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Unitary and Open Scattering Quantum Walks on Graphs

Alain Joye*

Abstract

We study a class of Unitary Quantum Walks on arbitrary graphs, parameterized by a family of scattering matrices. These Scattering Quantum Walks model the discrete dynamics of a system on the edges of the graph, with a scattering process at each vertex governed by the scattering matrix assigned to it. We show that Scattering Quantum Walks encompass several known Quantum Walks. Additionally, we introduce two classes of Open Scattering Quantum Walks on arbitrary graphs, also parameterized by scattering matrices: one class defined on the edges and the other on the vertices of the graph. We show that these walks give rise to proper Quantum Channels and describe their main spectral and dynamical properties, relating them to naturally associated classical Markov chains.

1 Introduction

Quantum Walks (QWs) defined on graphs or lattices are popular discrete time linear dynamical systems which are used in different scientific fields under different guises and for various applications, see *e.g.* the books and reviews [Ke, V-A, P, ABJ3, GZ, QMS, J4], and references therein. For example, in quantum optics or condensed matter physics, QWs provide a versatile tool to approximate the complex dynamics of certain systems in some physically relevant regimes, [KFC+, ZKG+, CC, WM, TMT]. QWs are used in the field of quantum computing and information processing, notably as quantum search algorithms, see [C, Sa, P, KMOR]. From a probabilistic perspective, QWs are considered as non commutative extensions of classical random walks and Markov chains, see *e.g.* [Sz, Ko2, G, APSS1].

The success and diversity of the different types of QWs have sparked the interest of the mathematical community which has rigorously addressed several of their properties. For example, the spectral and dynamical properties of certain QWs, [Ko1, BHJ, HKSS2, MS-B, JMa, HS, AG-PS, HSS, RST1, RST2, T, RT, CJWW], the Anderson (de-)localization in various models of random and quasiperiodic QWs [Kos, HJS1, HJS2, JMe, ASW, ABJ1, ABJ2, HJ1, BM, CFGW, CFO, CFL+, J2, J3], the many-body systems of QWs [AAM+, HJ2, R, AJR], or the topological properties of QWs [ABJ4, DFT, CGG+, SS-B, ST, D, ABJ5], to mention a few.

In this paper, we introduce and study the notion of Scattering Quantum Walks (SQWs) on arbitrary graphs, a class of QWs broad enough to encompass many QWs present in the literature, and which moreover admits both unitary and open versions. Unitary SQWs are used to address closed quantum systems, while open SQWs are relevant in the analysis of open quantum systems and are known as Quantum Channels.

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Let us describe informally the definition of a unitary SQW on a graph G . It is a unitary operator on a Hilbert space associated with G , which models the linear dynamics of a quantum system, or quantum walker, over a single time step. For a simple directed graph $G = (V, E)$ with vertex set V and edge set E , the edges come with two directions and we attach to each directed edge a canonical basis vector of a Hilbert space $l^2(D)$. The SQW on $l^2(D)$ is parameterized by a family of scattering matrices, each assigned to a vertex in V . Informally, we say that the quantum walker lives on the directed edges of the graph, as its quantum state is represented by a normalized vector of $l^2(D)$.

At each time step, the state of the quantum walker on a given edge with a specific direction undergoes a scattering process at the vertex towards which the edge points, say $x \in V$. This process is governed by the scattering matrix $S(x)$ assigned to x . The walker's state is then transformed into the corresponding linear combination of states on adjacent edges, where the directions now point away from the vertex x where the scattering process took place, see Figure 1.

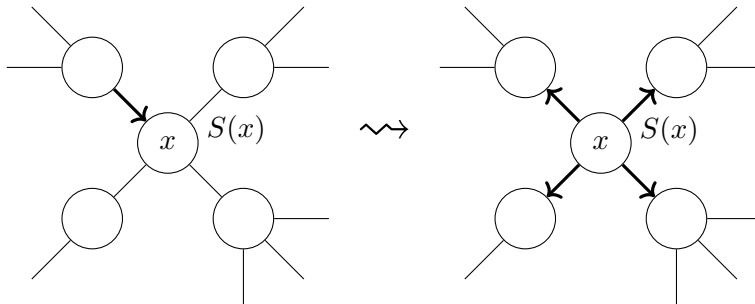


Figure 1: The scattering process at work in SQWs

The freedom in choosing the directed graph and the unitary scattering matrices at its vertices explains why SQWs encompass a significant set of unitary QWs considered in the literature. We explicitly show that Coined QWs, the Chalker-Coddington model, and a slight generalization of the Grover Walk belong to this class. Following [HKSS2, HSS] we revisit the spectral properties of the latter by relating them to those of a self-adjoint operator defined on $l^2(V)$, the Hilbert space associated with the graph's vertices, through natural boundary operators. We also study SQWs on the star-graph.

Let us informally describe the definition of an open SQW on the edges of G , by considering its action on density matrices on $l^2(D)$ representing the states of a quantum walker. We start with an initial state, and measure the position of the quantum walker. This quantum measurement yields a new state depending on the outcome, with a certain quantum mechanical probability. We then evolve this new state using the unitary SQW, resulting in another state. The final state is obtained by taking the expectation value of this state with respect to the quantum mechanical probability distribution of the position observable, which induces decoherence. The open SQW is the map from the initial state to the final state obtained this way. Additionally, passing from $l^2(D)$ associated with the edges of G to $l^2(V)$ associated with its vertices by means of boundary operators, which are instrumental in the analysis of the Grover Walk, we define a second open SQW on the vertices of G , we call induced by the open SQW on its edges.

Our analysis of the dynamical properties of both these open SQWs shows they are related to those of natural Markov processes defined on the graph, as in [G, APSS1], which depend on the choice of the scattering matrices. A few examples are worked out to demonstrate the variety of these constructions.

The paper is organized as follows. Section 2 is devoted to the definition of unitary SQWs on the edges of an arbitrary directed graph, their quantum mechanical interpretation, and their general properties. Particular cases such as the Chalker-Coddington model, Coined Quantum Walks, the star-graph case and the generalized Grover Walk are discussed in Section 3. The notion of open SQWs on the edges of a graph and their quantum mechanical interpretation are introduced in Section 4, while their spectral and dynamical properties are addressed in Section 5. Finally, Section 6 presents the definition and analysis of induced open SQWs on the vertices of the graph. Both notions of open SQWs are illustrated by examples. An appendix containing technical proofs closes the paper.

2 Unitary Scattering Quantum Walks on a Graph

Let us set the notation. A directed graph $G = (V, E)$ is specified by the set of its vertices V and the set of its edges E . The order of the graph G is $|V|$, the cardinal of V , which may be infinite. In the latter case, V is assumed to be countable and G is called infinite. For two vertices $x \in V, y \in V$ forming an edge, we will write $x \sim y$ the fact that $(xy) \in E$. The graphs we consider have no loop, *i.e.* $(xx) \notin E$ and to avoid trivialities, we will always assume that $|V| \geq 2$ and that G is connected. Each edge gives rise to two directed edges of opposite direction. A directed edge from vertex x to vertex y is denoted by (yx) , and the set of directed edges is D . Finally, the degree of a vertex $x \in V$ is $d_x \in \mathbb{N}^*$, and we have $\sum_{x \in V} d_x = 2|E| = |D|$. If G is infinite, we further assume that $\sup_{x \in V} d_x = \bar{d} < \infty$. Furthermore, we pick a vertex $r \in V$ we call the root and for any $x \in V$, we denote by $|x|$ the graph distance between x and r . For any $n \in \mathbb{N}$, the set $B_n = \{x \in V \text{ s.t. } |x| \leq n\}$ has finite cardinal bounded above by $\bar{d}(\bar{d} - 1)^{n-1}$.

We associate to G the Hilbert space $l^2(D)$ as follows. To each directed edge (yx) from vertex x to vertex y , we associate a canonical basis vector of $l^2(D)$, denoted by $|yx\rangle$, so that, for a finite graph, $l^2(D) = \text{span}\{|yx\rangle\}_{\substack{x, y \in V \\ x \sim y}}$, with $\dim l^2(D) = \sum_{x \in V} d_x < \infty$. In case G is infinite with countably many vertices, we set

$$l^2(D) = \left\{ \psi = \sum_{x \in V} \sum_{y \sim x} \psi_{xy} |xy\rangle \mid \sum_{x \in V} \sum_{y \sim x} |\psi_{xy}|^2 < \infty \right\}. \quad (2.1)$$

For later purposes, we note the direct sum decompositions

$$l^2(D) = \oplus_{x \in V} \mathcal{H}_x^I = \oplus_{x \in V} \mathcal{H}_x^O, \quad \text{where} \\ \mathcal{H}_x^I = \text{span}\{|xy\rangle\}_{y \sim x}, \quad \mathcal{H}_x^O = \text{span}\{|yx\rangle\}_{y \sim x}. \quad (2.2)$$

The d_x -dimensional subspaces \mathcal{H}_x^I , resp. \mathcal{H}_x^O , are the incoming, resp. outgoing, subspaces attached to the vertex $x \in V$, spanned by incoming, resp. outgoing, edges to x . We will need below the corresponding orthogonal projectors P_x^I , resp. P_x^O onto these subspaces. With the notation $|\varphi\rangle\langle\psi| \in \mathcal{B}(l^2(D))$ to denote, for any pair of vectors $\varphi, \psi \in l^2(D)$, the rank one operator such that $|\varphi\rangle\langle\psi|\chi = \varphi\langle\psi|\chi\rangle$, $\forall \chi \in l^2(D)$, these projectors read and satisfy

$$P_x^I = \sum_{y \sim x} |xy\rangle\langle xy|, \quad P_x^O = \sum_{y \sim x} |yx\rangle\langle yx| \quad \text{s.t.} \quad P_x^\# P_y^\# = \delta_{x,y} P_x^\#, \quad \# \in \{I, O\}, \quad (2.3) \\ P_x^I P_y^O = P_y^O P_x^I = \begin{cases} |xy\rangle\langle xy| & \text{if } x \sim y \\ 0 & \text{otherwise.} \end{cases}$$

We proceed with the definition of QWs defined on $l^2(D)$ as unitary operators parameterized by a family of scattering matrices. To each vertex $x \in V$ of degree d_x , we associate a unitary matrix called a scattering matrix

$$S(x) \in U(d_x), \text{ with matrix elements } S(x) = (S_{zy}(x))_{\substack{y \sim x \\ z \sim x}}. \quad (2.4)$$

Definition 2.1 Given the set of scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$, the QW operator on the graph G , $U_{\mathcal{S}}$, is defined on $l^2(D)$ by its action on the basis vectors

$$U_{\mathcal{S}}|xy\rangle = \sum_{z \sim x} S_{zy}(x)|zx\rangle, \text{ for all } x, y \in V, x \sim y, \quad (2.5)$$

or, equivalently,

$$U_{\mathcal{S}} = \sum_{x \in V} \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x)|zx\rangle\langle xy|. \quad (2.6)$$

The set of scattering matrices \mathcal{S} parameterizing the QW operator $U_{\mathcal{S}}$ is emphasized in the notation. We call the QW defined by (2.6) a Scattering Quantum Walk, SQW for short. We note that for all $x \in V$, $U_{\mathcal{S}}$ intertwines between the projectors P_x^{I} and P_x^{O}

$$U_{\mathcal{S}}P_x^{\text{I}} = P_x^{\text{O}}U_{\mathcal{S}} = P_x^{\text{O}}U_{\mathcal{S}}P_x^{\text{I}} = \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x)|zx\rangle\langle xy|. \quad (2.7)$$

Remark 2.2 If V is an infinite graph, the sum in (2.6) is to be understood as $\lim_{n \rightarrow \infty} \sum_{\substack{x \in V \\ |x| \leq n}} (\dots)$ in the strong sense. The convergence is ensured by the unitarity of $S(x)$: for any $x \in V$, any $\psi \in l^2(D)$,

$$\begin{aligned} \left\| \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x)|zx\rangle\langle xy|\psi \right\|^2 &= \sum_{\substack{y \sim x \\ z \sim x}} \sum_{\substack{y' \sim x \\ z' \sim x}} \overline{S_{zy'}(x)} S_{zy}(x) \langle \psi | xy' \rangle \langle z'x | zx \rangle \langle xy | \psi \rangle \\ &= \sum_{\substack{y \sim x \\ y' \sim x}} \left(\sum_{z \sim x} \overline{S_{zy'}(x)} S_{zy}(x) \right) \langle \psi | xy' \rangle \langle xy | \psi \rangle \\ &= \sum_{\substack{y \sim x \\ y' \sim x}} \delta_{yy'} |\langle \psi | xy \rangle|^2 = \|P_x^{\text{I}}\psi\|^2, \end{aligned} \quad (2.8)$$

where the orthogonal projectors $\{P_x^{\#}\}_{x \in V}$, $\# \in \{\text{I}, \text{O}\}$ form resolutions of the identity.

Lemma 2.3 For a graph $G = (V, E)$ and a set $\mathcal{S} = \{S(x)\}_{x \in V}$, the operator $U_{\mathcal{S}}$ acting on the Hilbert space $l^2(D)$ defined by (2.6) is a unitary operator.

Proof : The property follows from the unitarity of $S(x)$:

$$\begin{aligned} U_{\mathcal{S}}^*U_{\mathcal{S}} &= \sum_{x' \in V} \sum_{\substack{y' \sim x' \\ z' \sim x'}} \overline{S_{zy'}(x')} |x'y'\rangle\langle z'x'| \sum_{x \in V} \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) |zx\rangle\langle xy| \\ &= \sum_{x \in V} \sum_{\substack{y \sim x \\ y' \sim x'}} \left(\sum_{z \sim x} \overline{S_{zy'}(x)} S_{zy}(x) \right) |xy'\rangle\langle xy| \\ &= \sum_{x \in V} \sum_{\substack{y \sim x \\ y' \sim x}} \delta_{yy'} |xy'\rangle\langle xy| = \sum_{x \in V} P_x^{\text{I}} = \mathbb{I}, \end{aligned} \quad (2.9)$$

and the reverse identity $U_{\mathcal{S}}U_{\mathcal{S}}^* = \mathbb{I}$ is proven similarly. \square

The relations (2.3) show that $U_{\mathcal{S}}$ couples subspaces \mathcal{H}_x^I attached at neighbouring vertices of the graph.

Quantum mechanical interpretation: The quantum system at hand, or quantum walker, has configuration space given by the directed edges (xy) of the graph G , giving rise to the canonical basis of the Hilbert space $l^2(D)$. In a state described by a normalized vector $\psi \in l^2(D)$, the probability of the quantum walker to be on the directed edge (xy) of the graph G is $|\langle xy|\psi\rangle|^2 = |\psi_{xy}|^2$. The operator $U_{\mathcal{S}}$ defines the one time step evolution of the quantum system. By construction, the state $|xy\rangle$ of a quantum walker incoming at the vertex $x \in V$ along the edge (xy) undergoes a local scattering process monitored by the unitary matrix $S(x)$ which sends it to a linear combination of outgoing states along the edges (zx) , according to (2.5). This local scattering point of view on the quantum dynamics is at work in several physically motivated specific models that, as we will show, are special cases of our definition (2.6).

The questions of interest concern the determination of the spectrum of $U_{\mathcal{S}}$ and of the related properties of the discrete time dynamical system $(U_{\mathcal{S}}^n)_{n \in \mathbb{Z}}$ on $l^2(D)$, as a function of the characteristics of G , and of the set $\mathcal{S} = \{S(x)\}_{x \in V}$ that parametrize the quantum evolution. The behaviour in time of the probability distribution $\mathbb{P}_n^{\psi_0}(\cdot)$ on the set of directed edges $\{(xy)\}_{x \sim y}$ induced by the quantum dynamics is also of interest: let $\psi_0 \in l^2(D)$ be an initial state and $\psi_n = U_{\mathcal{S}}^n \psi_0 \in l^2(D)$ be the corresponding state at time $n \in \mathbb{Z}$. For (xy) a directed edge of G , $\mathbb{P}_n^{\psi_0}(\cdot)$ defined by

$$\mathbb{P}_n^{\psi_0}(xy) = |\langle xy|U_{\mathcal{S}}^n \psi_0\rangle|^2 = |\langle xy|\psi_n\rangle|^2 \quad (2.10)$$

yields the probability to find the quantum walker at time n on the oriented edge (xy) by a measurement of its position. Another important time dependent distribution on the vertices $x \in V$ of the graph, $\mathbb{Q}_n^{\psi_0}(\cdot)$, is the probability to find the quantum walker at time $n \in \mathbb{Z}$ in the subspace \mathcal{H}_x^I or, improperly, on the vertex $x \in V$, by a measurement of its position. It is defined by

$$\mathbb{Q}_n^{\psi_0}(x) = \|P_x^I U_{\mathcal{S}}^n \psi_0\|^2 = \|P_x^I \psi_n\|^2 = \sum_{y \sim x} \mathbb{P}_n^{\psi_0}(xy). \quad (2.11)$$

2.1 General Properties

We proceed with a few general considerations before discussing some special cases.

Perturbation theory: To compare two SQWs defined on the same graph with different sets of scattering matrices, we can resort to the following result which holds in infinite dimension. Such estimates have proven to be instrumental in the analyses of currents in the Chalker-Coddington model, [ABJ4, ABJ5], and other network models.

Lemma 2.4 *For a graph $G = (V, E)$ and two sets of scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$, resp. $\mathcal{S}' = \{S'(x)\}_{x \in V}$, let $U_{\mathcal{S}}$, resp. $U_{\mathcal{S}'}$, be defined on $l^2(D)$ according to (2.6). Then,*

$$\|U_{\mathcal{S}} - U_{\mathcal{S}'}\| \leq \sup_{x \in V} \|S(x) - S'(x)\|_{\text{HS}}, \quad (2.12)$$

where $\|\cdot\|_{\text{HS}}$ denotes the Hilbert-Schmidt norm on finite matrices.

Proof : For any $\psi = \sum_{x \in V} \sum_{y \sim x} \psi_{xy} |xy\rangle \in l^2(D)$,

$$\begin{aligned}
\|(U_S - U_{S'})\psi\|^2 &= \sum_{x \in V} \left\| P_x^O \sum_{\substack{y \sim x \\ z \sim x}} (S(x) - S'(x))_{zy} |zx\rangle \langle xy| \psi \right\|^2 \\
&= \sum_{x \in V} \left| \sum_{\substack{y \sim x \\ z \sim x}} (S(x) - S'(x))_{zy} \psi_{xy} \right|^2 \\
&\leq \sum_{x \in V} \sum_{z \sim x} \left(\sum_{y \sim x} |(S(x) - S'(x))_{zy}|^2 \right) \left(\sum_{y \sim x} |\psi_{xy}|^2 \right) \\
&\leq \sup_{x \in V} \|S(x) - S'(x)\|_{\text{HS}}^2 \|\psi\|^2.
\end{aligned} \tag{2.13}$$

□

The graph G as subgraph of K : Any finite graph $G = (V, E)$ of order $|V|$ can be viewed as a subgraph of the complete graph of order $|V|$, denoted by K . Defining $\widehat{G} = (V, \widehat{E})$ as the graph with same set of vertices V and set of edges \widehat{E} distinct from E such that $K = (G, E \cup \widehat{E})$, we will denote that situation as $K = G \cup \widehat{G}$. Accordingly, denoting by $l^2(\widehat{D})$ and $l^2(D_K)$ the Hilbert spaces associated with the directed edges of \widehat{G} and K , we show that $l^2(D_K) = l^2(D) \oplus l^2(\widehat{D})$ and that U_S can be viewed as the restriction to $l^2(D)$ of a unitary SQW, U_{S_K} , defined on $l^2(D_K)$.

Indeed, we note that for any $x, y \in V$, (xy) is an edge of K and is associated with the basis vector $|xy\rangle$ of $l^2(D_K)$. Since (xy) either belongs to E or to \widehat{E} , then either $|xy\rangle \in l^2(D)$ or $|xy\rangle \in l^2(\widehat{D})$. Sorting the basis vectors $\{|xy\rangle\}_{x, y \in V}$ accordingly, we have $l^2(D) = \text{span}\{|xy\rangle\}_{(xy) \in E} \subset l^2(D_K)$, $l^2(\widehat{D}) = \text{span}\{|xy\rangle\}_{(xy) \in \widehat{E}} \subset l^2(D_K)$ with $l^2(D_K) = l^2(D) \oplus l^2(\widehat{D})$.

Then, for each $x \in V$, let $\widehat{d}_x \in \mathbb{N}$ be such that $d_x + \widehat{d}_x = |V| - 1$ and consider $\mathbb{C}^{|V|-1} = \mathbb{C}^{d_x} \oplus \mathbb{C}^{\widehat{d}_x}$. In addition to $\mathcal{S} = \{S(x)\}_{x \in V}$, with $S(x) \in U(d_x)$ acting on \mathbb{C}^{d_x} , we consider $\widehat{\mathcal{S}} = \{\widehat{S}(x)\}_{x \in V}$, where $\widehat{S}(x) \in U(\widehat{d}_x)$ acts on $\mathbb{C}^{\widehat{d}_x}$. This allows us to define $U_{\widehat{\mathcal{S}}}$ on $l^2(\widehat{D})$. Now, for $K = G \cup \widehat{G}$, we use the direct sums of scattering matrices $\mathcal{S}_K = \{S(x) \oplus \widehat{S}(x)\}_{x \in V}$ acting on $\mathbb{C}^{|V|-1}$ for each $x \in V$, to construct U_{S_K} on $l^2(D_K)$ so that for any $x, y \in V$,

$$U_{S_K} |xy\rangle = \begin{cases} \sum_{\substack{z \sim y \\ (zx) \in E}} S_{zy}(x) |zx\rangle & \text{if } (xy) \in G \\ \sum_{\substack{z \sim y \\ (zx) \in \widehat{E}}} \widehat{S}_{zy}(x) |zx\rangle & \text{if } (xy) \in \widehat{G}. \end{cases} \tag{2.14}$$

We have thus shown:

Lemma 2.5 *For G finite and with the notation above,*

$$U_{S_K} = U_S \oplus U_{\widehat{\mathcal{S}}} \text{ acting on } l^2(D_K) = l^2(D) \oplus l^2(\widehat{D}). \tag{2.15}$$

Remark 2.6 *The graph $\widehat{G} = (V, \widehat{E})$ is not necessarily connected, in which case it provides $U_{\widehat{\mathcal{S}}}$ with a direct sum structure, regardless of the choice of $\widehat{\mathcal{S}} = \{\widehat{S}(x)\}_{x \in V}$.*

Asymptotics of $\mathbb{Q}_n^{\psi_0}(x)$: The large n behaviour of $\mathbb{Q}_n^{\psi_0}(x)$, the probability to find the quantum walker on the vertex $x \in V$ at time n , is oscillatory in case G is finite. We get a finite limit considering the Cesàro mean, which suppresses the oscillations. In the infinite dimensional case, the Cesàro mean limit involves the nature of $\sigma(U_S)$, according to the RAGE theorem, see e.g. [Si], Theorem 5.5.6, and [RT], Theorems B1 and B2.

More precisely, let $E(\cdot)$ defined on $] -\pi, \pi]$ denote the self-adjoint spectral projectors of U_S so that the spectral theorem reads in the resolution of the identity form $U_S = \int_{]-\pi, \pi]} e^{i\theta} dE(\theta)$. In particular, $E(\{\theta\})$ is the spectral projector on $\text{Ker}(U_S - e^{i\theta}\mathbb{I})$. Denoting by $\sigma_p(U_S)$ the set of eigenvalues of U_S , we have

Lemma 2.7 *Let U_S have spectral projectors $E(\cdot)$ and $\mathbb{Q}_n^{\psi_0}(x)$ be defined by (2.11). Then*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=0}^{N-1} \mathbb{Q}_n^{\psi_0}(x) = \sum_{e^{i\theta} \in \sigma_p(U_S)} \|P_x^I E(\{\theta\}) \psi_0\|^2. \quad (2.16)$$

Remark 2.8 *i) In case G is infinite and ψ_0 belongs to the continuous spectral subspace of U_S , if any, the limit vanishes.*

ii) For G finite, the finite N Cesàro mean and the RHS differ by an $O(N^{-1})$ term.

Proof : We write U for U_S below, to lighten the notation. The proof is a direct consequence Theorem B2 in [RT],

$$\text{s-} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} U^n |\psi_0\rangle \langle \psi_0| U^{-n} = \sum_{e^{i\theta} \in \sigma_p(U_S)} E(\{\theta\}) |\psi_0\rangle \langle \psi_0| E(\{\theta\}), \quad (2.17)$$

and of the cyclicity of the trace which yields

$$\mathbb{Q}_n^{\psi_0}(x) = \text{tr}(P_x^I U^n |\psi_0\rangle \langle \psi_0| U^{-n}) \quad (2.18)$$

and

$$\text{tr}(P_x^I E(\{\theta\}) |\psi_0\rangle \langle \psi_0| E(\{\theta\})) = \|P_x^I E(\{\theta\}) \psi_0\|^2. \quad (2.19)$$

□

An application of this result to the star-graph is presented in Section 3.3.

3 Particular Cases

3.1 The Chalker-Coddington Model

The Chalker-Coddington model [CC], providing a simplified description of the Quantum Hall effect, can be cast in the framework of SQW defined on $G = \mathbb{Z}^2$, as we briefly show. See [ABJ1, ABJ2] for a mathematical approach of this model, and references therein for background.

Let

$$\{\mathbb{S}_{j,2k}\}_{j,k \in \mathbb{Z}}, \text{ with } \mathbb{S}_{j,2k} \in U(2), \forall j, k, \quad (3.1)$$

be a collection of scattering matrices, called even or odd according to the parity of j . The unitary operator which defines the Chalker-Coddington model

$$U_{CC} : l^2(\mathbb{Z}^2) \rightarrow l^2(\mathbb{Z}^2) \quad (3.2)$$

reads as follows: Let $\{|j, k\rangle\}_{j,k \in \mathbb{Z}}$ be the canonical basis vectors of $l^2(\mathbb{Z}^2)$; U_{CC} is defined according to figure 2 by:

$$\begin{aligned} \begin{pmatrix} U_{CC}|2j, 2k\rangle \\ U_{CC}|2j+1, 2k-1\rangle \end{pmatrix} &= \mathbb{S}_{2j,2k} \begin{pmatrix} |2j+1, 2k\rangle \\ |2j, 2k-1\rangle \end{pmatrix}, \\ \begin{pmatrix} U_{CC}|2j+2, 2k+1\rangle \\ U_{CC}|2j+1, 2k\rangle \end{pmatrix} &= \mathbb{S}_{2j+1,2k} \begin{pmatrix} |2j+1, 2k+1\rangle \\ |2j+2, 2k\rangle \end{pmatrix}. \end{aligned} \quad (3.3)$$

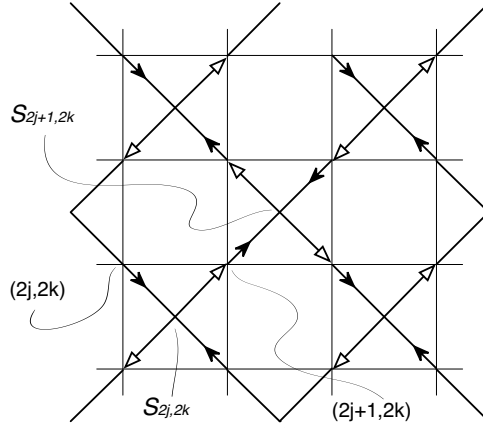


Figure 2: A Chalker–Coddington model with its incoming (solid arrows) and outgoing links.

The convention above is as follows (without indices):

$$\begin{pmatrix} U|a\rangle \\ U|b\rangle \end{pmatrix} = \mathbb{S} \begin{pmatrix} |c\rangle \\ |d\rangle \end{pmatrix} \Leftrightarrow \begin{cases} U|a\rangle = S_{11}|c\rangle + S_{21}|d\rangle \\ U|b\rangle = S_{12}|c\rangle + S_{22}|d\rangle \end{cases}, \quad (3.4)$$

where S_{ij} are the matrix elements of \mathbb{S} , in line with (2.5).

The underlying graph is $G = \mathbb{Z}^2$, with vertices at the intersections of the diagonal lines, where the scattering matrices sit. On the grid of Figure 2, the vertices carrying even matrices $S_{2j,2k}$, respectively odd matrices $S_{2j+1,2k}$, have coordinates

$$\begin{aligned} x^e(j, k) &= (2j, 2k) + (1/2, -1/2), \quad \text{respectively} \\ x^o(j, k) &= (2j + 1, 2k) + (1/2, 1/2), \quad \forall (j, k) \in \mathbb{Z}^2. \end{aligned} \quad (3.5)$$

The edges are the diagonal segments labelled by their center (j, k) on that grid and they have one direction only given by their arrow.

Note that we are missing half the directed edges with respect to the construction of $l^2(D)$, where each edge comes with two orientations. So we associate with each $(j, k) \in \mathbb{Z}^2$ the canonical basis vectors $|j, k\rangle_-$ of $l^2(\mathbb{Z}^2)$, corresponding to edges labeled by (j, k) with orientation *opposite* to the arrow. These vectors span another copy of $l^2(\mathbb{Z}^2)$ we denote by $l^2_-(\mathbb{Z}^2)$. For example, $|2j, 2k\rangle$ and $|2j + 1, 2k - 1\rangle$ are incoming to $x^e(j, k)$ while $|2j, 2k\rangle_-$ is incoming to $x^o(j - 1, k)$ and $|2j + 1, 2k - 1\rangle_-$ is incoming to $x^o(j, k - 1)$, and similarly for the other directed edges. Moreover, we have $l^2(D) = l^2(\mathbb{Z}^2) \oplus l^2_-(\mathbb{Z}^2)$.

Since the degree of all vertices is 4, we need 4×4 scattering matrices at each vertex to realize the Chalker Coddington model as a SQW on $l^2(D)$. We label and order the canonical basis of \mathbb{C}^4 at each vertex as $\{e_{NW}, e_{SE}, e_{NE}, e_{SW}\}$, where the cardinal symbols indicate the incoming and outgoing directions at the vertices, see (2.6). Then for every vertex $x^\#(j, k)$, $(j, k) \in \mathbb{Z}^2$, $\# \in \{e, o\}$, we define

$$S(x^\#(j, k)) = \begin{pmatrix} \mathbb{O} & S_{2j+1,2k} \\ S_{2j,2k} & \mathbb{O} \end{pmatrix} \in U(4) \quad (3.6)$$

with respect to the chosen ordered basis, and set $\mathcal{S}_{CC} = \{S(x^\#(j, k))\}_{\substack{(j,k) \in \mathbb{Z}^2 \\ \# \in \{e,o\}}}$.

Proposition 3.1 *With the notation and choices made above, the SQW defined on $l^2(D)$ according to (2.6) and parameterized by S_{CC} , denoted by $U_{S_{CC}}$, satisfies*

$$U_{S_{CC}} = U_{CC} \oplus \tilde{U}_{CC} \quad \text{on } l^2(D) = l^2(\mathbb{Z}^2) \oplus l^2_-(\mathbb{Z}^2) \quad (3.7)$$

where $U_{CC} = U_{S_{CC}}|_{l^2(\mathbb{Z}^2)}$ is the Chalker-Coddington operator (3.3).

The restriction $\tilde{U}_{CC} = U_{S_{CC}}|_{l^2_-(\mathbb{Z}^2)}$ is a copy of this model, where all orientations are reversed and for all $(j, k) \in \mathbb{Z}^2$, the scattering matrices $S_{2j,2k}$ and $S_{2j+1,2k}$ are exchanged.

Remark 3.2 *i) Casting the Chalker-Coddington model into a SQW amounts to add another independent copy of the model in the process of completing the set of directed edges.*

ii) The operator \tilde{U}_{CC} is unitarily equivalent to U_{CC} .

Proof : It is a matter of computation to check that the action of $U_{S_{CC}}$ on basis vectors of the form $|j, k\rangle$ coincides with (3.3) while its action on vectors $|j, k\rangle_-$ yields

$$\begin{aligned} \begin{pmatrix} U_{\mathbb{Z}^2}^{S_{CC}} |2j+1, 2k\rangle_- \\ U_{\mathbb{Z}^2}^{S_{CC}} |2j, 2k-1\rangle_- \end{pmatrix} &= S_{2j+1,2k} \begin{pmatrix} |2j, 2k\rangle_- \\ |2j+1, 2k-1\rangle_- \end{pmatrix}, \\ \begin{pmatrix} U_{\mathbb{Z}^2}^{S_{CC}} |2j+1, 2k+1\rangle_- \\ U_{\mathbb{Z}^2}^{S_{CC}} |2j+2, 2k\rangle_- \end{pmatrix} &= S_{2j,2k} \begin{pmatrix} |2j+2, 2k+1\rangle_- \\ |2j+1, 2k\rangle_- \end{pmatrix}. \end{aligned} \quad (3.8)$$

Therefore both $l^2(\mathbb{Z}^2)$ and $l^2_-(\mathbb{Z}^2)$ are invariant under $U_{S_{CC}}$ and, by inspection, \tilde{U}_{CC} coincides with a Chalker-Coddington model as described. \square

The Chalker-Coddington model is one of many quantum networks models. While this appellation is not universal, it often refers to QWs defined on graphs in a similar fashion as (2.5) with the understanding that the edges can be travelled by the quantum walker in one direction only. This imposes the degrees d_x to be even for all $x \in V$, so that the scattering matrix $S(x) \in U(d_x)$ assigned to $x \in V$ maps the $d_x/2$ incoming edges at x to the $d_x/2$ outgoing edges from x , see [D] for example. The Scattering Zippers, introduced and studied in [MS-B,BM] provide an other example related to the Chalker-Coddington model defined on a strip.

Without going into the details, such quantum network models can be viewed as restrictions of SQW defined on a doubled Hilbert space, as we saw for the Chalker-Model model.

3.2 Coined Quantum Walks

Coined QWs defined on graphs as introduced by [AAKV], have provides a useful concept in quantum computing and a versatile modeling tool in quantum dynamics. We shown that they also belong to the class of SQWs on regular graphs.

Let us consider the case where all scattering matrices are identity $d_x \times d_x$ matrices, $S(x) = \mathbb{I}_{d_x}$, which reduces (2.6) to

$$F = \sum_{x \in V} \sum_{y \sim x} |yx\rangle \langle xy| = F^* = F^{-1}. \quad (3.9)$$

The notation F is justified by the flip property $F|xy\rangle = |yx\rangle$, for all $x \sim y$. Therefore F is reduced by all orthogonal two-dimension subspaces $\mathcal{H}_{xy} = \text{span}\{|xy\rangle, |yx\rangle\}$, where $x \sim y$, with matrix representation in the ordered basis $\{|xy\rangle, |yx\rangle\}$,

$$F|_{\mathcal{H}_{xy}} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow F = \bigoplus_{(xy) \in E} F|_{\mathcal{H}_{xy}} \quad \text{and } \sigma(F) = \{-1, 1\}. \quad (3.10)$$

This trivial case allows for the decomposition of the general case according to

$$U_S = F(FU_S) \text{ where } F : \mathcal{H}_x^O \rightarrow \mathcal{H}_x^I, \text{ and } FU_S : \mathcal{H}_x^I \rightarrow \mathcal{H}_x^I, \forall x \in V, \quad (3.11)$$

such that

$$FU_S = \bigoplus_{x \in V} S(x) \text{ where } S(x) \simeq \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) |xz\rangle \langle xy| : \mathcal{H}_x^I \rightarrow \mathcal{H}_x^I. \quad (3.12)$$

In the decomposition (3.11), F is responsible for the motion of the quantum walker between different subspaces \mathcal{H}_x^I , while FU_S changes its state locally within each \mathcal{H}_x^I .

The general structure (3.11) of U_S as the composition of a local unitary operator and an operator that implements the motion is that of a Coined QW. However, in many models of quantum dynamics by Coined QWs on infinite regular graphs derived from the Schrödinger equation, the operator responsible for the motion of the walker is unitarily equivalent to a direct sum of shifts, analogous to the effect of the Laplacian, and therefore has absolutely continuous spectrum. The effect of the potential is local and analogous to the action of FU_S . These specificities are relevant when analyzing the spectral and dynamical (de-)localization properties of Random QWs, see *e.g.* [Kos, HJ1, JMe, ABJ2, ABJ3, ABJ4, ABJ5, J3]. Coined QWs of this sort defined on regular infinite graphs can be viewed as SQW:

Assume G is an infinite d regular graph, and let $\theta : \{1, 2, \dots, d\}$ be a permutation. Each vertex $x \in V$ forms exactly d edges with vertices in V that are labeled x_1, x_2, \dots, x_d . Set F_θ , the operator defined by its action on the basis vectors of $l^2(D)$

$$F_\theta : \mathcal{H}_x^I \rightarrow \mathcal{H}_x^O \text{ s.t. } F_\theta |xx_j\rangle = |x_{\theta(j)}x\rangle, \quad \forall j \in \{1, 2, \dots, d\}. \quad (3.13)$$

By definition, F_θ is unitary, as a change of basis, and its adjoint F_θ^* acts as

$$F_\theta^* : \mathcal{H}_x^O \rightarrow \mathcal{H}_x^I \text{ s.t. } F_\theta^* |x_jx\rangle = |xx_{\theta^{-1}(j)}\rangle, \quad \forall j \in \{1, 2, \dots, d\}. \quad (3.14)$$

We have a decomposition similar to (3.11) thanks to F_θ

$$U_S = F_\theta(F_\theta^*U_S) \text{ where } F_\theta^*U_S : \mathcal{H}_x^I \rightarrow \mathcal{H}_x^I, \quad \forall x \in V, \quad (3.15)$$

and, with the shorthand $S_{jk}(x) = S_{x_jx_k}(x)$,

$$F_\theta^*U_S |xx_j\rangle = \sum_k S_{\theta(k)j}(x) |xx_k\rangle. \quad (3.16)$$

Then we observe that for each $x \in V$, the matrix $S_\theta(x) = (S_{\theta(k)j}(x))_{k,j} \in U(d)$ is a scattering matrix as well, obtained by permuting the rows of $S(x)$, so that

$$F_\theta^*U_S = \bigoplus_{x \in V} S_\theta(x), \text{ where } S_\theta(x) : \mathcal{H}_x^I \rightarrow \mathcal{H}_x^I \quad (3.17)$$

is a local (coin) operator with arbitrary scattering matrices $S_\theta(x)$. The spectral properties of F_θ depend on the specificities of the graph and permutation θ .

We spell out the case of $G = \mathbb{Z}^d$, where the degree of each vertex $x \in \mathbb{Z}^d$ is $2d$. Set $I = \{\pm 1, \pm 2, \dots, \pm d\}$ and let $\{e_1, e_2, \dots, e_d\}$ be the canonical basis of \mathbb{R}^d . We denote a generic basis vector of $\mathcal{H}_x^I \subset l^2(D)$ as

$$|xx_\tau\rangle, \text{ where } \tau \in I, \text{ and } x_\tau = x - \text{sign}(\tau)e_{|\tau|} \in \mathbb{Z}^d. \quad (3.18)$$

The next lemma shows that the SQW U_S on $l^2(D)$ is unitarily equivalent to a Coined QW:

Lemma 3.3 *Let $G = \mathbb{Z}^d$ and $l^2(D)$ with canonical basis given by $\{|xx_\tau\rangle\}_{x \in \mathbb{Z}^d, \tau \in I}$, as in (3.18). We have the unitary equivalence*

$$l^2(D) \simeq l^2(V) \otimes \mathbb{C}^{2d} = \text{span} \{|x\rangle \otimes |\tau\rangle, x \in V, \tau \in I\}, \quad (3.19)$$

with the identification

$$|xx_\tau\rangle \simeq |x\rangle \otimes |\tau\rangle \quad (3.20)$$

where $\{|\tau\rangle\}_{\tau \in I}$ labels an orthonormal basis of \mathbb{C}^{2d} .

Let θ defined by

$$\theta : I \rightarrow I \quad \text{s.t.} \quad \theta(\tau) = -\tau, \quad \forall \tau \in I, \quad (3.21)$$

then we have the unitary equivalences

$$F_\theta \simeq T, \quad F_\theta^* U_S \simeq C, \quad (3.22)$$

where for all $x \in V, \tau \in I$,

$$\begin{aligned} C(|x\rangle \otimes |\tau\rangle) &= |x\rangle \otimes \sum_{\tau' \in I} S_\theta(x)_{\tau'\tau} |\tau'\rangle, \\ T(|x\rangle \otimes |\tau\rangle) &= |x + \text{sign}(\tau)e_{|\tau|}\rangle \otimes |\tau\rangle, \end{aligned} \quad (3.23)$$

so that U_S is unitarily equivalent to the Coined QW defined by the composition TC .

Proof : With our convention that (xx_τ) points in the direction of x , the basis vectors of \mathcal{H}_x^I are independent of $x \in \mathbb{Z}^d$

$$|xx_\tau\rangle = |\text{sign}(\tau)e_{|\tau|}\rangle, \quad \tau \in I, \quad (3.24)$$

and point in the $2d$ directions of the lattice. Denoting by $\{|\tau\rangle\}_{\tau \in I}$ an orthonormal basis of \mathbb{C}^{2d} , we have

$$\mathcal{H}_x^I = \text{span} \{|xx_\tau\rangle, \tau \in I\} \simeq \mathbb{C}^{2d} = \text{span} \{|\tau\rangle \in I\}. \quad (3.25)$$

Making use of $l^2(D) = \oplus_{x \in V} \mathcal{H}_x^I$, see (2.2), we deduce the announced unitary equivalence (3.19). Now, considering (3.13), we get with (3.21) and (3.18)

$$F_\theta |xx_\tau\rangle = |x_{-\tau}x\rangle = |yy_\tau\rangle, \quad (3.26)$$

with $y = x + \text{sign}(\tau)e_{|\tau|}$. In the space $l^2(V) \otimes \mathbb{C}^{2d}$, this amounts to the action of T , the translation by $\text{sign}(\tau)e_{|\tau|}$ in V , leaving the component in \mathbb{C}^{2d} invariant. Finally, (3.16) yields for each $x \in V, \tau \in I$

$$(F_\theta^* U_S) |xx_\tau\rangle = \sum_{\tau' \in I} S_\theta(x)_{\tau'\tau} |xx_{\tau'}\rangle \in \mathcal{H}_x^I, \quad (3.27)$$

which gives the equivalence with C . □

Remark 3.4 *i) The composition TC is the prototypical Coined QW on \mathbb{Z}^d .
ii) Other choices of the permutation θ , besides the identity permutation, may lead F_θ to be reduced by infinitely many finite dimensional subspaces and to be pure point spectrum.*

Similar considerations, which we don't make explicit here, show that the Coined QWs on the d -regular tree, studied in [HJ1, JMa, T] for example, are also special cases of SQWs.

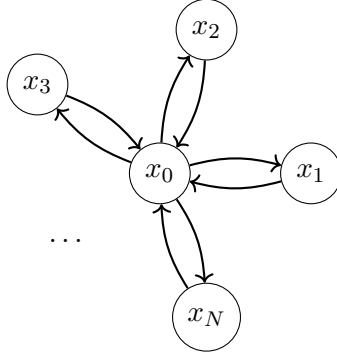


Figure 3: Star-graph SG with N branches.

3.3 Star-graph

Consider G to be the star-graph SG with N branches characterized by vertices x_0, x_1, \dots, x_N , with edges between x_0 and x_j , $1 \leq j \leq N$, only, see Figure 3.

To lighten the notation, we denote the vertices x_j by their label j only. Hence we have $d_0 = N$, and $d_j = 1$, $1 \leq j \leq N$, and the $2N$ canonical basis vectors of $l^2(D)$ are $\{|0j\rangle, |j0\rangle\}_{1 \leq j \leq N}$. To the center vertex 0 we associate the scattering matrix $S(0) = (S_{kj}(0))_{1 \leq k, j \leq N} \in U(N)$, and to the vertices j , $0 \leq j \leq N$, we associate $S(j) = e^{i\theta_j} \in U(1)$, denoting this set of matrices by \mathcal{S}_{SG}

The matrix of $U_{SG} \in U(2N)$ in the basis $\{|01\rangle, \dots, |0N\rangle, |10\rangle, \dots, |N0\rangle\}$ then reads

$$U_{\mathcal{S}_{SG}} \simeq \begin{pmatrix} 0 & 0 & \dots & 0 & e^{i\theta_1} & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & e^{i\theta_2} & \dots & 0 \\ \vdots & & \ddots & \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & \dots & e^{i\theta_N} \\ S_{11}(0) & S_{12}(0) & \dots & S_{1N}(0) & 0 & 0 & \dots & 0 \\ S_{21}(0) & S_{22}(0) & \dots & S_{2N}(0) & 0 & 0 & \dots & 0 \\ \vdots & & \ddots & \vdots & \vdots & & \ddots & \vdots \\ S_{N1}(0) & S_{N2}(0) & \dots & S_{NN}(0) & 0 & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} 0 & D(\theta) \\ S(0) & 0 \end{pmatrix}, \quad (3.28)$$

where $D(\theta) \in U(N)$ and $0 \in M_N(\mathbb{C})$ are defined by the bloc structure of U_{SG_N} . As

$$U_{\mathcal{S}_{SG}}^2 = \begin{pmatrix} D(\theta)S(0) & 0 \\ 0 & S(0)D(\theta) \end{pmatrix}, \quad (3.29)$$

where $S(0)D(\theta)$ and $D(\theta)S(0)$ are unitarily equivalent,

$$\sigma(D(\theta)S(0)) = \sigma(S(0)D(\theta)) = \{e^{i\alpha_j}\}_{1 \leq j \leq N}, \quad (3.30)$$

with eigenvalues repeated according to multiplicity, we deduce that

$$\sigma(U_{\mathcal{S}_{SG}}) = \{\pm e^{i\alpha_j/2}\}_{1 \leq j \leq N}. \quad (3.31)$$

Remark 3.5 We can allow $d_0 = N = \infty$ in this case, with $l^2(D) = l^2(\mathbb{N}^*) \oplus l^2(\mathbb{N}^*)$, $S(0)$ a unitary operator on $l^2(\mathbb{N}^*)$, and $D(\theta)$ a diagonal unitary operator on $l^2(\mathbb{N}^*)$. It is also possible to consider $l^2(D) = l^2(\mathbb{Z}) \oplus l^2(\mathbb{Z})$, labelling the branches of the star graph from $-\infty$ to ∞ , with $S(0)$ and $D(\theta)$ being unitary operators on $l^2(\mathbb{Z})$.

Therefore, the restriction $U_{S_{SG}}^2|_{\mathcal{H}_0^1} \simeq D(\theta)S(0)$ yields a general unitary operator acting on the (in-)finite dimensional Hilbert space \mathcal{H}_0^1 , that can be cast under the form of a QW, by designing $S(0)$ appropriately. Operators of this kind are the starting point for the analysis of certain deterministic unitary operators $S(0)$ perturbed by random phases $D(\theta) = \text{diag}(e^{i\theta_j})$, appearing in models displaying Anderson localization [Kos, HJS2, JMe, ABJ2, ABJ3, ABJ4, ABJ5, J3].

We proceed with the case of the finite star-graph to illustrate Lemma 2.7. We thus need to determine the spectrum and eigenprojectors of (3.28). Since the main steps hold in the infinite dimensional case, consider the following slightly more abstract framework:

Let \mathcal{H} be a separable Hilbert space and let $S \in \mathcal{B}(\mathcal{H})$, $D \in \mathcal{B}(\mathcal{H})$ be unitary operators. We consider U defined on the direct sum of Hilbert spaces $\mathcal{K} = \mathcal{H} \oplus \mathcal{H}$ by the bloc representation

$$U = \begin{pmatrix} 0 & D \\ S & 0 \end{pmatrix}. \quad (3.32)$$

Lemma 3.6 *For any $|z| \neq 1$ we have*

$$(U - z\mathbb{I}_{\mathcal{K}})^{-1} = \begin{pmatrix} z(DS - z^2\mathbb{I}_{\mathcal{H}})^{-1} & D(SD - z^2\mathbb{I}_{\mathcal{H}})^{-1} \\ S(DS - z^2\mathbb{I}_{\mathcal{H}})^{-1} & z(SD - z^2\mathbb{I}_{\mathcal{H}})^{-1} \end{pmatrix}, \quad (3.33)$$

and $\sigma(U) = \{\lambda \in \mathbb{S} \mid \lambda^2 \in \sigma(DS)\}$.

If $e^{i\alpha}$ is an eigenvalue of DS with associated spectral projector $P(\{\alpha\})$, then $\pm e^{i\alpha/2}$ is an eigenvalue of U with associated spectral projector

$$E^\pm(\{\alpha/2\}) = \frac{1}{2} \begin{pmatrix} P(\{\alpha\}) & \pm DQ(\{\alpha\})e^{-i\alpha/2} \\ \pm D^{-1}P(\{\alpha\})e^{i\alpha/2} & Q(\{\alpha\}) \end{pmatrix}, \quad (3.34)$$

where $Q(\{\alpha\}) = D^{-1}P(\{\alpha\})D$ is the spectral projector of SD associated with $e^{i\alpha} \in \sigma(SD)$. The multiplicity of $\pm e^{i\alpha/2} \in \sigma(U)$ equals that of $e^{i\alpha} \in \sigma(DS)$.

Remark 3.7 *i) We have*

$$E^\pm(\{\alpha/2\}) = \begin{pmatrix} \mathbb{I}_{\mathcal{H}} & 0 \\ 0 & D^{-1} \end{pmatrix} \frac{1}{2} \begin{pmatrix} P(\{\alpha\}) & \pm P(\{\alpha\})e^{-i\alpha/2} \\ \pm P(\{\alpha\})e^{i\alpha/2} & P(\{\alpha\}) \end{pmatrix} \begin{pmatrix} \mathbb{I}_{\mathcal{H}} & 0 \\ 0 & D \end{pmatrix}, \quad (3.35)$$

where the operator in the middle is the spectral projector of $\begin{pmatrix} 0 & \mathbb{I}_{\mathcal{H}} \\ DS & 0 \end{pmatrix}$, which is unitarily equivalent to U .

ii) The expression for the resolvent of U holds for bounded operators S and D .

iii) In case \mathcal{H} is finite dimensional and DS admits the spectral decomposition

$$DS = \sum_{j=1}^n e^{i\alpha_j} P_j, \quad \text{with } P_j = P(\{\alpha_j\}), \quad (3.36)$$

U admits the following spectral decomposition

$$U = \sum_{j=1}^n e^{i\alpha_j/2} \Pi_j^+ - e^{i\alpha_j/2} \Pi_j^-, \quad \text{where } \Pi_j^\tau = E^\tau(\{\alpha_j\}), \quad \tau \in \{+, -\}. \quad (3.37)$$

Proof : The expression of the resolvent can be derived using the formulae for $p \in \mathbb{N}$

$$U^{2p} = \begin{pmatrix} (DS)^p & 0 \\ 0 & (SD)^p \end{pmatrix}, \quad U^{2p+1} = \begin{pmatrix} 0 & D(SD)^p \\ S(DS)^p & 0 \end{pmatrix}, \quad (3.38)$$

and $(U - z\mathbb{I}_{\mathcal{K}})^{-1} = -\frac{1}{z} \sum_{j=0}^{\infty} U^j/z^j$, for $|z| > 1$, and one checks it holds for $|z| < 1$ as well. Since $\sigma(DS) = \sigma(SD)$, the statement of $\sigma(U)$ follows. The spectral projector is obtained by the Riesz formula in case $\pm e^{i\alpha/2}$ is isolated in the spectrum, or by direct verification. \square

Let us come back to the star-graph with N branches, and the ordered basis chosen before (3.28). The structure of that basis allows us to express $l^2(D) = \mathcal{H}_{x_0}^I \oplus \mathcal{H}_{x_0}^O$, where both subspaces can be identified to \mathbb{C}^N . Accordingly, we write $\psi = \begin{pmatrix} \psi^I \\ \psi^O \end{pmatrix}$, where the indices I, O refer to $\mathcal{H}_{x_0}^I, \mathcal{H}_{x_0}^O$. To keep things simple, we assume $\psi_0 = \psi_0^I$ and that the spectrum of $D(\theta)S(0)$ is simple. This allows us to compute the asymptotic (Cesàro mean) probabilities to find the quantum walker on the center x_0 and on the branch x_k of the star-graph.

Proposition 3.8 *Consider the SQW $U_{S_{SG}}$ defined by (3.28) and assume the spectrum $\sigma(D(\theta)S(0))$ is simple, with corresponding orthonormal basis of eigenvectors $\{\phi_j\}_{1 \leq j \leq N}$. Consider a normalized initial vector $\psi_0 = \psi_0^I \in \mathcal{H}_{x_0}^I$. Then,*

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=0}^{N-1} \mathbb{Q}_n^{\psi_0^I}(x_0) &= \frac{1}{2} \\ \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{j=0}^{N-1} \mathbb{Q}_n^{\psi_0^I}(x_k) &= \sum_{j=1}^N \frac{1}{2} | \langle k0 | \phi_j \rangle |^2 | \langle \phi_j | \psi_0^I \rangle |^2. \end{aligned} \quad (3.39)$$

Proof : We use the lighter notation (3.32) and that of Lemma 3.6 in this proof. To make use of Lemma 2.7, we compute $\|P_{x_0}^I \Pi_j^\tau \psi_0\|^2$, for $\tau \in \{+, -\}$, $1 \leq j \leq N$. As a matrix in the chosen basis, we have $P_{x_0}^I = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & 0 \end{pmatrix}$, so that

$$P_{x_0}^I \Pi_j^\tau \psi_0 = \frac{1}{2} \begin{pmatrix} P_j \psi_0^I \\ 0 \end{pmatrix} \Rightarrow \|P_{x_0}^I \Pi_j^\tau \psi_0\|^2 = \frac{1}{4} \|P_j \psi_0^I\|^2. \quad (3.40)$$

Consider now $P_{x_k} = |k0\rangle\langle k0|$, $1 \leq k \leq N$, such that for any $\phi \in l^2(D)$, $\|P_{x_k} \phi\|^2 = |\langle k0 | \phi \rangle|^2$. We compute

$$P_{x_k} \Pi_j^\tau \psi_0^I = \begin{pmatrix} 0 \\ |k0\rangle\langle k0| (\Pi_j^\tau \psi_0^I)^O \end{pmatrix}, \quad \text{where } (\Pi_j^\tau \psi_0^I)^O = \frac{1}{2} \tau D^{-1} P_j e^{i\alpha_j/2} \psi_0^I. \quad (3.41)$$

Eventually, making use of the fact that D is diagonal and unitary, and the assumption $P_j = |\phi_j\rangle\langle \phi_j|$, we get

$$\|P_{x_k} \Pi_j^\tau \psi_0^I\|^2 = \frac{1}{4} | \langle k0 | \phi_j \rangle |^2 | \langle \phi_j | \psi_0^I \rangle |^2. \quad (3.42)$$

Then Lemma 2.7 yields the results. \square

3.4 Generalized Grover Walk

A popular unitary QW used in quantum computing is the so called Grover QW, which corresponds to the following set of scattering matrices, see *e.g.* [P, HKSS2]

$$S(x) = \frac{2}{d_x} A - \mathbb{I} \in U(d_x), \quad \text{for all } x \in V, \quad (3.43)$$

where \mathbb{I} denotes the identity matrix and, for all $x \in V$, A is the all-ones matrix, $A_{zy} = 1$, $y \sim x, z \sim x$. In this Section, we introduce and analyze a slight generalization of the Grover walk and we prove a spectral mapping theorem between this QW and the adjacency matrix of the graph G . This kind of result has been shown in various setups in a series of papers, see [HKSS2, HS, HSS], for the Grover walk, by means of boundary operators. Our approach of the generalized Grover walk based on the Feshbach-Schur method proposes an alternative route to that used in these references, that we believe is interesting in its own right. We provide a first result for finite graphs, that we then generalize to the infinite dimensional case in an abstract setting.

Note that the boundary operator method developed in [HKSS2, HS, HSS] to reduce the problem originally stated on $l^2(D)$ to an operator on $l^2(V)$, will be used again in Section 6 to define induced open SQWs.

Let G be finite and let $\alpha \in (-\pi, \pi]$. For each $x \in V$, let $\omega(x) \in \mathbb{C}^{d_x}$ such that $\|\omega(x)\| = 1$. The generalized Grover walk of parameter α , or α -Grover walk, is defined by the set $\mathcal{S} = \{S(x), x \in V\}$ where:

$$S(x) = |\omega(x)\rangle\langle\omega(x)| + e^{i\alpha}(\mathbb{I}_{d_x} - |\omega(x)\rangle\langle\omega(x)|), \quad \forall x \in V. \quad (3.44)$$

For $\alpha = 0$, $S(x) = \mathbb{I}_{d_x}$, and $\alpha = \pi$ corresponds to the Grover walk. Note that in case $d_x = 1$, $S(x) = 1$.

We thus assume $\alpha \neq 0$ in the following and note that (3.44) yields the spectral decomposition of $S(x)$, with $\sigma(S(x)) = \{1, e^{i\alpha}\}$, where 1 has multiplicity 1 and $e^{i\alpha}$ has multiplicity $1 - d_x$. The corresponding SQW is denoted by U_α in this section. As in (3.12), we identify \mathbb{C}^{d_x} and \mathcal{H}_x^I , and abuse slightly notations to write

$$\omega(x) = \sum_{y \sim x} \omega_y(x) |xy\rangle. \quad (3.45)$$

Accordingly, with F given in (3.9),

$$FU_\alpha = (\Pi + e^{i\alpha}(\mathbb{I} - \Pi)), \quad (3.46)$$

see (3.12), where

$$\Pi = \bigoplus_{x \in V} |\omega(x)\rangle\langle\omega(x)| = \Pi^2 = \Pi^* \quad (3.47)$$

is the spectral projector corresponding to the eigenvalue 1 of FU_α , and $\mathbb{I} - \Pi$ is that corresponding to the eigenvalue $e^{i\alpha}$ of that unitary operator, with

$$\dim \Pi = |V|, \text{ and } \dim(\mathbb{I} - \Pi) = |D| - |V|. \quad (3.48)$$

We introduce the orthogonal subspaces $\mathcal{H}_1 = \Pi l^2(D)$, $\mathcal{H}_2 = (\mathbb{I} - \Pi) l^2(D)$ and express the operator F in matrix form according to $l^2(D) = \mathcal{H}_1 \oplus \mathcal{H}_2$ as

$$F = \begin{pmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{pmatrix}, \text{ where } F_{ij} : \mathcal{H}_j \rightarrow \mathcal{H}_i. \quad (3.49)$$

In particular, $F_{jj} = F_{jj}^*$ on \mathcal{H}_j and since F is unitary, F_{jj} is a contraction on \mathcal{H}_j : $\|F_{jj}\| \leq 1$, $j \in \{1, 2\}$.

The following map will be important for the result to come:
Let $\alpha \in (-\pi, \pi] \setminus \{0\}$ and $\varphi_\alpha : \mathbb{S}^1 \rightarrow \mathbb{R}$, with \mathbb{S}^1 the unit circle, defined by

$$\varphi_\alpha(\lambda) = \frac{\lambda^2 - e^{i\alpha}}{\lambda(1 - e^{i\alpha})}. \quad (3.50)$$

It is readily seen, writing $\lambda = e^{i\theta}$, $\theta \in (-\pi, \pi]$, that we have

$$\phi_\alpha(e^{i\theta}) = \mu = \frac{\sin(\alpha/2 - \theta)}{\sin(\alpha/2)} \in [-|\sin(\alpha/2)^{-1}|, |\sin(\alpha/2)^{-1}|]. \quad (3.51)$$

Moreover, for $\alpha \neq \pi$, $\varphi_\alpha^{-1}(\{\mu\})$ always consists of two distinct values $\lambda_+ \neq \lambda_-$ such that $\lambda_+\lambda_- = -e^{i\alpha}$. For $\alpha = \pi$, the same is true, except for $\varphi_\pi^{-1}(\{\pm 1\}) = \pm 1$.

Here is our first spectral mapping result between U_α and $\Pi F \Pi|_{\Pi^2(D)} = F_{11}$ in the finite dimensional case:

Theorem 3.9 *Let $\alpha \in (-\pi, \pi] \setminus \{0\}$, φ_α be defined by (3.50), and $\dim l^2(D) < \infty$. Then,*

$$\lambda \in \sigma(U_\alpha) \setminus \{\pm e^{i\alpha}\} \Rightarrow \mu \in \sigma(F_{11}), \text{ where } \mu = \varphi_\alpha(\lambda) \quad (3.52)$$

$$\mu \in \sigma(F_{11}) \setminus \{\pm 1\} \Rightarrow \lambda_-, \lambda_+ \in \sigma(U_\alpha), \text{ where } \varphi_\alpha^{-1}(\{\mu\}) = \{\lambda_-, \lambda_+\}. \quad (3.53)$$

Moreover, for $\mu \in (-1, 1)$, $\varphi_\alpha^{-1}(\{\mu\}) = \{\lambda_-, \lambda_+\}$,

$$\dim \text{Ker}(U_\alpha - \lambda_\pm \mathbb{I}) = \dim \text{Ker}(F_{11} - \mu \mathbb{I}_2) = \dim \text{Ker}(F_{22} + \mu \mathbb{I}_2), \quad (3.54)$$

and, for $\alpha \neq \pi$,

$$\text{Ker}(U_\alpha \pm \mathbb{I}) = \text{Ker}(F_{11} \pm \mathbb{I}_1), \quad \text{Ker}(U_\alpha \pm e^{i\alpha} \mathbb{I}) = \text{Ker}(F_{22} \pm \mathbb{I}_2). \quad (3.55)$$

For $\alpha = \pi$,

$$\text{Ker}(U_\pi \pm \mathbb{I}) = \text{Ker}(F_{11} \pm \mathbb{I}_1) + \text{Ker}(F_{22} \mp \mathbb{I}_2). \quad (3.56)$$

Remark 3.10 *i) The result only depends on the factorization (3.46).*

ii) Writing $\lambda = e^{i\theta}$, $\theta \in (-\pi, \pi]$, as in (3.51), we have $|\sin(\alpha/2 - \theta)| \leq |\sin(\alpha/2)|$, since F_{11} is a contraction and $|\mu| \leq 1$.

iii) We have $\text{Ker}(F_{11} \mp \mathbb{I}_1) = \Pi \text{Ker}(F \mp \mathbb{I})$, $\text{Ker}(F_{22} \mp \mathbb{I}_1) = (\mathbb{I} - \Pi) \text{Ker}(F \mp \mathbb{I})$.

iv) It follows from (3.48) that

$$\begin{aligned} \dim \text{Ker}(K_{22} - \mathbb{I}) + \dim \text{Ker}(K_{22} + \mathbb{I}) \\ = \dim \text{Ker}(K_{11} - \mathbb{I}) + \dim \text{Ker}(K_{11} + \mathbb{I}) + |D| - 2|V|. \end{aligned} \quad (3.57)$$

The proof of the Theorem is given in Appendix A.

As an illustration of this result, consider for $\theta \in (-\pi, \pi]$ and $\alpha \in (-\pi, \pi]$

$$U = \begin{pmatrix} -\cos(\theta) & e^{i\alpha} \sin(\theta) & 0 \\ \sin(\theta) & e^{i\alpha} \cos(\theta) & 0 \\ 0 & 0 & e^{i\alpha} \end{pmatrix} \text{ and } F = \begin{pmatrix} -\cos(\theta) & \sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (3.58)$$

which satisfy $F = F^* = F^{-1}$ and $U = F(\Pi + e^{i\alpha}(\mathbb{I} - \Pi))$, where

$$\Pi = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \Pi^2 = \Pi^*. \quad (3.59)$$

We compute for $\theta \neq 0$ and $\alpha \neq \pi$,

$$\sigma(F_{11}) = \{-\cos(\theta)\}, \quad \sigma(F_{22}) = \{\cos(\theta), 1\}, \quad \sigma(U) = \{e^{i\alpha}, \lambda_+, \lambda_-\} \quad (3.60)$$

where $\{\lambda_+, \lambda_-\} = \phi_\alpha^{-1}(\{-\cos(\theta)\})$. For $\theta \notin \{0, \pi\}$ and $\alpha = \pi$, we have

$$\sigma(F_{11}) = \{-\cos(\theta)\}, \sigma(F_{22}) = \{\cos(\theta), 1\}, \sigma(U) = \{-1, -e^{i\theta}, -e^{-i\theta}\}, \quad (3.61)$$

while for $\theta = \pi$ and $\alpha = \pi$, $+1$ is a double eigenvalue of U :

$$\sigma(F_{11}) = \{1\}, \sigma(F_{22}) = \{-1, 1\}, \sigma(U) = \{-1, 1\}. \quad (3.62)$$

When $\theta = 0$, $+1$ is a double eigenvalue of F_{22} , $e^{i\alpha}$ is a double eigenvalue of U and for $\alpha \neq \pi$,

$$\sigma(F_{11}) = \{-1\}, \sigma(F_{22}) = \{1\}, \sigma(U) = \{e^{i\alpha}, -1\}, \quad (3.63)$$

while for $\theta = 0$ and $\alpha = \pi$ we have $U = -\mathbb{I}$ and

$$\sigma(F_{11}) = \{-1\}, \sigma(F_{22}) = \{1\}, \sigma(U) = \{-1\}. \quad (3.64)$$

We now turn to a description of the spectral mapping in a more abstract infinite dimensional framework by means of the Feshbach-Schur map. Keeping the same notation and conventions as above, the starting point is again

$$U = F(\Pi + e^{i\alpha}(\mathbb{I} - \Pi)), \text{ with } F = F^* = F^{-1}, e^{i\alpha} \neq 1, \quad (3.65)$$

defined on $\mathcal{H} = \Pi\mathcal{H} \oplus (\mathbb{I} - \Pi)\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$, where $\Pi = \Pi^* = \Pi^2 \neq 0$ and $\dim \mathcal{H} = \infty$ is allowed. In bloc form we have for any $z \in \mathbb{C}$

$$U - z = \begin{pmatrix} F_{11} - z & e^{i\alpha}F_{12} \\ F_{21} & e^{i\alpha}F_{22} - z \end{pmatrix}. \quad (3.66)$$

We consider the two Schur complements or Feshbach maps defined as linear maps on \mathcal{H}_1 , respectively \mathcal{H}_2 , by

$$\begin{aligned} \tilde{S}_1(z) &= (F_{11} - z) - e^{i\alpha}F_{12}(e^{i\alpha}F_{22} - z)^{-1}F_{21}, \text{ for } z \in \rho(e^{i\alpha}F_{22}) \\ \tilde{S}_2(z) &= (e^{i\alpha}F_{22} - z) - e^{i\alpha}F_{21}(F_{11} - z)^{-1}F_{12}, \text{ for } z \in \rho(F_{11}). \end{aligned} \quad (3.67)$$

The isospectrality of the Feshbach-Schur maps states that

$$\text{for } z \in \rho(e^{i\alpha}F_{22}), z \in \rho(U) \Leftrightarrow 0 \in \rho(\tilde{S}_1(z)), \quad (3.68)$$

$$\text{for } z \in \rho(F_{11}), z \in \rho(U) \Leftrightarrow 0 \in \rho(\tilde{S}_2(z)), \quad (3.69)$$

see *e.g.* [BFS] Section IV, or the proof of Proposition 3.15.11 in [Si].

In our setup, the Feshbach-Schur method yields the following

Theorem 3.11 *Let the unitary operator U be defined by (3.65), and the maps F_{jj} on \mathcal{H}_j , $j = 1, 2$ be defined by the bloc decomposition (3.66) for $z = 0$. With φ_α defined by (3.50), we have*

for $\lambda \in \mathbb{S}^1 \setminus \{\pm e^{i\alpha}\}$,

$$\lambda \in \sigma(U) \Leftrightarrow \varphi_\alpha(\lambda) \in \sigma(F_{11}), \quad (3.70)$$

for $\lambda \in \mathbb{S}^1 \setminus \{\pm 1\}$,

$$\lambda \in \sigma(U) \Leftrightarrow \varphi_\alpha(\lambda) \in -\sigma(F_{22}). \quad (3.71)$$

Remark 3.12 *i) For the values $\{\pm 1, \pm e^{i\alpha}\}$, we have, as in the finite dimensional case,*

$$\text{Ker}(U \pm \mathbb{I}) = \text{Ker}(F_{11} \pm \mathbb{I}_1), \text{Ker}(U \pm e^{i\alpha}\mathbb{I}) = \text{Ker}(F_{22} \pm \mathbb{I}_2), \quad (3.72)$$

for $\alpha \neq \pi$ while, for $\alpha = \pi$,

$$\text{Ker}(U \pm \mathbb{I}) = \text{Ker}(F_{11} \pm \mathbb{I}_1) + \text{Ker}(F_{22} \mp \mathbb{I}_2). \quad (3.73)$$

ii) The spectra of F_{11} and F_{22} are related by $\sigma(F_{11}) \cup \{\pm 1\} = \sigma(-F_{22}) \cup \{\pm 1\}$, as the proof below shows. The values ± 1 may or may not belong to one or both spectra.

Proof : We first make use of the properties of F which imply

$$(F - z)^{-1} = \frac{F + z}{1 - z^2}, \quad z \in \mathbb{C} \setminus \{\pm 1\}, \quad (3.74)$$

to reduce the expressions of the Feshbach-Schur maps $\tilde{S}_1(z)$, respectively $\tilde{S}_2(z)$ to a simple expression in terms of the resolvent of F_{11} , respectively F_{22} .

The Schur complements of the diagonal blocs of the operator $F - z$ read

$$S_1(z) = (F_{11} - z) - F_{12}(F_{22} - z)^{-1}F_{21} \text{ for } z \in \rho(F_{22}) \quad (3.75)$$

$$S_2(z) = (F_{22} - z) - F_{21}(F_{11} - z)^{-1}F_{12} \text{ for } z \in \rho(F_{11}), \quad (3.76)$$

defined as operators of \mathcal{H}_1 , respectively \mathcal{H}_2 . Consequently, considering the bloc expression of the resolvent $(F - z)^{-1}$

$$(F - z)^{-1} = \begin{pmatrix} S_1^{-1}(z) & * \\ * & * \end{pmatrix}, \text{ for } z \in \rho(F_{22}) \setminus \{\pm 1\}$$

$$(F - z)^{-1} = \begin{pmatrix} * & * \\ * & S_2^{-1}(z) \end{pmatrix}, \text{ for } z \in \rho(F_{11}) \setminus \{\pm 1\}, \quad (3.77)$$

where the isospectrality property ensures the Schur complements $S_j(z)$, $j = 1, 2$, have bounded inverses for the values of z considered. Identity (3.74) yields

$$S_1(z)^{-1} = \frac{(F_{11} + z)}{1 - z^2}, \text{ for } z \in \rho(F_{22}) \setminus \{\pm 1\}, \quad (3.78)$$

which implies that $z \in \rho(-F_{11}) \setminus \{\pm 1\}$. By similar considerations on the second Schur complement, we get

$$\rho(F_{11}) \setminus \{\pm 1\} = \rho(-F_{22}) \setminus \{\pm 1\} \Leftrightarrow \sigma(F_{11}) \cup \{\pm 1\} = \sigma(-F_{22}) \cup \{\pm 1\}. \quad (3.79)$$

Therefore we deduce that

$$S_1(z) = (1 - z^2)(F_{11} + z)^{-1}, \text{ respectively } S_2(z) = (1 - z^2)(F_{22} + z)^{-1}, \quad (3.80)$$

for $z \in \rho(-F_{11}) \setminus \{\pm 1\}$, respectively $z \in \rho(F_{11}) \setminus \{\pm 1\}$. Hence, together with (3.75), we can write

$$-F_{12}(F_{22} - z)^{-1}F_{21} = (1 - z^2)(F_{11} + z)^{-1} - (F_{11} - z), \quad z \in \rho(-F_{11}) \setminus \{\pm 1\}$$

$$-F_{21}(F_{11} - z)^{-1}F_{12} = (1 - z^2)(F_{22} + z)^{-1} - (F_{22} - z), \quad z \in \rho(F_{11}) \setminus \{\pm 1\}, \quad (3.81)$$

which we substitute in (3.67) to get with (3.79)

$$\tilde{S}_1(z) = (1 - z^2 e^{-2i\alpha})(F_{11} + z e^{-i\alpha})^{-1} + z(e^{-i\alpha} - 1), \quad e^{-i\alpha} z \in \rho(-F_{11}) \setminus \{\pm 1\}$$

$$\tilde{S}_2(z) = e^{i\alpha} \{(1 - z^2)(F_{22} + z)^{-1} + z(1 - e^{-i\alpha})\}, \quad z \in \rho(F_{11}) \setminus \{\pm 1\}. \quad (3.82)$$

At this point we invoke the spectral mapping theorem for the selfadjoint operators F_{11} and F_{22} to determine the values of z such that $0 \in \rho(\tilde{S}_j(z))$, $j = 1, 2$.

We have that $\tilde{S}_2(z)$ is boundedly invertible for $z \in \rho(F_{11}) \setminus \{\pm 1\}$ if and only if

$$-\frac{z(1 - e^{-i\alpha})}{1 - z^2} \in \rho((F_{22} + z)^{-1}), \quad (3.83)$$

where

$$\sigma((F_{22} + z)^{-1}) = \{(\nu + z)^{-1}, \nu \in \sigma(F_{22}) \subset [-1, 1]\}. \quad (3.84)$$

Hence, for $z \in \rho(F_{11}) \setminus \{\pm 1\}$, $0 \in \rho(\tilde{S}_2(z))$ iff

$$-\frac{z(1 - e^{-i\alpha})}{1 - z^2} \neq \frac{1}{\nu + z}, \quad \forall \nu \in \sigma(F_{22}). \quad (3.85)$$

In other words, $\lambda \in \mathbb{S}^1 \setminus \{\pm 1\}$ belongs to $\sigma(U)$ iff $\varphi_\alpha(\lambda) = -\nu \in \sigma(F_{22})$, recall (3.50).

An analogous computation based on the first equation (3.82) yields $\lambda \in \mathbb{S}^1 \setminus \{\pm e^{i\alpha}\}$ belongs to $\sigma(U)$ iff $\varphi_\alpha(\lambda) = \mu \in \sigma(F_{11})$. \square

Coming back to $\mathcal{H} = l^2(D)$, we now relate the compression F_{11} defined on $\mathcal{H}_1 = \Pi l^2(D)$ to an operator T defined on $l^2(V)$, following [HKSS2, HSS]. Recall that $\dim \Pi = |V| = \dim l^2(V)$.

Let $\{|x\rangle\}_{x \in V}$ denote a fixed orthonormal basis of $l^2(V)$, where $|x\rangle$ is a vector attached to the vertex $x \in V$, and recall the convention $\omega(x) = \sum_{y \sim x} \omega_y(x) |xy\rangle \in \mathcal{H}_x^1 \subset l^2(D)$, where $\|\omega(x)\| = 1$, for all $x \in V$. We introduce

$$R = \sum_{x \in V} |x\rangle \langle \omega(x)| : l^2(D) \rightarrow l^2(V), \quad \text{and} \quad R^* = \sum_{x \in V} |\omega(x)\rangle \langle x| : l^2(V) \rightarrow l^2(D), \quad (3.86)$$

which are readily shown to satisfy

$$R^*R = \sum_{x \in V} |\omega(x)\rangle \langle \omega(x)| = \Pi : l^2(D) \rightarrow l^2(D) \quad (3.87)$$

$$RR^* = \sum_{x \in V} |x\rangle \langle x| = \mathbb{I} : l^2(V) \rightarrow l^2(V) \quad (3.88)$$

$$R\Pi = R, \quad R^* = \Pi R^*, \quad \text{and} \quad (3.89)$$

$$\|R\| = \|R^*\| = 1, \quad (3.90)$$

where $\|\cdot\|$ is the operator norm. The operator R is the *boundary operator* of [HSS]. We define

$$T = RFR^* = RU_\alpha R^* : l^2(V) \rightarrow l^2(V). \quad (3.91)$$

Thanks to the properties of R , $T = T^*$ is a contraction and we have

$$T = RF_{11}R^*, \quad R^*TR = F_{11}. \quad (3.92)$$

The spectral properties of T and F are related by the

Proposition 3.13 *With \mathbb{I}_1 denoting the identity in $\mathcal{H}_1 = \Pi l^2(D)$, \mathbb{I}_V the identity in $l^2(V)$, we have for all $z \in \rho(T) \cap \rho(F_{11})$,*

$$R^*(T - z\mathbb{I}_V)^{-1}R = (F_{11} - z\mathbb{I}_1)^{-1} \quad (3.93)$$

$$(T - z\mathbb{I}_V)^{-1} = R(F_{11} - z\mathbb{I}_1)^{-1}R^*. \quad (3.94)$$

Consequently $\sigma(T) = \sigma(F_{11})$ and for $\lambda \in [-1, 1]$ a common eigenvalue of T and F_{11} , the respective spectral projectors P_T^λ and P_1^λ , satisfy

$$P_1^\lambda = R^*P_T^\lambda R, \quad P_T^\lambda = RP_1^\lambda R^*, \quad (3.95)$$

and

$$\dim P_1^\lambda = \dim P_T^\lambda. \quad (3.96)$$

Remark 3.14 *i) The results above are also true for G infinite, i.e. $|V| = \infty$, $|D| = \infty$. The series defining R , R^* , R^*R and RR^* are meant in the strong sense in this case.*
ii) Together with Theorems 3.9 and 3.11, we get a spectral mapping result between U and T . In particular,

$$F_{11}\psi_1 = \mu\psi_1 \Leftrightarrow T\varphi = \mu\varphi, \text{ with } \varphi = R\psi_1 \Leftrightarrow \psi_1 = R^*\varphi. \quad (3.97)$$

Proof : We first note that thanks to (3.87) and (3.92)

$$T^2 = RF_{11}R^*RF_{11}R^* = RF_{11}\Pi F_{11}R^* = RF_{11}^2R^*, \quad (3.98)$$

so that by induction $T^k = RF_{11}^kR^*$, $\forall k \in \mathbb{N}$. Then, for any $z \in \mathbb{C}$ such that $|z| > 1$, we have the convergent Neumann series

$$(T - z\mathbb{I}_V)^{-1} = -\frac{1}{z} \sum_{k=0}^{\infty} \frac{T^k}{z^k} = -\frac{1}{z} \sum_{k=0}^{\infty} R \frac{F_{11}^k}{z^k} R^*, \quad (3.99)$$

where $F_{11}^0 = \Pi|_{\mathcal{H}_1} = \mathbb{I}_1$. Therefore (3.94) holds for all $z \in \rho(T) \cap \rho(F_{11})$. Now (3.88) and (3.92) imply

$$F_{11}^2 = R^*TRR^*TR = R^*T\mathbb{I}_V TR = R^*T^2R, \quad (3.100)$$

so that by induction $F_{11}^k = R^*T^kR$, $\forall k \in \mathbb{N}$. As above, we consider the Neumann series for $(F_{11} - \mathbb{I}_1)^{-1}$ to deduce that (3.93) holds for all $z \in \rho(T) \cap \rho(F_{11})$.

Now, (3.94) and (3.93) show that the resolvents are singular on the same set, so that $\sigma(T) = \sigma(F_{11})$. The relations (3.95) between spectral projectors associated with λ follow from their expressions via the Riesz formula for isolated eigenvalues, or via the strong limit of $-i\epsilon(A - \lambda - i\epsilon)^{-1}$ as $\epsilon \rightarrow 0$, for $A = T$ and $A = F_{11}$, for embedded eigenvalues, see *e.g.* Theorem 6.10 in [HiSi]. The equality of their ranges is a consequence of the cyclicity of the trace and (3.88). \square

4 Scattering Open Quantum Walk on a Graph

4.1 Definition and Properties

We define in this section an open QW on a graph G , $\Phi_{\mathcal{S}}$, parameterized by the set of scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$, in the same spirit as we defined $U_{\mathcal{S}}$, the unitary QW. An open QW is a Completely Positive Trace Preserving (CPTP) linear map $\Phi_{\mathcal{S}}$ on $\mathcal{T}(l^2(D))$, the set of trace class maps acting on $l^2(D)$, also known as a Quantum Channels.

Let us briefly recall these notions in our framework, referring the reader to the books [A, AJP, AL, Kr, Sc, Wa], for more information. Let \mathcal{H} be a separable Hilbert space on \mathbb{C} and $\mathcal{B}(\mathcal{H})$ the C^* algebra of all bounded operators on \mathcal{H} equipped with the operator norm. A positive map $\Phi : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ is characterized by $\Phi(A) \geq 0$ for all $A \geq 0$, $A \in \mathcal{B}(\mathcal{H})$, while it is called n -positive if $\Phi \otimes \mathbb{I}_n : \mathcal{B}(\mathcal{H}) \otimes M_n(\mathbb{C}) \rightarrow \mathcal{B}(\mathcal{H}) \otimes M_n(\mathbb{C})$ is positive, where $M_n(\mathbb{C})$ is the set of square complex matrices on \mathbb{C}^n and \mathbb{I}_n denotes the identity map on $M_n(\mathbb{C})$. A map Φ is completely positive (CP), if it is n -positive for all $n \in \mathbb{N}$ and it is called unital if $\Phi(\mathbb{I}) = \mathbb{I}$.

Let $\mathcal{T}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$ be the set of trace class operators on \mathcal{H} , which is a Banach space when endowed with the trace norm $\|\cdot\|_1$. For a map $\Phi : \mathcal{T}(\mathcal{H}) \rightarrow \mathcal{T}(\mathcal{H})$, the notions of (complete) positivity are defined as above and such a map is called trace preserving (TP) if $\text{tr}\Phi(A) = \text{tr}A$ for all $A \in \mathcal{T}(\mathcal{H})$. The set of CPTP maps is convex and the

composition of CPTP maps is CPTP. Kraus's Representation Theorem states that any CPTP map Φ on $\mathcal{T}(\mathcal{H})$ can be represented by means of a non unique set of *Kraus operators* $\{K_j\}_{j \in J}$, $K_j \in \mathcal{B}(\mathcal{H})$, with index set J at most countable, as follows:

$$\Phi(A) = \sum_{j \in J} K_j A K_j^*, \quad \text{with} \quad \sum_{j \in J} K_j^* K_j = \mathbb{I}, \quad (4.1)$$

where the convergence of the second sum is understood in the strong sense, implying the first sum converges in the trace norm sense. Conversely, any map Φ defined by (4.1) yields a CPTP map on $\mathcal{T}(\mathcal{H})$. Moreover such maps have operator norms equal to one:

$$\sup_{\substack{A \in \mathcal{T}(\mathcal{H}) \\ A \neq 0}} \frac{\|\Phi(A)\|_1}{\|A\|_1} = 1. \quad (4.2)$$

If $\dim \mathcal{H} < \infty$, the index set J can be chosen so that $|J| \leq (\dim \mathcal{H})^2$. In this case, CPTP maps can be unital since $\mathbb{I} \in \mathcal{T}(\mathcal{H})$; consider the map defined by $\Phi(A) = U A U^*$, where U a unitary operator on \mathcal{H} , for example.

Furthermore, since $\mathcal{B}(\mathcal{H})$ is the dual of $\mathcal{T}(\mathcal{H})$ with duality bracket

$$\mathcal{B}(\mathcal{H}) \times \mathcal{T}(\mathcal{H}) \ni (B, A) \mapsto \text{tr}(BA) \in \mathbb{C}, \quad (4.3)$$

any map $\Phi : \mathcal{T}(\mathcal{H}) \rightarrow \mathcal{T}(\mathcal{H})$ admits an adjoint $\Phi^* : \mathcal{B}(\mathcal{H}) \rightarrow \mathcal{B}(\mathcal{H})$ defined by

$$\text{tr}(B\Phi(A)) = \text{tr}(\Phi^*(B)A), \quad \forall (B, A) \in \mathcal{B}(\mathcal{H}) \times \mathcal{T}(\mathcal{H}). \quad (4.4)$$

By Kraus's Theorem, one also gets that the adjoint of a CPTP map given by (4.1) has the form

$$\Phi^*(B) = \sum_{j \in J} K_j^* B K_j, \quad \text{with} \quad \sum_{j \in J} K_j^* K_j = \mathbb{I}, \quad (4.5)$$

where the first sum converges in the strong sense, a consequence of the second one converging in the strong sense. The map Φ^* is CP and unital and, moreover, any CP unital map on $\mathcal{B}(\mathcal{H})$ has the form (4.5). Also Φ^* has operator norm bounded by one

$$\sup_{\substack{B \in \mathcal{B}(\mathcal{H}) \\ B \neq 0}} \frac{\|\Phi^*(B)\|}{\|B\|} \leq 1. \quad (4.6)$$

We finally introduce the set of states or density matrices, a subset of $\mathcal{T}(\mathcal{H})$, by

$$\mathcal{DM}(\mathcal{H}) = \{\rho \in \mathcal{T}(\mathcal{H}), \text{ s.t. } \rho = \rho^* \geq 0 \text{ and } \text{tr}(\rho) = 1\}, \quad (4.7)$$

which is invariant under CPTP maps.

Given a graph G and a set of scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$, with the notions introduced above, we first define a set of Kraus operators labelled by $x \in V$:

$$K(x) = \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) |zx\rangle \langle xy| \quad \text{s.t.} \quad K(x) = K(x) P_x^I = P_x^O K(x), \quad \forall x \in V. \quad (4.8)$$

Note that $U_{\mathcal{S}} = \sum_{x \in V} K(x)$, see (2.6), so that,

$$U_{\mathcal{S}} A U_{\mathcal{S}}^* = \sum_{x, x' \in V} K(x) A K^*(x'), \quad \forall A \in \mathcal{B}(l^2(D)). \quad (4.9)$$

in the strong sense, by Remark 2.2.

Lemma 4.1

$$K^*(x)K(x) = P_x^{\mathbb{I}}, \quad K(x)K^*(x) = P_x^{\mathbb{O}}, \quad (4.10)$$

and

$$\sum_{x \in V} K^*(x)K(x) = \sum_{x \in V} K(x)K^*(x) = \mathbb{I}, \quad (4.11)$$

with strong convergence in case $|V| = \infty$.

Proof : The first identities are proven along the lines of Lemma 2.3 while the second identities hold since $\{P_x^\#\}_{x \in V}$, $\# \in \{\mathbb{I}, \mathbb{O}\}$ form resolutions of the identity. \square

We can now proceed with definitions.

Definition 4.2 Given the set of Kraus operators $\{K(x)\}_{x \in V}$, the open QW on the graph G is defined by the map $\Phi_{\mathcal{S}}$ on $\mathcal{T}(l^2(D))$

$$\Phi_{\mathcal{S}}(A) = \sum_{x \in V} K(x)AK^*(x), \quad \forall A \in \mathcal{T}(l^2(D)). \quad (4.12)$$

We further introduce two maps on $\mathcal{T}(l^2(D))$

$$D^\#(A) = \sum_{x \in V} P_x^\# AP_x^\#, \quad \# \in \{\mathbb{I}, \mathbb{O}\}. \quad (4.13)$$

Proposition 4.3 The maps $\Phi_{\mathcal{S}}$ and $D^\#$, $\# \in \{\mathbb{I}, \mathbb{O}\}$ are CPTP, and they all can be extended to unital maps on $\mathcal{B}(l^2(D))$.

Moreover,

$$\Phi_{\mathcal{S}} = \Phi_{\mathcal{S}} \circ D^{\mathbb{I}} = D^{\mathbb{O}} \circ \Phi_{\mathcal{S}} = D^{\mathbb{O}} \circ \Phi_{\mathcal{S}} \circ D^{\mathbb{I}}, \quad (4.14)$$

and the link with $U_{\mathcal{S}}$ reads

$$\Phi_{\mathcal{S}}(\cdot) = D^{\mathbb{O}}(U_{\mathcal{S}} \cdot U_{\mathcal{S}}^*) = U_{\mathcal{S}} D^{\mathbb{I}}(\cdot) U_{\mathcal{S}}^*. \quad (4.15)$$

Proof : Using criterion (4.1) and Lemma 4.1, we get that $\Phi_{\mathcal{S}}$ and $D^\#$ are CPTP maps. By criterion (4.5) with $K^*(x)$ in place of $K(x)$ and Lemma 4.1 again, we see that these three maps can be extended to $\mathcal{B}(l^2(D))$ and are unital.

The second statement follows directly from properties (4.8) and (2.3), whereas the last statement stems from formula (2.7) for $U_{\mathcal{S}} A U_{\mathcal{S}}^*$. Applying $D^{\mathbb{O}}$ to this expression and replacing A by $D^{\mathbb{I}}(A)$ yields (4.15) thanks to (4.8) and (2.3) again. \square

Remark 4.4 *i) The operators $D^\#$ are projectors.*

ii) In finite dimension, Unital Quantum Channels are known to be affine combinations of Unitary Quantum Channels, see [MW], and to be entropy non-decreasing:

$$S(\rho) \leq S(\Phi_{\mathcal{S}}(\rho)), \quad \text{for all } \rho \in \mathcal{DM}(l^2(D)), \quad (4.16)$$

where $S : \mathcal{DM}(l^2(D)) \rightarrow [0, \ln(\dim l^2(D))]$ is the Von Neumann entropy $S(\rho) = -\text{tr}(\rho \ln \rho)$.

Note that thanks to (2.3), $D^{\mathbb{O}}$ and $D^{\mathbb{I}}$ commute and the CPTP map on $\mathcal{T}(l^2(D))$, and its extension to $\mathcal{B}(l^2(D))$, defined by

$$\text{Diag}(\cdot) = D^{\mathbb{O}} \circ D^{\mathbb{I}}(\cdot) = D^{\mathbb{I}} \circ D^{\mathbb{O}}(\cdot) = \sum_{\substack{x, y \in V \\ x \sim y}} |xy\rangle\langle xy| \cdot |xy\rangle\langle xy|, \quad (4.17)$$

is a projector as well. To address the dynamics, we consider the restriction

$$\Phi^{\text{Diag}} = \text{Diag} \circ \Phi_{\mathcal{S}}|_{\text{Diag}(\mathcal{T}(l^2(D)))}, \quad (4.18)$$

where we dropped mention to \mathcal{S} in order to lighten the notation.

Corollary 4.5 *The map Φ^{Diag} determines the dynamics in the sense that for any $n \geq 2$*

$$\Phi_{\mathcal{S}}^n = \Phi_{\mathcal{S}} \circ \Phi^{\text{Diag}^{n-2}} \circ \text{Diag} \circ \Phi_{\mathcal{S}} \quad (4.19)$$

Proof : Proposition 4.3 yields

$$\Phi_{\mathcal{S}}^n = \Phi_{\mathcal{S}} \circ (D^{\text{I}} \circ D^{\text{O}} \circ \Phi_{\mathcal{S}})^{n-2} D^{\text{I}} \circ D^{\text{O}} \circ \Phi_{\mathcal{S}}, \quad (4.20)$$

and (4.17) with the fact that Diag is a projector proves the statement. \square

Remark 4.6 *i) When acting on $\mathcal{T}(l^2(D))$, $\Phi_{\mathcal{S}}^n$, $n \geq 2$, leaves the subspace $\text{Diag}\mathcal{T}(l^2(D))$ only at the last time step. The essential part of the dynamics is thus driven by Φ^{Diag} and takes place in $\text{Diag}\mathcal{T}(l^2(D))$.*

ii) The extension of Φ^{Diag} to $\mathcal{B}(l^2(D))$ reads

$$\Phi^{\text{Diag}}(\cdot) = \sum_{x \in V} \sum_{\substack{y \sim x \\ z \sim x}} |S_{zy}(x)|^2 |zx\rangle\langle xy| \cdot |xy\rangle\langle zx| \quad (4.21)$$

with Kraus operators $K_{zy}(x) = S_{zy}(x)|zx\rangle\langle xy| : \mathcal{H}_x^{\text{I}} \rightarrow \mathcal{H}_x^{\text{O}}$ satisfying

$$\sum_{x \in V} \sum_{\substack{y \sim x \\ z \sim x}} K_{zy}^*(x) K_{zy}(x) = \sum_{x \in V} P_x^{\text{I}} = \mathbb{I}, \quad \sum_{x \in V} \sum_{\substack{y \sim x \\ z \sim x}} K_{zy}(x) K_{zy}^*(x) = \sum_{x \in V} P_x^{\text{O}} = \mathbb{I}, \quad (4.22)$$

with convergence in the strong sense.

When restricted to $\mathcal{DM}(l^2(D))$, the set of density matrices, the CPTP map $\Phi_{\mathcal{S}}$ describes the one time step quantum evolution of a quantum walker in a mixed states, now characterized by a density matrix. Again, the dynamical system $(\Phi_{\mathcal{S}}^n)_{n \in \mathbb{N}}$ on $\mathcal{T}(l^2(D))$ or $\mathcal{DM}(l^2(D))$, and the related spectral properties of the CPTP map $\Phi_{\mathcal{S}} \in \mathcal{B}(\mathcal{T}(l^2(D)))$ are of interest. We will address the spectrum of $\Phi_{\mathcal{S}}$, making use of the specifics of our construction.

Quantum Mechanical Interpretation: Similarly to the case of pure states considered in Section 2, quantum mechanical considerations induce natural time dependent distribution probabilities in the framework of density matrices. Given an initial state $\rho_0 \in \mathcal{DM}(l^2(D))$, the state at time n , is $\rho_n = \Phi_{\mathcal{S}}^n(\rho_0) \in \mathcal{DM}(l^2(D))$. The quantum mechanical probability to find the corresponding quantum walker at time n on the oriented edge (xy) of G , by a measurement of its position, is

$$\mathbb{P}_n^{\rho_0}(xy) = \text{tr}(|xy\rangle\langle xy| \Phi_{\mathcal{S}}^n(\rho_0)) = \text{tr}(|xy\rangle\langle xy| \rho_n) = \langle xy | \rho_n | xy \rangle. \quad (4.23)$$

The probability to find the quantum walker at time $n \in \mathbb{N}$ in the subspace \mathcal{H}_x^{I} or on the vertex $x \in V$, by a measurement of its position, is given by

$$\mathbb{Q}_n^{\rho_0}(x) = \text{tr}(P_x^{\text{I}} \Phi_{\mathcal{S}}^n(\rho_0)) = \text{tr}(P_x^{\text{I}} \rho_n) = \sum_{y \sim x} \mathbb{P}_n^{\rho_0}(xy). \quad (4.24)$$

Proposition 4.3 yields the following operational interpretation of the Quantum Channel defined by $\Phi_{\mathcal{S}}$. Given an initial quantum state $\rho_0 \in \mathcal{DM}(l^2(D))$, with $\rho_0 > 0$, one measures the position of the quantum walker on the vertices V . The probability to get the outcome $x \in V$ by this measurement is $\mathbb{Q}_0^{\rho_0}(x) = \text{tr}(P_x^{\text{I}} \rho_0) > 0$ and the wave packet reduction postulate says that after getting the outcome x in the measurement process,

the state immediately becomes $P_x^I \rho_0 P_x^I / \text{tr}(P_x^I \rho_0)$. The expectation value $\bar{\rho}$ of the state obtained after a position measurement is then

$$\bar{\rho} = \sum_{x \in V} \frac{P_x^I \rho_0 P_x^I}{\text{tr}(P_x^I \rho_0)} \mathbb{Q}_0^{\rho_0}(x) = \sum_{x \in V} P_x^I \rho_0 P_x^I = D^I(\rho_0), \quad (4.25)$$

inducing decoherence. Hence, the action of the Quantum Channel Φ_S on the state ρ_0 results in first taking its expectation value with respect to a position measurement, so that the state becomes $D^I(\rho_0)$, followed by evolving the result by means of the unitary Quantum Channel $U_S \cdot U_S^*$.

4.2 Quantum Trajectory

We strengthen this interpretation by considering the *Quantum Trajectory* associated with the measurement of the position on V . See [BJPP] for a recent account of this topic. The iterative protocol is as follows (dropping unessential indices from the notation and writing \mathcal{H} for $l^2(D)$).

- At time 0, the state is $\rho_0 \in \mathcal{DM}(\mathcal{H})$. We measure the position on V and get an outcome $x_1 \in V$, with probability $\text{tr}(P_{x_1} \rho_0)$ and evolve the reduced state by $U \cdot U^*$ to get at time 1

$$\rho_1 = U P_{x_1} \rho_0 P_{x_1} U^* / \text{tr}(P_{x_1} \rho_0). \quad (4.26)$$

Denoting $\mathbb{P}_1(x_1) = \text{tr}(P_{x_1} \rho_0)$ the probability to get the outcome $x_1 \in V$, we get

$$\rho_1 \mathbb{P}_1(x_1) = U P_{x_1} \rho_0 P_{x_1} U^*. \quad (4.27)$$

- At time 1, the state is $\rho_1 \in \mathcal{DM}(\mathcal{H})$. We measure the position on V , get an outcome $x_2 \in V$ with probability

$$\text{tr}(P_{x_2} \rho_1) = \text{tr}(P_{x_2} U P_{x_1} \rho_0 P_{x_1} U^* P_{x_2}) / \text{tr}(P_{x_1} \rho_0) \quad (4.28)$$

and evolve the reduced state by $U \cdot U^*$ to get at time 2

$$\rho_2 = U P_{x_2} \rho_1 P_{x_2} U^* / \text{tr}(P_{x_2} \rho_1). \quad (4.29)$$

Here, $\text{tr}(P_{x_2} \rho_1) = \mathbb{P}(x_2|x_1)$ is the probability to get the outcome x_2 , given the first outcome is x_1 , so that the probability to get the sequence of outcomes $(x_1, x_2) \in V^2$ reads

$$\mathbb{P}_2(x_1, x_2) = \text{tr}(P_{x_2} U P_{x_1} \rho_0 P_{x_1} U^* P_{x_2}). \quad (4.30)$$

Hence we have

$$\rho_2 \mathbb{P}_2(x_1, x_2) = U P_{x_2} \rho_1 P_{x_2} U^*. \quad (4.31)$$

- At time j , $j \geq 1$, the state is $\rho_j \in \mathcal{DM}(\mathcal{H})$. We measure the position on V , get an outcome $x_{j+1} \in V$, with probability $\text{tr}(P_{x_{j+1}} \rho_j)$ and evolve the reduced state by $U \cdot U^*$ to get at time $j+1$

$$\rho_{j+1} = U P_{x_{j+1}} \rho_j P_{x_{j+1}} U^* / \text{tr}(P_{x_{j+1}} \rho_j). \quad (4.32)$$

By induction, the probability to get the sequence of outcomes $(x_1, x_2, \dots, x_{j+1}) \in V^{j+1}$ is

$$\mathbb{P}_{j+1}(x_1, x_2, \dots, x_{j+1}) = \text{tr}(P_{x_{j+1}} U \dots P_{x_2} U P_{x_1} \rho_0 P_{x_1} U^* P_{x_2} \dots U^* P_{x_{j+1}}), \quad (4.33)$$

and

$$\rho_{j+1} \mathbb{P}_{j+1}(x_1, x_2, \dots, x_{j+1}) = U P_{x_{j+1}} \dots P_{x_2} U P_{x_1} \rho_0 P_{x_1} U^* P_{x_2} \dots P_{x_{j+1}} U^*. \quad (4.34)$$

The sequence of outcomes and states $\{(x_j, \rho_j)\}_{1 \leq j \leq n} \in (V \times \mathcal{DM}(\mathcal{H}))^n$, $n \in \mathbb{N}^*$, is a realization of a quantum trajectory of length n of the quantum walker under repeated measurement of the position on V , with corresponding probability

$$\mathbb{P}_n(x_1, x_2, \dots, x_n) = \text{tr}(P_{x_n} U \dots P_{x_2} U P_{x_1} \rho_0 P_{x_1} U^* P_{x_2} \dots U^* P_{x_n}) \geq 0. \quad (4.35)$$

Remark 4.7 *i) We did not pay attention to the possibility that some denominators $\text{tr}(P_{x_{j+1}} \rho_j)$ could vanish. This is harmless since the quantities of interest, $\mathbb{P}_n(x_1, x_2, \dots, x_n)$ and $\rho_n \mathbb{P}_n(x_1, x_2, \dots, x_n)$, are always well defined.*

ii) Note that $\mathbb{P}_j(x_1, x_2, \dots, x_j)$ is indeed a probability on V^j for all $j \in \mathbb{N}^$: setting $\mathcal{U}(\cdot) = U \cdot U^*$ and $D(\cdot) = \sum_{x \in V} P_x \cdot P_x$ on $\mathcal{B}(\mathcal{H})$ we get for each j ,*

$$\sum_{x_1, x_2, \dots, x_j \in V^j} \mathbb{P}_j(x_1, x_2, \dots, x_j) = \text{tr}(D^I \circ \mathcal{U} \dots \circ D^I \circ \mathcal{U} \circ D^I(\rho_0)) = \text{tr}(\rho_0) = 1, \quad (4.36)$$

as \mathcal{U} and D are CPTP maps and $\rho_0 \in \mathcal{DM}(\mathcal{H})$.

We are ready to provide a probabilistic interpretation of $\Phi_{\mathcal{S}}^n$, for all $n \in \mathbb{N}^*$.

Proposition 4.8 *Let $\rho_0 \in \mathcal{DM}(l^2(D))$ be an initial state and consider the quantum trajectory of length $n \in \mathbb{N}^*$ corresponding to repeated measurement of the position on V according to the protocol above. Let*

$$\bar{\rho}_n = \sum_{x_1, x_2, \dots, x_n \in V^n} \rho_n \mathbb{P}_n(x_1, x_2, \dots, x_n) \quad (4.37)$$

be the expectation value of the state obtained at time n with respect to the probability distribution \mathbb{P}_n on V^n defined by (4.35). We have

$$\bar{\rho}_n = \Phi_{\mathcal{S}}^n(\rho_0), \quad \forall n \in \mathbb{N}^*. \quad (4.38)$$

Proof : By definition and using (4.34) (with the lighter notation above),

$$\bar{\rho}_n = \sum_{x_1, x_2, \dots, x_n \in V^n} U P_{x_n} \dots U P_{x_1} \rho_0 P_{x_1} U^* \dots P_{x_n} U^* = \mathcal{U} \circ D^I \circ \mathcal{U} \dots \circ D^I \circ \mathcal{U} \circ D^I(\rho_0), \quad (4.39)$$

which yields the result thanks to (4.15) in Proposition 4.3. For G infinite, the convergence takes place in trace norm, thanks to (4.1) and (4.2): let the positive map

$$D_m^I(\cdot) = \sum_{\substack{x \in V \\ |x| \leq m}} P_x^I \cdot P_x^I \quad (4.40)$$

such that for $0 \leq A \in \mathcal{T}(l^2(D))$, we have $D_m^I(A) \leq D^I(A)$, $(D^I - D_m^I)(A) \leq D^I(A)$ and $(D^I - D_m^I)(A) \geq 0$ converges in trace norm to zero when $m \rightarrow \infty$. The difference $(\mathcal{U} \circ D^I)^n(\rho_0) - (\mathcal{U} \circ D_m^I)^n(\rho_0)$ is a finite sum of trace class positive terms of the form

$$(\mathcal{U} \circ D_m^I)^{n_1} \circ (\mathcal{U} \circ (D^I - D_m^I))^{n_2} \circ \dots \circ (\mathcal{U} \circ D_m^I)^{n_{2p-1}} \circ (\mathcal{U} \circ (D^I - D_m^I))^{n_{2p}}(\rho_0), \quad (4.41)$$

where p is finite, $\sum_{i=1}^{2p} n_i = n$, $n_i \geq 0$, and $n_{2k} \geq 1$, for some $k \leq p$. Using the inequalities above on each of the positive maps that compose (4.41), except $(\mathcal{U} \circ (D^I - D_m^I))^{n_{2k}}$, we get that its trace is bounded above by

$$\text{tr}\left((\mathcal{U} \circ D^I)^{n_1} (\mathcal{U} \circ (D^I - D_m^I))^{n_{2k}} (\mathcal{U} \circ D^I)^{n_2}(\rho_0)\right) \leq \text{tr}\left((D^I - D_m^I) \circ (\mathcal{U} \circ D^I)^{n_2}(\rho_0)\right), \quad (4.42)$$

where $n'_1, n'_2 \in \mathbb{N}$ are such that $n'_1 + n'_2 + n_{2k} = n$, and where we used that $\mathcal{U} \circ D^I$, and \mathcal{U} are trace preserving. The last term vanishes as $m \rightarrow \infty$, which ends the proof. \square

Comparison with the open QW of [APSS1]. Let us finally show that open SQWs are distinct from the open QWs devised in [APSS1]. To do so, we need to consider regular graphs G with $d_x = d$ for all $x \in V$, which we further assume be finite, for simplicity. We have the identification $l^2(D) = \bigoplus_{x \in V} \mathcal{H}_x^I \simeq l^2(V) \otimes \mathbb{C}^d$. Let $\{|\tau\rangle\}_{\tau \in I}$ with $|I| = d$, be an ONB of $\mathcal{H}_x^I \simeq \mathbb{C}^d$, and consider a labelling of the vertices so that the following identification holds, for each $x \in V$ fixed,

$$|xy\rangle \simeq |x\rangle \otimes |\tau\rangle, \quad \text{where } y \sim x, \tau \in I. \quad (4.43)$$

Hence the identification of basis vectors of $\mathcal{B}(l^2(D)) \simeq \mathcal{B}(l^2(V) \otimes \mathbb{C}^d)$

$$|xy\rangle\langle x'y'| \simeq |x\rangle\langle x'| \otimes |\tau\rangle\langle \tau'|. \quad (4.44)$$

The open QWs introduced in [APSS1] are denoted by \mathcal{M} , and act on density matrices on $l^2(V) \otimes \mathbb{C}^d$. Their defining characteristic is that they leave the following subset of states invariant

$$\mathcal{V} = \left\{ \rho \in \mathcal{DM}(l^2(V) \otimes \mathbb{C}^d) \mid \rho = \sum_{x \in V} |x\rangle\langle x| \otimes \rho(x), \rho(x) \in \mathcal{B}(\mathbb{C}^d) \right\}, \quad (4.45)$$

see Corollary 2.5 in [APSS1]. Now, $|xy\rangle\langle xy| \simeq |x\rangle\langle x| \otimes |\tau\rangle\langle \tau| \in \mathcal{V}$, while the computation

$$\Phi_S(|xy\rangle\langle xy|) = \sum_{\substack{z \sim x \\ t \sim x}} S_{zy}(x) \overline{S_{ty}(x)} |zx\rangle\langle tx| \quad (4.46)$$

shows $\Phi_S(|xy\rangle\langle xy|)$ is not equivalent to an element of \mathcal{V} , unless $S(x) = \mathbb{I}$.

We now turn to the spectral properties of Φ_S .

5 Spectral and Dynamical Properties of Φ_S

We will mainly consider the finite dimensional case corresponding to finite graphs G in this section, and will comment along the way on the infinite graph case.

For G finite, we will not distinguish $\mathcal{T}(l^2(D))$ and $\mathcal{B}(l^2(D))$. Let us equip $\mathcal{B}(l^2(D))$ with the Hilbert-Schmidt scalar product to make it a Hilbert space,

$$\langle A, B \rangle_{HS} = \text{tr}(A^* B), \quad \forall A, B \in \mathcal{B}(l^2(D)), \quad \text{s.t. } \|A\|_{HS} = \sqrt{\text{tr}(A^* A)}. \quad (5.1)$$

We denote the adjoint of a map $\Phi \in \mathcal{B}(l^2(D))$ with respect to this scalar product by Φ^\dagger . In particular, we have

$$\Phi_S^\dagger(\cdot) = \sum_{x \in V} K^*(x) \cdot K(x), \quad (U_S \cdot U_S^*)^\dagger = U_S^* \cdot U_S, \quad D^\# = D^{\#\dagger}, \quad \# \in \{O, I\}, \quad (5.2)$$

which makes $D^\#$ and Diag , recall (4.17), orthogonal projectors on $\mathcal{B}(l^2(D))$ and implies $\Phi_S^\dagger = D^I \circ \Phi_S^\dagger \circ D^O$.

Theorem 5.1 *Let G be finite. The open SQW Φ_S is a partial isometry on $\mathcal{B}(l^2(D))$ with $\text{Ker } \Phi_S = \text{Ran}(\mathbb{I} - D^I)$, where $\dim \text{Ker } \Phi_S = (\sum_{x \in V} d_x)^2 - \sum_{x \in V} d_x^2$. Moreover, $\sigma(\Phi_S) \setminus \{0\} = \sigma(\text{Diag} \circ \Phi_S|_{\text{Diag}\mathcal{B}(l^2(D))}) \setminus \{0\}$, with identical geometric multiplicities.*

$$\sum_{\lambda \in \sigma(\Phi_S) \setminus \{0\}} \dim \text{Ker}(\Phi_S - \lambda) \leq \text{Rank } \text{Diag}, \quad (5.3)$$

so that Φ_S is not diagonalizable if $\exists x \in V$ such that $d_x \geq 2$.

Proof : Thanks to Proposition (4.3),

$$\Phi_{\mathcal{S}} = \Phi_{\mathcal{S}} \circ D^{\mathbb{I}} \quad \text{and} \quad \Phi_{\mathcal{S}}^{\dagger} \circ \Phi_{\mathcal{S}} = D^{\mathbb{I}}, \quad (5.4)$$

so that $\Phi_{\mathcal{S}}((\mathbb{I} - D^{\mathbb{I}})(A)) = 0$ and $\text{Ran}(\mathbb{I} - D^{\mathbb{I}}) \subset \text{Ker} \Phi_{\mathcal{S}}$.

Moreover, for any $A \in \mathcal{B}(l^2(D))$,

$$\|\Phi_{\mathcal{S}}(A)\|_{HS} = \langle A | \Phi_{\mathcal{S}}^{\dagger} \circ \Phi_{\mathcal{S}}(A) \rangle_{HS} = \langle A | D^{\mathbb{I}}(A) \rangle_{HS} = \|D^{\mathbb{I}}(A)\|_{HS}, \quad (5.5)$$

so that on $\text{Ran}(\mathbb{I} - D^{\mathbb{I}})^{\perp} = \text{Ker}(\mathbb{I} - D^{\mathbb{I}}) = \text{Ran} D^{\mathbb{I}}$, $\Phi_{\mathcal{S}}$ is an isometry and $\text{Ker} \Phi_{\mathcal{S}} = \text{Ran}(\mathbb{I} - D^{\mathbb{I}})$.

Then, $\text{Ran} D^{\mathbb{I}}$ is spanned by $\{|xy\rangle\langle xz|, x \in V, y \sim x, z \sim x\}$, and thus has dimension $\sum_{x \in V} d_x^2$, which yields the first statement.

Let us turn to the nonzero eigenvalues of $\Phi_{\mathcal{S}}$. If $\lambda \in \sigma(\Phi_{\mathcal{S}}) \setminus \{0\}$, there exists $A \in \mathcal{B}(l^2(D)) \setminus \{0\}$ such that $D^{\mathbb{I}}(A) \neq 0$ and

$$\Phi_{\mathcal{S}}(A) = D^{\mathbb{O}} \circ \Phi_{\mathcal{S}} \circ D^{\mathbb{I}}(A) = \lambda(D^{\mathbb{I}}(A) + (\mathbb{I} - D^{\mathbb{I}})(A)), \quad (5.6)$$

by Proposition 4.3. Projecting onto $D^{\mathbb{I}}\mathcal{B}(l^2(D))$ and $(\mathbb{I} - D^{\mathbb{I}})\mathcal{B}(l^2(D))$, we get

$$D^{\mathbb{I}} \circ D^{\mathbb{O}} \circ \Phi_{\mathcal{S}} \circ D^{\mathbb{I}}(A) = \lambda D^{\mathbb{I}}(A), \quad (\mathbb{I} - D^{\mathbb{I}})(A) = \frac{1}{\lambda}(\mathbb{I} - D^{\mathbb{I}}) \circ \Phi_{\mathcal{S}} \circ D^{\mathbb{I}}(A). \quad (5.7)$$

The first equation implies that $D^{\mathbb{I}}(A)$ is an eigenvector associated with $\lambda \neq 0$ for the restriction $D^{\mathbb{I}} \circ D^{\mathbb{O}} \circ \Phi_{\mathcal{S}}|_{D^{\mathbb{I}}\mathcal{B}(l^2(D))}$ which, with (4.17), implies $D^{\mathbb{I}}(A) = \text{Diag}(A)$. Hence $\text{Diag}(A)$ is an eigenvector of the restriction $\text{Diag} \circ \Phi_{\mathcal{S}}|_{\text{Diag}\mathcal{B}(l^2(D))}$ associated with $\lambda \neq 0$.

Conversely, if $\text{Diag}(A)$ is a an eigenvector of $\text{Diag} \circ \Phi_{\mathcal{S}}|_{\text{Diag}\mathcal{B}(l^2(D))}$ associated with an eigenvalue $\lambda \neq 0$, then

$$B = \text{Diag}(A) + \frac{1}{\lambda}(\mathbb{I} - D^{\mathbb{I}}) \circ \Phi_{\mathcal{S}} \circ \text{Diag}(A) \quad (5.8)$$

satisfies thanks to Proposition 4.3, $\text{Ker} \Phi_{\mathcal{S}} = \text{Ran}(\mathbb{I} - D^{\mathbb{I}})$, and $\mathbb{I} - \text{Diag} = \mathbb{I} - D^{\mathbb{I}} \circ D^{\mathbb{O}}$

$$\begin{aligned} \Phi_{\mathcal{S}}(B) &= \Phi_{\mathcal{S}}(\text{Diag}(A)) + \frac{1}{\lambda}\Phi_{\mathcal{S}}((\mathbb{I} - D^{\mathbb{I}}) \circ \Phi_{\mathcal{S}} \circ \text{Diag}(A)) \\ &= \text{Diag} \circ \Phi_{\mathcal{S}}(\text{Diag}(A)) + (\mathbb{I} - D^{\mathbb{I}}) \circ D^{\mathbb{O}} \circ \Phi_{\mathcal{S}}(\text{Diag}(A)) \\ &= \lambda \left(\text{Diag}(A) + \frac{1}{\lambda}(\mathbb{I} - D^{\mathbb{I}}) \circ \Phi_{\mathcal{S}} \circ \text{Diag}(A) \right) = \lambda B. \end{aligned} \quad (5.9)$$

Finally, since $\dim \text{Diag} = \sum_{x \in V} d_x$, the total geometric multiplicity of $\Phi_{\mathcal{S}}$ cannot exceed $(\sum_{x \in V} d_x)^2 - \sum_{x \in V} d_x^2 + \sum_{x \in V} d_x$, which agrees with $\dim(\mathcal{B}(l^2(D))) = (\sum_{x \in V} d_x)^2$ iff $d_x = d_x^2, \forall x \in V$. \square

Remark 5.2 *Similar statements hold for $\Phi_{\mathcal{S}}^{\dagger}$.*

Equation (5.8) provides the explicit one to one correspondence between eigenvectors of $\text{Diag} \circ \Phi_{\mathcal{S}}|_{\text{Diag}\mathcal{B}(l^2(D))}$ and of $\Phi_{\mathcal{S}}$ associated with the same nonzero eigenvalues.

Denoting by $\|\cdot\|$ the operator norm induced on $\mathcal{B}(l^2(D))$ by $\|\cdot\|_{HS}$, we recover

$$\|\Phi_{\mathcal{S}}\| = \|\Phi_{\mathcal{S}}^{\dagger}\| = 1, \quad (5.10)$$

which holds for all CPTP unital maps, and all p -norms, $1 < p$, see [P-GWPR].

In particular, the spectrum of $\Phi_{\mathcal{S}}$ satisfies $\sigma(\Phi_{\mathcal{S}}) \subset \{z \in \mathbb{C}, \text{ s.t } |z| \leq 1\}$, where all eigenvalues of modulus one are semi-simple, and both 0 and 1 belong to the spectrum, since $|V| \geq 2$.

Also, $\sigma(\Phi_{\mathcal{S}}) = \overline{\sigma(\Phi_{\mathcal{S}})}$, as a consequence of $\Phi_{\mathcal{S}}(A)^ = \Phi_{\mathcal{S}}(A^*), \forall A \in \mathcal{B}(l^2(D))$.*

We address now the computation of nonzero eigenvalues of Φ_S . Recall (4.18),

$$\Phi^{\text{Diag}} = \text{Diag} \circ \Phi_S|_{\text{Diag}(\mathcal{B}(l^2(D)))}, \text{ so that } \Phi^{\text{Diag}\dagger} = \text{Diag} \circ \Phi_S^\dagger|_{\text{Diag}(\mathcal{B}(l^2(D)))}. \quad (5.11)$$

We view Φ^{Diag} as a matrix in the ONB basis $\text{Diag}(\mathcal{B}(l^2(D))) = \text{span}\{|xy\rangle\langle xy|\}_{\substack{x,y \in V \\ x \sim y}}$:

Lemma 5.3 *The restriction Φ^{Diag} has a matrix representation with respect to the orthonormal basis $\{|xy\rangle\langle xy|\}_{\substack{x,y \in V \\ x \sim y}}$ which is entry-wise positive and bistochastic.*

Proof : We have, see (4.21),

$$\Phi^{\text{Diag}}(|xy\rangle\langle xy|) = \sum_{z \sim x} |S_{zy}(x)|^2 |zx\rangle\langle zx|. \quad (5.12)$$

Hence, labelling the matrix elements by the directed edges (xy) ,

$$\Phi^{\text{Diag}} \simeq (\Phi_{zt\,xy}^{\text{Diag}})_{x,y,z,t \in V} \text{ where } \Phi_{zt\,xy}^{\text{Diag}} = \begin{cases} |S_{zy}(x)|^2 & \text{if } t = x, y \sim x, z \sim x \\ 0 & \text{otherwise.} \end{cases} \quad (5.13)$$

Since $S(x) = (S_{zy}(x))_{\substack{z \sim x \\ y \sim x}}$ is unitary for all $x \in V$, we have

$$\sum_{zt} \Phi_{zt\,xy}^{\text{Diag}} = \sum_{z \sim x} |S_{zy}(x)|^2 = 1 \quad \text{and} \quad \sum_{xy} \Phi_{zt\,xy}^{\text{Diag}} = \sum_{y \sim t} |S_{zy}(t)|^2 = 1. \quad (5.14)$$

□

Remark 5.4 *i) The operator $\Phi^{\text{Diag}\dagger}$ being the adjoint of Φ^{Diag} has a matrix representation given by the transpose of $(\Phi_{zt\,xy}^{\text{Diag}})_{x,y,z,t \in V}$.*

ii) The map Φ^{Diag} is the transition matrix of a naturally related classical Markov process on D , the set of directed edges, parameterized by S .

The main spectral properties of Φ^{Diag} , determining $\sigma(\Phi_S) \setminus \{0\}$, read as follows according to Perron-Frobenius Theorem, see *e.g.* [KS, N, Wo]:

- $\sigma(\Phi^{\text{Diag}}) \subset \{z \in \mathbb{C}, \text{ s.t. } |z| \leq 1\}$, with semi-simple modulus one eigenvalues.
- If Φ^{Diag} is irreducible, 1 is a simple eigenvalue with corresponding eigenvector $\sum_{x \sim y} |xy\rangle\langle xy|$. If Φ^{Diag} has period $p > 1$, $\sigma(\Phi^{\text{Diag}}) \cap S^1 = \{e^{i2\pi k/p}\}_{0 \leq k < p}$ are simple eigenvalues. Moreover, the whole spectrum is invariant under rotation by the angle $2\pi/p$.
- If Φ^{Diag} is irreducible and aperiodic, 1 is the only eigenvalue of modulus one and is simple.

In particular, we have

Proposition 5.5 *Assume $S_{zy}(x) \neq 0$, for all $x, y, z \in V$, $y \sim x, z \sim x$. Then the bistochastic map Φ^{Diag} is irreducible. Moreover, Φ^{Diag} is aperiodic if the graph G contains a cycle with an odd number of vertices, and it is irreducible with period 2 otherwise.*

Remark 5.6 *Irreducibility may hold under weaker assumptions on the scattering matrices, see the example of the tree with three vertices discussed in Section 5.1.*

Proof : Let Γ be the graph associated with the matrix Φ^{Diag} as follows. It has vertices labelled by the directed edges of G , (xy) , $x \sim y$, and directed edges from (xy) to (zt) iff $\Phi_{zt,xy}^{\text{Diag}} = \delta_{xt}|S_{zy}(x)|^2 > 0$. Under the assumption on the elements of $S(x)$, we get that Γ has an edge from (xy) to (zx) for all $z \sim x$, $y \sim x$, $x \in V$, *i.e.* between any incoming edge of G at x and any outgoing edge of G from x . The matrix Φ^{Diag} is irreducible iff there exists a path of directed edges of Γ between any two of its vertices (xy) and (zt) . Since G is connected, there exists a path from x to t , made of oriented edges (x_1x) , (x_2x_1) , \dots , (tx_n) . But (xy) and (x_1x) are connected in Γ , as are (x_1x) and (x_2x_1) , up to (x_nx_{n-1}) and (tx_n) , so that Φ^{Diag} is irreducible.

Because for any directed edge (xy) of G , (xy) and (yx) form a directed edge of Γ , the matrix element $(\Phi^{\text{Diag}^2})_{xy,xy} > 0$, so that either the irreducible matrix Φ^{Diag} has period 2, or it is aperiodic. When G contains a cycle with n vertices, for any edge (xy) of G between vertices of the cycle, we have $(\Phi^{\text{Diag}^n})_{xy,xy} > 0$, estimating the matrix element by the product of the elements along consecutive edges. Since an edge (xy) satisfies $(\Phi^{\text{Diag}^{2p+1}})_{xy,xy} > 0$, $p \in \mathbb{N}^*$, iff G contains a cycle with $2p+1$ vertices including x and y , this yields the result. \square

Consequently, the discrete asymptotic dynamics induced by $\Phi_{\mathcal{S}}$ is essentially independent of the set of scattering matrices \mathcal{S} that parameterize $\Phi_{\mathcal{S}}$:

Corollary 5.7 *Let $\Phi_{\mathcal{S}}$ be defined on $\mathcal{B}(l^2(D))$ with $|V| < \infty$. If $S_{zy}(x) \neq 0$, for all $x, y, z \in V$, $y \sim x, z \sim x$, then*

$$\frac{1}{N} \sum_{n=0}^{N-1} \Phi_{\mathcal{S}}^n(\cdot) = \frac{\mathbb{I}}{\sum_{x \in V} d_x} \text{tr}(\cdot) + \mathcal{O}(1/N). \quad (5.15)$$

If, furthermore, G contains a cycle with an odd number of vertices, $\exists \gamma > 0$ such that

$$\Phi_{\mathcal{S}}^n(\cdot) = \frac{\mathbb{I}}{\sum_{x \in V} d_x} \text{tr}(\cdot) + \mathcal{O}(e^{-\gamma n}). \quad (5.16)$$

Proof : Since $\Phi_{\mathcal{S}}$ is a unital CPTP map, the identity $\mathbb{I} \in \mathcal{B}(l^2(D))$ is invariant under $\Phi_{\mathcal{S}}$ and $\Phi_{\mathcal{S}}^\dagger$. Moreover, the irreducibility of Φ^{Diag} and Theorem 5.1 imply that \mathbb{I} spans the invariant space. Consequently, the rank one self-adjoint spectral projector of $\Phi_{\mathcal{S}}$ associated with the eigenvalue one is self-adjoint with respect to the Hilbert Schmidt inner product (5.1) and reads

$$P_{\{1\}}(\cdot) = \frac{\mathbb{I}}{\sum_{x \in V} d_x} \text{tr}(\cdot). \quad (5.17)$$

If Φ^{Diag} has period 2, $-1 \in \sigma(\Phi_{\mathcal{S}})$ is simple, and since all other eigenvalues have moduli strictly smaller than 1, the spectral decomposition of $\Phi_{\mathcal{S}}$, see [Ka], and the Cesàro average yield the result. In case Φ^{Diag} is aperiodic, 1 is the only eigenvalue of modulus one, so that the spectral decomposition yields (5.16), which ends the proof. \square

This Corollary implies that the asymptotics in time of the (Cesàro mean) probability $\mathbb{Q}_n^{\rho_0}(x)$ to find the quantum walker in the subspace \mathcal{H}_x^I , see (4.24), satisfies

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \mathbb{Q}_n^{\rho_0}(x) = \frac{d_x}{\sum_{y \in V} d_y}. \quad (5.18)$$

Of course, in case $\Phi_{\mathcal{S}}^n(\cdot)$ converges exponentially fast to its invariant spectral projector, no Cesàro mean is necessary and the convergences are exponential as well.

Remark 5.8 *i) For an alternative argument providing the asymptotic behaviour of $\Phi_{\mathcal{S}}^n$ on the basis of the spectral properties of Φ^{Diag} , see Appendix C.*

ii) The asymptotic CPTP map shows that if G is infinite, the existence of a non trivial large times asymptotics for Φ^{Diag^n} is not guaranteed. We consider such an infinite dimensional case at the end of the present Section.

5.1 Tree with three vertices

For illustration purposes, we consider the special case of $G = T_3$, the tree with three vertices, see figure 4. Note that this case coincides with the star-graph SG_2 , with central vertex y .

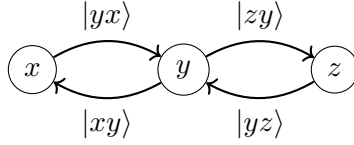


Figure 4: The graph $G = T_3$ with basis vectors of \mathcal{H}_{T_3} .

The degrees of the vertices are $d_x = d_z = 1$ and $d_y = 2$, so that $\dim l^2(D) = 4$ and $\dim \mathcal{B}(l^2(D)) = 16$. The associated scattering matrices in $\mathcal{S} = \{S(x), S(y), S(z)\}$ are

$$\begin{aligned} S(x) &= e^{i\theta_x} \in U(1), \quad S(z) = e^{i\theta_z} \in U(1) \\ S(y) &= \begin{pmatrix} S_{xx}(y) & S_{xz}(y) \\ S_{zx}(y) & S_{zz}(y) \end{pmatrix} \in U(2) \end{aligned} \quad (5.19)$$

according to our notation. The matrix representation of $U_{\mathcal{S}}$ in the ordered basis

$$\{|yx\rangle, |yz\rangle, |xy\rangle, |zy\rangle\} \quad (5.20)$$

is given by, see (3.28),

$$U_{\mathcal{S}} = \begin{pmatrix} 0 & 0 & e^{i\theta_x} & 0 \\ 0 & 0 & 0 & e^{i\theta_z} \\ S_{xx}(y) & S_{xz}(y) & 0 & 0 \\ S_{zx}(y) & S_{zz}(y) & 0 & 0 \end{pmatrix}. \quad (5.21)$$

Set $D = \text{Diag}(e^{i\theta_x}, e^{i\theta_z}) \in U(2)$. Then, the spectrum of $U_{\mathcal{S}}$ satisfies

$$\sigma(U_{\mathcal{S}}^2) = \sigma(DS(y)) = \{e^{i\alpha_1}, e^{i\alpha_2}\}, \quad \text{i.e.} \quad \sigma(U_{\mathcal{S}}) = \{\pm e^{i\alpha_1/2}, \pm e^{i\alpha_2/2}\}. \quad (5.22)$$

To express $\Phi_{\mathcal{S}}$, we observe that

$$\begin{aligned} P_x^{\text{I}} &= |xy\rangle\langle xy|, \quad P_z^{\text{I}} = |zy\rangle\langle zy| \quad \text{and} \quad P_y^{\text{I}} = |yx\rangle\langle yx| + |yz\rangle\langle yz|, \\ P_x^{\text{O}} &= |yx\rangle\langle yx|, \quad P_z^{\text{O}} = |yz\rangle\langle yz| \quad \text{and} \quad P_y^{\text{O}} = |xy\rangle\langle xy| + |zy\rangle\langle zy|, \end{aligned} \quad (5.23)$$

so that

$$\begin{aligned} \text{Ran } D^{\text{I}} &= \text{span}\{|xy\rangle\langle xy|, |zy\rangle\langle zy|, |yx\rangle\langle yx|, |yz\rangle\langle yz|, |yx\rangle\langle yz|, |yz\rangle\langle yx|\} \\ \text{Ran } D^{\text{O}} &= \text{span}\{|yx\rangle\langle yx|, |yz\rangle\langle yz|, |xy\rangle\langle xy|, |zy\rangle\langle zy|, |xy\rangle\langle zy|, |zy\rangle\langle xy|\}. \end{aligned} \quad (5.24)$$

Consequently, with the shorthand $D_{\perp}^{\#} = \mathbb{I} - D^{\#}$, $\# \in \{O, I\}$,

$$\begin{aligned} \text{Ran Diag} &= \text{span}\{|xy\rangle\langle xy|, |zy\rangle\langle zy|, |yx\rangle\langle yx|, |yz\rangle\langle yz|\}, \\ \text{Ran } D^I \circ D_{\perp}^O &= \text{span}\{|yx\rangle\langle yz|, |yz\rangle\langle yx|\} \\ \text{Ran } D^O \circ D_{\perp}^I &= \text{span}\{|xy\rangle\langle zy|, |zy\rangle\langle xy|\}, \end{aligned} \quad (5.25)$$

and we refrain from spelling out the eight basis vectors of $\text{Ran } D_{\perp}^O \circ D_{\perp}^I$. Recall that $\text{Ker } \Phi_S = \text{Ran}(\mathbb{I} - D^I)$ has dimension 10. We express Φ_S as a bloc matrix in the following ordered list of subspaces, with their respective ordered bases listed above

$$\text{Ran Diag} \quad \text{Ran } D^I \circ D_{\perp}^O \quad \text{Ran } D^O \circ D_{\perp}^I \quad \text{Ran } D_{\perp}^O \circ D_{\perp}^I. \quad (5.26)$$

Below, the symbol $\mathbf{0} \in \mathbb{C}^8$ denotes a vector of zeros and the vertical and horizontal lines delimitate blocs with respect to the projectors D^I and D_{\perp}^I

$$\Phi_S = \begin{array}{c} \left(\begin{array}{cccc|cc} 0 & 0 & |S_{xx}(y)|^2 & |S_{xz}(y)|^2 & S_{xx}(y)\overline{S_{xz}(y)} & S_{xz}(y)\overline{S_{xx}(y)} & 0 & 0 & \mathbf{0}^T \\ 0 & 0 & |S_{zx}(y)|^2 & |S_{zz}(y)|^2 & S_{zx}(y)\overline{S_{zz}(y)} & S_{zz}(y)\overline{S_{zx}(y)} & 0 & 0 & \mathbf{0}^T \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{0}^T \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{0}^T \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{0}^T \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \mathbf{0}^T \\ \hline 0 & 0 & S_{xx}(y)\overline{S_{zx}(y)} & \overline{S_{zz}(y)}S_{xz}(y) & S_{xx}(y)\overline{S_{zz}(y)} & S_{xz}(y)\overline{S_{zx}(y)} & 0 & 0 & \mathbf{0}^T \\ 0 & 0 & \overline{S_{xx}(y)}S_{zx}(y) & S_{zz}(y)\overline{S_{xz}(y)} & S_{zx}(y)\overline{S_{zz}(y)} & S_{zz}(y)\overline{S_{xx}(y)} & 0 & 0 & \mathbf{0}^T \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0}\mathbf{0}^T \end{array} \right). \end{array} \quad (5.27)$$

We observe that the Hilbert-Schmidt norm of each nonzero column equals one, as it should. The four by four upper left corner of the matrix corresponds to the bistochastic matrix representation of Φ^{Diag} in the chosen basis of Ran Diag

$$\Phi^{\text{Diag}} \simeq \begin{pmatrix} 0 & 0 & |S_{xx}(y)|^2 & |S_{xz}(y)|^2 \\ 0 & 0 & |S_{zx}(y)|^2 & |S_{zz}(y)|^2 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \quad (5.28)$$

The spectral data of Φ^{Diag} as a function of the scattering matrix $S(y)$ are readily determined. Without going into the details, we have

- If the matrix elements of $S(y)$ are all nonzero, Φ^{Diag} is irreducible with period 2. For $S(y) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$, the Hadamard matrix, Φ^{Diag} is not diagonalisable, has simple spectrum $\sigma(\Phi^{\text{Diag}}) = \{1, -1, 0\}$, with an eigennilpotent associated with the spectral projector on its kernel.
- If $S(y) = \mathbb{I}$, Φ^{Diag} is reducible with spectrum $\sigma(\Phi^{\text{Diag}}) = \{1, -1\}$, each eigenvalue being of multiplicity 2.
- For $S(y) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, Φ^{Diag} is irreducible with period 4, so that $\sigma(\Phi^{\text{Diag}}) = \{1, -1, i, -i\}$.

5.2 The graph \mathbb{Z} with Hadamard Scattering Matrices

We consider the infinite graph $G = \mathbb{Z}$ with $S(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \in U(2)$, the Hadamard matrix for each x , to illustrate the difference in the asymptotics given in Corollary 5.7 for finite graphs. Hence, the nonzero matrix elements of the infinite stochastic matrix Φ^{Diag} , see (4.21), are all equal to $1/2$.

To analyze Φ^{Diag} , we label the vertices of G by $x \in \mathbb{Z}$, and we find it convenient to denote the vectors corresponding to incoming edges at x from the left as $|2x-1\rangle$, and those associated with outgoing edges from x to the left as $|2x\rangle$, see Figure 5.

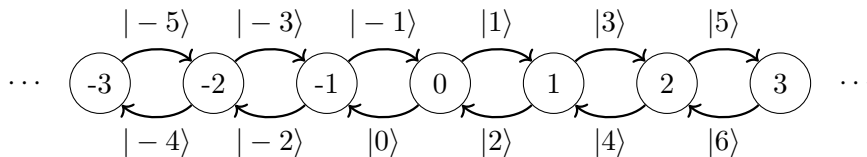


Figure 5: The graph $G = \mathbb{Z}$ with incoming and outgoing edges at the vertices.

We further write the basis vectors of $\text{Diag}\mathcal{T}(l^2(D))$ as $|x\rangle\langle x| = e_x$, $x \in \mathbb{Z}$, so that $\text{Diag}\mathcal{T}(l^2(D)) \simeq l^1(\mathbb{Z})$, with ordered basis

$$\{\dots, e_{-2}, e_{-1}, e_0, e_1, e_2, \dots\}. \quad (5.29)$$

Accordingly, the matrix elements of Φ^{Diag} in the ordered basis (5.29) are denoted by Φ_{xy}^{Diag} . More precisely, we have

$$\begin{aligned} \Phi^{\text{Diag}}(e_{2x}) &= \frac{1}{2}(e_{2(x-1)} + e_{2(x-1)+1}), \\ \Phi^{\text{Diag}}(e_{2x+1}) &= \frac{1}{2}(e_{2(x+1)} + e_{2(x+1)+1}). \end{aligned} \quad (5.30)$$

This shows that Φ^{Diag} is an irreducible stochastic matrix of period 2, looking at the graph Γ associated with Φ^{Diag} in Figure 6; see also the proof of Proposition 5.5.

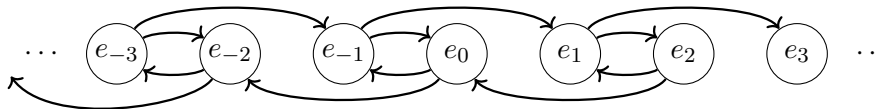


Figure 6: The graph Γ with the specified incoming and outgoing edges.

As a simple computation reveals, Φ^{Diag} admits no invariant vector in $l^1(\mathbb{Z})$. We prove the following property of its matrix elements in Appendix B:

Lemma 5.9 *There exists $c < \infty$ such that for any $x, y \in \mathbb{Z}$,*

$$0 \leq \Phi_{xy}^{\text{Diag}^n} \leq c/\sqrt{n}, \quad \text{for all } n \geq N_0(x-y) \quad (5.31)$$

where $N_0(x-y) \in \mathbb{N}$.

As a consequence, the map provided in Corollary 4.5

$$\Phi_{\mathcal{S}}^n = \Phi_{\mathcal{S}} \circ \Phi^{\text{Diag}^{n-2}} \circ \text{Diag} \circ \Phi_{\mathcal{S}}, \quad (5.32)$$

converges to zero in the weak sense. More precisely, $\forall (xy), (x'y'), (zt), (z't') \in D$,

$$\lim_{n \rightarrow \infty} \text{tr}(|x'y'\rangle\langle z't'| \Phi_{\mathcal{S}}^n(|xy\rangle\langle zt|)) = 0, \quad (5.33)$$

since the matrix elements of $\Phi_{\mathcal{S}}$ connect P_x^I and P_x^O , so that the argument of the trace is a sum of finitely many matrix elements of $\Phi^{\text{Diag}^{n-2}}$. Hence, for infinite graph, the dynamics can send the state at infinity, preventing the existence of an asymptotic state.

6 Induced Open Quantum Walk on G

The open QW $\Phi_{\mathcal{S}} \in \mathcal{T}(l^2(D))$ defined above lives on the directed edges of G . We provide here an open QW $\Psi_{\mathcal{S}} \in \mathcal{T}(l^2(V))$ defined via $\Phi_{\mathcal{S}}$ which lives on the vertices of G , by reducing each incoming subspaces \mathcal{H}_x^I , $x \in V$ to the vectors $|x\rangle \in l^2(V)$ associated with the vertex $x \in V$. To do so, we make use of the natural boundary operator R and its adjoint R^* between $l^2(D)$ to $l^2(V)$, see (3.86), generalizing the approach [HKSS2] of the unitary Grover Walk to open QW.

We recall the expressions of R and R^* given by

$$R = \sum_{x \in V} |x\rangle\langle \omega(x)| : l^2(D) \rightarrow l^2(V), \quad R^* = \sum_{x \in V} |\omega(x)\rangle\langle x| : l^2(V) \rightarrow l^2(D), \quad (6.1)$$

where $\{\omega(x)\}_{x \in V}$ is a family of normalized vectors of $l^2(D)$ indexed by $x \in V$ such that

$$\omega(x) = \sum_{y \sim x} \omega_y(x) |xy\rangle \in P_x^I l^2(D), \quad \text{with } \langle \omega(x) | \omega(x') \rangle = \delta_{xx'}, \quad \forall x, x' \in V. \quad (6.2)$$

Then we consider the map

$$\mathcal{R}(\cdot) = R^* \cdot R : \mathcal{T}(l^2(V)) \rightarrow \mathcal{T}(l^2(D)) \quad (6.3)$$

which is CPTP thanks to (3.88). Note that for G infinite, the series in (3.88) converges in the strong sense. Also, (3.87) converges strongly so that the following map is well defined

$$\mathcal{R}^\dagger(\cdot) = R \cdot R^* : \mathcal{T}(l^2(D)) \rightarrow \mathcal{T}(l^2(V)) \quad (6.4)$$

and can be extended as a map on $\mathcal{B}(l^2(D))$, which coincides with \mathcal{R}^* , the adjoint of \mathcal{R} , and is CP and unital. We now set

$$\tilde{\Phi}_{\mathcal{S}} = \mathcal{R}^\dagger \circ \Phi_{\mathcal{S}} \circ \mathcal{R} : \mathcal{T}(l^2(V)) \rightarrow \mathcal{T}(l^2(V)), \quad (6.5)$$

which in terms of the expression (4.12) for $\Phi_{\mathcal{S}}$ reads

$$\tilde{\Phi}_{\mathcal{S}}(B) = \sum_{x \in V} RK(x)R^*BRK^*(x)R^*, \quad \forall B \in \mathcal{T}(l^2(V)). \quad (6.6)$$

To assess the properties of $\tilde{\Phi}_{\mathcal{S}}$, we compute

$$RK(x)R^* = \sum_{x', x'' \in V} |x'\rangle\langle \omega(x') | K(x) \omega(x'') \rangle \langle x''|, \quad (6.7)$$

where

$$\begin{aligned} \langle \omega(x') | K(x) | \omega(x'') \rangle &= \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) \langle \omega(x') | zx \rangle \langle xy | \omega(x'') \rangle \\ &= \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) \overline{\omega_x(z)} \omega_y(x) \delta_{x'z} \delta_{zx''}, \end{aligned} \quad (6.8)$$

so that

$$RK(x)R^* = \sum_{\substack{y \sim x \\ z \sim x}} S_{zy}(x) \overline{\omega_x(z)} \omega_y(x) |z\rangle \langle x|. \quad (6.9)$$

This leads us to introduce

$$v(x) = \sum_{z \sim x} v_z(x) |z\rangle \in l^2(V), \text{ with } v_z(x) = (S(x)\omega(x))_z = \sum_{y \sim x} S_{zy}(x) \omega_y(x), \quad (6.10)$$

where we view $\omega(x)$ and $S(x)\omega(x)$ as vectors in \mathbb{C}^{d_x} above, and

$$\theta(x) = \sum_{z \sim x} \overline{\omega_x(z)} v_z(x) |z\rangle \in l^2(V). \quad (6.11)$$

Note that $v(x)$ and $\theta(x)$ have finitely many nonzero components and since $S(x)$ is unitary and $\|\omega(x)\| = 1$, we have

$$\|v(x)\|^2 = 1, \quad \|\theta(x)\|^2 = \sum_{z \sim x} |\omega_x(z)|^2 |v_z(x)|^2 \leq \sum_{z \sim x} |v_z(x)|^2 = 1. \quad (6.12)$$

Thus, the Kraus operators associated with the CP map $\tilde{\Phi}_S$ have rank one

$$RK(x)R^* = |\theta(x)\rangle \langle x|, \quad RK^*(x)R^* = |x\rangle \langle \theta(x)|. \quad (6.13)$$

From the computations above we deduce that

$$\Phi_S^*(\mathbb{I}_V) = \sum_{x \in V} RK^*(x)R^* RK(x)R^* = \sum_{x \in V} |x\rangle \langle x| \|\theta(x)\|^2 \leq \mathbb{I}_V, \quad (6.14)$$

which makes $\tilde{\Phi}_S$ a quantum operation, characterized by the inequality (6.14), rather than a CPTP map. Incidentally, we get from (6.12) that $\tilde{\Phi}_S$ is a CPTP map iff $|\omega_x(z)|^2 = 1$ for all $x \in V$ and all $z \sim x$, which is possible only if $|V| = 2$.

To cure this defect, we modify the vector $\theta(x)$, observing $\langle \theta(x) | x \rangle = 0$: set

$$\chi(x) = \theta(x) + e^{i\beta_x} \sqrt{1 - \|\theta(x)\|^2} |x\rangle, \text{ where } \beta_x \in \mathbb{R}, \quad (6.15)$$

and, recall (6.13), define rank one operators on $l^2(V)$

$$\mathcal{G}(x) = |\chi(x)\rangle \langle x|, \quad \mathcal{G}^*(x) = |x\rangle \langle \chi(x)|. \quad (6.16)$$

Definition 6.1 For each $x \in V$, let $\theta(x)$, $\chi(x)$ and $\mathcal{G}(x)$ be given by (6.11), (6.15) and (6.16). We define the map $\Psi_S(\cdot) : \mathcal{T}(l^2(V)) \rightarrow \mathcal{T}(l^2(V))$ by

$$\Psi_S(\cdot) = \sum_{x \in V} \mathcal{G}(x) \cdot \mathcal{G}^*(x). \quad (6.17)$$

To assess the properties of Ψ_S , it is useful to introduce a stochastic matrix $P \in M_{|V|}(\mathbb{C})$ by its elements, where $|V| = \infty$ if G is infinite.

$$P_{xy} = |\langle y | \chi(x) \rangle|^2 \geq 0, \text{ for } x, y \in V. \quad (6.18)$$

Note that $P_{xy} = 0$ if $x \not\sim y$ and $x \neq y$, which makes P sparse. The matrix P is the transition matrix of a discrete time Markov chain M on V , $M : \mathbb{N} \rightarrow V$ such that at time $t \in \mathbb{N}$ and for $x, y \in V$,

$$\mathbb{P}(M(t) = y | M(t-1) = x) = |\langle y | \chi(x) \rangle|^2 = P_{xy}. \quad (6.19)$$

A probability vector on V is a row vector of the form $p = (p_x)_{x \in V}$, *i.e.*, given an ordering of the vertices,

$$p = (p_{x_1}, p_{x_2}, \dots, p_{x_{|V|}}), \quad (6.20)$$

with $p_x \geq 0$ and $\sum_{x \in V} p_x = 1$. The support of p is the set $\{x \in V \text{ s.t. } p_x > 0\}$, and p is strictly positive if its support is V . For a set of vertices $S \subset V$, we denote the probability of this set by $p(S) = \sum_{x \in S} p_x$.

Given an initial probability vector p we have for all $t \in \mathbb{N}$,

$$\mathbb{P}(M(0) = x) = p_x, \forall x \in V, \Rightarrow \mathbb{P}_p(M(t) = x) = (pP^t)_x, \quad (6.21)$$

where the subscript p indicates the initial distribution of the Markov chain M , see [N, KS, Wo] for example.

Theorem 6.2 *The map Ψ_S defined in (6.17) is a CPTP map on $\mathcal{T}(l^2(V))$. With P given by (6.18), we have for all $n \geq 1$*

$$\Psi_S^n(\cdot) = \sum_{x, y \in V} |\chi(y)\rangle\langle x| \cdot |x\rangle\langle\chi(y)| P^{n-1}_{xy}. \quad (6.22)$$

Moreover, for any initial state $\rho_0 \in \mathcal{DM}(l^2(V))$, the probability to find the quantum walker on the vertex $x \in V$ at time $n \geq 1$, $\mathbb{Q}_n^{\rho_0}(x)$ reads

$$\mathbb{Q}_n^{\rho_0}(x) = (r_0 P^n)_x, \quad (6.23)$$

where $r_0 = (\langle x_1 | \rho_0 x_1 \rangle, \langle x_2 | \rho_0 x_2 \rangle, \dots, \langle x_{|V|} | \rho_0 x_{|V|} \rangle)$.

Remark 6.3 *i) For $A \in \mathcal{T}(l^2(V))$, the sum over $x, y \in V$ defining $\Psi_S^n(A)$ converges in trace norm.*

ii) For $\rho_0 \in \mathcal{DM}(l^2(V))$, $n \geq 1$, we can write

$$\Psi_S^n(\rho_0) = \sum_{y \in V} |\chi(y)\rangle\langle\chi(y)| \mathbb{P}_{r_0}(M(n-1) = y), \quad (6.24)$$

the expectation of the matrix valued random variable $|\chi(\cdot)\rangle\langle\chi(\cdot)|$ on V with respect to the law of the Markov chain M at time $n-1$.

iii) Similarly, the probability of presence of the quantum walker at $x \in V$ at time n is given by the law of the Markov chain M :

$$\mathbb{Q}_n^{\rho_0}(x) = \mathbb{P}_{r_0}(M(n) = x). \quad (6.25)$$

iv) There are other possibilities to modify the Kraus operators in order to promote $\tilde{\Phi}_S$ to a CPTP map. A well-known modification consists in adding the extra Kraus operator $(\mathbb{I}_V - \Phi_S^\dagger(\mathbb{I}_V))^{1/2} \geq 0$ to $\{RK(x)R^\}_{x \in V}$. However, since*

$$(\mathbb{I}_V - \Phi_S^\dagger(\mathbb{I}_V))^{1/2} = \sum_{x \in V} (1 - \|\theta(x)\|^2)^{1/2} |x\rangle\langle x| \quad (6.26)$$

has a priori a large rank, this supplementary Kraus operator gives the corresponding CPTP map less structure than Ψ_S has.

Proof : By construction, $\|\chi(x)\|^2 = 1$ for all $x \in V$, so that the Kraus operators defining Ψ_S satisfy

$$\sum_{x \in V} \mathcal{G}^*(x)\mathcal{G}(x) = \sum_{x \in V} |x\rangle\langle x| = \mathbb{I}_V, \quad (6.27)$$

with convergence in the strong sense if G is infinite, which ensure Ψ_S is CPTP. Then, for any $n \in \mathbb{N}$ we compute

$$\begin{aligned} \Psi_S^n(\cdot) &= \sum_{x_1, x_2, \dots, x_n \in V} |\chi(x_n)\rangle\langle x_1| \cdot |x_1\rangle\langle \chi(x_n)| \times \\ &\quad |\langle x_2|\chi(x_1)\rangle|^2 |\langle x_3|\chi(x_2)\rangle|^2 \dots |\langle x_n|\chi(x_{n-1})\rangle|^2, \end{aligned} \quad (6.28)$$

which, with (6.18), implies (6.22) immediately. Finally,

$$\begin{aligned} \mathbb{Q}_n^{\rho_0}(x) &= \langle x | \Psi_S^n(\rho_0) x \rangle \\ &= \sum_{x', y' \in V} \langle x | \chi(y') \rangle \langle x' | \rho_0 x' \rangle \langle \chi(y') | x \rangle P^{n-1}_{x' y'} \\ &= \sum_{x', y' \in V} \langle x' | \rho_0 x' \rangle P^{n-1}_{x' y'} P_{y' x} = (r_0 P^n)_x, \end{aligned} \quad (6.29)$$

where

$$r_0 = (\langle x_1 | \rho_0 x_1 \rangle, \langle x_2 | \rho_0 x_2 \rangle, \dots, \langle x_{|V|} | \rho_0 x_{|V|} \rangle) \quad (6.30)$$

which, with (6.21), ends the proof. \square

We mainly consider G finite in the rest of this section, and will comment along the way on the infinite graph case.

In this case, we can thus easily deduce the large n behaviour of the map $\Psi_S^n(\cdot)$ from the properties of the stochastic matrix P .

Corollary 6.4 *Let G be finite. If P is irreducible, there exists a strictly positive probability vector $\pi = (\pi_{x_1}, \pi_{x_2}, \dots, \pi_{x_{|V|}})$ such that with $\mathbf{1}^T = (1, 1, \dots, 1)$ and for N large enough $\frac{1}{N} \sum_{n=0}^{N-1} P^n = \mathbf{1}\pi + O(N^{-1})$ and*

$$\frac{1}{N} \sum_{n=0}^{N-1} \Psi_S^n(\cdot) = \sum_{y \in V} |\chi(y)\rangle\langle \chi(y)| \pi_y \text{tr}(\cdot) + O(N^{-1}). \quad (6.31)$$

If P is irreducible and moreover aperiodic, there exists $\gamma > 0$ such that for n large, $P^n = \mathbf{1}\pi + O(e^{-\gamma n})$ and

$$\Psi_S^n(\cdot) = \sum_{y \in V} |\chi(y)\rangle\langle \chi(y)| \pi_y \text{tr}(\cdot) + O(e^{-\gamma n}). \quad (6.32)$$

Moreover, for any initial state $\rho_0 \in \mathcal{DM}(l^2(V))$, $\mathbb{Q}_n^{\rho_0}(x)$, the probability to find the quantum walker on the vertex $x \in V$ at time n , satisfies for P irreducible

$$\frac{1}{N} \sum_{n=0}^{N-1} \mathbb{Q}_n^{\rho_0}(x) = \pi_x + O(N^{-1}). \quad (6.33)$$

If P is irreducible and aperiodic,

$$\mathbb{Q}_n^{\rho_0}(x) = \pi_x + O(e^{-\gamma n}). \quad (6.34)$$

Proof: If P is irreducible, Perron-Frobenius Theorem ensures the existence of a strictly positive probability row vector $\pi = (\pi_{x_1}, \pi_{x_2}, \dots, \pi_{x_{|V|}})$ such that with $\mathbf{1}^T = (1, 1 \dots, 1)$ and for N large enough

$$\frac{1}{N} \sum_{n=0}^{N-1} P^n = \mathbf{1}\pi + O(N^{-1}), \quad (6.35)$$

see e.g. [N,KS,Wo]. Hence, the matrix elements of the projector $\mathbf{1}\pi$ read $(\mathbf{1}\pi)_{xy} = \pi_y > 0$. Inserting this in (6.22) yields

$$\frac{1}{N} \sum_{n=0}^{N-1} \Psi_{\mathcal{S}}^n(\cdot) = \sum_{x,y \in V} |\chi(y)\rangle\langle x| \cdot |x\rangle\langle \chi(y)| \pi_y + O(N^{-1}), \quad (6.36)$$

which, with $\sum_{x \in V} \langle x| \cdot |x\rangle = \text{tr}(\cdot)$, proves the result in the irreducible case. The irreducible and aperiodic case is proven the same way.

Consider now the probability $Q_n^{\rho_0}$ given by formula (6.29). Inserting in this expression the large time asymptotics (6.35) for the Cesàro mean of P^n in the irreducible case proves (6.33). Formula (6.34) is proven similarly in the irreducible and aperiodic case. \square

Remark 6.5 *i) Up to the strict positivity of π , the Corollary can be given a purely spectral proof that we sketch in Appendix B for completeness.*

ii) Since the asymptotic state typically differs from $\mathbb{I}_V \text{tr}(\cdot)$, which has maximal von Neuman entropy, it shows that $\Psi_{\mathcal{S}}$ is not entropy non-decreasing.

iii) If P fails to be irreducible, the limiting behaviour of $\Psi_{\mathcal{S}}(\rho_0)$ and $Q_n^{\rho_0}$ depend on the initial state $\rho_0 \in \mathcal{DM}(l^2(V))$, as shown on the example in Section 6.1.2.

iv) The form of the asymptotic state is likely to hold true for certain infinite graphs. We show that this is the case on the example of the next section.

The results presented in Theorem 6.2 and Corollary 6.4 only depend on the form (6.16) of the rank one Kraus operators of $\Psi_{\mathcal{S}}$. In particular, the asymptotic state of $\Psi_{\mathcal{S}}^n$ and corresponding probabilities to find the walker on each vertex are monitored by the invariant probability vector π of the Markov chain associated with P . This is to be contrasted with the corresponding asymptotic quantities stated in Corollary 5.7 and (5.18) for the open QW $\Phi_{\mathcal{S}}^n$ which only depend on the degrees of the vertices of G .

The non trivial dependence of the invariant probability vector π on the parameters of the construction, i.e. the graph G , the scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$ and the vectors $\{\omega(x)\}_{x \in V}$ appearing in R , is illustrated by the examples of the next section.

6.1 Examples

We illustrate the variety of behaviours induced open SQW on graphs can display as a function of the scattering matrices, by working out the cases where they correspond to the α -Grover Walk, and to the Discrete Fourier Transform.

Let G be an arbitrary finite graph and consider the boundary operator R and its adjoint (6.1) parameterized by the family of unit vectors

$$\omega(x) = \frac{\mathbf{1}}{\sqrt{d_x}} \in \mathbb{C}^{d_x}, \quad \forall x \in V. \quad (6.37)$$

This choice is motivated by the fact that it yields an equal weight to each of the vectors spanning \mathcal{H}_x^1 , and thus is likely to make P irreducible. The components of the vector $v(x)$ (6.10) thus satisfy

$$v_z(x) = \frac{1}{\sqrt{d_x}} \sum_{y \sim x} S_{zy}(x) := \frac{1}{\sqrt{d_x}} L_z(x), \quad \forall x \in V, z \sim x. \quad (6.38)$$

Consequently, see (6.11), (6.15),

$$\begin{aligned} \theta(x) &= \frac{1}{\sqrt{d_x}} \sum_{z \sim x} \frac{L_z(x)}{\sqrt{d_z}} |z\rangle, \quad \text{with } \|\theta(x)\|^2 = \frac{1}{d_x} \sum_{z \sim x} \frac{|L_z(x)|^2}{d_z}, \\ \chi(x) &= \theta(x) + e^{i\beta_x} \sqrt{1 - \|\theta(x)\|^2} |x\rangle, \end{aligned} \quad (6.39)$$

which leads to the stochastic matrix P (6.18):

$$P_{xy} = \begin{cases} \frac{|L_y(x)|^2}{d_x d_y} & \text{if } x \sim y \\ 1 - \|\theta(x)\|^2 & \text{if } x = y \\ 0 & \text{otherwise} \end{cases}, \quad \forall x, y \in V. \quad (6.40)$$

For this choice of boundary operator, we now consider two families of scattering matrices $\mathcal{S} = \{S(x)\}_{x \in V}$.

6.1.1 The α -Grover Scattering Matrices

Following (3.44), we set $\forall x \in V$,

$$S(x) = \frac{1}{d_x} |\mathbf{1}\rangle \langle \mathbf{1}| + e^{i\alpha} \left(\mathbb{I}_{d_x} - \frac{1}{d_x} |\mathbf{1}\rangle \langle \mathbf{1}| \right), \quad (6.41)$$

the matrix elements of which read, with $\nu(\alpha) = 1 - e^{i\alpha} \neq 0$,

$$S_{zy}(x) = \begin{cases} e^{i\alpha} + \frac{\nu(\alpha)}{d_x} & \text{if } y = z \sim x \\ \frac{\nu(\alpha)}{d_x} & \text{if } y \neq z, y \sim x, z \sim x \\ 0 & \text{otherwise.} \end{cases} \quad (6.42)$$

Thus, for $z \sim x$

$$L_z(x) = (d_x - 1) \frac{\nu(\alpha)}{d_x} + e^{i\alpha} + \frac{\nu(\alpha)}{d_x} = 1, \quad (6.43)$$

and, $\forall x, y \in V$,

$$P_{xy} = \begin{cases} \frac{1}{d_x d_y} & \text{if } x \sim y \\ 1 - \frac{1}{d_x} \sum_{z \sim x} \frac{1}{d_z} & \text{if } x = y \\ 0 & \text{otherwise.} \end{cases} \quad (6.44)$$

We observe that $P = P^T$ is independent of α and is actually bistochastic. Since G is connected, P is irreducible. We have shown

Lemma 6.6 *The invariant probability vector of the stochastic matrix P associated with the open QW on G induced by the α -Grover walk is uniform on the vertices of G :*

$$\pi_y = 1/|V|, \quad \forall y \in V. \quad (6.45)$$

Thus the asymptotic probability of presence of the walker on the sites of G is uniform as well. Also, the asymptotic state in Cesàro mean, is $\frac{1}{|V|} \sum_{y \in V} |\chi(y)\rangle \langle \chi(y)|$, see Corollary 6.4, where

$$|\chi(y)\rangle = \frac{1}{\sqrt{d_y}} \sum_{z \sim y} \frac{1}{\sqrt{d_z}} |z\rangle + e^{i\beta_y} \sqrt{1 - \frac{1}{d_y} \sum_{z' \sim x} \frac{1}{d_{z'}}} |y\rangle. \quad (6.46)$$

Remark 6.7 *i) The value $\alpha = 0$ is allowed in the arguments that lead to these results. Hence they hold in particular for $S(x) = \mathbb{I}_x$, for all $x \in V$.*

ii) Any unitary matrix with constant diagonal elements and constant off-diagonal elements coincides, up to a phase, with (6.41), so that its associated stochastic matrix P is identical to (6.44). The same holds if the unitary matrix is multiplied from the left by any unitary diagonal matrix, thanks to (6.40).

6.1.2 The Discrete Fourier Transform Scattering Matrices

For any $x \in V$, let $\Omega_x = e^{-2\pi i/d_x}$ and consider

$$S(x) = \frac{1}{\sqrt{d_x}} \begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \Omega_x & \Omega_x^2 & \cdots & \Omega_x^{d_x-1} \\ 1 & \Omega_x^2 & \Omega_x^4 & \cdots & \Omega_x^{2(d_x-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \Omega_x^{d_x-1} & \Omega_x^{2(d_x-1)} & \cdots & \Omega_x^{(d_x-1)(d_x-1)} \end{pmatrix} \quad (6.47)$$

written in the canonical basis of \mathbb{C}^{d_x} . Here, the jk matrix element of $S(x)$ corresponds to $S_{x_j x_k}(x)$, for a labelling of the d_x adjacent vertices x_1, x_2, \dots, x_{d_x} of x . Since the rows of a unitary matrix are orthogonal, we get for $x_j \sim x$,

$$L_{x_j}(x) = \begin{cases} \sqrt{d_x} & \text{if } j = 1, \\ 0 & \text{if } j \geq 2, \end{cases} \quad (6.48)$$

so that $\theta(x) = \frac{1}{\sqrt{d_{x_1}}} |x_1\rangle$, with $x_1 \sim x$. Consequently, $\forall x, y \in V$,

$$P_{xy} = \begin{cases} \frac{1}{d_{x_1}} & \text{if } y = x_1 \sim x \\ 1 - \frac{1}{d_{x_1}} & \text{if } y = x \\ 0 & \text{otherwise.} \end{cases} \quad (6.49)$$

This stochastic matrix is in general not irreducible, but its invariant probability vectors can be determined. Once the labelling of the adjacent vertices to x is fixed for all $x \in V$, P defines the map N on V such that

$$N : V \rightarrow V \\ x \mapsto N(x) = y, \quad \text{where } y \sim x \text{ is uniquely determined by } P_{xy} > 0. \quad (6.50)$$

We can then construct a directed subgraph $\Sigma \subset G$ (without loops) associated with P or equivalently with N : Σ has same vertex set V as G and (yx) form an edge of Σ iff $y = N(x)$. Σ is also known as a *functional graph* or *successor graph*, and may or may not be connected.

Consider the set of the connected components of Σ ,

$$\text{CC}(\Sigma) = \cup_{i=1}^r C_i \quad \text{where } C_i \subseteq V \text{ is connected in } \Sigma, \quad i = 1, \dots, r. \quad (6.51)$$

Each component $C_i \in \text{CC}(\Sigma)$, $i = 1, \dots, r$, consists of one cycle, the vertices of which are possibly the roots of a finite tree. See Figure 7 for an example corresponding to the map N on $\{s, t, u, v, w, x, y, z\}$ with values

$$\{N(s) = y, N(t) = x, N(u) = x, N(v) = t, N(w) = t, N(x) = y, N(y) = z, N(z) = x\}. \quad (6.52)$$

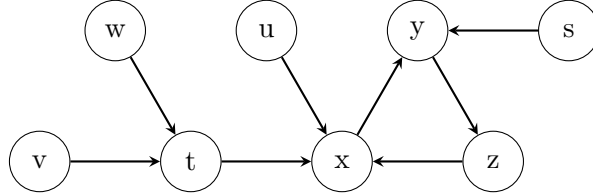


Figure 7: The functional graph Σ associated with the map N (6.52)

Given the stochastic matrix P (6.49), we first determine the dimension of $\text{Ker}(P - \mathbb{I})$, which equals the dimension of the subspace of left invariant vectors of P .

Lemma 6.8 *The stochastic matrix associated with DFT scattering matrices satisfies*

$$\dim \text{Ker}(P - \mathbb{I}) = |\text{CC}(\Sigma)|. \quad (6.53)$$

Proof : We set $E = P - \mathbb{I}$, with matrix elements E_{xy} , $x, y \in V$

$$E_{xy} = \begin{cases} \varepsilon_{N(x)} & \text{if } y = N(x) \sim x \\ -\varepsilon_{N(x)} & \text{if } y = x \\ 0 & \text{otherwise} \end{cases}, \quad \forall x, y \in V, \quad \text{with } \varepsilon_x = 1/d_x \in (0, 1]. \quad (6.54)$$

Labelling the vertices by $V = \{1, 2, \dots, n\}$, with $n = |V|$, we get that

$$v = (v_1, v_2, \dots, v_n)^T \in \text{Ker}(P - \mathbb{I}) = \text{Ker } E \quad (6.55)$$

if and only if

$$\varepsilon_{N(j)} v_j = \varepsilon_{N(j)} v_{N(j)}, \quad \forall j \in V. \quad (6.56)$$

Hence, writing $V = C_1 \cup C_2 \cup \dots \cup C_r$, where $r < n$, we get for each $i \in \{1, \dots, r\}$ and all $k \in C_i \in \text{CC}(\Sigma)$, $v_k = v(C_i) \in \mathbb{C}$ arbitrary, since $\varepsilon_j > 0$ for all $j \in V$. Thus $\text{Ker}(P - \mathbb{I})$ has dimension r , the number of connected components of Σ . \square

Thus, if Σ is connected, P admits a unique invariant row probability vector π .

Lemma 6.9 *Assume Σ is connected and denote by $\text{Cyc} \subseteq V$ the set of its vertices belonging to the cycle of Σ . Then the invariant row probability vector π of P is supported on Cyc and has components*

$$\pi_x = \begin{cases} d_{N(x)} / \sum_{y \in \text{Cyc}} d_y & \text{if } x \in \text{Cyc} \\ 0 & \text{otherwise.} \end{cases} \quad (6.57)$$

Remark 6.10 *The lack of strict positivity of π shows P is not irreducible.*

Proof : As above, we use the labelling $V = \{1, 2, \dots, n\}$, with $n = |V|$ and look for $\pi = (\pi_1, \dots, \pi_n)$ such that $\pi E = 0$. Assuming the vertices $\{1, \dots, s\} = \text{Cyc} \subseteq V$ satisfy

$$N(1) = 2, N(2) = 3, \dots, N(s-1) = s, N(s) = 1, \quad (6.58)$$

we get the following bloc structure for E

$$E = \begin{pmatrix} A & \mathbb{O} \\ B & C \end{pmatrix} \quad (6.59)$$

where $A \in M_s(\mathbb{C})$ reads

$$A = \begin{pmatrix} -\varepsilon_2 & \varepsilon_2 & & & & \\ & -\varepsilon_3 & \varepsilon_3 & & & \\ & & \ddots & & & \\ & & & -\varepsilon_s & \varepsilon_s & \\ \varepsilon_1 & & & & & -\varepsilon_1 \end{pmatrix}, \quad (6.60)$$

$B \in M_{n-s} \times s(\mathbb{C})$ and $C \in M_{n-s} \times n-s(\mathbb{C})$ and $\mathbb{O} \in M_s \times n-s(\mathbb{C})$ is the matrix with zero elements. Writing $\pi = (\pi^{(1)}, \pi^{(2)})$ where $\pi^{(1)}$ is a length s row vector and $\pi^{(2)}$ a length $n-s$ row vector, the equation $E\pi = 0$ reads

$$(\pi^{(1)}A + \pi^{(2)}B, \pi^{(2)}C) = 0. \quad (6.61)$$

Knowing the subspace of solutions is of dimension 1, we set $\pi^{(2)} = 0$ and look for non trivial solutions to $\pi^{(1)}A = 0$:

$$\begin{aligned} \pi_1^{(1)}\varepsilon_2 &= \pi_s^{(1)}\varepsilon_1 \\ \pi_{j-1}^{(1)}\varepsilon_j &= \pi_j^{(1)}\varepsilon_{j+1}, \quad 2 \leq j \leq s-1 \\ \pi_{s-1}^{(1)}\varepsilon_s &= \pi_s^{(1)}\varepsilon_1 \end{aligned} \quad (6.62)$$

Such a solution is given by

$$\pi_j^{(1)} = c/\varepsilon_{j+1}, \quad \forall 1 \leq j \leq s-1, \quad \text{and} \quad \pi_s^{(1)} = c/\varepsilon_1, \quad (6.63)$$

where $c \in \mathbb{C}^*$ is arbitrary, which after normalization and with $\varepsilon_j = 1/d_j$ and (6.58) yields (6.57). \square

As a consequence, with the DFT scattering matrix and under the assumption that Σ is connected, we obtain that the asymptotic state in Cesàro mean reads

$$\sum_{y \in \text{Cyc}} |\chi(y)\rangle \langle \chi(y)| \frac{d_{N(y)}}{\sum_{z \in \text{Cyc}} d_z} \quad (6.64)$$

with

$$|\chi(y)\rangle = \frac{1}{\sqrt{d_{N(y)}}} |N(y)\rangle + e^{i\beta y} \sqrt{1 - \frac{1}{d_{N(y)}}} |y\rangle. \quad (6.65)$$

The asymptotic probability of presence at x in Cesàro mean is $\pi_x = \frac{d_{N(x)}}{\sum_{y \in \text{Cyc}} d_y}$ if $x \in \text{Cyc}$ and zero otherwise.

Finally, if $\#\text{CC}(\Sigma) \geq 2$, we have $V = C_1 \cup \dots \cup C_r$ and we consider $\mathbb{C}^{|V|} = \bigoplus_{i=1}^r \mathbb{C}^{|C_i|}$, where $\mathbb{C}^{|C_i|}$ is associated with the vertices in C_i . Therefore we can write

$$P = \bigoplus_{i=1}^r P_i, \quad (6.66)$$

where P_i is the restriction of P to the invariant subspaces $\mathbb{C}^{|C_i|}$ for $i \in \{1, 2, \dots, r\}$. Moreover, the results derived above in case Σ is connected apply to each of the P_i 's. In particular, for each $i \in \{1, 2, \dots, r\}$, there exists a unique invariant probability row vector $\pi_i \in \mathbb{C}^{|C_i|}$ for P_i , supported on Cyc_i , the cycle of C_i , according to Lemma 6.9. In the following, we view $\pi_i \in \mathbb{C}^{|C_i|} \subset \mathbb{C}^{|V|}$ as a probability vector on $\mathbb{C}^{|V|}$ and, accordingly, P_i as a matrix on $\mathbb{C}^{|V|}$. We also introduce the corresponding column vectors $\mathbf{1}_i \in \mathbb{C}^{|V|}$ supported on Cyc_i with nonzero components equal to one.

From the decomposition (6.66) and Lemma 6.9, we deduce

$$\frac{1}{N} \sum_{n=0}^{N-1} P^n = \sum_{1 \leq i \leq r} \mathbf{1}_i \pi_i + O(N^{-1}), \quad (6.67)$$

where the sum of the right hand side is the spectral projector of P on its eigenvalue 1, which is of dimension $r = |\text{CC}(\Sigma)|$. Gathering these observations, we obtain in the general case for DFT scattering matrices:

Lemma 6.11 *For $\rho_0 \in \mathcal{DM}(l^2(V))$, the asymptotic probability of presence at x , $Q_n^{\rho_0}(x)$ given by (6.29), satisfies*

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} Q_n^{\rho_0}(x) = \begin{cases} r_0(\text{Cyc}_i) \pi_i(x) & \text{if } x \in \text{Cyc}_i, \\ 0 & \text{otherwise,} \end{cases} \quad (6.68)$$

where π_i is given in Lemma 6.9 the index $i \in \{1, 2, \dots, r\}$ is uniquely determined by x so that $\pi_i(x) > 0$, r_0 is defined by ρ_0 in (6.30) and $r_0(\text{Cyc}_i) = \sum_{y \in \text{Cyc}_i} r_0(y)$.

Moreover, the corresponding asymptotic state (6.22) applied to ρ_0 satisfies

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=0}^{N-1} \Psi_S^n(\rho_0) = \sum_{i=1}^r r_0(\text{Cyc}_i) \sum_{y \in \text{Cyc}_i} |\chi(y)\rangle \langle \chi(y)| \pi_i(y). \quad (6.69)$$

Remark 6.12 *i) The difference between the finite N and asymptotic Cesàro mean probabilities and states is again $O(N^{-1})$.*

ii) Because P is stochastic, (6.67) implies in the limit $N \rightarrow \infty$

$$1 = r_0 \sum_{i=1}^r \mathbf{1}_i \pi_i \mathbf{1} = \sum_{i=1}^r r_0(\text{Cyc}_i), \quad (6.70)$$

so that $\{r_0(\text{Cyc}_i)\}_{1 \leq i \leq r}$ defines a probability on the cycles of Σ .

iii) The asymptotic state is thus the expectation with respect to the probability on the cycles above of the asymptotic states (6.64) for each cycle.

6.2 An infinite Graph with DFT scattering matrices

To complete the picture, we consider a simple example of infinite graph, in the framework of the discrete Fourier transform.

Let G with a set of vertices denoted by \mathbb{Z} with edges between each consecutive integers plus an extra edge between the vertices 0 and +1. Take the scattering matrices given by (6.47) at each vertex, and consider a labelling of the adjacent vertices of $x \in V = \mathbb{Z}$, see (6.48), such that

$$\begin{cases} x_1 = x + 1 & \text{if } x \leq 0, \\ x_1 = x - 1 & \text{if } x \geq 1. \end{cases} \quad (6.71)$$

Accordingly, the only off diagonal nonzero entries of P are, see (6.49),

$$P_{-10} = 1/3, P_{01} = 1/3, P_{21} = 1/3, P_{10} = 1/3 \quad (6.72)$$

and

$$\begin{cases} P_{x-1x} = 1/2 & \text{if } x \leq -1, \\ P_{x+1x} = 1/2 & \text{if } x \geq 2, \end{cases} \quad (6.73)$$

These relations define the map N (6.50), and the diagonal elements are determined by the stochasticity condition. This yields the infinite matrix, where the dots mark the main diagonal, and underlined 00 element $2/3$:

$$P = \begin{pmatrix} \ddots & 1/2 & & & & & \\ & 1/2 & 1/2 & & & & \\ & & 1/2 & 1/2 & & & \\ & & & \underline{2/3} & 1/3 & 0 & \\ & & & 0 & \underline{2/3} & 1/3 & \\ & & & 0 & \underline{1/3} & \underline{2/3} & \\ & & & & & 1/3 & 2/3 & \\ & & & & & & 1/2 & 1/2 & \\ & & & & & & & 1/2 & \ddots \end{pmatrix} \quad (6.74)$$

To this reducible matrix corresponds the situation depicted as Figure 8

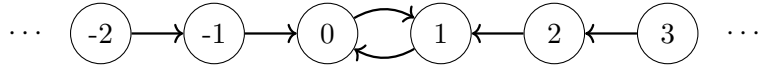


Figure 8: The infinite graph Σ associated with the stochastic matrix P (6.74).

It is readily verified that the only probability vector $\pi \in l^1(\mathbb{Z})$ such that $\pi P = \pi$ has nonzero components

$$\pi_0 = 1/2, \quad \pi_1 = 1/2. \quad (6.75)$$

Incidentally, this is the invariant probability vector of the central 2×2 stochastic bloc

$$G = \begin{pmatrix} 2/3 & 1/3 \\ 1/3 & 2/3 \end{pmatrix}. \quad (6.76)$$

Lemma 6.13 *There exists $\gamma > 0$ and $c > 0$ such that for any $x, y \in \mathbb{Z}$, and $n \geq N(x, y)$*

$$|P_{xy}^n - \pi_y| \leq ce^{-\gamma n}, \quad (6.77)$$

with the understanding that $\pi_y = 0$ for $y \leq -1$ or $y \geq 2$.

The proof of this technical lemma is provided in Appendix C.

As a consequence, thanks to Theorem (6.2), we have in this infinite dimensional example

$$\Psi_S^n(\cdot) = \sum_{y=0}^1 \frac{1}{2} |\chi(y)\rangle \langle \chi(y)| \text{tr}(\cdot) + O(e^{-\gamma n}), \quad (6.78)$$

in where $\chi(y)$ are defined by (6.65), in the weak sense. This result is in keeping with the finite dimensional result Lemma 6.9.

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7 Appendices

Appendix A: This appendix is devoted to the proof of Theorem 3.9. We denote U_α by U for short below, and we occasionally drop the identity symbols in expressions like $F_{jj} - z\mathbb{I}_j$, $z \in \mathbb{C}$, writing $F_{jj} - z$ instead.

Proof: Let us assume that $U\psi = \lambda\psi$, $\lambda \in \mathbb{S}^1$, $\psi \neq 0$. With $\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$, where $\psi_1 = \Pi\psi$, $\psi_2 = (\mathbb{I} - \Pi)\psi$, and (3.11), (3.46), we have, equivalently

$$\begin{cases} F_{11}\psi_1 + e^{i\alpha}F_{12}\psi_2 = \lambda\psi_1 \\ F_{21}\psi_1 + e^{i\alpha}F_{22}\psi_2 = \lambda\psi_2. \end{cases} \quad (7.1)$$

Composing the eigenvalue equation with F , we obtain similarly

$$\begin{cases} \lambda F_{11}\psi_1 + \lambda F_{12}\psi_2 = \psi_1 \\ \lambda F_{21}\psi_1 + \lambda F_{22}\psi_2 = e^{i\alpha}\psi_2. \end{cases} \quad (7.2)$$

Expressing $F_{12}\psi_2$ from the first equation (7.2) and inserting in the first equation (7.1), we get

$$F_{11}\psi_1 = \frac{\lambda^2 - e^{i\alpha}}{\lambda(1 - e^{i\alpha})}\psi_1 = \mu\psi_1, \quad (7.3)$$

while using the last equations (7.2), (7.1) to eliminate $F_{21}\psi_1$ yields similarly

$$F_{22}\psi_2 = -\frac{\lambda^2 - e^{i\alpha}}{\lambda(1 - e^{i\alpha})}\psi_2 = -\mu\psi_2. \quad (7.4)$$

We also note that $\psi_1 = 0$ implies $\psi_2 \neq 0$ and, with $F_{22} = F_{22}^*$,

$$F_{22}\psi_2 = e^{-i\alpha}\lambda\psi_2 = \bar{\lambda}e^{i\alpha}\psi_2 \Rightarrow \lambda = \pm e^{i\alpha} \ \& \ \mu = \mp 1. \quad (7.5)$$

Similarly, $\psi_2 = 0$ implies $\psi_1 \neq 0$ and

$$F_{11}\psi_1 = \lambda\psi_1 = \bar{\lambda}\psi_1 \Rightarrow \lambda = \mu = \pm 1. \quad (7.6)$$

Assume $\lambda \notin \{\pm e^{i\alpha}\}$. Since $\psi_1 \neq 0$ by our choice of λ , (7.3) implies $\mu \in \sigma(F_{11})$. Also, if $\lambda \notin \{\pm 1\}$, then $\psi_2 \neq 0$ so that by (7.4), $-\mu \in \sigma(F_{22})$.

Consider here $\alpha \in (-\pi, \pi) \setminus \{0\}$ and suppose $\lambda = \pm 1$. Then $\mu = \pm 1$, so that $\|F_{11}\psi_1\| = \|\psi_1\| \neq 0$. Since F is unitary and $\Pi, \mathbb{I} - \Pi$ are orthogonal projectors, we deduce that

$$\|\psi_1\|^2 = \|F\psi_1\|^2 = \|F_{11}\psi_1\|^2 + \|F_{21}\psi_1\|^2 = \|\psi_1\|^2 + \|F_{21}\psi_1\|^2 \Rightarrow F_{21}\psi_1 = 0. \quad (7.7)$$

Hence, the second equation (7.1) implies $\psi_2 = 0$, since $F_{22} \mp e^{-i\alpha}\mathbb{I}_2$ is invertible, as $F_{22} = F_{22}^*$. Altogether, $U\psi = \pm\psi$ implies $\psi = \Pi\psi = \psi_1 \neq 0$ and $F_{11}\psi_1 = \pm\psi_1$, *i.e.*

$$\text{Ker}(U \mp \mathbb{I}) \subset \text{Ker}(F_{11} \mp \mathbb{I}_1). \quad (7.8)$$

If $\lambda = \pm e^{i\alpha}$, then $\mu = \mp 1$ and $\psi_2 \neq 0$. Hence $\pm 1 \in \sigma(F_{22})$, and by an argument similar to the one above, $F_{12}\psi_2 = 0$, so that $\psi_1 = 0$ by the first equation (7.1), since $F_{11} \mp e^{i\alpha}\mathbb{I}_1$ is invertible. Hence, $U\psi = \pm e^{i\alpha}\psi$ implies $\psi = (\mathbb{I} - \Pi)\psi = \psi_2$ and $F_{22}\psi_2 = \pm\psi_2$, *i.e.*

$$\text{Ker}(U \mp e^{i\alpha}\mathbb{I}) \subset \text{Ker}(F_{22} \mp \mathbb{I}_2). \quad (7.9)$$

Conversely, assume

$$F_{11}\psi_1 = \mu\psi_1, \quad (7.10)$$

with, for now, $\mu \in (-1, 1)$, $\psi_1 \neq 0$. Then $\phi_\alpha^{-1}(\{\mu\}) = \{\lambda_+, \lambda_-\}$, where $\lambda_\epsilon \neq \pm e^{i\alpha}$, $\epsilon \in \{+, -\}$. We construct two eigenvectors of U associated with λ_+ and λ_- respectively, as follows. With λ denoting λ_+ or λ_- , we set

$$\psi_2 = -e^{-i\alpha}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21}\psi_1, \quad (7.11)$$

which is well defined and consider

$$\psi = \psi_1 + \psi_2 = (\mathbb{I} - e^{-i\alpha}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21})\psi_1. \quad (7.12)$$

Therefore, using $F_{22}\psi_2 = -e^{-i\alpha}F_{21}\psi_1 + \lambda e^{-i\alpha}\psi_2$,

$$\begin{aligned} U\psi &= F_{11}\psi_1 + e^{i\alpha}F_{12}\psi_2 + F_{21}\psi_1 + e^{i\alpha}F_{22}\psi_2 \\ &= \mu\psi_1 + \lambda\psi_2 - F_{12}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21}\psi_1. \end{aligned} \quad (7.13)$$

It thus remains to show that $-F_{12}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21}\psi_1 = (\lambda - \mu)\psi_1$ to get eventually $U\psi = \lambda\psi$. We proceed by considering the Schur complement of the 22 bloc of the invertible operator

$$F - \lambda e^{-i\alpha} = \begin{pmatrix} F_{11} - \lambda e^{-i\alpha} & F_{12} \\ F_{21} & F_{22} - \lambda e^{-i\alpha} \end{pmatrix}, \quad (7.14)$$

given by

$$S_1 = F_{11} - \lambda e^{-i\alpha} - F_{12}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21} : \mathcal{H}_1 \rightarrow \mathcal{H}_1. \quad (7.15)$$

Recall that since $F - \lambda e^{-i\alpha}$ and $F_{11} - \lambda e^{-i\alpha}$ are both invertible, S_1 is invertible as well and such that

$$(F - \lambda e^{-i\alpha})^{-1} = \begin{pmatrix} S_1^{-1} & * \\ * & * \end{pmatrix}, \quad (7.16)$$

where a $*$ denotes a bloc we do not need to know here. Then, since the resolvent of $F = F^* = F^{-1}$ reads for $z \neq \pm 1$

$$(F - z)^{-1} = \frac{F + z}{1 - z^2}, \quad (7.17)$$

we get an alternative expression for S_1^{-1} by considering

$$\frac{F + \lambda e^{-i\alpha}}{1 - \lambda^2 e^{-2i\alpha}} = \begin{pmatrix} S_1^{-1} & * \\ * & * \end{pmatrix}, \quad (7.18)$$

which yields

$$S_1 = (1 - \lambda^2 e^{-2i\alpha})(F_{11} + \lambda e^{-i\alpha})^{-1}. \quad (7.19)$$

Altogether, we deduce from (7.15) and (7.19)

$$-F_{12}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21} = (1 - \lambda^2 e^{-2i\alpha})(F_{11} + \lambda e^{-i\alpha})^{-1} - (F_{11} - \lambda e^{-i\alpha}), \quad (7.20)$$

which applied to ψ_1 gives

$$\begin{aligned} -F_{12}(F_{22} - \lambda e^{-i\alpha})^{-1}F_{21}\psi_1 &= \frac{(1 - \lambda^2 e^{-2i\alpha})}{\mu + \lambda e^{-i\alpha}}\psi_1 - (\mu - \lambda e^{-i\alpha})\psi_1 \\ &= -\mu\psi_1 + \frac{1 + \lambda e^{-i\alpha}\mu}{\mu + \lambda e^{-i\alpha}}\psi_1. \end{aligned} \quad (7.21)$$

Using $\mu = \varphi_\alpha(\lambda)$ under the form $e^{-i\alpha}\lambda^2 + \mu\lambda = 1 + e^{-i\alpha}\mu\lambda$, the last fraction reduces to λ which, together with (7.13), shows $U\psi = \lambda\psi$.

Also, if $\dim \text{Ker}(F_{11} - \mu\mathbb{I}_1) = m_1^\mu > 1$, and $\{\psi_1^{(1)}, \dots, \psi_1^{(m_1^\mu)}\}$ form a basis of this eigenspace, the previous construction yields for each $\psi_1^{(j)}$ two eigenvectors of U associated with λ_- and λ_+ denoted by $\psi_\pm^{(j)}$ via (7.12). Then $\{\psi_\pm^{(1)}, \dots, \psi_\pm^{(m_1^\mu)}\}$ are linearly independent since their projections $\{\Pi\psi_\pm^{(j)}\}$ are, so that

$$\dim \text{Ker}(U - \lambda_\pm \mathbb{I}) \geq \dim \text{Ker}(F_{11} - \mu\mathbb{I}_1). \quad (7.22)$$

With $\mu \in (-1, 1)$ again, so that $\lambda_\pm \notin \{\pm 1\}$, we can start from

$$F_{22}\psi_2 = -\mu\psi_2 \quad (7.23)$$

with $\psi_2 \neq 0$ to construct eigenvectors for U associated with $\lambda \in \{\lambda_-, \lambda_+\} = \varphi_\alpha^{-1}(\{\mu\})$ in a similar way as above. Indeed, setting

$$\psi_1 = -e^{i\alpha}(F_{11} - \lambda)^{-1}F_{12}\psi_2, \quad (7.24)$$

which is well defined, we check using the Schur complement of the 11 bloc of the invertible operator $F - \lambda$, (7.17), and the relation $\varphi_\alpha(\mu) = \lambda$, that

$$\psi = \psi_1 + \psi_2 = (\mathbb{I} - e^{-i\alpha}(F_{11} - \lambda)^{-1}F_{12})\psi_2 \quad (7.25)$$

satisfies $U\psi = \lambda\psi$, for $\lambda = \lambda_-$ and $\lambda = \lambda_+$. And by an argument similar to that just given,

$$\dim \text{Ker}(U - \lambda_\pm \mathbb{I}) \geq \dim \text{Ker}(F_{22} + \mu\mathbb{I}_2). \quad (7.26)$$

We consider now the cases $\mu = \pm 1$ excluded above, assuming $F_{11}\psi_1 = \pm\psi_1 \neq 0$. Equation (7.7) implies $F_{21}\psi_1 = 0$, and we get from (7.13) $U\psi_1 = F_{11}\psi_1 = \pm\psi_1$, *i.e.* $\lambda_\pm = \pm 1 \in \sigma(U)$, where $\pm 1 \in \varphi_\alpha^{-1}(\{\pm 1\})$. This yields

$$\text{Ker}(F_{11} \mp \mathbb{I}_1) \subset \text{Ker}(U \mp \mathbb{I}). \quad (7.27)$$

Note that the vector ψ_2 given in (7.11) is well defined for $\lambda_\pm = \pm 1$ and equals zero, as it should.

Next, we consider $\psi_2 \in \text{Ker}(F_{22} \mp \mathbb{I}_2)$. The equation corresponding to (7.7) with indices exchanged yields $F_{12}\psi_2 = 0$, so that (7.13) implies $U\psi_2 = \pm e^{i\alpha}\psi_2$ and

$$\text{Ker}(F_{22} \mp \mathbb{I}_2) \subset \text{Ker}(U \mp e^{i\alpha}\mathbb{I}). \quad (7.28)$$

Together with (7.8) and (7.9), the last two inclusions prove (3.55).

At this point, we note with (3.48) that

$$\begin{aligned} \sum_{\mu \in \sigma(F_{11})} \dim \text{Ker}(F_{11} - \mu) &= \dim \Pi = |V| \\ \sum_{\mu \in \sigma(F_{22})} \dim \text{Ker}(F_{22} - \mu) &= \dim(\mathbb{I} - \Pi) = |D| - |V|, \end{aligned} \quad (7.29)$$

and that (7.22), (7.26) yield for $\mu \in (-1, 1)$

$$\dim \text{Ker}(U - \lambda_- \mathbb{I}) + \dim \text{Ker}(U - \lambda_+ \mathbb{I}) \geq \dim \text{Ker}(F_{11} - \mu \mathbb{I}_2) + \dim \text{Ker}(F_{22} + \mu \mathbb{I}_2). \quad (7.30)$$

With (3.55), we deduce

$$\begin{aligned} |D| &= \sum_{\lambda \in \sigma(U)} \dim \text{Ker}(U - \lambda) \\ &= \sum_{\lambda \in \sigma(U) \setminus \{\pm 1, \pm e^{i\alpha}\}} \dim \text{Ker}(U - \lambda) + \sum_{\lambda \in \{\pm 1, \pm e^{i\alpha}\}} \dim \text{Ker}(U - \lambda) \\ &\geq \sum_{\mu \in \sigma(F_{11})} \dim \text{Ker}(F_{11} - \mu) + \sum_{\mu \in \sigma(F_{22})} \dim \text{Ker}(F_{22} - \mu) = |D|. \end{aligned} \quad (7.31)$$

Therefore, we have equality in (7.30) for all $\mu \in (-1, 1)$. In turn, with (7.22), (7.26) this implies

$$\dim \text{Ker}(U - \lambda_{\pm} \mathbb{I}) = \dim(\text{Ker } F_{11} - \mu \mathbb{I}_2) = \dim(\text{Ker } F_{22} + \mu \mathbb{I}_2). \quad (7.32)$$

This ends the proof in the case $\alpha \in (-\pi, \pi) \setminus \{0\}$.

When $\alpha = \pi$, the potential eigenvalues $\pm e^{i\alpha}$ and ∓ 1 for U are degenerate, which requires revisiting the argument. Assuming $U\psi = \lambda\psi$ with $\psi \neq 0$ and $\lambda = \pm 1$, we do not have necessarily $\psi_1 \neq 0$. However we derive from (7.1) and (7.2) that

$$F_{11}\psi_1 \mp \psi_1 = 0 \quad \text{and} \quad F_{22}\psi_2 \pm \psi_2 = 0, \quad (7.33)$$

which implies

$$\Pi \text{Ker}(U \mp \mathbb{I}) \subset \text{Ker}(F_{11} \mp \mathbb{I}_1), \quad \text{and} \quad (\mathbb{I} - \Pi) \text{Ker}(U \mp \mathbb{I}) \subset \text{Ker}(F_{22} \mp \mathbb{I}_2). \quad (7.34)$$

Conversely, if $0 \neq \psi_1 \in \text{Ker}(F_{11} \mp \mathbb{I}_1)$, then $F_{21}\psi_1 = 0$, see (7.7), so that $U\psi_1 = \pm\psi_1$. Similarly, $0 \neq \psi_2 \in \text{Ker}(F_{22} \mp \mathbb{I}_2)$ implies $U\psi_2 = \mp\psi_2$. In other words,

$$\text{Ker}(F_{11} \mp \mathbb{I}_1) \subset \text{Ker}(U \mp \mathbb{I}), \quad \text{and} \quad \text{Ker}(F_{22} \pm \mathbb{I}_2) \subset \text{Ker}(U \mp \mathbb{I}), \quad (7.35)$$

where the subspaces $\text{Ker}(F_{11} \mp \mathbb{I}_1)$ and $\text{Ker}(F_{22} \pm \mathbb{I}_2)$ are orthogonal. Hence the validity of (3.56). Since (7.30) also holds for $\alpha = \pi$ and $-1 < \mu < 1$, we can argue as (7.31) to deduce the validity of (3.54) for $\alpha = \pi$. \square

Appendix B: Let us prove Lemma 5.9. We first observe that (5.30) implies

$$\Phi^{\text{Diag}}(e_{2x+1}) = \Phi^{\text{Diag}}(e_{2(x+2)}), \quad (7.36)$$

which allows us to focus on $\Phi^{\text{Diag}^n}(e_{2x})$, for $n \in \mathbb{N}$. Consequently,

$$\Phi^{\text{Diag}^2}(e_{2x}) = \frac{1}{2}(\Phi^{\text{Diag}}(e_{2(x-1)}) + \Phi^{\text{Diag}}(e_{2(x+1)})). \quad (7.37)$$

By induction one gets for any $n \in \mathbb{N}$

$$\Phi^{\text{Diag}^n}(e_{2x}) = \frac{1}{2^{n-1}} \sum_{k=0}^{n-1} \binom{n-1}{k} \Phi^{\text{Diag}}(e_{2(x-(n-1)+2k)}), \quad (7.38)$$

where

$$\Phi^{\text{Diag}}(e_{2(x-(n-1)+2k)}) = \frac{1}{2}(e_{2(x-n+2k)} + e_{2(x-n+2k+1)}). \quad (7.39)$$

Therefore, the matrix elements of Φ^{Diag} read, using (7.36),

$$\begin{aligned}\Phi_{2y\ 2x}^{\text{Diag}^n} &= \Phi_{2y+1\ 2x}^{\text{Diag}^n} = \frac{1}{2^n} \binom{n-1}{\frac{n+y-x}{2}} \\ \Phi_{2y\ 2x+1}^{\text{Diag}^n} &= \Phi_{2y\ 2x+1}^{\text{Diag}^n} = \frac{1}{2^n} \binom{n-1}{\frac{n+y-x}{2} - 1}.\end{aligned}\quad (7.40)$$

with the understanding that $\binom{r}{s} = 0$ if $r < s$, or $(r, s) \notin \mathbb{N} \times \mathbb{N}$. It remains to establish the asymptotics for n large of the right hand sides. Consider the (nonzero) binomial coefficient

$$\binom{N}{\frac{N+\Delta}{2}} = \frac{N!}{\frac{N+\Delta}{2}! \frac{N-\Delta}{2}!}, \quad (7.41)$$

for Δ fixed, as $N \rightarrow \infty$, with N and Δ of identical parity. Using Stirling's formula $N! = \sqrt{2\pi N} (N/e)^N (1 + o(N))$, we infer

$$\frac{1}{2^{N+1}} \binom{N}{\frac{N+\Delta}{2}} = \frac{1}{\sqrt{2\pi N}} + o(N) \leq c/\sqrt{N}, \quad \forall N \geq N_0(\Delta), \quad (7.42)$$

which proves the statement. \square

Appendix C: This appendix sketches an alternative spectral argument to show Corollary 6.4. Since the stochastic matrix P satisfies $\|P^n\|_\infty \leq 1$ for all $n \in \mathbb{N}$, where $\|M\|_\infty = \max_{1 \leq i \leq d} \sum_{j=1}^n |M_{ij}|$, for any $M \in M_d(\mathbb{C})$, and admits $\mathbf{1}$ as an invariant vector, it has spectral radius 1. Moreover, all its eigenvalues of modulus 1 are semi-simple. In case the eigenvalue 1 is simple, the rank one matrix $\mathbf{1}\pi$ is the corresponding spectral projector such that $\pi P = \pi$. Since the eigenvalues of P have either modulus strictly smaller than 1, or have modulus one and are semi-simple, the Cesàro mean (6.35) holds thanks to functional calculus, see [Ka]. In case no other eigenvalue than 1 has modulus 1, one gets $P^n = \mathbf{1}\pi + O(e^{-\gamma n})$, $\gamma > 0$, by functional calculus again. Finally, noting that P^n and its Cesàro mean are stochastic matrices, the xy matrix element of (6.35) satisfies $0 \leq \frac{1}{N} \sum_{n=0}^{N-1} P^n_{xy} = \pi_y + O(N^{-1})$, which yields $\pi_y \geq 0$, in the limit $N \rightarrow \infty$.

When $\dim \text{Ker}(P - 1) > 1$, the same result holds, with the spectral projector $P_{\{1\}}$ onto $\text{Ker}(P - 1)$ in place of $\mathbf{1}\pi$.

Appendix D: We prove Lemma 6.13 here. Let us decompose the operator (6.74) as

$$P = B + C, \quad \text{where } C = \frac{1}{3}(|-1\rangle\langle 0| + |2\rangle\langle 1|), \quad (7.43)$$

and B has the bloc decomposition

$$B = \begin{pmatrix} \sigma_- & 0 & 0 \\ 0 & G & 0 \\ 0 & 0 & \sigma_+ \end{pmatrix} = \sigma + G. \quad (7.44)$$

Here G is defined in (6.76) and σ_\pm correspond, up to a factor 1/2 and except for one diagonal element, to the identity plus a one sided shift. The immediate properties

$$\sigma G = G \sigma = 0, \quad C^2 = 0, \quad C \sigma^n = 0, \quad G^n C = 0, \quad (7.45)$$

yield

$$P^n = (B + C)^n = B^n + \sum_{k=0}^{n-1} \sigma^k C G^{n-(k+1)}. \quad (7.46)$$

Moreover, this implies that the general term of the sum satisfies

$$\langle x | \sigma^k C G^{n-(k+1)} y \rangle = 0 \quad \text{if } 0 \leq x \leq 1 \text{ or } y \in \{0, 1\}^C, \quad (7.47)$$

which with the bloc structure of B^n shows that $P_{xy}^n = 0$ for $x \geq 0$ and $y \leq -1$, or for $x \leq 1$ and $y \geq 2$.

We check by induction that for $y \geq 3$

$$P^n |y\rangle = B^n |y\rangle = \sigma^n |y\rangle = \frac{1}{2^n} \sum_{k=0}^n \binom{n}{k} |y+k\rangle, \quad (7.48)$$

while for $y \leq -2$, the same formula holds with $|y-k\rangle$ in place of $|y+k\rangle$. Hence $P_{xy}^n = 0$ for $x < y$ and $y \geq 3$, and for $x > y$ and $y \leq -2$.

For $y = 2$, the expression is a little different due to the value $2/3$ of the entry 22 of σ_+ . By induction

$$P^n |2\rangle = \left(\frac{2}{3}\right)^n \left\{ |2\rangle + \frac{1}{2} \sum_{k=0}^{n-1} \left(\frac{2}{3}\right)^{-k-1} P^k |3\rangle \right\}, \quad (7.49)$$

while the same expression holds for $P^n | -1\rangle$, with $| -2\rangle$ in place of $|3\rangle$.

The spectral decomposition of the 2×2 bloc G (6.76) reads

$$G = Q_{\{1\}} + \frac{1}{3} Q_{\{1/3\}}, \quad (7.50)$$

where $\sigma(G) = \{1, 1/3\}$ and the corresponding eigenprojectors are $Q_{\{1\}} = \frac{1}{2} |\mathbf{1}\rangle \langle \mathbf{1}| = \mathbf{1}\pi$, with π given in (6.75), and $Q_{\{1/3\}} = \mathbb{I} - Q_{\{1\}}$.

This yields for $0 \leq x \leq 1, 0 \leq y \leq 1$

$$P_{xy}^n = B_{xy}^n = G_{xy}^n = Q_{1xy} + O(e^{-\gamma n}) = \pi_y + O(e^{-\gamma n}), \quad (7.51)$$

for $0 < \gamma \leq \ln 3$. For $x, y \geq 3$, with $x \geq y$,

$$P_{xy}^n = \sigma_{xy}^n = \frac{1}{2^n} \binom{n}{x-y} \leq \frac{1}{2^n} \frac{n^{x-y}}{(x-y)!} \leq e^{-\gamma n}, \quad (7.52)$$

for $0 < \gamma < \ln 2$, and $n \geq N'(x-y)$, for some $N'(x-y) > 0$. A similar bound holds in case $x, y \leq -2$. Equation (7.49) implies $P_{22}^n = P_{-1-1}^n = (2/3)^n \leq e^{-n \ln(3/2)}$, and together with (7.48) for $x \geq 3$,

$$P_{x2}^n = \left(\frac{2}{3}\right)^n \frac{1}{2} \sum_{k=0}^{n-1} \left(\frac{2}{3}\right)^{-k-1} P_{x3}^k = \left(\frac{2}{3}\right)^{n-1} \frac{1}{2} \sum_{k=x-3}^{n-1} \left(\frac{3}{4}\right)^k \binom{k}{x-3}. \quad (7.53)$$

Thanks to the relation for any $z \in \mathbb{C}$, s.t. $|z| < 1, j \geq 0$,

$$\left| \sum_{k=j}^M z^k \binom{k}{j} - \frac{z^j}{(1-z)^{j+1}} \right| \leq c e^{-\gamma_z M}, \quad (7.54)$$

for $0 < \gamma_z < |\ln |z||$, $c = c(\gamma_z)$ and $M \geq N_0(j)$, we eventually obtain for $n \geq N''(x)$,

$$P_{x2}^n = \left(\frac{2}{3}\right)^n (3^{x-2} + O(e^{-\gamma_z n})) \leq (3^{x-2} + 1) e^{-n \ln(3/2)} \leq C_0 e^{-\gamma n}, \quad (7.55)$$

where $0 < \gamma < \ln(3/2)$, and C_0 is independent of x . Note that the error term can be made uniform in x by lowering the value of γ , and choosing n large enough, in an x dependent way. A similar estimate holds for P_{x-1}^n , $x \leq -2$.

We are left to consider the sum in (7.46) for $x \in \{0, 1\}^C$ and $y \in \{0, 1\}$. Assume $x \geq 2$, the case $x \leq -1$ being similar.

For $x \geq 3$, we have thanks to (7.43) and (7.53)

$$\sum_{k=0}^{n-1} \langle x | \sigma^k C G^{n-(k+1)} y \rangle = \sum_{k=x-2}^{n-1} \frac{1}{3} \left(\frac{2}{3}\right)^{k-1} \frac{1}{2} \sum_{l=x-3}^{k-1} \left(\frac{3}{4}\right)^l \binom{l}{x-3} \langle 1 | G^{n-(k+1)} y \rangle. \quad (7.56)$$

Inserting the spectral decomposition of G into the scalar product, we get $\langle 1 | Q_{\{1\}} y \rangle = \pi_y$ for the contribution stemming from the eigenprojector $Q_{\{1\}}$. Exchanging the summation indices, the remaining double sum reads

$$\frac{1}{4} \sum_{l=x-3}^{n-2} \left(\frac{3}{4}\right)^l \binom{l}{x-3} \sum_{k=l+1}^{n-1} \left(\frac{2}{3}\right)^k = \frac{3}{4} \sum_{l=x-3}^{n-2} \left(\frac{3}{4}\right)^l \binom{l}{x-3} \left\{ \left(\frac{2}{3}\right)^{l+1} - \left(\frac{2}{3}\right)^n \right\}. \quad (7.57)$$

Using (7.54), the first contribution equals $1 + O(e^{-\gamma n})$ while, the second is $O(e^{-\gamma n})$, for some $0 < \gamma < \ln(3/2)$. Let us show that the contribution from the second spectral projector to (7.56) is exponentially decreasing. The corresponding scalar product in the right hand side of the sum reads

$$\frac{3^{(k+1)}}{3^n} \langle 1 | Q_{\{1/3\}} y \rangle \quad (7.58)$$

so that performing the same steps as above, the double sum is now of order

$$\begin{aligned} \frac{1}{3^n} \sum_{l=x-3}^{n-2} \left(\frac{3}{4}\right)^l \binom{l}{x-3} \sum_{k=l+1}^{n-1} 2^k &= \frac{1}{3^n} \sum_{l=x-3}^{n-2} \left(\frac{3}{4}\right)^l \binom{l}{x-3} (2^n - 2^{l+1}) \\ &\leq \frac{1}{3^n} \sum_{l=x-3}^{n-2} \left(\frac{3}{4}\right)^l \binom{l}{x-3} 2^n. \end{aligned} \quad (7.59)$$

The last series is of order $(2/3)^n$ by (7.54), so that we eventually get for $x \geq 3$, $y \in \{0, 1\}$

$$P_{xy}^n = \pi_y + O(e^{-\gamma n}), \quad (7.60)$$

where $0 < \gamma < \ln 2$, for $n \geq N'''(x)$.

Eventually, we address the entry P_{2y}^n , $y \in \{0, 1\}$, which reads thanks to (7.48), (7.49) and (7.50)

$$\begin{aligned} P_{2y}^n &= \sum_{k=0}^{n-1} \frac{1}{3} \langle 2 | \sigma^k 2 \rangle \left(\langle 1 | Q_{\{1\}} y \rangle + \frac{1}{3^{n-(k+1)}} \langle 1 | Q_{\{1/3\}} y \rangle \right) \\ &= \sum_{k=0}^{n-1} \frac{1}{3} \left(\frac{2}{3}\right)^k \left(\pi_y + \frac{3^{k+1}}{3^n} \langle 1 | Q_{\{1/3\}} y \rangle \right). \end{aligned} \quad (7.61)$$

Computing the geometric series, one gets $P_{2y}^n = \pi_y + O(e^{-\gamma n})$, for $\gamma > 0$, which finishes the proof of the lemma. \square

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