bmatrix} a & b \\ b^* & 1 - a \end{bmatrix}$, we have

$$\lim_{z \uparrow 0} \text{Tr} [\text{vec}^{-1} \Pi_0 (B(z, \Sigma) \text{vec}(\rho))] = \lim_{z \uparrow 0} (\pi_1 \sigma_1(z) a + \pi_2 \sigma_2(z) (1 - a)),$$

where $\pi_1, \pi_2 > 0$. Therefore, if $\{|e_0\rangle, |e_1\rangle\}$ is the canonical basis of \mathbb{C}^2 , then an application of Corollary 2.14 shows that

- $a_1 \leq c_1$ and $a_2 \leq c_2 \Rightarrow$ vertex $|0\rangle$ is recurrent;
- $a_1 \leq c_1$ and $a_2 > c_2 \Rightarrow$ vertex $|0\rangle$ is $|e_1\rangle \langle e_1|$ -transient and ρ -recurrent for $\rho \neq |e_1\rangle \langle e_1|$;

- $a_1 > c_1$ and $a_2 \leq c_2 \Rightarrow$ vertex $|0\rangle$ is $|e_0\rangle\langle e_0|$ -transient and ρ -recurrent for $\rho \neq |e_0\rangle\langle e_0|$;
- $a_1 > c_1$ and $a_2 > c_2 \Rightarrow$ vertex $|0\rangle$ is transient.

The Perron-Stieltjes inversion formula (Proposition 1.1 of [19]) gives

$$d\Sigma(x) = \frac{1}{\pi} \begin{bmatrix} \left[\frac{\sqrt{4a_1^2c_1^2 - (x - a_1^2 - c_1^2)^2}}{2c_1^2x} \right]_+ & 0 & 0 & 0 \\ 0 & * & 0 & 0 \\ 0 & 0 & * & 0 \\ 0 & 0 & 0 & \left[\frac{\sqrt{4a_2^2c_2^2 - (x - a_2^2 - c_2^2)^2}}{2c_2^2x} \right]_+ \end{bmatrix} dx,$$

thus an application of the Karlin-McGregor formula for CTOQWs gives for $\rho = \begin{bmatrix} a & b \\ b^* & 1 - a \end{bmatrix}$,

$$p_{00;\rho}(t) = a \int_0^\infty e^{-xt} \left[\frac{\sqrt{4a_1^2c_1^2 - (x - a_1^2 - c_1^2)^2}}{2c_1^2x} \right]_+ dx + (1 - a) \int_0^\infty e^{-xt} \left[\frac{\sqrt{4a_2^2c_2^2 - (x - a_2^2 - c_2^2)^2}}{2c_2^2x} \right]_+ dx.$$

Moreover, assume that $r := a_1 = c_1$ and $s := a_2 = c_2$, then the weight matrix $d\Sigma(x)$ is

$$d\Sigma(x) = \frac{1}{\pi} \begin{bmatrix} \left[\frac{\sqrt{-x^2 + 4xr^2}}{2r^2x} \right]_+ & 0 & 0 & 0 \\ 0 & w_{r,s}(x) & 0 & 0 \\ 0 & 0 & w_{r,s}(x) & 0 \\ 0 & 0 & 0 & \left[\frac{\sqrt{-x^2 + 4xs^2}}{2s^2x} \right]_+ \end{bmatrix} dx$$

where

$$w_{r,s}(x) = \left[\frac{2\sqrt{((r+s)^2 - x)(x - (r-s)^2)}}{2(r^2 + s^2)x - (r^2 - s^2)^2} \right]_+ + \left(\frac{(r+s)(r-s)}{r^2 + s^2} \right)^2 \delta_{x_0}(z), \quad x_0 = \frac{(r+s)^2(r-s)^2}{2(r^2 + s^2)}.$$

Finally, we describe the associated walk on the integer line.

Let us consider the homogeneous CTOQW on \mathbb{Z} with

$$R_i^{i+1} = A = \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix}, \quad R_i^{i-1} = C = \begin{bmatrix} c_1 & 0 \\ 0 & c_2 \end{bmatrix}, \quad \forall i \in \mathbb{Z}, \quad a_1, a_2, c_1, c_2 > 0.$$

In this case we have

$$G_i = - \begin{bmatrix} a_1^2 + c_1^2 & 0 & 0 & 0 \\ 0 & \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2} & 0 & 0 \\ 0 & 0 & \frac{a_1^2 + c_1^2 + a_2^2 + c_2^2}{2} & 0 \\ 0 & 0 & 0 & a_2^2 + c_2^2 \end{bmatrix}, \quad i \in \mathbb{Z}.$$

Using the first equation on (2.3.18) with $A_{-1} = A$ and $C_0 = C$, we obtain

$$B(z; W_{11}) = \begin{bmatrix} \frac{\sqrt{(z - a_1^2 - c_1^2)^2 - 4a_1^2c_1^2}}{(z - a_1^2 - c_1^2)^2 - 4a_1^2c_1^2} & 0 & 0 & 0 \\ 0 & * & 0 & 0 \\ 0 & 0 & * & 0 \\ 0 & 0 & 0 & \frac{\sqrt{(z - a_2^2 - c_2^2)^2 - 4a_2^2c_2^2}}{(z - a_2^2 - c_2^2)^2 - 4a_2^2c_2^2} \end{bmatrix},$$

where we used $dW_+ = dW_- = d\tilde{\Sigma}(x)$, $d\tilde{\Sigma}(x)$ being the weight matrix given by (2.4.2).

It is easily seen that

$$\lim_{z \uparrow 0} \frac{\sqrt{(z - a_k^2 - c_k^2)^2 - 4a_k^2c_k^2}}{(z - a_k^2 - c_k^2)^2 - 4a_k^2c_k^2} = \infty \Leftrightarrow a_k = c_k, \quad k = 1, 2,$$

therefore, for $\rho = \begin{bmatrix} a & b \\ b^* & 1 - a \end{bmatrix}$, we obtain that

- $a_1 = c_1$ and $a_2 = c_2$ implies that the walk is recurrent;
- $a_1 \neq c_1$ and $a_2 \neq c_2$ implies that the walk is transient;
- $a_1 = c_1$ and $a_2 \neq c_2$ implies that the walk is ρ -transient for $a = 0$ and ρ -recurrent for $a > 0$;
- $a_1 \neq c_1$ and $a_2 = c_2$ implies that the walk is ρ -transient for $a = 1$ and ρ -recurrent for $a < 1$.

Moreover, the measure dW_{11} is obtained by applications of the Perron-Stieltjes inversion formula:

$$dW_{11}(x) = \begin{bmatrix} \left[\frac{\sqrt{(x-a_1^2-c_1^2)^2-4a_1^2c_1^2}}{(x-a_1^2-c_1^2)^2-4a_1^2c_1^2} \right]_+ & 0 & 0 & 0 \\ 0 & * & 0 & 0 \\ 0 & 0 & * & 0 \\ 0 & 0 & 0 & \left[\frac{\sqrt{(x-a_2^2-c_2^2)^2-4a_2^2c_2^2}}{(x-a_2^2-c_2^2)^2-4a_2^2c_2^2} \right]_+ \end{bmatrix}.$$

The case of simultaneous unitarily diagonalizable transitions. The above analysis can be applied to the simultaneous unitary diagonalizable coins, that is, we can take an unitary matrix U and coins given by

$$A = U \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix} U^*, \quad C = U \begin{bmatrix} c_1 & 0 \\ 0 & c_2 \end{bmatrix} U^*, \quad a_1, a_2, c_1, c_2 > 0$$

to obtain analogous conclusions about the recurrence of vertex $|0\rangle$. In this case, we have

- $a_1 \leq c_1$ and $a_2 \leq c_2 \Rightarrow$ vertex $|0\rangle$ is recurrent;
- $a_1 \leq c_1$ and $a_2 > c_2 \Rightarrow$ vertex $|0\rangle$ is $U|e_1\rangle\langle e_1|U^*$ -transient and ρ -recurrent for $\rho \neq U|e_1\rangle\langle e_1|U^*$;
- $a_1 > c_1$ and $a_2 \leq c_2 \Rightarrow$ vertex $|0\rangle$ is $U|e_0\rangle\langle e_0|U^*$ -transient and ρ -recurrent for $\rho \neq U|e_0\rangle\langle e_0|U^*$;
- $a_1 > c_1$ and $a_2 > c_2 \Rightarrow$ vertex $|0\rangle$ is transient.

Let us describe an example of this and, in addition, let us consider a perturbation on the first vertex. In this case, the walk can be represented by Figure 2.4, where B_0 represents the rate of jumping from vertex $|0\rangle$ to itself. Moreover, since we are taking B_0 as the operator containing the rate of remaining on site $|0\rangle$, one may

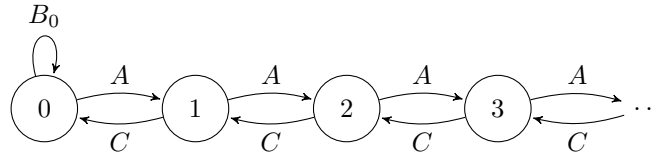


Figure 2.4: A slight modification on the first vertex.

think that $B_0 \neq 0$ should increase the probability of recurrence on site $|0\rangle$, however the exactly opposite may happen as the following example illustrates.

Example 2.21. Let $U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}$ and consider the CTOQW with generator

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0 + [B_0] & [C] & & & \\ [A] & G & [C] & & \\ & [A] & G & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad A = C = U \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} U^*, \quad B_0 = U \begin{bmatrix} b_1 & b_2 \\ b_2 & b_3 \end{bmatrix} U^*,$$

$b_k \in \mathbb{R}$, $k = 1, 2, 3$, $G = -\mathcal{U} \text{diag}(8, 5, 5, 2) \mathcal{U}^*$ and

$$G_0 = -2\mathcal{U} \begin{bmatrix} 8 + 2b^2 & b_2(b_3 - b_1) & b_2(b_3 - b_1) & -2b_2^2 \\ b_2(b_3 - b_1) & 5 + (b_1 - b_3)^2 + 2b_2^2 & -2b_2^2 & b_2(b_1 - b_3) \\ b_2(b_3 - b_1) & -2b_2^2 & 5 + (b_1 - b_3)^2 + 2b_2^2 & b_2(b_1 - b_3) \\ -2b_2^2 & b_2(b_1 - b_3) & b_2(b_1 - b_3) & 2 + 2b_2^2 \end{bmatrix} \mathcal{U}^*,$$

where $\mathcal{U} = U \otimes U$.

We remark that the matrix B_0 is a multiplication $B_0 = UTU^*$, where T is Hermitian, therefore unitary diagonalizable. In this case we have $B_0 = UVDV^*U^*$, where D is diagonal and V is unitary, however we preserve the representation $B_0 = UTU^*$ in order to preserve the products involving the coins and to assure that the transitions of the walk do not have a diagonal dynamics when $b_2 \neq 0$.

The Stieltjes transform of the weight matrix associated to $\tilde{\mathcal{L}}$ ($\hat{\mathcal{L}}$ with $G_0 + [B_0]$ switched by G) is then, by equation (2.4.3),

$$B(z, \tilde{\Sigma}) = \frac{1}{32} \mathcal{U} \begin{bmatrix} w_1(z) & 0 & 0 & 0 \\ 0 & w_2(z) & 0 & 0 \\ 0 & 0 & w_3(z) & 0 \\ 0 & 0 & 0 & w_4(z) \end{bmatrix} \mathcal{U}^*, \quad \begin{aligned} w_1(z) &= 8 - z - \sqrt{z(z-16)} \\ w_2(z) &= w_3(z) = 20 - 4z - 4\sqrt{z^2 - 10z + 9} \\ w_4(z) &= 32 - 16z - 16\sqrt{z^2 - 4z} \end{aligned} \quad (2.4.4)$$

The Stieltjes transform of $-\hat{\mathcal{L}}$ is obtained by

$$B(z, \Sigma) = \left(B(z, \tilde{\Sigma})^{-1} + (G_0 + [B_0] - G) \right)^{-1} \\ = \mathcal{U} \begin{bmatrix} 4 - b_2^2 + \frac{w_1(z)}{32} & \frac{b_2(b_1-b_3)}{2} & \frac{b_2(b_1-b_3)}{2} & b_2^2 \\ \frac{b_2(b_1-b_3)}{2} & \frac{5-b_1^2-b_2^2-b_3^2+2b_1b_3}{2} + \frac{w_2(z)}{32} & b_2^2 & \frac{b_2(b_1-b_3)}{2} \\ \frac{b_2(b_1-b_3)}{2} & b_2^2 & \frac{5-b_1^2-b_2^2-b_3^2+2b_1b_3}{2} + \frac{w_3(z)}{32} & \frac{b_2(b_1-b_3)}{2} \\ b_2^2 & \frac{b_2(b_1-b_3)}{2} & \frac{b_2(b_1-b_3)}{2} & 1 - b_2^2 + \frac{w_4(z)}{32} \end{bmatrix}^{-1} \mathcal{U}^*.$$

After some calculus using the limit given in Corollary 2.14, we obtain the following results:

- $b_2 = 0$ and $b_1 \notin \{b_3 + 3\sqrt{2}/2, b_3 - 3\sqrt{2}/2, b_3\} \Rightarrow$ vertex $|0\rangle$ is recurrent;
- $b_2 = 0$ and $b_1 \in \{b_3 + 3\sqrt{2}/2, b_3 - 3\sqrt{2}/2, 1\} \Rightarrow$ vertex $|0\rangle$ is ρ -recurrent if and only if $\rho = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$;
- $b_2 \neq 0 \Rightarrow$ vertex $|0\rangle$ is transient.

Now we point out that the choice $b_2 = 0$ keeps some recurrence properties of site $|0\rangle$, however a non-null b_2 assures that vertex $|0\rangle$ is transient for any choice of ρ .

A perturbation on the vertex $|0\rangle$ for the CTOQW on \mathbb{Z} : We consider CTOQW on Z with the same transitions as above with a perturbation on vertex $|0\rangle$, that is, the we are taking the walk given by Figure 2.5, where

$$A = C = U \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} U^*, \quad B_0 = U \begin{bmatrix} b_1 & b_2 \\ b_2 & b_3 \end{bmatrix} U^*, \quad U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix}, \quad b_1, b_2, b_3 \in \mathbb{R}.$$

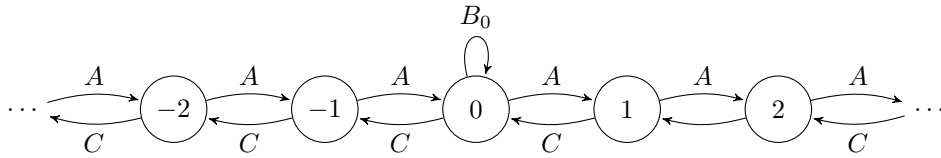


Figure 2.5: Generator $\hat{\mathcal{L}}$ of a CTOQW on \mathbb{Z} with a perturbation on vertex $|0\rangle$.

We want to apply Equation (2.3.17) to verify if vertex $|0\rangle$ is recurrent. To do this, we notice that

$$\hat{\mathcal{L}}^+ = \begin{bmatrix} G_0^\alpha + [B_0] & [C] & & & \\ [A] & G^\alpha & [C] & & \\ & [A] & G^\alpha & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad \hat{\mathcal{L}}^- = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ & [A] & G^\alpha & [C] & \\ & & [A] & G^\alpha & [C] \\ & & & [A] & G^\alpha \end{bmatrix},$$

where $G^\alpha = -\mathcal{U} \text{diag}(8, 5, 5, 2) \mathcal{U}^*$ and

$$G_0^\alpha = -\frac{1}{2} [(A^*A + B_0^*B_0 + C^*C) \otimes I + I \otimes (A^*A + B_0^*B_0 + C^*C)].$$

The Stieltjes transform of the weight matrix associated to $\hat{\mathcal{L}}^-$ is given on Equation (2.4.4)(since $A = C$) while the Stieltjes transform of the weight matrix associated to $\hat{\mathcal{L}}^+$ is

$$\begin{aligned} B(z, W_+) &= (B(z, W_-)^{-1} + (G_0^\alpha + [B_0] - G^\alpha))^{-1} \\ &= \mathcal{U} \begin{bmatrix} s_1(z) & \frac{b_2(b_1-b_3)}{2} & \frac{b_2(b_1-b_3)}{2} & b_2^2 \\ \frac{b_2(b_1-b_3)}{2} & s_2(z) & b_2^2 & \frac{b_2(b_1-b_3)}{2} \\ \frac{b_2(b_1-b_3)}{2} & b_2^2 & s_2(z) & \frac{b_2(b_1-b_3)}{2} \\ b_2^2 & \frac{b_2(b_1-b_3)}{2} & \frac{b_2(b_1-b_3)}{2} & s_3(z) \end{bmatrix}^{-1} \mathcal{U}^*. \end{aligned}$$

where $s_1(z) = \frac{z - \sqrt{z^2 - 16z}}{2} - 4 - b_2^2$, $s_2(z) = \frac{5 - z - (b_1 - b_3)^2 + \sqrt{z^2 - 10z + 9}}{2} - b_2^2$, $s_3(z) = \frac{z - \sqrt{z^2 - 4z}}{2} - 1 - b_2^2$.

Some calculus show that

$$-\lim_{z \uparrow 0} \text{Tr}(B(z, W_{11})\rho) = \infty$$

for any choice of $b_1, b_2, b_3 \in \mathbb{R}$ and $\rho \in \mathbb{M}_2(\mathbb{C})$, therefore vertex $|0\rangle$ is always recurrent for this CTOQW.

The same can be done with vertex $|-1\rangle$, however in this case we have to evaluate $-\lim_{z \uparrow 0} \text{Tr}(B(z, W_{22})\rho) = \infty$, which is always infinite for any choice of $b_1, b_2, b_3 \in \mathbb{R}$ and $\rho \in \mathbb{M}_2(\mathbb{C})$, therefore vertex $|-1\rangle$ is also always recurrent for this CTOQW.

2.4.2 Noncommuting transitions

Let

$$A = \begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix}, \quad C = \begin{bmatrix} 1 & 1 \\ 0 & -1 \end{bmatrix},$$

where

$$G_1 = -3I_4, \quad G_0 = \frac{1}{2} \begin{bmatrix} -4 & 1 & 1 & 0 \\ 1 & -3 & 0 & 1 \\ 1 & 0 & -3 & 1 \\ 0 & 1 & 1 & -2 \end{bmatrix}, \quad G_2 = -\frac{1}{2} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 1 & 3 & 0 & 1 \\ 1 & 0 & 3 & 1 \\ 0 & 1 & 1 & 4 \end{bmatrix}.$$

Consider the CTOQW with $V = \{0, 1, 2, 3\}$ induced by the generator

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0 & [C] & 0 & 0 \\ [A] & G_1 & [C] & 0 \\ 0 & [A] & G_1 & [C] \\ 0 & 0 & [A] & G_2 \end{bmatrix}.$$

Note that this generator satisfies the conditions (2.3.5) with $R_n = I_4$, $n = 0, 1, 2, 3$, thus there exists a positive weight matrix associated to $\hat{\mathcal{L}}$, which will be evaluated now.

The eigenvalues of $-\hat{\mathcal{L}}$ are

$$\begin{aligned} \lambda_1 &= 0, \quad \lambda_2 = 3 - \sqrt{5}, \quad \lambda_3 = 3 + \sqrt{5}, \quad \lambda_4 = 3 - \sqrt{7}, \quad \lambda_5 = 3 + \sqrt{7} \\ \lambda_6 &= \frac{7 - \sqrt{17}}{4}, \quad \lambda_7 = \frac{7 + \sqrt{17}}{4}, \quad \lambda_8 = \frac{11 - \sqrt{41}}{4}, \quad \lambda_9 = \frac{11 + \sqrt{41}}{4}, \end{aligned}$$

($\lambda_1, \lambda_4, \lambda_5, \lambda_6, \lambda_7, \lambda_8$ and λ_9 have multiplicity 2) with weights

$$\begin{aligned} W_1 &= \frac{1}{20} \begin{bmatrix} 3 & -1 & -1 & 2 \\ -1 & 2 & 2 & 1 \\ -1 & 2 & 2 & 1 \\ 2 & 1 & 1 & 3 \end{bmatrix}, \quad W_2 = \frac{1}{2} \left(W_1 + \frac{\sqrt{5}}{20} Y \right), \quad W_3 = \frac{1}{2} \left(W_1 - \frac{\sqrt{5}}{20} Y \right), \\ W_4 &= \frac{1}{14} \left((14 + 3\sqrt{7}) W_1 + \frac{\sqrt{7}}{4} Y \right), \quad W_5 = \frac{1}{14} \left((14 - 3\sqrt{7}) W_1 - \frac{\sqrt{7}}{4} Y \right), \\ W_6 &= \frac{1}{4} \left(1 + \frac{\sqrt{17}}{17} \right) (I_4 - 4W_1), \quad W_7 = \frac{1}{4} \left(1 - \frac{\sqrt{17}}{17} \right) (I_4 - 4W_1) \\ W_8 &= \frac{1}{4} \left(1 + \frac{4\sqrt{41}}{41} \right) (I_4 - 4W_1), \quad W_9 = \frac{1}{4} \left(1 - \frac{4\sqrt{41}}{41} \right) (I_4 - 4W_1). \end{aligned}$$

As usually, the next step is to obtain the Stieltjes transform of $d\Sigma$, the weight matrix associated to J . By equation (2.20) of [17], we have

$$B(z, \Sigma) = \left(B(z, \tilde{\Sigma})^{-1} + (G_0 - G) \right)^{-1} = \text{diag}(f_1(z), f_2(z), f_3(z), f_4(z)),$$

where

$$f_k(z) = \frac{1}{2} \frac{\psi_k(z)m_{1,k} - m_{1,k}\sqrt{\psi_k(z)^2 + 4\gamma_k(z)^2} - 2\tilde{g}_k\gamma_k(z) + 2g_k\gamma_k(z)}{m_{1,k}^2\gamma_k(z) - \tilde{g}_k^2\gamma_k(z) - g_k^2\gamma_k(z) + 2\tilde{g}_kg_k\gamma_k(z) - m_{1,k}g_k\psi_k(z) + m_{1,k}\tilde{g}_k\psi_k(z)},$$

and we have put $G_0 = \text{diag}(g_1, g_2, g_3, g_4)$, $\psi_k(z) = -(z + g_k)^2 + m_{1,k}^2 - m_{0,k}^2$, $\gamma_k(z) = (z + g_k)m_{1,k}$.

Now, we are able to consider an antidiagonal transition in the following terms: consider a CTOQW on \mathbb{Z}_+ whose generator is of the form

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0 & [C] & & & \\ [A] & G & [C] & & \\ & [A] & G & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}, \quad A = \begin{bmatrix} 0 & a_1 \\ a_2 & 0 \end{bmatrix}, \quad C = \begin{bmatrix} 0 & c_1 \\ c_2 & 0 \end{bmatrix},$$

$$G_0 = - \begin{bmatrix} a_2^2 & 0 & 0 & 0 \\ 0 & \frac{a_1^2 + a_2^2}{2} & 0 & 0 \\ 0 & 0 & \frac{a_1^2 + a_2^2}{2} & 0 \\ 0 & 0 & 0 & a_1^2 \end{bmatrix}, \quad G = - \begin{bmatrix} a_2^2 + c_2^2 & 0 & 0 & 0 \\ 0 & \frac{a_1^2 + a_2^2 + c_1^2 + c_2^2}{2} & 0 & 0 \\ 0 & 0 & \frac{a_1^2 + a_2^2 + c_1^2 + c_2^2}{2} & 0 \\ 0 & 0 & 0 & a_1^2 + c_1^2 \end{bmatrix}.$$

We have the symmetrization

$$J = R(-\hat{\mathcal{L}})R^{-1} = \begin{bmatrix} -G_0 & [P_0] & & & \\ [P_0] & -G & [P_1] & & \\ & [P_1] & -G & [P_0] & \\ & & [P_0] & -G & [P_1] \\ & & [P_1] & -G & [P_0] \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \quad R = \text{diag}([R_0], [R_1], \dots),$$

where

$$R_{2k} = \begin{bmatrix} \left(\frac{c_2}{a_1}\right)^{\frac{k}{2}} & \left(\frac{c_1}{a_2}\right)^{\frac{k-2}{2}} & & 0 \\ & 0 & \left(\frac{c_2}{a_1}\right)^{\frac{k-2}{2}} & \left(\frac{c_1}{a_2}\right)^{\frac{k}{2}} \end{bmatrix}, \quad R_{2k+1} = \left(\frac{c_1 c_2}{a_1 a_2}\right)^{\frac{k}{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad k = 0, 1, 2, \dots,$$

and P_0 and P_1 are the ones given above. Thus J and $\hat{\mathcal{L}}$ have the same associated weight matrix and we obtain, for $d\Sigma(x)$ given above that

$$\lim_{z \uparrow 0} \text{Tr}(B(z, \Sigma)\rho) = \lim_{z \uparrow 0} (f_1(z)a + f_4(z)(1-a)),$$

where $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$. After some calculus we obtain that

$$\lim_{z \uparrow 0} f_1(z) = \infty \Leftrightarrow a_1 = \sqrt{\frac{2c_2^4 - a_2^2 c_1^2 + a_2^4 + 3a_2^2 c_2^2}{a_2^2 + 2c_2^2}}, \quad 2c_2^4 + a_2^4 + 3a_2^2 c_2^2 > a_2^2 c_1^2,$$

$$\lim_{z \uparrow 0} f_4(z) = \infty \Leftrightarrow a_2 = \sqrt{\frac{2c_1^4 - a_1^2 c_2^2 + a_1^4 + 3a_1^2 c_1^2}{a_1^2 + 2c_1^2}}, \quad 2c_1^4 + a_1^4 + 3a_1^2 c_1^2 > a_1^2 c_2^2,$$

giving the following conclusion (see Corollary 2.14):

- $a_1 = \sqrt{\frac{2c_2^4 - a_2^2 c_1^2 + a_2^4 + 3a_2^2 c_2^2}{a_2^2 + 2c_2^2}}$ and $a_2 = \sqrt{\frac{2c_1^4 - a_1^2 c_2^2 + a_1^4 + 3a_1^2 c_1^2}{a_1^2 + 2c_1^2}} \Rightarrow$ vertex $|0\rangle$ is recurrent;

- $a_1 = \sqrt{\frac{2c_2^4 - a_2^2 c_1^2 + a_2^4 + 3a_2^2 c_2^2}{a_2^2 + 2c_2^2}}$ and $a_2 \neq \sqrt{\frac{2c_1^4 - a_1^2 c_2^2 + a_1^4 + 3a_1^2 c_1^2}{a_1^2 + 2c_1^2}} \Rightarrow$ vertex $|0\rangle$ is ρ -transient when $a = 0$ and ρ -recurrent when $a > 0$;
- $a_1 \neq \sqrt{\frac{2c_2^4 - a_2^2 c_1^2 + a_2^4 + 3a_2^2 c_2^2}{a_2^2 + 2c_2^2}}$ and $a_2 = \sqrt{\frac{2c_1^4 - a_1^2 c_2^2 + a_1^4 + 3a_1^2 c_1^2}{a_1^2 + 2c_1^2}} \Rightarrow$ vertex $|0\rangle$ is ρ -transient when $a = 1$ and ρ -recurrent when $a < 1$;
- $a_1 \neq \sqrt{\frac{2c_2^4 - a_2^2 c_1^2 + a_2^4 + 3a_2^2 c_2^2}{a_2^2 + 2c_2^2}}$ and $a_2 \neq \sqrt{\frac{2c_1^4 - a_1^2 c_2^2 + a_1^4 + 3a_1^2 c_1^2}{a_1^2 + 2c_1^2}} \Rightarrow$ vertex $|0\rangle$ is transient.

The last example of this section will consider CTOQWs with non-null Hamiltonian part.

Example 2.22. Let us consider $r, s > 0$ such that $rs = 1$. We set the matrices

$$A = rI_2, \quad C = sI_2, \quad H_0 = \begin{bmatrix} v & u \\ u & v \end{bmatrix}, \quad B = \begin{bmatrix} 1 & ui \\ ui & 1 \end{bmatrix}, \quad u, v \in \mathbb{R}.$$

The CTOQW with $V = \{0, 1\}$: we consider the case $H_1 = H_0$ and let

$$G_0^\alpha = \begin{bmatrix} -r^2 - u^2 & 0 & 0 & u^2 \\ 0 & -r^2 - u^2 & u^2 & 0 \\ 0 & u^2 & -r^2 - u^2 & 0 \\ u^2 & 0 & 0 & -r^2 - u^2 \end{bmatrix}, \quad G_1^\alpha = \begin{bmatrix} -s^2 - u^2 & 0 & 0 & u^2 \\ 0 & -s^2 - u^2 & u^2 & 0 \\ 0 & u^2 & -s^2 - u^2 & 0 \\ u^2 & 0 & 0 & -s^2 - u^2 \end{bmatrix}.$$

On this case,

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0^\alpha + [B] & [C] \\ [A] & G_1^\alpha + [B] \end{bmatrix},$$

thus the semigroup preserves trace. Also, the eigenvalues of $\hat{\mathcal{L}}$ are

$$\lambda_1 = 0, \quad \lambda_2 = -\frac{1+r^4}{r^2}, \quad \lambda_3 = -\frac{1+2u^2r^2+r^4}{r^2}, \quad \lambda_4 = -2u^2,$$

and the corresponding weights are

$$W_1 = \frac{1}{2(1+r^4)} \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}, \quad W_2 = r^4 W_1, \quad W_3 = \frac{r^4}{2(1+r^4)} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}, \quad W_4 = \frac{1}{r^4} W_3.$$

For instance,

$$p_{00;\rho}(t) = \frac{1 + e^{\lambda_2 r^4 t}}{1 + r^4},$$

for any density $\rho \in \mathbb{M}_2(\mathbb{C})$.

The CTOQW with $V = \mathbb{Z}_{\geq 0}$: we consider the case $H_i = H_0 \forall i \in V$, then the trace-preserving case has

$$G_0^\alpha = \begin{bmatrix} -r^2 - u^2 & 0 & 0 & u^2 \\ 0 & -r^2 - u^2 & u^2 & 0 \\ 0 & u^2 & -r^2 - u^2 & 0 \\ u^2 & 0 & 0 & -r^2 - u^2 \end{bmatrix}, \quad G_i^\alpha = G := \begin{bmatrix} -2 - u^2 & 0 & 0 & u^2 \\ 0 & -2 - u^2 & u^2 & 0 \\ 0 & u^2 & -2 - u^2 & 0 \\ u^2 & 0 & 0 & -2 - u^2 \end{bmatrix}, \quad i \geq 1.$$

By the technique of [21], the matrix weight associated to

$$\tilde{\mathcal{L}} = \begin{bmatrix} G & [C] & & & \\ [A] & G & [C] & & \\ & [A] & G & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}$$

is given by

$$d\tilde{W}(x) = \frac{\sqrt{[4(xu^2 - 2u^2 - u^4 + x) - x^2]_+} + \sqrt{[4x - x^2]_+}}{4\pi} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix}.$$

The Stieltjes transform of $d\tilde{\Sigma}$ is

$$B(z, \tilde{\Sigma}) = \frac{\sqrt{-4(-zu^2 + u^2 + u^4 - z) + z^2 - 4 + 2z - 2u^2 - \sqrt{-4z + z^2}}}{4} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix},$$

thus an application of formula given by Equation 2.20 of [17] gives the Stieltjes transform $B(z, \Sigma)$, where $d\Sigma$ is the matrix weight associated to the CTOQW whose generator is

$$\hat{\mathcal{L}} = \begin{bmatrix} G_0^\alpha & [C] & & & \\ [A] & G & [C] & & \\ & [A] & G & [C] & \\ & & \ddots & \ddots & \ddots \end{bmatrix}.$$

After some calculus, we obtain

$$-\lim_{z \uparrow 0} \text{Tr}(B(z, \Sigma)\rho) = \frac{1 + r^4 + |1 - r^4|}{1 - r^4 + |1 - r^4|} r^2,$$

for any choice of ρ , which allows us to conclude that the CTOQW is recurrent if and only if $r \geq 1$, that is, $r \geq s$. If $r < s$, then the walk is transient for every density ρ .

The CTOQW with $V = \mathbb{Z}$: the Stieltjes transform of the matrix weight W_{11} associated to the walk on \mathbb{Z} is obtained by Equation (2.3.18) and we have

$$-\lim_{z \uparrow 0} \text{Tr}(B(z, W_{11})\rho) = \frac{1 + r^4 + |1 - r^4|}{1 - 2r^4 + (r^4 + 1)|1 - r^4| + r^8} r^2,$$

which is finite if and only if $r = s = 1$. Therefore this CTOQW in \mathbb{Z} is recurrent if and only if $r = s$ and transient for every density if and only if $r \neq s$.

2.5 Jumps and Holding Time

In this section we treat the recurrence of homogeneous CTOQW based on its jump chain. The probability distribution of the jumps will appear as values bounded by CP maps defined on terms of R_j^i and G_i which characterize the generator \mathcal{L} . Before that, let us recall some properties of the discrete and continuous-time Markov chains (DTMC and CTMC respectively) on the set of vertices $V = \mathbb{Z}$.

Proposition 2.23 ([32]). *Consider a CTMC on \mathbb{Z} generated by a Q -matrix $Q = (q_{ij})_{i,j \in \mathbb{Z}}$. A vertex $i \in \mathbb{Z}$ is recurrent if and only if it is recurrent for its jump chain $\Pi = (\pi_{ij})_{i,j \in \mathbb{Z}}$, which is a DTMC, where*

$$\pi_{ij} = \begin{cases} q_{ij}/q_{ii}, & \text{if } j \neq i \text{ and } q_{ii} \neq 0 \\ 0, & \text{if } j \neq i \text{ and } q_{ii} = 0 \\ 0, & \text{if } j = i \text{ and } q_{ii} \neq 0 \\ 1, & \text{if } j = i \text{ and } q_{ii} = 0 \end{cases}.$$

If the CTMC is homogeneous with non-negative rates ($q_{ij} > 0$ for $|j - i| = 1$), then

$$\Pi = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ & \lambda & 0 & \gamma & \\ & & \lambda & 0 & \gamma \\ & & & \ddots & \ddots & \ddots \end{bmatrix}, \quad \lambda = \frac{q_{0,-1}}{q_{0,-1} + q_{0,1}}, \quad \gamma = \frac{q_{0,1}}{q_{0,-1} + q_{0,1}}, \quad (2.5.1)$$

thus the walk is recurrent if and only if $\lambda = \gamma$.

For simplicity, we will assume $R_i^i = 0$ for all $i \in V$, in order to apply the results obtained on [5]. We follow [5, 33] to discuss the quantum trajectory describing the indirect measurement of the position of a CTOQW Λ of the more general form (2.2.1) in order to obtain probabilistic properties of Λ . So, let $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$ be a probability space where independent Poisson point processes $N^{ij}, i, j \in V, i \neq j$ on \mathbb{R}^2 are defined.

Definition 2.24. Let Λ be a CTOQW with generator of the form (2.2.1) and an initial density operator $\mu = \sum_{i \in V} \rho(i) \otimes |i\rangle \langle i| \in \mathcal{D}$. The quantum trajectory describing the indirect measurement of the position of the CTOQW is the Markov chain described by the density operators $(\mu_t)_{t \geq 0}$ such that

$$\mu_0 = \rho_0 \otimes |X_0\rangle \langle X_0|,$$

where X_0 and ρ_0 are random variables with distribution

$$\mathbb{P} \left((X_0, \rho) = \left(i, \frac{\rho(i)}{\text{Tr}(\rho(i))} \right) \right) = \text{Tr}(\rho(i)) \text{ for all } i \in V,$$

and such that $\mu_t =: \rho_t \otimes |X_t\rangle \langle X_t|$ satisfies the stochastic differential equation

$$\begin{aligned} \mu_t = & \mu_0 + \int_0^t M(\mu_{s-}) ds \\ & + \sum_{ij} \int_0^t \int_{\mathbb{R}} \left(\frac{S_i^j \mu_{s-} S_i^{j*}}{\text{Tr}(S_i^j \mu_{s-} S_i^{j*})} - \mu_{s-} \right) 1_{0 < y < \text{Tr} S_i^j \mu_{s-} S_i^{j*}} N^{ij}(dy, ds) \end{aligned} \quad (2.5.2)$$

for all $t \geq 0$, where

$$M(u) = \mathcal{L}(u) - \sum_{ij} \left(S_i^j \mu S_i^{j*} - \mu \text{Tr}(S_i^j \mu S_i^{j*}) \right).$$

Hence, for a fixed $\mu = \sum_i \rho(i) \otimes |i\rangle \langle i| \in \mathcal{D}$,

$$M(\mu) = \sum_i (G_i \rho(i) + \rho(i) G_i^* - \rho(i) \text{Tr}(G_i \rho(i) + \rho(i) G_i^*)) \otimes |i\rangle \langle i|.$$

The evolution of the solution μ_t of (2.5.2) is described as follows: suppose $X_0 = i_0$ for some $i_0 \in V$ and fix $\rho_0 \in V(\mathfrak{h}_{i_0})$. For all $t \geq 0$, consider the solution

$$\eta_t = \rho_0 + \int_0^t (G_{i_0} \eta_s + \eta_s G_{i_0}^* - \eta_s \text{Tr}(G_{i_0} \eta_s + \eta_s G_{i_0}^*)) ds,$$

which is a density operator on acting on \mathfrak{h}_{i_0} . For $j \neq i_0$, define

$$T_1^j = \inf\{t \geq 0; N^{i_0, j} \left(u, y | 0 \leq u \leq t, 0 \leq y \leq \text{Tr}(R_{i_0}^j \eta_u R_{i_0}^{j*}) \right) \geq 1\}.$$

Since the random variables T_1^j are mutually independent and nonatomic, we can define $T_1 = \inf_{j \neq i_0} \{T_1^j\}$ once there exists a unique $j \in V$ such that $T_1^j = T_1$. The random variable T_1 is said to be the **first jump time** of the CTOQW conditional on $X_0 = i_0$.

The first jump time to site $|j\rangle$ is then denoted by T_1^j and has distribution

$$\mathbb{P}(T_1^j > \varepsilon) = e^{-\int_0^\varepsilon \text{Tr}(R_{i_0}^j \eta_u R_{i_0}^{j*}) du},$$

thus

$$\mathbb{P}(T_1 \leq \varepsilon) \leq \varepsilon \sum_{j \neq i_0} \|R_{i_0}^{j*} R_{i_0}^j\|.$$

The strongly convergence of $\sum_{ij} S_i^{j*} S_i^j$ implies that $\mathbb{P}(T_1 > 0) = 1$. Thereby, on $[0, T_1]$, we can define the solution $(X_t, \rho_t)_{t \geq 0}$ as

$$\begin{aligned} (X_t, \rho_t) &= (i_0, \eta_t) \text{ for } t \in [0, T_1] \text{ and} \\ (X_{T_1}, \rho_{T_1}) &= \left(j, \frac{R_{i_0}^j \eta_{T_1} R_{i_0}^{j*}}{\text{Tr}(R_{i_0}^j \eta_{T_1} R_{i_0}^{j*})} \right) \text{ if } T_1 = T_1^j. \end{aligned}$$

Now we solve

$$\eta_t = \rho_{T_1} + \int_0^t (G_j \eta_s + \eta_s G_j^* - \eta_s \text{Tr}(G_j \eta_s + \eta_s G_j^*)) ds$$

and then obtain the second jump time T_2 . So on we obtain an increasing sequence of jumps $(T_n)_n$ with $\lim_{n \rightarrow \infty} T_n = \infty$ almost surely (see section 18.2.3 of [5] for more details). This means that the walk do not explode, that is, Λ does not makes infinitely many jumps in a finite interval. For details concerned about explosions in the classical case, see section 2.2 of [32].

Set $\tau_i^{(0)} = 0$, then the time at which X_t reaches $|i\rangle$ for the n -th time is defined as

$$\tau_i^{(n)} = \inf\{t > \tau_{n-1}^i : X_t = i \text{ and } X_{t-} \neq i\}, \quad n = 1, 2, 3, \dots, \quad (2.5.3)$$

thus the **holding time** on the n -th step is given by

$$S_n = \begin{cases} \tau_i^{(n)} - \tau_i^{(n-1)}, & \text{if } \tau_i^{(n-1)} < \infty \\ 0, & \text{otherwise.} \end{cases}$$

The next result is obtained following the idea of Proposition 1.2.2 of [1].

Proposition 2.25. *Let Λ be a CTOQW on a set of vertices V . Given $i \in V$ and $\rho \in \mathcal{S}(\mathfrak{h}_i)$, the following limit exists*

$$q_{i;\rho} := \lim_{t \downarrow 0} \frac{1 - p_{ii;\rho}(t)}{t}.$$

Moreover, $p_{ii;\rho}(t) = 1$ for all $t \geq 0$ if and only if $q_{i;\rho} = 0$.

On the sequel, we will say that i is a ρ -**absorbing** vertex if $q_{i;\rho} = 0$ (equivalently $p_{ii;\rho}(t) = 1$ for all $t \geq 0$) and **absorbing** if $q_{i;\rho'} = 0$ for every density operator $\rho' \in \mathcal{S}(\mathfrak{h}_i)$.

For instance, let λ be a CTOQW on $V = \{0, 1\}$ such that its generator is $\mathcal{L} = \Phi - I$, Φ quantum channel with Kraus operators

$$R_0^0 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad R_1^0 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_0^1 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad R_1^1 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

We have for a density operator $\rho = \begin{bmatrix} a & b \\ b^* & 1-a \end{bmatrix}$ on \mathbb{C}^2 the transition

$$p_{00;\rho}(t) = \frac{1 + a + e^{-2t}(1-a)}{2}, \quad t \in [0, \infty).$$

Hence, i is ρ -absorbing if and only if $a = 1$, which happens only for $\rho = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$. Therefore the definition of absorbing vertex indeed depends on the quantum states.

The existence of the limit $q_{i;\rho}$ is proved above. Now we will give an explicit expression for it directly from the generator of Λ .

Proposition 2.26. *The value $q_{i;\rho}$ obtained as the limit on Proposition 2.25 has the form*

$$q_{i;\rho} = \lim_{t \downarrow 0} \frac{1 - p_{ii;\rho}(t)}{t} = -\text{Tr}(\mathbb{P}_i \mathcal{L} \mathbb{P}_i \rho) = -\text{Tr}(G_i \rho + \rho G_i^*) = \sum_{j \neq i} \text{Tr}(R_i^{j*} R_i^j \rho). \quad (2.5.4)$$

Moreover, for $j \neq i$,

$$q_{ji;\rho} := \lim_{t \downarrow 0} \frac{p_{ji;\rho}(t)}{t} = \text{Tr}(\mathbb{P}_j \mathcal{L} \mathbb{P}_i \rho) = \text{Tr}(R_i^j \rho R_i^{j*}). \quad (2.5.5)$$

2.6 The $G_i = -q_i I/2$ case

In this section we will consider the special class of CTOQW with generator of the form

$$\mathcal{L}(\rho) = \sum_{i \in V} \left(\sum_{j \in V} R_j^i \rho(j) R_j^{i*} - q_i \rho(i) \right) \otimes |i\rangle \langle i|, \quad (2.6.1)$$

that is, we are assuming that $\sum_{j \in V} R_j^{i*} R_j^i = q_i I$, $q_i \geq 0$ and $H = 0$, thus $G_i = -\frac{q_i}{2} I$. In this case, the value $q_{i;\rho}$ of Proposition 2.26 is just q_i , since it does not depend on the density.

If $q_i > 0$ for all $i \in V$, then the generator (2.6.1) is of the form $\mathcal{L} = \Phi - Q$, where $Q = \text{diag}(q_j I)_{j \in V}$ and thus ΦQ^{-1} is a quantum channel.

Theorem 2.27. Let Λ be a CTOQW with generator of the form (2.6.1). Suppose that the chain starts on $i \in V$ with initial density operator $\rho \in \mathcal{S}(\mathfrak{h}_i)$. Then, for $j \neq i$,

$$\mathbb{P}_{i,\rho}(F_1 = j) := \mathbb{P}_{i,\rho}(\text{first jump is to } j) = \begin{cases} \frac{q_{ji,\rho}}{q_i}, & \text{if } q_i \neq 0 \\ 0, & \text{otherwise.} \end{cases} \quad (2.6.2)$$

We already know the distribution of F_1 , in the sequel we present the distribution for all F_n , $n = 1, 2, \dots$.

Theorem 2.28. Let Λ be a CTOQW with generator of the form (2.6.1) starting on vertex $|i\rangle$ with initial density operator $\rho \in \mathcal{S}(\mathfrak{h}_i)$. The distribution

$$\mathbb{P}_{i,\rho}(F_n = k) := \mathbb{P}_{i,\rho}(\text{the } n\text{-th jump is to } k) \quad (2.6.3)$$

is given by

$$\mathbb{P}_{i,\rho}(F_n = k) = \sum_{i_1, \dots, i_n \in V} \frac{\text{Tr}(R_{i_n}^k \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_n}^{k*})}{q_{i_1} \dots q_{i_n}}. \quad (2.6.4)$$

We will call the discrete random variable $\{F_n, n \geq 0\}$ by **quantum jump chain** of the CTOQW Λ . Let us describe this chain for the case where the generator is of the form (2.6.1). First we rewrite (2.6.1) by

$$\mathcal{L} = \Phi - Q, \quad \Phi(\rho) = \sum_{i,j \in V} B_j^i \rho(j) B_j^{i*}, \quad B_j^i = R_j^i \otimes |i\rangle \langle j|, \quad (2.6.5)$$

where $Q = \sum_{k \in V} q_k I_k \otimes |k\rangle \langle k|$, $q_k \geq 0$, and I_k is the identity matrix of \mathfrak{h}_k .

On this case we put $M_i^j := \frac{1}{\sqrt{q_i}} R_i^j$, then

$$\mathbb{P}_{i,\rho}(F_n = k) = \text{Tr}\left(\Pi_{ki}^{(n)} \rho\right),$$

where Π is a discrete OQW given by

$$\Pi(\rho) = \sum_{i,j \in V} M_j^i \rho(j) M_j^{i*} \otimes |i\rangle \langle i|.$$

It is easy to see that the quantum jump chain of Λ with such a generator represents a discrete OQW, because for each $i \in V$,

$$\sum_{j \in V} M_j^{i*} M_j^i = \sum_{j \in V} \frac{R_j^{i*}}{\sqrt{q_i}} \frac{R_j^i}{\sqrt{q_i}} = \frac{1}{q_i} \sum_{j \in V} R_j^{i*} R_j^i = I_j.$$

Lemma 2.29. Consider a CTOQW that starts the walk on site $|i\rangle$ with initial density operator $\rho \in \mathcal{S}(\mathfrak{h}_i)$. There exist $r, s > 0$ such that

$$r \leq \mathbb{E}_{i,\rho'}(T_1) \leq s, \quad \forall i \in V, \quad \forall \rho' \in \mathcal{S}(\mathfrak{h}). \quad (2.6.6)$$

We recall that a vertex $|i\rangle$ is ρ -recurrent if

$$\int_0^\infty p_{ii;\rho}(t) dt = \mathbb{E}_{i,\rho}(n_i) = \infty,$$

where n_i is the time spent on site $|i\rangle$, that is,

$$n_i = \int_0^\infty 1_{\{X_t=i\}} dt.$$

Remark 2.30. Let us look to the graphic representation of a random walk on \mathbb{Z}^+ , starting on vertex $|2\rangle$, represented on Figure 2.6. The walker spends a time S_1 on $|2\rangle$ before the first jump, which is to $|3\rangle$. Then it spends a time S_2 on $|3\rangle$ before the second jump, which is to $|5\rangle$, and goes on. Note that after 8 jumps, the walker spent time on $|2\rangle$ three times, thus the walker occupied site $|2\rangle$, until J_8 , for a time $S_1 + S_4 + S_7$. Therefore the time spent on any site $|i\rangle$ is

$$n_i = \int_0^\infty 1_{\{X_t=i\}} dt = S_1 + \sum_{n=1}^\infty S_{n+1} 1_{\{F_n=i\}},$$

that is, we sum the holding times S_n in which the n -th jump is to $|i\rangle$.

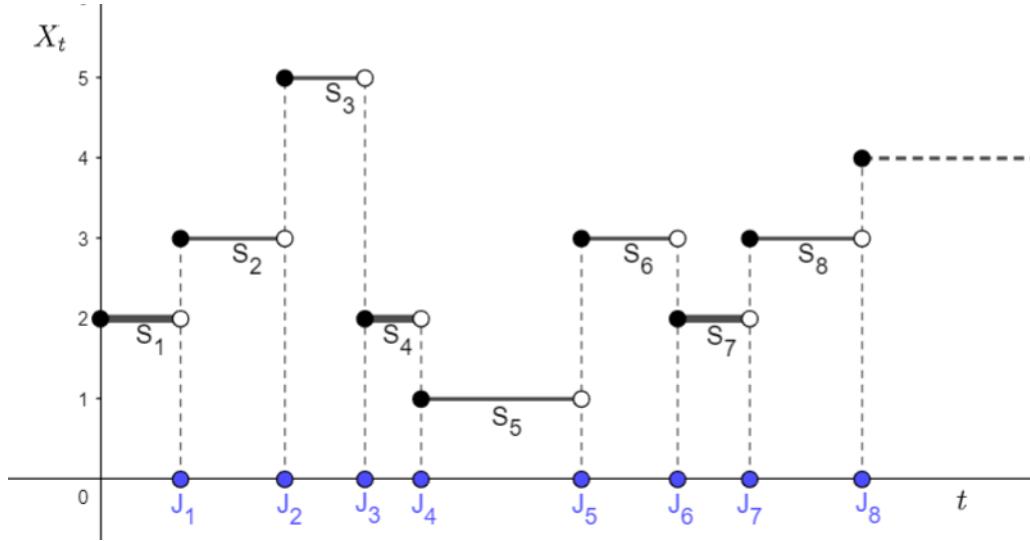


Figure 2.6: Holding Times of a right-continuous chain.

The following Theorem gives a complete recurrence criterion for a semifinite CTOQW based on its quantum jump chain.

Theorem 2.31 (Recurrence Equivalence with the Quantum Jump Chain). *Consider a CTOQW Λ with generator of the form (2.6.1). A vertex $|i\rangle$ is ρ -recurrent if and only if*

$$\sum_{n=0}^{\infty} P_{i,\rho}(F_n = i) = \infty.$$

Consider a CTOQW on a set V . For $i, j \in V$, the set of continuous-time trajectories going from vertex i to vertex j in n jumps is defined by

$$\mathcal{P}^n(i, j) = \{\xi = (i_0, \dots, i_n; t_1, \dots, t_n) \mid i_0 = i, i_n = j\}.$$

We set $\mathcal{P}(i, j) = \cup_{n \in \mathbb{N}} \mathcal{P}^n(i, j)$, then for $\xi = (i_0, \dots, i_n; t_1, \dots, t_n) \in \mathcal{P}(i, j)$, define the operator $T_t : \mathfrak{h}_i \rightarrow \mathfrak{h}_j$ by

$$T_t(\xi) = e^{(t-t_n)G_{i_n}} R_{i_{n-1}}^j e^{(t_n-t_{n-1})G_{i_{n-1}}} \dots e^{(t_2-t_1)G_{i_1}} R_i^{i_1} e^{t_1 G_i}. \quad (2.6.7)$$

This notation allows us to give an equivalent definition of irreducible CTOQWs. We say that a CTOQW with generator \mathcal{L} is **irreducible** when for all $X \in \mathcal{I}_1(\mathcal{H})$ with $X \geq 0$ and $X \neq 0$, there exists $t > 0$ such that $e^{t\mathcal{L}}(X) > 0$.

Proposition 2.32 ([5]). *A CTOQW with generator (2.2.2) is irreducible if and only if, for every $i, j \in V$, and for any $\phi \in \mathfrak{h}_i \setminus \{0\}$, the set*

$$\{T_t(\xi)\phi, t \geq 0, \xi \in \mathcal{P}(i, j)\}$$

is total in \mathfrak{h}_j .

Proposition 2.33. *A CTOQW with generator of the form (2.6.1) is irreducible if and only if its quantum jump chain is irreducible.*

Proof. By hypothesis, for each $i \in V$, there exists a $q_i \geq 0$ such that $G_i = -q_i/2$, thus the operator $T_t(\xi)$ in equation (2.6.7) is

$$\begin{aligned} T_t(\xi) &= e^{(t-t_n)G_{i_n}} R_{i_{n-1}}^j e^{(t_n-t_{n-1})G_{i_{n-1}}} \dots e^{(t_2-t_1)G_{i_1}} R_i^{i_1} e^{t_1 G_i} \\ &= e^{-(t-t_n)q_{i_n}/2 - (t_n-t_{n-1})q_{i_{n-1}}/2 - \dots - t_1 q_i/2} \frac{R_{i_{n-1}}^j}{\sqrt{q_{i_{n-1}}}} \dots \frac{R_i^{i_1}}{\sqrt{q_i}}. \end{aligned}$$

Thus, for $\phi \in \mathfrak{h}_i \setminus \{0\}$, the set

$$\{T_t(\xi)\phi, t \geq 0, \xi \in \mathcal{P}(i, j)\}$$

is total in \mathfrak{h}_j if and only if the set $\{L_\pi \phi | \pi \in \mathcal{P}(i, j)\}$ is total in \mathfrak{h}_j , where

$$L_\pi = L_{i_n, i_{n-1}} \cdots L_{i_1, i_0}$$

is the set of paths from i to j for the quantum jump chain. □

The CTOQWs of our interest on this work will be defined now: a CTOQW is called **homogeneous** if there exist matrices A, B and C such that $R_{i+1, i} = A$, $R_{i, i} = B$ and $R_{i, i+1} = C$ for all $i \in V$. When $B = 0$, as we are assuming ($R_i^i = 0$), then we say that the walk Λ is **induced by a coin** (C, A) .

We notice that the generator of a CTOQW induced by a coin (C, A) satisfying $A^*A + C^*C = qI$, $q > 0$, is given by

$$\mathcal{L} \left(\sum_{i \in V} \rho(i) \otimes |i\rangle \langle i| \right) = \sum_{i \in V} (A\rho(i-1)A^* + C\rho(i+1)C^* - q\rho(i)) \otimes |i\rangle \langle i|. \quad (2.6.8)$$

A CTOQW with a generator of the form (2.6.8) will be called a CTOQW induced by a **trace-preserving coin** (C, A) .

Corollary 2.34 (Recurrence criteria for a trace-preserving coin of dimension n). *Consider a CTOQW with $\dim(\mathfrak{h}) = n$ and generator of the form (2.6.5). Then a vertex $|i\rangle \in V$ is ρ -recurrent for the CTOQW if and only if it is ρ -recurrent for its quantum jump chain (which is an OQW).*

This corollary gives a complete criteria for the site recurrence of a CTOQW induced by a trace-preserving coin of dimension 2. In the sequel we expand the generator of CTOQWs induced by coins of dimension 2 where the coin is not necessarily trace-preserving.

Example 2.35. *Consider a CTOQW Λ with generator of the form (2.6.5) on $V = \mathbb{Z}$, with $R_i^{i+1} = E$ and $R_i^i = F$ for every $i \in \mathbb{Z}$,*

$$E = \frac{1}{9} \begin{bmatrix} \sqrt{3} + 2\sqrt{6} & -\sqrt{6} + 2\sqrt{3} \\ -\sqrt{6} + 2\sqrt{3} & 2\sqrt{3} + \sqrt{6} \end{bmatrix}, \quad F = \frac{1}{9} \begin{bmatrix} 2\sqrt{3} + \sqrt{6} & -2\sqrt{3} + \sqrt{6} \\ -2\sqrt{3} + \sqrt{6} & \sqrt{3} + 2\sqrt{6} \end{bmatrix}.$$

The quantum jump chain of Λ is then the OQW induced by the coin (E, F) . ◇

Proposition 2.36. *A CTOQW induced by a coin with generator of the form (2.6.1) is irreducible if and only if the operators CA and AC have no common eigenvectors.*

Proof. By proposition 2.33, the CTOQW is irreducible if and only if its quantum jump chain is irreducible. The quantum jump chain is the OQW induced by the coin $(C/\sqrt{q}, A/\sqrt{q})$, where $q > 0$, which is irreducible if and only if the operators CA/q and AC/q have no common eigenvectors, by Proposition 7.3 of [12]. □

We define the **auxiliary map** $\mathcal{T} : \mathbb{M}_n(\mathbb{C}) \rightarrow \mathbb{M}_n(\mathbb{C})$ of the CTOQW induced by a coin (C, A) as

$$\mathcal{T}(\rho) = C\rho C^* + A\rho A^*.$$

When ρ is a density satisfying $\mathcal{T}(\rho) = q\rho$, then ρ is said to be **q -invariant** for \mathcal{T} .

The following consequence of Theorem 2.31 is obtained with Theorem 17 of [27]:

Corollary 2.37 (Recurrence criteria for trace-preserving coins of dimension 2). *Consider a CTOQW on \mathbb{Z} induced by a coin (C, A) of dimension 2 such that $A^*A + C^*C = qI$, $q > 0$.*

(1) If C and A have at most one common eigenvector, let ρ_∞ be the unique invariant density of the auxiliary map. Then, we have

$$\text{Tr}(C^*C\rho_\infty) \neq \frac{q}{2} \Rightarrow (C, A) \text{ is transient,}$$

$$\text{Tr}(C^*C\rho_\infty) = \frac{q}{2} \Rightarrow (C, A) \text{ is recurrent.}$$

(2) If C and A have two linearly independent eigenvectors in common, let u_1 be one of them and let u_2 be a norm one vector such that $u_2 \perp u_1$. Also let $\sigma_1 = |u_1\rangle\langle u_1|$ and $\sigma_2 = |u_2\rangle\langle u_2|$. Then we have

$$\begin{aligned} \operatorname{Tr}(C^*C\sigma_1) = \frac{q}{2} \text{ and } \operatorname{Tr}(C^*C\sigma_2) = \frac{q}{2} &\Rightarrow (C, A) \text{ is recurrent,} \\ \operatorname{Tr}(C^*C\sigma_1) \neq \frac{q}{2} \text{ and } \operatorname{Tr}(C^*C\sigma_2) \neq \frac{q}{2} &\Rightarrow (C, A) \text{ is transient,} \\ \operatorname{Tr}(C^*C\sigma_1) \neq \frac{q}{2} \text{ and } \operatorname{Tr}(C^*C\sigma_2) = \frac{q}{2} &\Rightarrow (C, A) \text{ is transient with respect to } \sigma_i \text{ and it is} \\ &\text{recurrent with respect to all densities but } \sigma_1, \\ &\text{for } (i, j) = (1, 2) \text{ or } (i, j) = (2, 1). \end{aligned}$$

2.7 Appendices

Proof of Proposition 2.6. Let $i, j \in V$ and $\alpha, \beta \geq 0$. As Λ_t is a semigroup and $\sum_k \mathbb{P}_k = I$,

$$\begin{aligned} p_{ji;\rho}(\alpha + \beta) &= \operatorname{Tr}(\mathbb{P}_j \Lambda_{\alpha+\beta} \mathbb{P}_i \rho) = \sum_k \operatorname{Tr}(\mathbb{P}_j \Lambda_\alpha \mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho) \\ &= \sum_k \operatorname{Tr}(\mathbb{P}_j \Lambda_\alpha \mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho) \frac{\operatorname{Tr}(\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho)}{\operatorname{Tr}(\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho)} \\ &= \sum_k \operatorname{Tr}\left(\mathbb{P}_j \Lambda_\alpha \mathbb{P}_k \frac{\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho}{\operatorname{Tr}(\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho)}\right) \operatorname{Tr}(\mathbb{P}_k \Lambda_\beta \mathbb{P}_i \rho) \\ &= \sum_k p_{jk;\rho'_{ki}(\beta)}(\alpha) p_{ki;\rho}(\beta). \end{aligned} \tag{2.7.1}$$

Proof of Proposition 2.8. Define the function $g : W_i \rightarrow [0, 1]$ by $g(\rho, s) = p_{ji;\rho}(s)$. Since $e^{t\mathcal{L}}$ is uniformly continuous, g is continuous on $[0, +\infty)$ for a fixed $\rho \in S_{\mathfrak{h}_i}$. By definition, for $t \in [0, +\infty)$, given $\varepsilon > 0$, there is an $\alpha > 0$ such that $|t - s| < \alpha$ implies $|g(\rho, t) - g(\rho, s)| < \varepsilon/2$.

For $\beta := \min(\alpha, \varepsilon/2)$, if $|t - s| < \beta$ and $\|\rho - \rho'\|_1 < \beta$, where $\|\cdot\|_1$ is the trace norm in \mathfrak{h}_i , we have

$$\begin{aligned} |g(\rho, t) - g(\rho', s)| &\leq |g(\rho, t) - g(\rho, s)| + |g(\rho, s) - g(\rho', s)| \\ &< \frac{\varepsilon}{2} + |\operatorname{Tr}(\mathbb{P}_j \Lambda_s \mathbb{P}_i (\rho - \rho'))| \\ &\leq \frac{\varepsilon}{2} + |\operatorname{Tr}(\Lambda_s \mathbb{P}_i (\rho - \rho'))| \\ &= \frac{\varepsilon}{2} + |\operatorname{Tr}(\mathbb{P}_i (\rho - \rho'))| \\ &= \frac{\varepsilon}{2} + |\operatorname{Tr}(\rho - \rho')| \\ &= \frac{\varepsilon}{2} + \|\rho - \rho'\|_1 \\ &< \varepsilon. \end{aligned}$$

This concludes the proof.

Proof of Proposition 2.9. (1) By contradiction, suppose that there exists $k > 0$ with $p_{ii;\rho}(k) = 0$. Since $p_{ii;\rho}(t)$ is jointly continuous on $(t, \rho) \in ([0, \infty) \times S_{\mathfrak{h}_i})$ and $p_{ii;\rho}(0) = 1$, we can assume $k = \min\{s > 0 : p_{ii;\rho}(s) = 0\}$. Moreover, there exists $\varepsilon > 0$ such that, for $t < k$,

$$k - t < \varepsilon \text{ and } \|\rho - \tilde{\rho}\| < \varepsilon \Rightarrow p_{ii;\tilde{\rho}}(t) > 0. \tag{2.7.2}$$

Now, note that

$$\rho'_{ii}(k/n) = \frac{\mathbb{P}_i \Lambda_{k/n} \mathbb{P}_i \rho}{\operatorname{Tr}(\mathbb{P}_i \Lambda_{k/n} \mathbb{P}_i \rho)} \xrightarrow{n \rightarrow \infty} \frac{\mathbb{P}_i I \mathbb{P}_i \rho}{\operatorname{Tr}(\mathbb{P}_i I \mathbb{P}_i \rho)} = \frac{\mathbb{P}_i \rho}{\operatorname{Tr}(\mathbb{P}_i \rho)} = \mathbb{P}_i \rho.$$

Now, take n such that $\frac{k}{n} < \varepsilon$ and $\|\mathbb{P}_i \rho - \rho'_{ii}(k/n)\| < \varepsilon$, then $p_{ii;\rho'_{ii}(k/n)}((kn - k)/n) > 0$, thus

$$p_{ii;\rho}(k) \geq p_{ii;\rho'_{ii}(k/n)}((kn - k)/n) p_{ii;\rho}(k/n) > 0,$$

which is a contradiction.

For item (2), let $x \geq 0$, then item (1) gives

$$p_{ij;\rho}(t+x) \geq p_{ii;\rho'_{ij}(t)}(x)p_{ij;\rho}(t) > 0.$$

Suppose $p_{ii;\rho}(t) = 1$ for some $t > 0$. If we had $p_{ji;\rho}(s) > 0$ for some $j \neq i$ and $s \in [0, t]$, then

$$0 = \sum_{k \neq i} p_{ki;\rho}(t) \geq p_{ji;\rho}(t-s+s) \geq p_{ii;\rho'_{ji}(s)}(t-s)p_{ji;\rho}(s) > 0,$$

which is a contradiction. This shows item (3).

To proof item (4), note that for fixed $0 \leq t_0 < \delta$, $W(i, \delta) := S_{\mathfrak{h}_i} \times [t_0, \delta]$ is a compact set in $W_i = S_{\mathfrak{h}_i} \times [0, +\infty)$. Hence, by the joint continuity, N_{ji} is attained on $(0, 1]$.

Proof of Theorem 2.10. If $p_{ji;\rho}(t) = 0$ for all t , then the result is obvious. Thus suppose $p_{ji;\rho}(t) > 0$, for some $t \geq 0$. The second item of Proposition 2.9 assures the existence of $N_\delta \in \mathbb{N}$ such that $p_{ji;\rho}(n\delta) > 0, \forall n \geq N$.

By the Mean Value Theorem for Integrals, we have

$$\int_0^\infty p_{ji;\rho}(t)dt = \sum_{n=0}^\infty \int_{n\delta}^{(n+1)\delta} p_{ji;\rho}(t)dt = \sum_{n=0}^\infty \delta p_{ji;\rho}(n\delta + s_n),$$

where $(s_n)_{n=0}^\infty$ is a sequence in $[0, \delta]$.

By Proposition 2.6,

$$p_{ji;\rho}(n\delta + s_n) \geq p_{ji;\rho}(n\delta)p_{jj;\rho'_{ji}(n\delta)}(s_n), \forall n \geq N, \quad (2.7.3)$$

and

$$p_{ji;\rho}(n\delta + \delta) = p_{ji;\rho}(n\delta + s_n + \delta - s_n) \geq p_{jj;\rho'_{ji}(n\delta+s_n)}(\delta - s_n)p_{ji;\rho}(n\delta + s_n), \forall n \geq N, \quad (2.7.4)$$

so that for any fixed ρ ,

$$\begin{aligned} \int_0^\infty p_{ji;\rho}(t)dt &= \delta \sum_{n=0}^\infty p_{ji;\rho}(n\delta + s_n)dt \\ &\geq \delta \sum_{n=N}^\infty p_{ji;\rho}(n\delta + s_n)dt \\ &\stackrel{(2.7.3)}{\geq} \delta \sum_{n=N}^\infty p_{ji;\rho}(n\delta)p_{jj;\rho'_{ji}(n\delta)}(s_n) \\ &\geq \delta N_j \sum_{n=N}^\infty p_{ji;\rho}(n\delta) \end{aligned} \quad (2.7.5)$$

and

$$\begin{aligned} \sum_{n=0}^\infty p_{ji;\rho}(n\delta + \delta) &\stackrel{(2.7.4)}{\geq} \sum_{n=0}^\infty p_{jj;\rho'_{ji}(n\delta+s_n)}(\delta - s_n)p_{ji;\rho}(n\delta + s_n) \\ &\geq \sum_{n=N}^\infty p_{jj;\rho'_{ji}(n\delta+s_n)}(\delta - s_n)p_{ji;\rho}(n\delta + s_n) \\ &\geq N_j \sum_{n=N}^\infty p_{ji;\rho}(n\delta + s_n) \\ &= \frac{N_j}{\delta} \sum_{n=N}^\infty \delta p_{ji;\rho}(n\delta + s_n) \\ &= \frac{N_j}{\delta} \sum_{n=0}^\infty \delta p_{ji;\rho}(n\delta + s_n) - \frac{N_j}{\delta} \sum_{n=0}^{N-1} \delta p_{ji;\rho}(n\delta + s_n) \\ &= \frac{N_j}{\delta} \int_0^\infty p_{ji;\rho}(t)dt - \frac{N_j}{\delta} \sum_{n=0}^{N-1} \delta p_{ji;\rho}(n\delta + s_n). \end{aligned} \quad (2.7.6)$$

Whence, for a state ρ , the divergence of the series in (2.7.5) implies the divergence of the integral on the left. Also, if we suppose the integral on (2.7.6) diverges, then the series on the left diverges, since the series on the right hand is finite.

Proof of Proposition 2.11. 1. Since ρ is faithful, there exists $\alpha > 0$ such that $\rho \geq \alpha \tilde{\rho}$, thus

$$\int_0^\infty p_{ii;\rho}(t)dt = \int_0^\infty \text{Tr}(\mathbb{P}_i \Lambda \mathbb{P}_i \rho) dt \geq \alpha \int_0^\infty \text{Tr}(\mathbb{P}_i \Lambda \mathbb{P}_i \tilde{\rho}) dt = \alpha \int_0^\infty p_{ii;\tilde{\rho}}(t) dt > \infty.$$

2. Suppose $\rho'_{ii}(\delta)$ is faithful for some $\delta \geq 0$. The item 1 gives that i is $\rho'_{ii}(\delta)$ -recurrent, therefore,

$$\int_0^\infty p_{ii;\rho}(t) dt \geq \int_0^\infty p_{ii;\rho}(t + \delta) dt \geq \int_0^\infty p_{ii;\rho}(\delta) p_{ii;\rho'_{ii}(\delta)}(t) dt = p_{ii;\rho}(\delta) \int_0^\infty p_{ii;\rho'_{ii}(\delta)}(t) dt = \infty.$$

3. Let $\rho \in \mathcal{S}_{\mathfrak{h}_i}$. By the Spectral Theorem, ρ can be written as

$$\rho = \sum_{x=1}^n \lambda_x |x\rangle \langle x|, \quad (2.7.7)$$

where the vectors $|x\rangle$ s are the eigenvectors of ρ with eigenvalues λ_x s. Since ρ is non-faithful, there is at least one null eigenvalue and the remainder eigenvalues are positive summing 1. Thus, (2.7.7) can be rewritten as

$$\rho = \sum_{x \in S} \lambda_x |x\rangle \langle x|, S \subsetneq \{1, \dots, n\}. \quad (2.7.8)$$

Take a sequence of positive numbers $(\alpha_r)_{r \in R}$, where $R := \{1, \dots, n\} / S \neq \emptyset$, whose sum is 1.

Defining

$$\rho_X = \sum_{x \in S} \frac{\lambda_x}{2} |x\rangle \langle x| + \sum_{x \in R} \frac{\alpha_x}{2} |x\rangle \langle x| = \sum_{x=1}^n \frac{\tilde{\alpha}_x}{2} |x\rangle \langle x|, \tilde{\alpha}_x = \begin{cases} \lambda_x, & \text{if } x \in S \\ \alpha_x, & \text{if } x \in R \end{cases},$$

we get by the first item that i is ρ_X -recurrent, since ρ_X is faithful.

Now, define

$$\rho_Y = \sum_{x \in R} \alpha_x |x\rangle \langle x|,$$

which is a non-faithful density operator and then we get $2\rho_X = \rho + \rho_Y$. This leads us to

$$\begin{aligned} \int_0^\infty p_{ii;\rho}(t) dt + \int_0^\infty p_{ii;\rho_Y}(t) dt &= \int_0^\infty (p_{ii;\rho}(t) + p_{ii;\rho_Y}(t)) dt \\ &= \int_0^\infty (\text{Tr}(\mathbb{P}_i \Lambda_t \mathbb{P}_i \rho) + \text{Tr}(\mathbb{P}_i \Lambda_t \mathbb{P}_i \rho_Y)) dt \\ &= \int_0^\infty \text{Tr}(\mathbb{P}_i \Lambda_t \mathbb{P}_i (\rho + \rho_Y)) \\ &= 2 \int_0^\infty \text{Tr}(\mathbb{P}_i \Lambda_t \mathbb{P}_i (\rho_X)) \\ &= 2 \int_0^\infty p_{ii;\rho_X}(t) dt. \end{aligned}$$

The integral on the right hand diverges once i is ρ_X -recurrent, this implies that at least one of the integrals on the left hand side diverges. Therefore, i is ρ -recurrent or ρ_Y -recurrent.

4. By item (3), vertex i is ρ -recurrent with respect to some non-faithful ρ . Since $n = 2$, the eigenvalues of ρ are 0 and 1, thus there exists a unit vector $|v\rangle \in \mathbb{C}^2$ such that $\rho = |v\rangle \langle v|$, that is, ρ is pure.

Proof of Proposition 2.25. The case $p_{ii;\rho}(t) = 1$ for all $t \geq 0$ is trivial, giving $q_{i;\rho} = 0$. If $p_{ii;\rho}(t) < 1$ for some $t > 0$, we still have that $p_{ii;\rho}(t)$ never vanishes (item 1 of Proposition 2.9). Let $\psi(t) = -\log p_{ii;\rho}(t)$ and $q = \sup_{t>0} \frac{\psi(t)}{t}$. We claim that

$$\lim_{t \downarrow 0} \frac{\psi(t)}{t} = q.$$

Since we have $\limsup_{t>0} \frac{\psi(t)}{t} \leq q$, showing that $\liminf_{t>0} \frac{\psi(t)}{t} \geq q$ will prove the claim.

Thus let $q' < q$ and take $s > 0$ such that $\frac{\psi(s)}{s} \geq q'$. For each $t > 0$, there exists a natural n and $h \in [0, t)$ such that $s = nt + h$. Analogous to the proof of Proposition 2.6, we have

$$\begin{aligned} p_{ii;\rho}(nt+h) &= \sum_{k_1, \dots, k_{n-1} \in V} \text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_{k_1} \Lambda_t \mathbb{P}_{k_2} \dots \Lambda_t \mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho \right) \\ &= \sum_{k_1, \dots, k_{n-1} \in V} \left[\text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_{k_1} \frac{\mathbb{P}_{k_1} \Lambda_t \mathbb{P}_{k_2} \dots \Lambda_t \mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho}{\text{Tr} \left(\mathbb{P}_{k_1} \Lambda_t \mathbb{P}_{k_2} \dots \Lambda_t \mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho \right)} \right) \times \right. \\ &\quad \text{Tr} \left(\mathbb{P}_{k_1} \Lambda_t \mathbb{P}_{k_2} \frac{\mathbb{P}_{k_2} \Lambda_t \mathbb{P}_{k_3} \dots \Lambda_t \mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho}{\text{Tr} \left(\mathbb{P}_{k_2} \Lambda_t \mathbb{P}_{k_3} \dots \Lambda_t \mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho \right)} \right) \times \dots \times \\ &\quad \left. \text{Tr} \left(\frac{\mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho}{\text{Tr} \left(\mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho \right)} \right) \text{Tr} \left(\mathbb{P}_{k_{n-1}} \Lambda_h \mathbb{P}_i \rho \right) \right], \end{aligned}$$

where we are considering, without loss of generality, only the traces which are non-null on the sum.

The positivity of the traces give the inequality

$$\begin{aligned} p_{ii;\rho}(nt+h) &\geq \text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_i \frac{\mathbb{P}_i \Lambda_t \mathbb{P}_i \dots \Lambda_t \mathbb{P}_i \Lambda_h \mathbb{P}_i \rho}{\text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_i \dots \Lambda_t \mathbb{P}_i \Lambda_h \mathbb{P}_i \rho \right)} \right) \dots \text{Tr} \left(\frac{\mathbb{P}_i \Lambda_h \mathbb{P}_i \rho}{\text{Tr} \left(\mathbb{P}_i \Lambda_h \mathbb{P}_i \rho \right)} \right) \text{Tr} \left(\mathbb{P}_i \Lambda_h \mathbb{P}_i \rho \right) \\ &= \prod_{k=1}^n p_{ii;\rho'_k}(t) p_{ii;\rho}(h), \end{aligned}$$

where

$$p_{ii;\rho'_k}(t) = \frac{\overbrace{\mathbb{P}_i \Lambda_t \mathbb{P}_i \Lambda_t \dots \mathbb{P}_i \Lambda_t \mathbb{P}_i \Lambda_h \mathbb{P}_i \rho}^{k \text{ times}}}{\underbrace{\text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_i \Lambda_t \dots \mathbb{P}_i \Lambda_t \mathbb{P}_i \Lambda_h \mathbb{P}_i \rho \right)}_{k \text{ times}}}.$$

It is easy to see that

$$q' < \frac{\psi(s)}{s} = \frac{-\log p_{ii;\rho}(s)}{s} = \frac{-\log p_{ii;\rho}(nt+h)}{s} \leq \frac{-\log \left(\prod_{k=1}^n p_{ii;\rho'_k}(t) p_{ii;\rho}(h) \right)}{s},$$

thus let $t \downarrow 0$, then observe that $nt/s \rightarrow 1$, $h \rightarrow 1$ and $p_{ii;\rho'_k}(t) \rightarrow \rho$ to obtain

$$\begin{aligned} q' &< \lim_{t \downarrow 0} \frac{-\log \left(\prod_{k=1}^n p_{ii;\rho'_k}(t) p_{ii;\rho}(h) \right)}{s} \leq \lim_{t \downarrow 0} \frac{-\log (p_{ii;\rho}(t)^n p_{ii;\rho}(h))}{s} \\ &= \lim_{t \downarrow 0} \frac{n\psi(t) + \psi(h)}{s} = \lim_{t \downarrow 0} \frac{nt}{s} \cdot \frac{\psi(t)}{t} + \frac{\psi(h)}{s}. \end{aligned}$$

Therefore $q' < \lim_{t \downarrow 0} \frac{\psi(t)}{t}$ for every $q' < q$, completing the proof of the claim.

Note that $q > 0$, otherwise we would have $p_{ii;\rho}(t) = 1$ for all $t \geq 0$. This means that $\psi(t) > 0$ for t sufficiently small, hence

$$\lim_{t \downarrow 0} \frac{1 - p_{ii;\rho}(t)}{t} = \lim_{t \downarrow 0} \frac{1 - e^{\psi(t)}}{\psi(t)} \cdot \frac{\psi(t)}{t} = \lim_{t \downarrow 0} \frac{1 - e^{\psi(t)}}{\psi(t)} \cdot \lim_{t \downarrow 0} \frac{\psi(t)}{t} = q,$$

and the proof is complete by putting $q_{i;\rho} = q$.

Proof of Proposition 2.26. Recall that semigroups operators satisfy

$$\Lambda'_t = \mathcal{L} \Lambda_t, \quad \Lambda'_0 = \mathcal{L},$$

thus

$$\begin{aligned} q_{i;\rho} &= \lim_{t \downarrow 0} \frac{1 - p_{ii;\rho}(t)}{t} = -\lim_{t \downarrow 0} \frac{\text{Tr} \left(\mathbb{P}_i \Lambda_t \mathbb{P}_i \rho \right) - \text{Tr} \left(\mathbb{P}_i \rho \right)}{t} = -\lim_{t \downarrow 0} \frac{\text{Tr} \left(\left(\mathbb{P}_i \Lambda_t \mathbb{P}_i - I \right) \rho \right)}{t} \\ &= -\text{Tr} \left(\mathbb{P}_i \Lambda'_0 \mathbb{P}_i \rho \right) = -\lim_{t \downarrow 0} \text{Tr} \left(\mathbb{P}_i \mathcal{L} \mathbb{P}_i \rho \right). \end{aligned}$$

Let $j \neq i$, then

$$\mathrm{Tr}(\mathbb{P}_j \mathcal{L} \mathbb{P}_i \rho) = \lim_{t \downarrow 0} \frac{\mathrm{Tr}(\mathbb{P}_j \Lambda_t \mathbb{P}_i \rho) - \mathrm{Tr}(\mathbb{P}_j \Lambda_0 \mathbb{P}_i \rho)}{t} = \lim_{t \downarrow 0} \frac{\mathrm{Tr}(\mathbb{P}_j \Lambda_t \mathbb{P}_i \rho)}{t} = \lim_{t \downarrow 0} \frac{p_{ji;\rho}(t)}{t} =: q_{ji;\rho},$$

thus the definition of this limit makes sense.

Proof of Theorem 2.27.

Firstly we recall that

$$T_1^j = \inf\{t \geq 0; N^{i_0,j} \left(u, y | 0 \leq u \leq t, 0 \leq y \leq \mathrm{Tr}(R_{i_0}^j \eta_u R_{i_0}^{j*}) \right) \geq 1\},$$

where η_t is the solution of

$$\eta_t = \rho_0 + \int_0^t (G_{i_0} \eta_s + \eta_s G_{i_0}^* - \eta_s \mathrm{Tr}(G_{i_0} \eta_s + \eta_s G_{i_0}^*)) ds.$$

By assumption, we have $G_{i_0} \eta_s + \eta_s G_{i_0}^* = -q_i \eta_s$ for any s , thus η_t is the solution of

$$\eta_t = \rho_0 + \int_0^t (-q_i \eta_s - \eta_s \mathrm{Tr}(-q_i \eta_s)) ds = \rho,$$

thus $\eta_t = \rho_0$ for every $t \geq 0$.

By Proposition 2.26, we have

$$T_1^j = \inf\{t \geq 0; N^{i_0,j} (u, y | 0 \leq u \leq t, 0 \leq y \leq q_{j i_0; \rho}) \geq 1\},$$

thus there is no dependence on the first variable of $N^{i_0,j}$, thus the process are just usual independent Poisson processes of intensity $q_{j i_0; \rho}$. Therefore, the first jump is to j with probability

$$\mathbb{P}_{i_0, \rho}(X(T_1) = j) = \frac{q_{j, i_0; \rho}}{\sum_k q_{k, i_0; \rho}} = \frac{q_{j, i_0; \rho}}{q_i}.$$

In a more rigorous way, suppose firstly that $\mathrm{Tr}(G_i \rho + \rho G_i^*) = 0$, then we have $\mathrm{Tr}(R_j^i \rho R_j^{i*}) = 0$ for every j , meaning that the walker never leaves i , thus $\mathbb{P}_{i, \rho}(F_1 = j) = 0$ for every $j \neq i$. Now suppose $q_i \neq 0$. Let $j \neq i$ and denote

$$R_{ji;\rho}(h) = \mathbb{P}_{i, \rho}(X(t+h) = j | X(t) = i, X(t+h) \neq i),$$

where we are assuming that t is so small that there is no jump until $t+h$. Hence

$$\begin{aligned} \mathbb{P}_{i, \rho}(X(T_1) = j) &= \text{the probability of a transition from } i \text{ to } j \text{ given that a transition} \\ &\quad \text{out of } i \text{ does occur.} \\ &= \lim_{h \rightarrow 0} R_{ji;\rho}(h). \end{aligned}$$

A calculation gives, for $t = 0$,

$$\begin{aligned} \lim_{h \rightarrow 0} R_{ji;\rho}(h) &= \lim_{h \rightarrow 0} \frac{\mathbb{P}_{i, \rho}(X(h) = j | X(h) \neq i)}{\mathbb{P}_{i, \rho}(X(h) \neq i)} \\ &= \lim_{h \rightarrow 0} \frac{\mathbb{P}_{i, \rho}(X(h) = j, X(h) \neq i)}{\mathbb{P}_{i, \rho}(X(h) \neq i)} \\ &= \lim_{h \rightarrow 0} \frac{\mathbb{P}_{i, \rho}(X(h) = j)}{\mathbb{P}_{i, \rho}(X(h) \neq i)} \\ &= \lim_{h \rightarrow 0} \frac{p_{ji;\rho}(h)}{1 - p_{ii;\rho}(h)} \\ &= \lim_{h \rightarrow 0} \frac{p_{ji;\rho}(h)}{h} \cdot \frac{h}{1 - p_{ii;\rho}(h)} \\ &= \lim_{h \rightarrow 0} \frac{p_{ji;\rho}(h)}{h} \lim_{h \rightarrow 0} \frac{h}{1 - p_{ii;\rho}(h)} \\ &= \frac{q_{ji;\rho}}{q_{i;\rho}}. \end{aligned}$$

Proof of Theorem 2.28. Let us suppose that we start a CTOQW of the form (2.6.1) on $(X_0, \rho_0) = (i, \rho)$ and it makes n jumps. We can then say that Λ has jumped at some trajectory $(i, i_1, i_2, \dots, i_n)$ for some vertices $i_1, \dots, i_n \in V$. The state on the n -th jump is then

$$\rho_{T_{i_n}} = \frac{R_{i_{n-1}}^{i_n} \rho_{T_{i_{n-1}}} R_{i_{n-1}}^{i_n*}}{\text{Tr}(R_{i_{n-1}}^{i_n} \rho_{T_{i_{n-1}}} R_{i_{n-1}}^{i_n*})}.$$

We claim that, if the n -th jump is to $j \in V$, then

$$\rho_{T_{i_n}} = \frac{R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n}}{\text{Tr}(R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n})}, \quad \forall n = 1, 2, \dots$$

It is easy to see that the claim is true for $n = 1$. So suppose it is valid for some $n \geq 1$, then

$$\begin{aligned} \rho_{T_{i_{n+1}}} &= \frac{R_{i_n}^{i_{n+1}} \rho_{T_{i_n}} R_{i_n}^{i_{n+1}*}}{\text{Tr}(R_{i_n}^{i_{n+1}} \rho_{T_{i_n}} R_{i_n}^{i_{n+1}*})} \\ &= \frac{R_{i_{n+1}}^{i_{n+1}} R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n} R_{i_n}^{i_{n+1}*}}{\text{Tr}(R_{i_{n+1}}^{i_{n+1}} R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n} R_{i_n}^{i_{n+1}*})} \\ &\times \left(\text{Tr} \left(\frac{R_{i_{n+1}}^{i_{n+1}} R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n} R_{i_n}^{i_{n+1}*}}{\text{Tr}(R_{i_{n+1}}^{i_{n+1}} R_{i_{n-1}}^{i_n} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_{n-1}}^{i_n} R_{i_n}^{i_{n+1}*})} \right) \right)^{-1} \\ &= \frac{R_{i_n}^{i_{n+1}} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_n}^{i_{n+1}}}{\text{Tr}(R_{i_n}^{i_{n+1}} \dots R_{i_1}^{i_2} R_{i_1}^{i_1} \rho R_{i_1}^{i_1*} R_{i_1}^{i_2*} \dots R_{i_n}^{i_{n+1}})}, \end{aligned}$$

proving the claim.

By Law of Total Probability applied n times we obtain

$$\begin{aligned} \mathbb{P}_{i,\rho}(F_{n+1} = i_{n+1}) &= \sum_{i_n \in V} \mathbb{P}_{i,\rho}(F_{n+1} = i_{n+1} | F_n = i_n) \mathbb{P}_{i,\rho}(F_n = i_n) \\ &\vdots \\ &= \sum_{i_1, \dots, i_n \in V} \mathbb{P}_{i,\rho}(F_{n+1} = i_{n+1} | F_n = i_n) \mathbb{P}_{i,\rho}(F_n = i_n | F_{n-1} = i_{n-1}) \dots \mathbb{P}_{i,\rho}(F_1 = i_1) \\ &= \sum_{i_1, \dots, i_n \in V} \mathbb{P}_{i_n, \rho_{T_{i_n}}}(F_1 = i_{n+1}) \mathbb{P}_{i_{n-1}, \rho_{T_{i_{n-1}}}}(F_1 = i_n) \dots \mathbb{P}_{i_1, \rho_{T_{i_1}}}(F_1 = i_1) \mathbb{P}_{i,\rho}(F_1 = i_1). \end{aligned} \tag{2.7.9}$$

The proof is finished by several applications of Theorem (2.27). \square

Proof of Lemma 2.29. By [5], we have for all $t > 0$ the identity

$$\mathbb{P}_{i,\rho}(T_1^i > t) = \exp \left[\int_0^t \text{Tr}((G_i + G_i^*) \eta_s^\rho) ds \right].$$

Also, $\text{Tr}((G_i + G_i^*) \rho) = -\text{Tr}(\sum_j R_i^{j*} R_i^j \rho) < -Y$ for some $Y > 0$, hence the compactness of $\mathcal{S}(\mathfrak{h})$ and a continuity argument allow us to evoke the Weierstrass Theorem to obtain $m, M > 0$ such that the following bound is valid

$$-mt \leq \int_0^t \text{Tr}((G_i + G_i^*) \eta_s^\rho) ds \leq -tM, \quad \forall t \geq 0.$$

Putting $r = m^{-1}$ and $s = M^{-1}$, the expected value $\mathbb{E}_{i,\rho'}(T_1) = \int_0^\infty \mathbb{P}_{i,\rho'}(T_1 > t) dt$ satisfies

$$r \leq \mathbb{E}_{i,\rho'}(T_1) \leq s$$

for every choice of $i \in V$ and $\rho \in \mathcal{S}(\mathfrak{h}_i)$. \square

Proof of Theorem 2.31. Suppose that the CTOQW starts on site $|i\rangle$ with initial density operator $\rho \in \mathcal{S}(\mathfrak{h}_i)$. Remark 2.30 and Fubini's Theorem give

$$\int_0^\infty p_{ii;\rho}(t)dt = \mathbb{E}_{i,\rho}(n_i) = \mathbb{E}_{i,\rho} \left(\sum_{n=0}^\infty S_{n+1} 1_{\{F_n=i\}} \right) = \sum_{n=0}^\infty \mathbb{E}_{i,\rho} (S_{n+1} 1_{\{F_n=i\}}).$$

Fix $n \in \{1, 2, 3, \dots\}$. Then an application of the Strong Markov Property to the stopping time S_n results on

$$\mathbb{E}_{i,\rho} (S_{n+1} 1_{\{F_n=i\}}) = \mathbb{E}_{i,\rho} (S_{n+1} | F_n = i) \mathbb{P}_{i,\rho} (F_n = i) = \mathbb{E}_{i,\rho} (\mathbb{E}_{i,\rho_i^n}(S_1)) \mathbb{P}_{i,\rho} (F_n = i),$$

where $\rho_i^n = \rho_{\tau_i^{(n)}}$. Since $T_1 = S_1$, we obtain the identity

$$\int_0^\infty p_{ii;\rho}(t)dt = \sum_{n=0}^\infty \mathbb{E}_{i,\rho} (\mathbb{E}_{i,\rho_i^n}(T_1)) \mathbb{P}_{i,\rho} (F_n = i),$$

thus we can use the boundaries obtained on Lemma 2.29 to obtain constants $r, s > 0$ which result on the inequalities

$$r \sum_{n=0}^\infty \mathbb{P}_{i,\rho} (F_n = i) \leq \int_0^\infty p_{ii;\rho}(t)dt \leq s \sum_{n=0}^\infty \mathbb{P}_{i,\rho} (F_n = i).$$

Chapter 3

Open questions

Below we state a few questions in connection with the results presented in this thesis.

- **Recurrence criteria for discrete dynamics if a measure is available.** In [27], recurrence criteria has been presented for homogeneous OQWs on the line and this is done in terms of spectral properties of the coin. On the other hand, the present work allows us to examine, in certain cases, recurrence of QMCs in terms of a matrix measure. A natural question is to ask how the spectral criterion given in [27] can be generalized to QMCs and how it is related with the existence of matrix measures. Is there a simple recurrence criterion in the case that a measure is available? As a first attempt, this problem can be broken into two parts, namely, a) the case for which the sides of the coin are diagonal or simultaneously diagonalizable, and b) the case for which there is no simultaneous diagonalization, i.e., the sides do not commute. On first sight, a central aspect of this problem seems to be a more thorough examination of Dette's criterion regarding the non-commuting case.
- **Site-recurrence criteria for homogeneous nearest-walk CTOQWs in 1 dimension in terms of Lindblad generators.** Given a valid Lindblad generator associated with a homogeneous tridiagonal matrix, when is such walk site-recurrent? The question is analogous to the one for the discrete-time case of OQWs studied in [27], where a complete criterion is obtained (both for the case of order 2 coins and for the case of irreducible coins). Regarding the continuous-time case, the question can be restated as: how to determine recurrence in terms of the entries (or spectra) of the transition effect matrices and hamiltonians? In this work, we have obtained partial results on such direction, but a general solution is unknown even for the case of order 2 effect matrices. Whenever one has simultaneous diagonalization of the matrices, one has clear answers, but we have seen that as soon as one abandons such assumption, the problem becomes more complicated.
- **Lindblad generators versus matrix measures.** If a matrix measure exists, one can resort to Karlin-McGregor methods in order to determine certain statistics of the walk such as recurrence. But with the above discussion in mind, this immediately raises the following questions: what conditions are imposed on the effect matrices and hamiltonians of the Lindblad generator so that one is able to obtain positive matrix measures? Is it possible to obtain matrix measures associated with Lindblad generators with nonzero hamiltonian parts? What about non-positive matrix measures?

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