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MEAN HITTING TIME STATISTICS OF QUANTUM DYNAMICS IN TERMS OF GENERALIZED INVERSES

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Resumo. Neste trabalho apresentamos métodos para calcular o tempo médio de primeira visita de partículas quânticas agindo em grafos finitos. As expressões obtidas são dadas em termos de inversas generalizadas associadas com dinâmicas completamente positivas que preservam traço, os chamados canais quânticos. O contexto considerado aqui pertence à área de informação e computação quântica, e os teoremas provados neste trabalho estendem resultados recentes no assunto, no sentido de que a suposição de irreducibilidade pode ser substituída por uma hipótese estritamente mais fraca, aumentando a aplicabilidade dos resultados para uma classe maior de exemplos incluindo, por exemplo, passeios quânticos unitários.

Palavras-chave: mecânica quântica; passeios quânticos; tempos médios de primeira visita; canais quânticos

Abstract. In this work we present methods for calculating the mean hitting time of first visit for quantum particles acting on finite graphs. The expressions obtained are given in terms of generalized inverses associated with trace-preserving, completely positive dynamics, the so-called quantum channels. The setting considered here belongs to the realm of quantum information and computation, and the theorems proved in the work extend recent results on the subject in that the technical assumption of irreducibility can be replaced by a strictly weaker one, allowing the applicability of the results to a larger class of examples, such as unitary quantum walks.

Keywords: quantum mechanics; quantum walks; mean time of first visit; quantum channels

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Contents

Introduction

The purpose of this thesis is to discuss basic statistics of quantum versions of random walks on graphs. The main question we will address is motivated by the following setting, coming from the classical theory of Markov chains: given a graph and transition probabilities between its vertices, what is the mean time for a walker to reach vertex j for the first time, given that it has started at vertex i? Formally, the mean hitting time is given by

$$E_i(T_j) = \sum_t t P_i(T_j = t)$$

where T_j is the random variable given by the time of first visit to vertex j, and $P_i(T_j = t)$ is the probability that $T_j = t$, given that the walk begins at position i.

From the theory of Markov chains we know that, alternatively, the mean hitting time can be calculated without resorting to its definition directly. A well-known method is via the fundamental matrix associated with a finite ergodic Markov chain with stochastic matrix P,

$$Z = (I - P + \Omega)^{-1}$$

where $\Omega = \lim_{n\to\infty} P^n$, and for which the following equation is valid:

$$E_i(T_j) = \frac{Z_{jj} - Z_{ij}}{\pi_j}. \tag{0.0.1}$$

Above, $\pi = (\pi_i)$ denotes the unique fixed probability associated with the walk. This is the **mean hitting time formula (MHTF)**, and is one of several expressions relating Z with statistical quantities of the walk [1, 8].

In the context of quantum information and computation, the problem of finding quantum versions of the MHTF has been studied in [23] in the context of open quantum walks on finite graphs, and later in [24] where quantum Markov chains are considered. Shortly after, a version of the MHTF was proved for positive maps [25]. We remark that in all such works we have the important assumption that the walks are irreducible, which can be seen as a kind of “connectivity” of the walk. As we will be considering particles with internal degrees of freedom, one should work with a careful, precise definition regarding the accessibility of the vertices.

We also remark that [23] and [25] present formulae in terms of a so-called fundamental matrix Z, whereas [24] also discusses expressions in terms of generalized inverses of the dynamics, following [20] (we remark that Z is a generalized inverse as well).

The results of this thesis concern the problem of obtaining mean hitting time expressions for more general quantum dynamics, namely, we consider a strictly larger set of operators, given by quantum channels, which are trace-preserving, completely positive maps acting on some finite-dimensional Hilbert space [31]. In addition, we will discuss how one is able to replace the assumption of irreducibility. This latter point is of crucial importance if one wishes to consider hitting time expressions in terms of generalized inverses for certain dynamics, such as unitary quantum walks: as conjugation operators, these are usually reducible. Nevertheless, their dynamics is quite nontrivial and, as we will see, we are able to find hitting time expressions in such cases as well. The key to such development is to make considerations on the spectra of certain generating functions associated with the walk.

In Chapter 1 we review basic definition regarding generalized inverses, Markov chains, discrete-time quantum walks and quantum Markov chains. Then we explain how to associate any quantum channel with a quantum Markov chain, so that one can make use of previous results regarding hitting times. Then, after a discussion of a more specific generalized inverse (the so-called group inverse), we will be in position to establish new results, by replacing the assumption of irreducibility with a strictly weaker assumption.

In Chapter 2, we discuss hitting times for continuous-time quantum walks. There, we are able to draw similarities and differences with respect to the discrete-time case, and we take the opportunity to present several examples. During the preparation of this work, the author has made use of the software Maple to make conjectures, verify calculations and present examples we believe are instructive to the reader.

Chapter 1

Discrete-time QMCs

1.1 Generalized inverses

Here we define two kinds of generalized inverses. The first one, which we will call g-inverse, has the property of solving equations involving matrices. The second one, the Drazin inverse, has other interesting properties and, in some cases, it is also a g-inverse. These facts will be explained more carefully in this section. The content presented here, along with a more comprehensive treatment on this subject, can be found in [4] and [12].

Let us denote matrices by uppercase letters A, B, C, and so on, over a field $\mathbb{F}$ which can stand for the real numbers or the complex numbers. If the matrices have m rows and n columns, we say that it is an $m \times n$ matrix. The set of $m \times n$ matrices over $\mathbb{F}$ will be denoted by $\mathbb{F}^{m\times n}$. We write $\mathbb{F}^n$ for the space of column vectors with entries in $\mathbb{F}$. In a multiplication of matrices where their dimensions are not specified, it is always assumed that they are such that the operation is well defined.

Definition 1.1. *A* **g-inverse** *of a matrix $A \in \mathbb{F}^{m\times n}$ is any matrix A^- such that*

$$AA^-A = A.$$

What we refer to as a g-inverse here is called a (1)-inverse in the literature cited above. The reason for this is because condition $AA^-A = A$ satisfied by A^- given in Definition 1.1 is conventionally numbered as equation (1) among a set of four equations called **Penrose equations** or **Penrose conditions**. Different combinations of these conditions define different kinds of generalized inverses. For example, inverses that satisfy conditions i, j and k are called (i, j, k)-inverses. We will not be concerned with those in this work, so we drop the notation with prefixed numbers and adopt instead the term 'g-inverse' used by Hunter [20].

We can see from Definition 1.1 that if a matrix A is invertible, then $A^- = A^{-1}$ is the only g-inverse of A.

A possible motivation for defining a g-inverse can be given by the following application to linear systems. Let $A \in \mathbb{F}^{m\times n}$ and $\mathbf{x} \in \mathbb{F}^n$ and $\mathbf{b} \in \mathbb{F}^m$, and consider the system

$$A\mathbf{x} = \mathbf{b}$$

which we are trying to solve for $\mathbf{x}$. We know that if A is non-singular, we can solve it and obtain the unique solution $\mathbf{x} = A^{-1}\mathbf{b}$. In the more general case where A is singular or non square, we might ask whether there is an $X \in \mathbb{F}^{n\times m}$ such that whenever $A\mathbf{x} = \mathbf{b}$ has a solution, it follows that $\mathbf{x} = X\mathbf{b}$ is a solution. If the answer is yes, then we consider equations $A\mathbf{e}_i = \mathbf{a}_i$, for $i = 1, 2, \dots, m$ where $\mathbf{e}_i \in \mathbb{F}^n$ are the standard basis vectors for $\mathbb{F}^n$ and $\mathbf{a}_i \in \mathbb{F}^m$ is the i-th column of A. These equations make clear that for $i = 1, \dots, m$, the system $A\mathbf{x} = \mathbf{a}_i$ has a solution. Then, as we are supposing, there exists for each one of these, respectively, a solution of the form $\mathbf{x} = X\mathbf{a}_i$. So substituting this $\mathbf{x}$ into $A\mathbf{x} = \mathbf{a}_i$, we have that $AX\mathbf{a}_i = \mathbf{a}_i$, which implies, because $\mathbf{a}_i = A\mathbf{e}_i$, that $AXA\mathbf{e}_i = A\mathbf{e}_i$ for each $\mathbf{e}_i$. Thus we have $AXA = A$.

On the other hand, suppose we have a matrix X such that $AXA = A$. If $A\mathbf{x} = \mathbf{b}$ has a solution, then

$$\mathbf{b} = A\mathbf{x} = AXA\mathbf{x} = AX\mathbf{b}$$

from which we see that $X\mathbf{b}$ is a solution.

In conclusion, we have that if X is a g-inverse of A, then it has the property of solving linear systems $A\mathbf{x} = \mathbf{b}$. And it is a fact that for any given matrix, it always has a g-inverse, as explained below.

Let A be any $m \times n$ matrix and suppose it has rank r. We can always perform a Gauss-Jordan elimination to transform the matrix into its **reduced row-echelon form**. In this form, the matrix will have the following properties:

1. each of the first r rows contain at least one non-zero element, and the remaining rows consist only of zero elements.
2. the first non-zero element in each row is 1, and it is strictly to the right of the first non-zero element of the row above.
3. each first non-zero element of a row is the only non-zero element of its column.

To illustrate, here is an example of a matrix in reduced row-echelon form:

$$\begin{bmatrix} 1 & a & 0 & 0 & b \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & c \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

The steps taken to reduce a $m \times n$ matrix to this form are elementary row operations, each of which can be achieved by multiplying the matrix on the left by an invertible $m \times m$ matrix E_i. So reducing our matrix A in k steps is equivalent to multiplying it on the left successively by k invertible matrices $E_1, \dots, E_k$, or equivalently, multiply it on the left by $E_k E_{k-1} \cdots E_1 = E$, an invertible matrix. In other words, given a matrix A, there always exists an invertible matrix E such that EA is in reduced row-echelon form.

Now given a matrix of rank r in reduced row-echelon form, we can perform a permutation on its columns to achieve a matrix of the form

$$R := \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} \tag{1.1.1}$$

where I_r is the $r \times r$ identity, the O's denote zero matrices, and K is any matrix, observing that the O's and K must be of suitable dimensions.

By noting that a permutation on the columns of a $m \times n$ matrix can be effected by multiplying it on the right by some $n \times n$ permutation matrix P, which is always invertible, we can do this to our reduced matrix EA and obtain

$$EAP = \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} \quad \Longrightarrow \quad A = E^{-1} \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} P^{-1} = E^{-1} R P^{-1}. \tag{1.1.2}$$

Now consider the $n \times m$ matrix

$$S := \begin{bmatrix} I_r & O \\ O & L \end{bmatrix}$$

where L is any $(n-r) \times (m-r)$ matrix. We have that

$$\begin{aligned} RSR &= \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} \cdot \begin{bmatrix} I_r & O \\ O & L \end{bmatrix} \cdot \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} \\ &= \begin{bmatrix} I_r & O \\ O & O \end{bmatrix} \cdot \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} = \begin{bmatrix} I_r & K \\ O & O \end{bmatrix} = R, \end{aligned}$$

so S satisfy the definition of a generalized inverse for R.

Finally, to obtain a generalized inverse for our $m \times n$ matrix A, we simply define $X := PSE$, and then we have

$$AXA = (E^{-1}RP^{-1})(PSE)(E^{-1}RP^{-1}) = E^{-1}RSRP^{-1} = E^{-1}RP^{-1} = A.$$

This discussion shows that there exists a g-inverse for any given matrix, and it also sketches a procedure for its construction.

We will mainly be interested in matricial equations of the form $AXB = C$ where A, B, C are given and we want to solve for X. For that purpose, we will use the results presented below.

Theorem 1.2. *A necessary and sufficient condition for the equation $AXB = C$ to be consistent is that $AA^-CB^-B = C$, where A^- and B^- are any g-inverses for A and B, respectively. In this case, the general solution is given by*

$$X = A^-CB^- + H - A^-AHBB^-,$$

where H is an arbitrary matrix.

Proof. Let A^- and B^- be generalized inverses for A and B, respectively. If $AXB = C$ has a solution X_0, then

$$AA^-CB^-B = AA^-AX_0BB^-B = AX_0B = C.$$

Conversely, if $AA^-CB^-B = C$, then X_0 given by $X_0 = A^-CB^-$ is a solution to $AXB = C$.

Now suppose that the equation is consistent. Then as we have seen, $X_0 = A^-CB^-$ is a solution, and it is easy to check that for arbitrary H,

$$A^-CB^- + H - A^-AHBB^- \tag{1.1.3}$$

is also a solution to the equation: just multiply it on the left by A and on the right by B, and it gives us $AA^-CBB^- + AHB - AA^-AHBB^-B = AA^-CBB^- + AHB - AHB = AA^-CB^-B = C$, where the last equality is due to the consistency condition.

Finally, if X_0 is any solution to $AXB = C$, then by choosing $H = X_0$ in 1.1.3, we obtain

$$A^-CB^- + X_0 - A^-AX_0BB^- = A^-CB^- + X_0 - A^-CB^- = X_0,$$

therefore every possible solution is of the given form, and this completes the proof.

□

In the case where in the equation $AXB = C$ either A or B are equal to the identity of the suitable dimension, we can apply Theorem 1.2 to this simpler case, and note that the only generalized inverse of the identity matrix is itself. This observation gives us the following:

Corollary 1.3. *A necessary and sufficient condition for the equation $AX = C$ to be consistent is that $AA^-C = C$, where A^- is any g-inverse of A, in which case the general solution is given by*

$$X = A^-C + (I - A^-A)U,$$

where U is an arbitrary matrix.

A necessary and sufficient condition for the equation $XB = C$ to be consistent is that $CB^-B = C$, where B^- is any g-inverse of B, in which case the general solution is given by

$$X = CB^- + V(I - BB^-),$$

where V is an arbitrary matrix.

We note that in general the g-inverse of a given matrix is not unique. The next theorem ([20], Section 3) characterizes all the g-inverses of a given matrix.

Theorem 1.4. *If A^- is any g-inverse of A, then all g-inverses of A can be characterized as members of the following equivalent sets:*

$$\{A^-AA^- + H - A^-AHAA^- \mid H \text{ arbitrary}\} \tag{1.1.4}$$
$$\{A^-AA^- + (I - A^-A)U + V(I - AA^-) \mid U, V \text{ arbitrary}\} \tag{1.1.5}$$
$$\{A^- + W - A^-AWAA^- \mid W \text{ arbitrary}\} \tag{1.1.6}$$
$$\{A^- + (I - A^-A)F + G(I - AA^-) \mid F, G \text{ arbitrary}\} \tag{1.1.7}$$

Proof. We apply Theorem 1.2 to solve $AXA = A$ for X by choosing $B = C = A$. The solution immediately gives us the set (1.1.4). To see the inclusion (1.1.4) $\subset$ (1.1.5), we simply choose $U = \frac{1}{2}HAA^- + \frac{1}{2}H$ and $V = \frac{1}{2}A^-AH + \frac{1}{2}H$ for an element of the set (1.1.5) so we get

$$\begin{aligned}
&A^-AA^- + (I - A^-A)\left(\frac{1}{2}HAA^- + \frac{1}{2}H\right) + \left(\frac{1}{2}A^-AH + \frac{1}{2}H\right)(I - AA^-) \\
=&A^-AA^- + 2\frac{1}{2}H - 2\frac{1}{2}A^-AHAA^- + \cancel{\frac{1}{2}HAA^-} - \cancel{\frac{1}{2}A^-AH} + \cancel{\frac{1}{2}A^-AH} - \cancel{\frac{1}{2}HAA^-} \\
=&A^-AA^- + H - A^-AHAA^-,
\end{aligned}$$

which is an element of (1.1.4). To show the reverse inclusion, choose $H = (I - A^-A)U + V(I - AA^-)$ for an element of the set (1.1.4) and we get

$$\begin{aligned}
&A^-AA^- + (I - A^-A)U + V(I - AA^-) - \cancel{A^-A((I - A^-A)U + V(I - AA^-))AA^-} \\
=&A^-AA^- + (I - A^-A)U + V(I - AA^-),
\end{aligned}$$

which is an element of (1.1.5). The terms above cancel out because $A^-A(I - A^-A) = 0$ and $(I - AA^-)AA^- = 0$. We have therefore the equivalence of the first 2 sets.

To obtain the inclusion (1.1.6)$\subset$ (1.1.4), choose $H = W + A^-$ for an element of (1.1.6) and we obtain

$$\begin{aligned}
&A^-AA^- + (W + A^-) - A^-A(W + A^-)AA^- \\
=&A^-AA^- + W + A^- - A^-AWAA^- - A^-AA^-AA^- \\
=&\cancel{A^-AA^-} + W + A^- - A^-AWAA^- - \cancel{A^-AA^-} \\
=&A^- + W - A^-AWAA^-,
\end{aligned}$$

which is an element of (1.1.6). To show the reverse inclusion, we choose $W = H + A^-AA^-$ for an element of (1.1.6) to obtain any given element of (1.1.4).

We have so far that the first three sets are all equivalent. The equivalence between (1.1.6) an (1.1.7) is shown in the same manner as the equivalence of the first two sets, completing the proof.

□

The next generalized inverse, unlike the previous definition, is only defined for square matrices. First, we define the index of a matrix.

Definition 1.5. *Given a matrix $A \in \mathbb{F}^{n\times n}$, the least nonnegative integer k such that* $\mathrm{Ran}(A^k) = \mathrm{Ran}(A^{k+1})$ *is the* **index** *of A, denoted by* $\mathrm{Ind}(A) = k$.

Observation: we consider A^0 to be the identity matrix for any matrix A. So, for example, nonsingular matrices are precisely those with index zero.

Definition 1.6. *If $A \in \mathbb{F}^{n\times n}$ with* $\mathrm{Ind}(A) = k$, *and if $A^D \in \mathbb{F}^{n\times n}$ is a matrix such that*

1. $A^DAA^D = A^D$
2. $A^DA = AA^D$
3. $A^{k+1}A^D = A^k$

then A^D is called the **Drazin inverse** *of A.*

It can be shown that the Drazin inverse of an $n \times n$ matrix always exists and is unique [p. 123, [12]].

We note that the Drazin inverse is not a g-inverse (Def. 1.1) in general. The next theorem [Theorem 7.2.4, [12]] specifies when that happens.

Theorem 1.7. *Let $A \in F^{n\times n}$. Then $AA^DA = A$ if, and only if* $\mathrm{Ind}(A) \leq 1$.

A Drazin inverse which is also a g-inverse receives a special name:

Definition 1.8. *Let $A \in \mathbb{F}^{n\times n}$ with $\operatorname{Ind}(A) \leq 1$. Then the Drazin inverse of A is denoted by $A^{\#}$ and called the* **group inverse** *of A.*

We could have alternatively defined the group inverse, given a square matrix A as the unique matrix $A^{\#}$, when it exists, satisfying the three following conditions:

$$A^{\#}AA^{\#} = A^{\#}, \quad A^{\#}A = AA^{\#}, \quad AA^{\#}A = A.$$

The group inverse of a given square matrix exists, by Theorem 1.7, precisely when its index is not greater than 1.

This inverse will be essential for the study of formulas for reducible open quantum walks and quantum Markov chains, as we will see later.

1.2 Classical Markov Chains

In this section we review some concepts of Markov chains, in particular mean hitting times, and how generalized inverses can be applied to obtain these quantities from the transition probabilities of the chain. This goes in parallel to what will be presented in the next sections, where we use generalized inverses to calculate related quantities in the quantum setting.

For notation, we will use in this section uppercase letters $A, M, P, \ldots$ to denote matrices, and lowercase boldface letters $\mathbf{e}, \mathbf{f}, \mathbf{g}, \ldots$ to denote column-vectors. We consider a prime in $\boldsymbol{\pi}', \mathbf{u}', \ldots$ to denote $\boldsymbol{\pi}^T, \boldsymbol{u}^T$, the transposed matrix of the column-vectors $\boldsymbol{\pi}, \mathbf{u}$, which are row-vectors.

Let $\{X_n\}$, $n = 0, 1, 2, \ldots, m$ be a discrete time Markov Chain with finite state space $S = \{1, 2, \ldots, m\}$ and transition probability matrix $P = [p_{ij}]$, where $p_{ij} := \mathbf{P}\{X_{n+1} = j \mid X_n = i\}$ $\forall n \in \mathbb{N}$, is the transition probability from state i to state j. Suppose P is irreducible, that is, for each pair of i and j, there is a $t \in \mathbb{N}$ such that $\mathbf{P}\{X_{n+t} = j \mid X_n = i\} > 0$. Next, we write $\mathbf{P}_i(\,\cdot\,) := \mathbf{P}(\,\cdot\,|X_0 = i)$ for the conditional probability and $\mathbf{E}_i$ the expected value relative to this probability.

Define

$$\begin{aligned} T_j &= \inf\{n \geq 1 : X_n = j\}, \\ m_{ij} &= \mathbf{E}_i T_j. \end{aligned}$$

The quantity m_{ij} is called **mean hitting time** to go from i to j. In case $i = j$, we call m_{ii} **mean first return time**, or recurrence time, to site i.

Since P is irreducible and finite, we know that $m_{ij} < \infty$ for all i, j (Lemma 1.13, [26]). Note that we can condition the expectation on the first step to obtain:

$$\begin{aligned} \mathbf{E}_i T_j &= \sum_{k\in S} \mathbf{E}_i(T_j|X_1 = k)\mathbf{P}_i(X_1 = k) \\ &= \sum_{k\in S\setminus\{j\}} \mathbf{E}_i(T_j|X_1 = k)p_{ik} \\ &\quad + \mathbf{E}_i(T_j|X_1 = j)p_{ij} \\ &= \sum_{k\in S\setminus\{j\}} (1 + \mathbf{E}_k(T_j))p_{ik} + p_{ij} \\ &= 1 + \sum_{\substack{k \\ k\neq j}} p_{ik}\mathbf{E}_k T_j. \end{aligned} \tag{1.2.1}$$

.

We can define the matrices $M = [m_{ij}]$, $M_d = [\delta_{ij} m_{ij}]$, where δ_{ij} is the Kronecker delta, and $E = [1]$ is the matrix which has every entry equal to 1. Equation (1.2.1) can be rewritten as

$$m_{ij} = 1 + \sum_{k\in S} p_{ik}\big(m_{kj} - \delta_{ik} m_{ik}\big)$$

which can be expressed in terms of the matrices defined above as $M = E + P(M - M_d)$ or, equivalently,

$$(I - P)M = E - PM_d. \tag{1.2.2}$$

We see that this is almost an equation of the form $AX = C$, with an unknown matrix X, which could be solved using a generalized inverse for the singular matrix $I - P$, except for the fact that the right-hand side also contains unknown terms of M. However, it is a fact of the Theory of Markov Chains that if P is irreducible and finite, then there is a unique vector $\boldsymbol{\pi}' = (\pi_1, \ldots, \pi_m)$ such that $\boldsymbol{\pi}'P = \boldsymbol{\pi}'$ with $\pi_i > 0$ for all i and $\sum_i \pi_i = 1$. So we can multiply equation (1.2.2) on the left by $\boldsymbol{e}\boldsymbol{\pi}'$ to obtain

$$0 = \boldsymbol{e}\boldsymbol{e}' - \boldsymbol{e}\boldsymbol{\pi}' M_d \quad \Longleftrightarrow \quad E = \Pi M_d,$$

where $\boldsymbol{e}' = (1, \ldots, 1)$ and $\Pi = \boldsymbol{e}\boldsymbol{\pi}'$. Observe that for square matrices A and D, where D is diagonal, we have

$$(AD)_d = (DA)_d = DA_d = A_d D.$$

Therefore taking the diagonal of $E = \Pi M_d$ we obtain

$$I = \Pi_d M_d \quad \Longleftrightarrow \quad M_d = (\Pi_d)^{-1},$$

which is the known Kac's Lemma [22].

Example 1.9. *Consider*

$$P = \begin{pmatrix} 1-a & a \\ b & 1-b \end{pmatrix},$$

where $0 < a, b \leq 1$*, so that the chain is irreducible. Equation (1.2.2) becomes*

$$\begin{pmatrix} a(m_{11} - m_{21}) & a(m_{12} - m_{22}) \\ -b(m_{11} - m_{21}) & -b(m_{12} - m_{22}) \end{pmatrix} = \begin{pmatrix} 1 - (1-a)m_{11} & 1 - am_{22} \\ 1 - bm_{11} & (1-b)m_{22} \end{pmatrix}.$$

Solving this system for the m_{ij} *we obtain.*

$$M = \begin{pmatrix} \frac{a+b}{b} & 1/a \\ 1/b & \frac{a+b}{a} \end{pmatrix}.$$

Example 1.10. *Consider the transition probability matrix*

$$P = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 \\ 0 & 1/2 & 0 & 1/2 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

We can solve $(I - P)M = E - PM_d$ *for* M *to obtain*

$$M = \begin{pmatrix} 6 & 1 & 4 & 9 \\ 5 & 3 & 3 & 8 \\ 8 & 3 & 3 & 5 \\ 9 & 4 & 1 & 6 \end{pmatrix}.$$

To use the theory of generalized inverses to solve problems such as these, we use the next key result, due to Hunter [20], for obtaining a g-inverse of $I - P$.

Theorem 1.11. *Let* P *be the transition probability matrix of a finite irreducible Markov Chain with stationary probabilty vector* $\boldsymbol{\pi}'$*. Let* $\boldsymbol{t}$ *and* $\boldsymbol{u}$ *be any vectors such that* $\boldsymbol{\pi}'\boldsymbol{t} \neq 0$ *and* $\boldsymbol{u}'\boldsymbol{e} \neq 0$*. Then:*

(a) $I - P + \boldsymbol{t}\boldsymbol{u}'$ *is nonsingular.*
(b) $[I - P + \boldsymbol{t}\boldsymbol{u}']^{-1}$ *is a g-inverse of* $I - P$*.*

Proof. Define $A = \mathrm{adj}(I-P)$, the adjugate matrix (A.0.1) of $I-P$. By the properties of the adjugate matrix, we have that $(I-P) = (I-P)A = \det(I-P)I = 0$, since $I-P$ is singular. This is equivalent to

$$AP = A = PA.$$

The first equality above implies that each line of A is a multiple of $\boldsymbol{\pi}'$. The second equality above implies that each column of A is a multiple of $\boldsymbol{e}$. Both combined imply that $A = k\boldsymbol{e}\boldsymbol{\pi}'$, where k is a scalar.

The scalar is k is not zero: By irreducibility, we know that the eigenvalues $\lambda_1, \ldots, \lambda_m$ of P are such that only $\lambda_1 = 1$, so $(I-P)$ has eigenvalues $1-\lambda_1, \ldots, 1-\lambda_m$ such that only $1-\lambda_1 = 0$. From (A.0.3) we know that we then have $\mathrm{Tr}(\mathrm{adj}(I-P)) = \prod_{j=2}^{m}(1-\lambda_j) \neq 0$. On the other hand, $\mathrm{Tr}(\mathrm{adj}(I-P)) = \mathrm{Tr}(k\boldsymbol{e}\boldsymbol{\pi}') = k$. Therefore, $k \neq 0$.

The matrix $I - P + \boldsymbol{t}\boldsymbol{u}'$ is nonsingular: By Lemma (A.1), we have

$$\det(I-P+\boldsymbol{t}\boldsymbol{u}') = \det(I-P) + \boldsymbol{u}'A\boldsymbol{t} = \boldsymbol{u}'(k\boldsymbol{e}\boldsymbol{\pi}')\boldsymbol{e} = k(\boldsymbol{u}'\boldsymbol{e})(\boldsymbol{\pi}'\boldsymbol{t}) \neq 0.$$

This concludes item (a). For (b), observe that $(I-P+\boldsymbol{t}\boldsymbol{u}')(I-P+\boldsymbol{t}\boldsymbol{u}')^{-1} = I$. Multiplying this equation on the left by $\boldsymbol{\pi}'$ and using $\boldsymbol{\pi}'(I-P) = \boldsymbol{0}'$ we obtain

$$\boldsymbol{\pi}'\boldsymbol{t}\boldsymbol{u}'(I-P+\boldsymbol{t}\boldsymbol{u}')^{-1} = \boldsymbol{\pi}' \quad \Longleftrightarrow \quad \boldsymbol{u}'(I-P+\boldsymbol{t}\boldsymbol{u}')^{-1} = \frac{\boldsymbol{\pi}'}{\boldsymbol{\pi}'\boldsymbol{t}}$$

so $(I-P)(I-P+\boldsymbol{t}\boldsymbol{u}')^{-1} = I - \frac{\boldsymbol{t}\boldsymbol{\pi}'}{\boldsymbol{\pi}'\boldsymbol{t}}$, and therefore

$$(I-P)(I-P+\boldsymbol{t}\boldsymbol{u}')^{-1}(I-P) = I-P,$$

proving item (b).

□

We are now able to solve equation (1.2.2) in terms of a g-inverse of $I-P$, and the solution is given by the theorem below, also due to Hunter [20].

Theorem 1.12. *Let G be a g-inverse of $I-P$, where P is irreducible and finite. Then*

$$M = \big[G\Pi - E(G\Pi)_d + I - G + EG_d\big]D, \tag{1.2.3}$$

where $D = M_d = (\Pi_d)^{-1}$.

We refer to equation (1.2.3) for mean hitting times of a Markov chain in terms of a generalized inverse G as Hunter's Mean Hitting Time Formula, or just Hunter's Formula, for short. In the next section we will define Quantum Markov Chains and present an analogous result to Theorem 1.12 in that context.

1.3 Discrete-time QMCs

The goal of this section is to define Quantum Markov Chains and its particular case of Open Quantum Walks. We start by fixing some notations and definitions for linear operators on a Hilbert space $\mathcal{H}$ over the complex numbers $\mathbb{C}$. We denote by $\mathcal{B}(\mathcal{H})$ the space of continuous linear operators on $\mathcal{H}$, also called bounded operators. For a $\rho \in \mathcal{B}(\mathcal{H})$, we write its Hilbert adjoint as ρ^*. We say that $\rho \in \mathcal{B}(\mathcal{H})$ is **positive semidefinite** (or positive, for short), denoted by $\rho \geq 0$, when $\langle v|\rho v\rangle \geq 0$ for all $v \in \mathcal{H}$, where $\langle \cdot | \cdot \rangle$ is the inner product of $\mathcal{H}$. If $\langle v|\rho v\rangle > 0$ for all $v \neq 0$, we say ρ is **positive definite** (or strictly positive), denoted by $\rho > 0$. We denote by $\mathcal{I}_1(\mathcal{H})$ the set of trace-class operators on $\mathcal{H}$ [30]. The norm of the space of trace-class operators is denoted by $\|\cdot\|_1$ defined as $\|\rho\|_1 := \mathrm{Tr}\left(|\rho|\right)$, where $|\rho| = \sqrt{\rho^*\rho}$. By definition, our **states**, or **densities**, will be operators $\rho \in \mathcal{I}_1(\mathcal{H})$ such that

$$\|\rho\|_1 = 1, \quad \text{and} \quad \rho \geq 0.$$

Next, let us consider linear maps $\Phi : \mathcal{I}_1(\mathcal{H}) \longrightarrow \mathcal{I}_1(\mathcal{H})$. By definition, a linear map Φ on $\mathcal{I}_1(\mathcal{H})$ is **trace-preserving** (TP) when $\mathrm{Tr}\,\big(\Phi(\rho)\big) = \mathrm{Tr}(\rho)$, for all $\rho \in \mathcal{I}_1(\mathcal{H})$. If the map Φ preserves the positive semidefinite property of the operators ρ on $\mathcal{H}$, that is, if $\Phi(\rho) \geq 0$ whenever $\rho \geq 0$, then we say Φ is a **positive** map. When the extended map $\Phi \otimes \mathrm{Id}$ to the space $\mathcal{I}_1(\mathcal{H}) \otimes \mathcal{B}(\mathbb{C}^m)$ is positive, then by definition Φ is m-**positive**. A linear map is said to be **completely positive** (CP) when it is m-positive for all $m \in \mathbb{N}$, see [7, 31] for more on these matters.

Now take V to be a countable set of vertices and consider a Hilbert space formed by a direct sum of the form $\mathcal{H} = \bigoplus_{i\in V} \mathfrak{h}_i$, where each $\mathfrak{h}_i$ is a separable Hilbert space. For an operator A on $\mathcal{H}$ with $\mathfrak{h}_j^{\perp} \subset \mathrm{Ker}\, A$ and $\mathrm{Ran}\, A \subset \mathfrak{h}_i$, we write A as $A = A_{ij} \otimes |i\rangle\langle j|$, where A_{ij} is seen as an operator from $\mathfrak{h}_j$ to $\mathfrak{h}_i$. So if a vector $x \in \mathcal{H}$ belongs to a certain $\mathfrak{h}_l$, we can denote it by $x \otimes |l\rangle$. When we apply A on x, we will have either $Ax = 0$, if $l \neq j$, or $Ax = (A_{ij} \otimes |i\rangle\langle j|)(x \otimes |j\rangle) = A_{ij}x \otimes |i\rangle$, for $l = j$. This is consistent with the notation used in [3] where $\mathfrak{h}_i = \mathfrak{h}$ for all i, and $\mathcal{H} = \mathfrak{h} \otimes \mathbb{C}^V$. In this case, we fix an orthonormal basis $\{|i\rangle\}_{i\in V}$ for $\mathbb{C}^V$ and the $|i\rangle\langle j|$ are operators on $\mathbb{C}^V$, in the sense that for vectors $|\phi\rangle, |\psi\rangle \in \mathbb{C}^V$, we can define

$$\begin{aligned} |\phi\rangle\langle\psi| \,:\, &\mathbb{C}^V \longrightarrow \mathbb{C}^V \\ &|\omega\rangle \mapsto \big(\langle\psi|\omega\rangle\big)|\phi\rangle. \end{aligned}$$

After these considerations, we may follow S. Gudder [17] and define a **Quantum Markov Chain** (QMC) as the operator $\Phi : \mathcal{I}_1(\mathcal{H}) \longrightarrow \mathcal{I}_1(\mathcal{H})$ that maps $\rho = \sum_{i,j\in V} \rho_{ij} \otimes |i\rangle\langle j|$ to

$$\Phi(\rho) = \sum_{i\in V} \left(\sum_{j\in V} \Phi_{ij}(\rho_{jj}) \right) \otimes |i\rangle\langle i|,$$

with the required property that each $\Phi_{ij} : \mathcal{I}_1(\mathfrak{h}_j) \longrightarrow \mathcal{I}_1(\mathfrak{h}_i)$ be a completely positive map, and also that the topological duals Φ_{ij}^* satisfy

$$\sum_{i\in V} \Phi_{ij}^*(\mathrm{Id}_{\mathfrak{h}_i}) = \mathrm{Id}_{\mathfrak{h}_j},$$

a condition which is equivalent to preservation of trace by the map Φ. Because of the complete positivity of the Φ_{ij}, they have a **Kraus representation** [2, 7] of the form

$$\Phi_{ij}(\rho) = \sum_{L} L\rho L^*, \quad \rho \in \mathcal{I}_1(\mathfrak{h}_j), \tag{1.3.1}$$

where we sum over a countable number of operators $L : \mathfrak{h}_j \to \mathfrak{h}_i$.

In the special case for which the Φ_{ij} are given simply by

$$\Phi_{ij}(\rho) = B_{ij}\rho B_{ij}^* \;, \quad \rho \in \mathcal{I}_1(\mathfrak{h}_j),$$

then the QMC reduces to what we call an **Open Quantum Walk** (OQW), following S. Attal et al. [3], and the map Φ is given by

$$\Phi(\rho) = \sum_{i,j\in V} M_{ij}\rho M_{ij}^* \;, \quad M_{ij} = B_{ij} \otimes |i\rangle\langle j|, \quad \rho \in \mathcal{I}_1(\mathcal{H}).$$

It can be shown in this case that the preservation of trace is equivalent to

$$\sum_{i\in V} B_{ij}^* B_{ij} = \mathrm{Id}_{\mathfrak{h}_j}, \quad \forall j.$$

We can think of our system as a simulation of Markov chain on a graph with a set of n **vertices**, or **sites** V, but the particle performing the walk also has an internal state represented by a linear operator on a Hilbert space of dimension k. We say that the system has k **internal degrees of freedom**, or that k is the dimension of the state space. QMCs and OQWs can be defined in more general complex Hilbert spaces where we do not have necessarily finitely many vertices and degrees of freedom. However, our focus will be on finite systems, so we will soon particularize the concepts to the finite case where the Hilbert spaces will be reduced to finite complex vector spaces $\mathbb{C}^m$ and spaces of complex matrices.

As we see in the definition of QMCs, its range depends only on the block-diagonal terms of ρ, i.e., only terms of the form ρ_{jj} appear in the image under Φ. Hence we are only interested in elements $\rho \in \mathcal{I}_1(\mathcal{H})$ of the form $\rho = \sum_{i\in V} \rho_i \otimes |i\rangle\langle i|$, where we drop the notation ρ_{ii} and write it just as ρ_i. For physical considerations, we focus only on elements of $\mathcal{I}_1(\mathcal{H})$ which are densities.

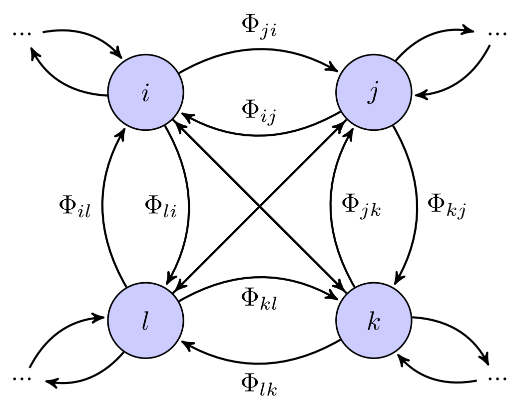

Figure 1.1: Schematic illustration of QMCs. The walk is realized on a graph with a set of vertices denoted by $i, j, k, l, \ldots$ and each operator Φ_{ij} is a completely positive map describing a transformation in the internal degree of freedom of the particle during the transition from vertex j to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

As we are restricted to the case where V has finite size n and the dimension of each $\mathfrak{h}_i$ is k, we can consider without loss of generality that each $\mathfrak{h}_i = \mathbb{C}^k$. In this case, the ρ_i will be operators on $\mathbb{C}^k$, which are $k \times k$ matrices. The space of complex $k \times k$ matrices is denoted by $M_k(\mathbb{C})$, or only M_k for short. We write the set of densities on n vertices and k internal degrees of freedom as

$$\mathcal{D}_{n,k} := \left\{ \rho = \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_n \end{bmatrix} \;:\; \rho_i \in M_k(\mathbb{C}), \;\; \rho_i \geq 0, \; i = 1, \ldots, n, \; \sum_{j=1}^{n} \mathrm{Tr}(\rho_j) = 1 \right\},$$

where $\rho = \sum_{i=1}^{n} \rho_i \otimes |i\rangle\langle i|$ is expressed as a block-column matrix, with n elements of $M_k(\mathbb{C})$ as blocks.

We can take advantage of this matrix representation for ρ by noting that

$$\Phi(\rho) = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} \Phi_{ij}(\rho_j) \right) \otimes |i\rangle\langle i|$$

so we can express the action of Φ on ρ matricially as

$$\Phi(\rho) = \begin{bmatrix} \Phi_{11} & \cdots & \Phi_{1n} \\ \Phi_{21} & \cdots & \Phi_{2n} \\ \vdots & \ddots & \vdots \\ \Phi_{n1} & \cdots & \Phi_{nn} \end{bmatrix} \cdot \begin{bmatrix} \rho_1 \\ \rho_2 \\ \vdots \\ \rho_n \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{n} \Phi_{1j}(\rho_j) \\ \sum_{j=1}^{n} \Phi_{2j}(\rho_j) \\ \vdots \\ \sum_{j=1}^{n} \Phi_{nj}(\rho_j) \end{bmatrix}. \tag{1.3.2}$$

Here the ρ_i are matrices, but the Φ_{ij} are operators on matrices, so the operations involved in the equation above are not usual matrix multiplication. Nevertheless, by looking at the proper matrix representations of the Φ_{ij} we will see shortly that, in practice, one can always perform block matrix multiplications that lead to the numerical results of interest. Finally, it is worth recalling that in the finite case, where we are taking each Φ_{ij} as a completely positive operator on $M_k(\mathbb{C})$, we have a result [7] stating that the expression (1.3.1) will involve only finitely many operators, and it becomes

$$\Phi_{ij}(\rho_m) = \sum_L L\rho_m L^*, \quad \rho_m \in M_k(\mathbb{C}), \tag{1.3.3}$$

where now we sum over a finite collection of matrices $L \in M_k(\mathbb{C})$.

1.4 Probability notions: basic statistics and hitting times

We consider the formalism of **monitoring** [15], under which we inspect whether the particle is found at a chosen vertex. In other words, we perform a measurement of the position. If the particle is detected, then the experiment is over. If not, then the particle is known to be in the subspace associated with the complement of the inspected vertex, and the process continues. Within this formalism, the following probabilistic notions for a QMC are defined:

$p_r(\rho \to j) =$ probability of reaching vertex j in r steps when starting at state ρ.
$\pi_r(\rho \to j) =$ probability of reaching vertex j for the first time in r steps when starting at state ρ.
$\pi(\rho \to j) =$ probability of ever reaching vertex j starting at state ρ.
$\tau(\rho \to j) =$ expected time of first visit to vertex j when starting at state ρ.

If we define for each vertex j a projector $\mathbb{P}_j$ that acts on densities by the relation

$$\mathbb{P}_j\left(\sum_i \rho_i \otimes |i\rangle\langle i|\right) = \rho_j \otimes |j\rangle\langle j|,$$

and if we let $\mathbb{Q}_j := I - \mathbb{P}_j$ be its complement, then the probabilistic notions above, associated with a QMC Φ, can be expressed as

$$\begin{aligned}
p_r(\rho \to j) &= \mathrm{Tr}\left(\mathbb{P}_j\Phi^r\rho\right)\\
\pi_r(\rho \to j) &= \mathrm{Tr}\left(\mathbb{P}_j\Phi(\mathbb{Q}_j\Phi)^{r-1}\rho\right)\\
\pi(\rho \to j) &= \sum_{r\geq 1}\pi_r(\rho \to j)\\
\tau(\rho \to j) &= \begin{cases}\infty, & \text{if } \pi(\rho \to j) < 1\\ \sum_{r\geq 1} r\pi_r(\rho \to j), & \text{if } \pi(\rho \to j) = 1\end{cases}
\end{aligned}$$

We call the $\pi(\rho \to j)$ **hitting probabilities** and the $\tau(\rho \to j)$ **mean hitting times**. When we refer to the mean hitting time of starting at a vertex i to reach a different vertex j, we also call it the **mean time of first visit**.

In order to calculate mean hitting times and hitting probabilities, we will use generating functions defined as

$$\mathbb{G}_{ij}(z) = \sum_{m\geq 1}\mathbb{P}_i\Phi(\mathbb{Q}_i\Phi)^{m-1}\mathbb{P}_j z^{m-1} = \mathbb{P}_i\Phi(I - z\mathbb{Q}_i\Phi)^{-1}\mathbb{P}_j, \quad z \in \mathbb{C},\ |z| < 1.$$

Such objects have been considered in [15], also see [25] and references therein. With this we define

$$H_{ij} := \begin{cases}\lim_{x\uparrow 1}\mathbb{G}_{ij}(x), & i \neq j\\ I, & i = j\end{cases}, \qquad K_{ij} := \lim_{x\uparrow 1}\frac{d}{dx}\mathbb{G}_{ij}(x).$$

The matrix of operators $H = [H_{ij}]$ and $K = [K_{ij}]$ are called, respectively, the **hitting probability** and **mean hitting time** operators, and we have that

$$\pi(\rho_j \to i) = \mathrm{Tr}(H_{ij}\rho_j),$$
$$\tau(\rho_j \to i) = \mathrm{Tr}(K_{ij}\rho_j),$$

where the index j on ρ_j denotes that it is a density concentrated at site j, i.e., a density of the form $\rho = \rho_j \otimes |j\rangle\langle j|$. To make more explicit the fact that ρ_j is concentrated at site j, we can also sometimes write $\tau(\rho_j \otimes |j\rangle \to |i\rangle)$ to denote that same quantity.

A state $\sum_i \rho_i \otimes |i\rangle\langle i|$ is said to be **faithful** if $\rho_i > 0$ for all i. We define a finite positive map Φ to be **irreducible** when it has a unique faithful state. Equivalently, a positive map Φ on $\mathcal{I}_1(\mathcal{H})$ is defined to be irreducible when the only orthogonal projections P such that $\Phi(P\mathcal{I}_1(\mathcal{H})P) \subset P\mathcal{I}_1(\mathcal{H})P$ are $P = 0$ or $P = I$. As we are in finite dimension, our map Φ being positive and trace-preserving implies that we always has an invariant state, so the theorem presented below, due to R. Carbone and Y. Pautrat [10, 11], provides us the following useful implications (the statement below extracted from [Theorem 1.1, [16]]):

Theorem 1.13. *Let Φ be a CP map on $\mathcal{I}_1(\mathcal{H})$.*

(a) If Φ is irreducible and has an invariant state, then it is unique and faithful.

(b) If Φ admits a unique invariant state and such state is faithful, then Φ is irreducible.

An irreducible and finite QMC is said to be **aperiodic** if 1 is its only eigenvalue with unit modulus. A finite QMC is by definition **ergodic** if it is irreducible and aperiodic. It is a well-known result that the iterates of an ergodic QMC acting on any initial density will converge to its invariant state [11]. We remark that in [11] the term ergodic refers to a slightly distinct notion than the one employed here.

The following theorem is a result presented in [6] which is analogous to the classical Kac's Lemma [22], and connects the invariant states of an OQW to its associated mean hitting times. It employs the notion of a **semifinite** OQW, which means that the internal degrees of freedom are finite, but the set of vertices could be possibly countably infinite.

Theorem 1.14. *[6] Let Φ be a semifinite irreducible OQW with invariant state*

$$\pi = \sum_{i\in V} \pi_i \otimes |i\rangle\langle i|.$$

Then for any $i, j \in V$ and $\rho \in \mathcal{S}(\mathfrak{h}_i)$, the sequence $(t_j^{(k)}/k)_k$, where $t_j^{(k)} = \inf\{n > t_j^{(k-1)} \mid x_n = j\}$, converges with respect to $\mathbb{P}_{i,\rho}$ both almost surely and in the L^1-sense to

$$\mathbb{E}_{i,\frac{\pi_i}{\mathrm{Tr}\,\pi_i}}(t_i) = \frac{1}{\mathrm{Tr}\,\pi_i},$$

where t_j denotes the mean first return time to site j, and $\mathbb{E}_{j,\rho}$ is the expected value conditional to a initial state concentrated at a site j with density ρ.

In order to write concrete calculations for QMCs, let $M_{m,n}(\mathbb{C})$ be the space of $m \times n$ complex matrices. We define the vec function for any $A \in M_{m,n}(\mathbb{C})$ as the map vec : $M_{m,n}(\mathbb{C}) \to \mathbb{C}^{mn}$ given by

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{n2} & \dots & a_{mn} \end{bmatrix} \mapsto \quad \mathrm{vec}(A) = \begin{bmatrix} a_{11} \\ a_{12} \\ \vdots \\ a_{1n} \\ \vdots \\ a_{m1} \\ \vdots \\ a_{mn} \end{bmatrix}. \tag{1.4.1}$$

Note that this function takes the rows of a matrix and stacks them vertically in a column vector. For a density $\rho = \sum_{i=1}^{n} \rho_i \otimes |i\rangle\langle i|$, $\rho_i \in M_k(\mathbb{C})$, we establish the correspondence

$$\rho = \begin{bmatrix} \rho_1 \\ \vdots \\ \rho_n \end{bmatrix} \qquad \longleftrightarrow \qquad |\rho\rangle := \begin{bmatrix} |\rho_1\rangle \\ \vdots \\ |\rho_n\rangle \end{bmatrix} = \begin{bmatrix} \mathrm{vec}\,(\rho_1) \\ \vdots \\ \mathrm{vec}\,(\rho_n) \end{bmatrix} \in \mathbb{C}^{nk^2},$$

where we define each $|\rho_i\rangle := \mathrm{vec}\,(\rho_i) \in \mathbb{C}^{k^2}$. Given two matrices $A = [a_{ij}] \in M_{m,n}(\mathbb{C})$ and $B \in M_{p,q}(\mathbb{C})$, we define their **Kronecker product** [18], denoted by $A \otimes B$, as the matrix

$$A \otimes B := [a_{ij}B] = \begin{bmatrix} a_{11}B & \cdots & a_{1n}B \\ \vdots & \ddots & \vdots \\ a_{m1}B & \cdots & a_{mn}B \end{bmatrix} \in M_{mp,nq}(\mathbb{C}).$$

We state without proof a few properties of the Kronecker product: for all $A, A' \in M_{m,n}(\mathbb{C})$, $B, B' \in M_{p,q}(\mathbb{C})$, $C \in M_{r,s}(\mathbb{C})$ and $\alpha \in \mathbb{C}$, we have

$$\begin{aligned}
&(\alpha A) \otimes B = A \otimes (\alpha B) \\
&(A \otimes B) = A^T \otimes B^T \\
&(A \otimes B) = A^* \otimes B^* \\
&(A \otimes B) \otimes C = A \otimes (B \otimes C) \\
&(A + A') \otimes B = A \otimes B + A' \otimes B \\
&A \otimes (B + B') = A \otimes B + A \otimes B'
\end{aligned}$$

where A^T is the notation for A transposed. It is a property of the vec function that for $A, X, B \in M_k(\mathbb{C})$, we have $\mathrm{vec}\,(AXB) = A \otimes B^T\,\mathrm{vec}\,(X)$, where $\otimes$ is the Kronecker product [18]. So, if we apply the vec function to equation (1.3.3), then we have

$$\mathrm{vec}\,(\Phi_{ij}(\rho_m)) = \mathrm{vec}\left(\sum_L L\rho L^*\right) = \sum_L L \otimes \overline{L}\,\mathrm{vec}\,(\rho_m) = \sum_L L \otimes \overline{L}|\rho_m\rangle.$$

This motivates us to define

$$\lceil \Phi_{ij} \rceil := \sum_L L \otimes \overline{L} \in M_{k^2}(\mathbb{C}),$$

so we can write more simply

$$\mathrm{vec}\,(\Phi_{ij}(\rho_m)) = \lceil \Phi_{ij} \rceil |\rho_m\rangle.$$

Finally, if we define the matrix

$$\lceil \Phi \rceil := \begin{bmatrix} \lceil \Phi_{11} \rceil & \cdots & \lceil \Phi_{1n} \rceil \\ \vdots & \ddots & \vdots \\ \lceil \Phi_{n1} \rceil & \cdots & \lceil \Phi_{nn} \rceil \end{bmatrix} \in M_{nk^2}(\mathbb{C}),$$

then we can express equation (1.3.2) as

$$\lceil \Phi \rceil |\rho\rangle = \begin{bmatrix} \lceil \Phi_{11} \rceil & \cdots & \lceil \Phi_{1n} \rceil \\ \lceil \Phi_{21} \rceil & \cdots & \lceil \Phi_{2n} \rceil \\ \vdots & \ddots & \vdots \\ \lceil \Phi_{n1} \rceil & \cdots & \lceil \Phi_{nn} \rceil \end{bmatrix} \cdot \begin{bmatrix} |\rho_1\rangle \\ |\rho_2\rangle \\ \vdots \\ |\rho_n\rangle \end{bmatrix} = \begin{bmatrix} \sum_{j=1}^{n} \lceil \Phi_{1j} \rceil |\rho_j\rangle \\ \sum_{j=1}^{n} \lceil \Phi_{2j} \rceil |\rho_j\rangle \\ \vdots \\ \sum_{j=1}^{n} \lceil \Phi_{nj} \rceil |\rho_j\rangle \end{bmatrix},$$

except now we have regular multiplication of matrices and vectors. However it is important to emphasize that these matrices are partitioned in n^2 blocks of dimension $k \times k$, and the vectors are partitioned in n blocks of dimensions $k \times 1$.

Consider the class of finite ergodic QMCs. It is a fact that the iterates $\lceil \Phi \rceil^m$ of the matrix of one such QMC converges to $|\pi\rangle\langle e_{I_k^n}|$ when m goes to infinity [24], where

$$|e_{I_k^n}\rangle := \begin{bmatrix} \operatorname{vec}(I_k) \\ \operatorname{vec}(I_k) \\ \vdots \\ \operatorname{vec}(I_k) \end{bmatrix} = \begin{bmatrix} |e_{I_k}\rangle \\ |e_{I_k}\rangle \\ \vdots \\ |e_{I_k}\rangle \end{bmatrix} \in \mathbb{C}^{nk^2}, \quad |e_{I_k}\rangle := \operatorname{vec}(I_k) \in \mathbb{C}^{k^2},$$

where $|\pi\rangle$ is the vector form of the limit density π of the QMC, $I_k \in M_k(\mathbb{C})$ is the identity matrix, and $\langle x| := |x\rangle^*$. We also write $|e_{I_k^n}\rangle$ only as $|e_I\rangle$ for simplicity. We call $\Omega := |\pi\rangle\langle e_{I_k^n}|$ the **limit map** associated with the ergodic QMC Φ.

The vec function also establishes a unitary equivalence between the Hilbert spaces $M_k(\mathbb{C})$ and $\mathbb{C}^{k^2}$ with their inner products $\langle \cdot \mid \cdot \rangle_{M_k}$ and $\langle \cdot \mid \cdot \rangle_{\mathbb{C}^{k^2}}$ [25] by the fact that

$$\langle B \mid A\rangle_{M_n} = \operatorname{Tr}(B^* A) = \sum_{i,j} \overline{B_{ij}} A_{ij} = \operatorname{vec}(B)^* \operatorname{vec}(A) = \langle \operatorname{vec}(B) \mid \operatorname{vec}(A)\rangle_{\mathbb{C}^{n^2}}, \quad A, B \in M_n.$$

With this we have that for $\rho_i \in M_k$

$$\operatorname{Tr}(\rho_i) = \langle e_{I_k} | \rho_i\rangle,$$

and for $\rho = \sum_i \rho_i \otimes |i\rangle\langle i|$,

$$\operatorname{Tr}(\rho) = \sum_i \operatorname{Tr}(\rho_i) = \sum_i \langle e_{I_k} | \rho_i\rangle = \langle e_{I_k^n} | \rho\rangle.$$

Now that we have established these probability notions and how to do calculations involving QMCs using matrices, we proceed to show a few results concerning generalized inverses for $I - \Phi$, where Φ is a QMC, and a quantum version of Hunter's Formula for irreducible QMCs. The following theorem [Proposition 6.3, [24]] gives us a g-inverse for $I - \lceil \Phi \rceil$. For completeness, we present its proof.

Theorem 1.15. *Let Φ be an irreducible QMC on a finite graph with stationary density π. Let $|t\rangle, |u\rangle \in \mathbb{C}^{nk^2}$ be such that $\langle e_I|t\rangle \neq 0$ and $\langle u|\pi\rangle \neq 0$. Then $I - \Phi + |t\rangle\langle u|$ is invertible and its inverse is a g-inverse of $I - \Phi$*

Proof. We denote the adjugate matrix of B by $\operatorname{adj}(B)$, as defined in (A.0.1). And let us define $A := \operatorname{adj}(I - \Phi)$.

By Lemma A.1, we have that $\det(X + |c\rangle\langle r|) = \det(X) + \langle r| \operatorname{adj}(X) |c\rangle$, for any vectors $|c\rangle, |r\rangle$. Then, because $I - \Phi$ is singular,

$$\det(I - \Phi + |t\rangle\langle u|) = \langle u|A|t\rangle. \tag{1.4.2}$$

We also have by a property of the adjugate that $A(I - \Phi) = (I - \Phi)A = 0$, so $A\Phi = A$ and $\Phi A = A$. Because Φ has only 1 fixed point, the first equation tells us that every row of A is a fixed row-vector of Φ, and the second equation tells us that every column of A is a fixed column-vector of Φ. We conclude $A = c|\pi\rangle\langle u|$ for some $c \in \mathbb{C}$.

Because Φ has only 1 fixed point, we have that $I - \Phi$ has only 1 eigenvalue equal to zero, say $\lambda_1 = 0$, therefore, by (A.0.3), we have that

$$\operatorname{Tr}(\operatorname{adj}(I - \Phi)) = \prod_{i \neq 1} \lambda_i \neq 0,$$

so we can conclude $c \neq 0$. Therefore $\det(I - \Phi) = c\langle u|\pi\rangle\langle e_I|t\rangle =\neq 0$.

Now note that

$$(I - \Phi + |t\rangle\langle u|)^{-1}(I - \Phi + |t\rangle\langle u|) = I, \tag{1.4.3}$$

and if we multiply it on the right by $|\pi\rangle$ then $(I - \Phi)|\pi\rangle = 0$ and we will have

$$(I - \Phi + |t\rangle\langle u|)^{-1}|t\rangle\langle u|\pi\rangle = |\pi\rangle \Longrightarrow (I - \Phi + |t\rangle\langle u|)^{-1}|t\rangle = \frac{|\pi\rangle}{\langle u|\pi\rangle}.$$

Replace this in equation (1.4.3) and we get

$$(I - \Phi + |t\rangle\langle u|)^{-1}(I - \Phi) = I - \frac{|\pi\rangle\langle u|}{\langle u|\pi\rangle}.$$

Finally, we multiply it on the left by $I - \Phi$ and use again the fact that $(I - \Phi)|\pi\rangle = 0$, so we obtain

$$(I - \Phi)(I - \Phi + |t\rangle\langle u|)^{-1}(I - \Phi) = I - \Phi,$$

proving that $(I - \Phi + |t\rangle\langle u|)^{-1}$ is a g-inverse for $I - \Phi$.

□

From this follows the next two results, proven in [24], which provides a characterization for any possible g-inverse of $I - \Phi$:

Corollary 1.16. *Let Φ be an irreducible QMC on a finite graph with stationary density π. Let $|t\rangle, |u\rangle \in \mathbb{C}^{nk^2}$ be such that $\langle e_I|t\rangle \neq 0$ and $\langle u|\pi\rangle \neq 0$. Then any g-inverse of $I - \Phi$ can be written as:*

$$G = \big(I - \Phi + |t\rangle\langle u|\big)^{-1} + |\pi\rangle\langle f| + |g\rangle\langle e_I|$$

where $|f\rangle, |g\rangle$ are arbitrary vectors.

Remark 1.17. *In the next theorem, we use the notation $(A)_d$ to denote the block-diagonal version of a matrix $A \in M_{nk^2}(\mathbb{C})$. The blocks will be of size n, which is the number of sites of the QMC considered. The notation $(\,\cdot\,)_d$ will be used throughout this work in theorems and examples.*

Theorem 1.18. (Hunter's formula for irreducible QMCs [24]) *Let Φ be an ergodic QMC on a finite graph with $n \geq 2$ vertices and $k \geq 2$ internal degrees of freedom, and let π be its stationary density and Ω its limit map. Let $K = (K_{ij})$ denote the matrix of mean hitting time operators to vertices $i = 1, \dots, n$, $D = K_d = \mathrm{diag}(K_{11}, \dots, K_{nn})$, G any g-inverse of $I - \Phi$, and let E denote the block matrix for which each block equals the identity of order k^2. (a) Then the mean hitting time for the walk to reach vertex i, beginning at vertex j with initial density ρ_j is given by*

$$\tau(\rho_j \otimes |j\rangle \to |i\rangle) = \mathrm{Tr}(K_{ij}\rho_j) = \mathrm{Tr}\Big(\big[D\big(\Omega G - (\Omega G)_d E + I - G + G_d E\big)\big]_{ij}\rho_j\Big). \tag{1.4.4}$$

(b) By setting $G = (I - \Phi + |u\rangle\langle e_I|)^{-1} + |f\rangle\langle e_I|$, with $|f\rangle$ arbitrary, and $|u\rangle$ such that $\langle u|\pi\rangle \neq 0$, then we have that for every vertex i and initial density ρ_j on vertex j,

$$\tau(\rho_j \otimes |j\rangle \to |i\rangle) = \mathrm{Tr}(K_{ij}\rho_j) = \mathrm{Tr}\Big(\big[D(I - G + G_d E)\big]_{ij}\rho_j\Big).$$

1.5 Applying Hunter's formula to any irreducible quantum channel

Here we consider quantum channels and we will be interested in the mean hitting time of reaching a certain subspace. By associating a QMC to such channel, we will obtain a formula for the mean hitting times of the channel using Hunter's Mean Hitting Time Formula for discrete time QMCs.

A finite-dimensional **quantum channel** is a linear, completely positive, trace-preserving map $T : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ on the space of order n complex matrices. Consider the space $\mathscr{H}_n$ in which the matrices of $M_n(\mathbb{C})$ act, which in this case is simply $\mathbb{C}^n$. For $V \subset \mathscr{H}_n$ subspace, let $P \in M_n(\mathbb{C})$ be the orthogonal projection onto V and $Q = I_n - P$. We define the operators $\mathbb{P}$ and $\mathbb{Q}$ on $M_n(\mathbb{C})$ by $\mathbb{P}X = PXP$ and $\mathbb{Q}X = QXQ$, respectively, for $X \in M_n(\mathbb{C})$. These operators are also orthogonal projections, but they act on $M_n(\mathbb{C})$.

For instance, we can take ψ to be any pure state (i.e., a unit vector on $\mathbb{C}$), so that V is the 1-dimensional subspace spanned by ψ, which implies that $P = |\psi\rangle\langle\psi|$.

If we take $\phi \in \mathscr{H}_n$ as an initial state, and V as the arrival subspace, we are interested in obtaining $\tau(\phi \to V)$, the expected time of first visit to subspace V given that we start in the state ϕ. We denote by $\pi_r(\phi \to V)$ the probability of reaching subspace V, starting at ϕ, in exactly r steps, given by

$$\pi_r(\phi \to V) = \mathrm{Tr}(\mathbb{P}T(\mathbb{Q}T)^{r-1}\rho_\phi),$$

where $\rho_\phi = |\phi\rangle\langle\phi|$ is the pure state density matrix associated with the state ϕ. If the probability of ever reaching V starting from ϕ, $\pi(\phi \to V) = \sum_{r\geq 1} \pi_r(\phi \to V)$, is 1, then we have the mean hitting time given by

$$\tau(\phi \to V) = \sum_{r\geq 1} r\pi_r(\phi \to V) = \sum_{r\geq 1} r\,\mathrm{Tr}(\mathbb{P}T(\mathbb{Q}T)^{r-1}\rho_\phi). \tag{1.5.1}$$

We could as well substitute $\mathbb{P} = I - \mathbb{Q}$ in the expression above, since both operators will give the same trace. In case $\pi(\phi \to V) < 1$, then $\tau(\phi \to V) = \infty$.

Now we form a new map $\Lambda = \Lambda_{T,V}$ dependent on both the quantum channel T and the arrival subspace V, given by a 2×2 matrix of operators (in the same way as in 1.3.2):

$$\Lambda = \begin{bmatrix} \Lambda_{11} & \Lambda_{12} \\ \Lambda_{21} & \Lambda_{22} \end{bmatrix} = \begin{bmatrix} (I-\mathbb{Q})T & (I-\mathbb{Q})T \\ \mathbb{Q}T & \mathbb{Q}T \end{bmatrix}, \tag{1.5.2}$$

where each Λ_{ij} is an operator on $M_n(\mathbb{C})$ defined on the right hand side. Another way of stating this is by defining the map

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \longmapsto \Lambda \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} \Lambda_{11}(X_1) + \Lambda_{12}(X_2) \\ \Lambda_{21}(X_1) + \Lambda_{22}(X_2) \end{bmatrix} = \begin{bmatrix} (I-\mathbb{Q})T(X_1+X_2) \\ \mathbb{Q}T(X_1+X_2) \end{bmatrix},$$

where $X_1, X_2 \in M_n(\mathbb{C})$. Note that

$$\begin{aligned} \mathrm{Tr}\left(\begin{bmatrix} (I-\mathbb{Q})T(X_1+X_2) \\ \mathbb{Q}T(X_1+X_2) \end{bmatrix}\right) &= \mathrm{Tr}((I-\mathbb{Q})T(X_1+X_2)) + \mathrm{Tr}(\mathbb{Q}T(X_1+X_2)) \\ &= \mathrm{Tr}(T(X_1+X_2)) = \mathrm{Tr}(X_1+X_2) = \mathrm{Tr}\left(\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}\right), \end{aligned} \tag{1.5.3}$$

hence we see that Λ preserves trace.

We can think of the sites on which Λ acts as being states relative to the arrival subspace V in the first component, and the states in the orthogonal complement $V^\perp$ in the second component.

Let us consider an initial state $\phi \in V^\perp$ orthogonal to the final subspace. What is the mean hitting time of reaching site 1 given that we start with density $\rho_\phi = |\phi\rangle\langle\phi|$ concentrated in site 2? In the notation of QMCs that we are using, this quantity is $\tau(\rho_\phi \otimes |2\rangle \to |1\rangle)$. Before proceeding, let $\mathbb{P}_1, \mathbb{P}_2$ be the projectors such that

$$\mathbb{P}_1 \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} X_1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbb{P}_2 \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 \\ X_2 \end{bmatrix},$$

and let $\mathbb{Q}_i = I - \mathbb{P}_i$, $i = 1, 2$, acting on this space of the form $\mathbb{C}^2 \otimes M_n(\mathbb{C})$ (the subindexes distinguish them from the previous projectors $\mathbb{P}$ and $\mathbb{Q}$ defined on $M_n(\mathbb{C})$). By the definition of mean hitting time for QMCs, we have

$$\begin{aligned} \tau(\rho_\phi \otimes |2\rangle \to |1\rangle) &:= \sum_{r\geq 1} r\,\mathrm{Tr}(\mathbb{P}_1\Lambda(\mathbb{Q}_1\Lambda)^{r-1}\rho) \\ &= \sum_{r\geq 1} r\,\mathrm{Tr}(\mathbb{P}_1\Lambda\mathbb{P}_2(\mathbb{P}_2\Lambda\mathbb{P}_2)^{r-1}\mathbb{P}_2\rho) \\ &= \sum_{r\geq 1} r\,\mathrm{Tr}(\Lambda_{12}\Lambda_{22}^{r-1}\rho_\phi) = \sum_{r\geq 1} r\,\mathrm{Tr}((I-\mathbb{Q})T(\mathbb{Q}T)^{r-1}\rho_\phi) \\ &= \sum_{r\geq 1} r\,\mathrm{Tr}(\mathbb{P}T(\mathbb{Q}T)^{r-1}\rho_\phi), \end{aligned} \tag{1.5.4}$$

and this shows, by comparing with (1.5.1) that $\tau(\rho_\phi \otimes |2\rangle \to |1\rangle) = \tau(\phi \to V)$, which is the mean hitting time for the quantum channel, provided the condition $\pi(\phi \to V) = 1$.

We summarize this in the following:

Lemma 1.19. *Let $T : M_n(\mathbb{C}) \to M_n(\mathbb{C})$ be a quantum channel, $V \subset \mathbb{C}^n$ a subspace, and let $|\phi\rangle$ be a state in $V^\perp$ and $\rho_\phi = |\phi\rangle\langle\phi|$. Let P be the orthogonal projector onto V and $Q = I - P$, and define the operator $\mathbb{Q} := Q \cdot Q$. Let $\Lambda = \Lambda_{T,V}$ be defined as in (1.5.2). We have*

a) Λ is a positive, trace-preserving map.

b) If T is irreducible, then Λ is irreducible, and if π is the stationary state of T, then

$$\begin{bmatrix} (I-\mathbb{Q})\pi \\ \mathbb{Q}\pi \end{bmatrix}$$

is the stationary state of Λ.

c) The mean hitting time for T to reach subspace V starting from a state $\phi \in V^\perp$ is the same as the mean hitting time for Λ starting at site $|2\rangle$ with initial density ρ_ϕ to reach state $|1\rangle$.

Proof. Item a) follows from (1.5.3) that Λ is trace preserving. Item c) follows from (1.5.4). To prove item b), consider a general density

$$\begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix},$$

and suppose it is stationary for Λ. Then we have

$$\begin{bmatrix} (I-\mathbb{Q})T & (I-\mathbb{Q})T \\ \mathbb{Q}T & \mathbb{Q}T \end{bmatrix} \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}$$
$$\Longrightarrow \begin{bmatrix} (I-\mathbb{Q})T(\rho_1+\rho_2) \\ \mathbb{Q}T(\rho_1+\rho_2) \end{bmatrix} = \begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix}.$$

If we add the two equations above, we obtain $T(\rho_1+\rho_2) = \rho_1+\rho_2$, hence $\rho_1+\rho_2 = \beta\pi$ for some scalar β. Taking the trace, we have $1 = \mathrm{Tr}(\rho_2+\rho_2) = \beta\,\mathrm{Tr}(\pi) = \beta$. So $\rho_1+\rho_2 = \pi$. Because $(I-\mathbb{Q})T(\rho_1+\rho_2) = \rho_1$, we deduce $(I-\mathbb{Q})T\pi = (I-\mathbb{Q})\pi = \rho_1$. Similarly, from $\mathbb{Q}T(\rho_1+\rho_2) = \rho_2$ we see that $\mathbb{Q}\pi = \rho_2$.

The operator Λ can be seen as a positive map on $\mathcal{I}_1(V \oplus V^\perp)$, and as we have just seen, the only fixed density of Λ will be

$$\begin{bmatrix} \rho_1 \\ \rho_2 \end{bmatrix} = \begin{bmatrix} (I-\mathbb{Q})\pi \\ \mathbb{Q}\pi \end{bmatrix},$$

where π is the fixed density of T. To see that this state is faithful, consider, for $0 \neq v \in V$:

$$\langle v|\rho_1 v\rangle = \langle v|(I-\mathbb{Q})\pi v\rangle = \langle v|\pi v\rangle - \langle Qv|\pi Qv\rangle = \langle v|\pi v\rangle > 0,$$

and also for $0 \neq u \in V^\perp$:

$$\langle u|\rho_2 u\rangle = \langle u|\mathbb{Q}\pi u\rangle = \langle Qu|\pi Qu\rangle = \langle u|\pi u\rangle > 0.$$

The strictly greater than zero inequalities follow because π is a faithful state, since T is irreducible. Hence, the only invariant state for Λ is faithful, and it follows from Theorem 1.13 that Λ is irreducible.

□

Now we can then apply Theorem 1.18 to the QMC $\Lambda = \Lambda_{T,V}$ to obtain the the mean hitting time for the quantum channel T. This can be stated as follows:

Theorem 1.20. *Let T be an irreducible completely positive quantum channel on $M_n(\mathbb{C})$ with, $V \subset \mathscr{H}_n$ a and $\phi \in V^\perp$. Let Λ be the T,V-dependent QMC associated with the channel, with stationary density π and limit map Ω. Let $K = (K_{ij})$ denote the matrix of mean hitting time operators of Λ for vertices $i = 1, 2$, $D = K_d = \mathrm{diag}(K_{11}, K_{22})$, let G be any g-inverse of $I - \Lambda$ and E be the block matrix where each block is the identity of order n^2. (a) The mean hitting time for the state ϕ to reach subspace V starting from ϕ, under the action of T, is given by*

$$\tau(\phi \to V) = \mathrm{Tr}\left(\left[D(\Omega G - (\Omega G)_d E + I - G + G_d E)\right]_{12}\rho_\phi\right).$$

(b) By setting $G = (I - \Lambda + |u\rangle\langle e_I|)^{-1} + |f\rangle\langle e_I|$ with arbitrary $|f\rangle$, and $|u\rangle$ such that $\langle u|\pi\rangle \neq 0$, then we have

$$\tau(\phi \to V) = \mathrm{Tr}\left(\left[D(I - G + G_d E)\right]_{12}\rho_\phi\right). \tag{1.5.5}$$

1.5.1 Example

Let us apply the results above to a specific example. Consider the quantum channel T acting on $M_2(\mathbb{C})$ given by $T(X) = AXA^* + BXB^*$, where A and B are 2×2 matrices given by

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

It is easy to check that $A^*A + B^*B = I_2$, so the map is trace preserving and unital (i.e., it is identity-preserving). By the definition given by T, it is a completely positive map, therefore positive. So T is a quantum channel.

The matrix representation of the channel is given by $\lceil T \rceil = A \otimes \bar{A} + B \otimes \bar{B}$,

$$\lceil T \rceil = \frac{1}{3} \begin{bmatrix} 2 & 1 & 1 & 1 \\ -1 & 2 & 0 & 1 \\ -1 & 0 & 2 & 1 \\ 1 & -1 & -1 & 2 \end{bmatrix}.$$

We can check that $\dim \ker(\lceil T \rceil - I_4) = 1$, so the channel is irreducible since T is unital. Now we choose two orthogonal states $\phi, \psi \in \mathscr{H}_2 = \mathbb{C}^2$,

$$\phi = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \quad \psi = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

and define the orthogonal projector matrices in $M_2(\mathbb{C})$

$$P = |\psi\rangle\langle\psi| = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}, \quad Q = |\phi\rangle\langle\phi| = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}.$$

With these, the orthogonal projector maps in $M_2(\mathbb{C})$, $\mathbb{P} = P \cdot P$ and $\mathbb{Q} = Q \cdot Q$ have matrix representations $\lceil \mathbb{P} \rceil = P \otimes \bar{P}$ and $\lceil \mathbb{Q} \rceil = Q \otimes \bar{Q}$:

$$\lceil \mathbb{P} \rceil = \frac{1}{4} \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}, \quad \lceil \mathbb{Q} \rceil = \frac{1}{4} \begin{bmatrix} 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}.$$

The matrix representation of the mean hitting time operator for T can be calculated by $\lceil K \rceil = \lceil T \rceil (I_4 - \lceil \mathbb{Q} \rceil \lceil T \rceil)^{-2}$, and it gives us

$$\lceil K \rceil = \frac{1}{6} \begin{bmatrix} 39 & -12 & -12 & 9 \\ -72 & 32 & 28 & -12 \\ -72 & 28 & 32 & -12 \\ 177 & -72 & -72 & 39 \end{bmatrix}.$$

With this, we can calculate $\tau(\phi \to V)$, where $V = \operatorname{span}\{\psi\} \subset \mathbb{C}^2$, and $\rho_\phi = |\phi\rangle\langle\phi|$=Q. We have

$$\tau(\phi \to V) = \operatorname{Tr}((I - \mathbb{Q})K\rho_\phi) = 6. \tag{1.5.6}$$

Now we turn to the use of Hunter's formula for mean hitting times to obtain the result above. First we define the QMC $\Lambda = \Lambda_{T,V}$ via equation (1.5.2), whose matrix representation is

$$\lceil \Lambda \rceil = \begin{bmatrix} (I_4 - \lceil \mathbb{Q} \rceil)\lceil T \rceil & (I_4 - \lceil \mathbb{Q} \rceil)\lceil T \rceil \\ \lceil \mathbb{Q} \rceil \lceil T \rceil & \lceil \mathbb{Q} \rceil \lceil T \rceil \end{bmatrix} = \frac{1}{12} \begin{bmatrix} 3 & 6 & 6 & 3 & 3 & 6 & 6 & 3 \\ 1 & 6 & -2 & 5 & 1 & 6 & -2 & 5 \\ 1 & -2 & 6 & 5 & 1 & -2 & 6 & 5 \\ -1 & -2 & -2 & 7 & -1 & -2 & -2 & 7 \\ 5 & -2 & -2 & 1 & 5 & -2 & -2 & 1 \\ -5 & 2 & 2 & -1 & -5 & 2 & 2 & -1 \\ -5 & 2 & 2 & -1 & -5 & 2 & 2 & -1 \\ 5 & -2 & -2 & 1 & 5 & -2 & -2 & 1 \end{bmatrix}.$$

This QMC is irreducible and its only stationary density is

$$|\pi\rangle = \frac{1}{4}\begin{bmatrix}1 & 1 & 1 & 1 & 1 & -1 & -1 & 1\end{bmatrix}^T.$$

Let $\mathbb{P}_1, \mathbb{P}_2$ be the projector matrices

$$\mathbb{P}_1 = \begin{bmatrix} I_4 & 0 \\ 0 & 0 \end{bmatrix}, \quad \mathbb{P}_2 = \begin{bmatrix} 0 & 0 \\ 0 & I_4 \end{bmatrix},$$

and $\mathbb{Q}_i = I_8 - \mathbb{P}_i$, $i = 1, 2$. We can calculate $K_d = D$, the diagonal of the mean hitting time operator for the QMC Λ and obtain

$$D = \frac{1}{6}\begin{bmatrix} -51 & 24 & 24 & -9 & 0 & 0 & 0 & 0 \\ 18 & -4 & -8 & 6 & 0 & 0 & 0 & 0 \\ 18 & -8 & -4 & 6 & 0 & 0 & 0 & 0 \\ 87 & -36 & -36 & 21 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 9 \\ 0 & 0 & 0 & 0 & -3 & 0 & 0 & -9 \\ 0 & 0 & 0 & 0 & -3 & 0 & 0 & -9 \\ 0 & 0 & 0 & 0 & 3 & 0 & 0 & 9 \end{bmatrix}.$$

We choose two arbitrary vectors $|u\rangle, |f\rangle \in \mathbb{C}^8$, say

$$|u\rangle = |f\rangle = \begin{bmatrix}1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\end{bmatrix}^T,$$

so we can define a generalized inverse G for $I - \Lambda$ as $G = (I - \Lambda + |u\rangle\langle e_I|)^{-1} + |f\rangle\langle e_I|$. In order for G to exist, we need to check that $\langle u|\pi\rangle \neq 0$, and in our case $\langle u|\pi\rangle = 1/4$, so the condition is satisfied. Calculating G by this definition, we obtain

$$G = \frac{1}{4}\begin{bmatrix} 2 & 2 & 2 & 2 & -2 & 2 & 2 & 2 \\ 1 & 8 & -4 & 3 & 1 & 4 & -4 & 3 \\ 1 & -4 & 8 & 3 & 1 & -4 & 4 & 3 \\ 1 & -2 & -2 & 5 & 1 & -2 & -2 & 1 \\ 1 & 0 & 0 & -1 & 5 & 0 & 0 & -1 \\ -1 & 0 & 0 & 1 & -1 & 4 & 0 & 1 \\ -1 & 0 & 0 & 1 & -1 & 0 & 4 & 1 \\ 1 & 0 & 0 & -1 & 1 & 0 & 0 & 3 \end{bmatrix} \implies G_d = \frac{1}{4}\begin{bmatrix} 5 & 2 & 2 & 5 & 0 & 0 & 0 & 0 \\ 1 & 8 & -4 & 3 & 0 & 0 & 0 & 0 \\ 1 & -4 & 8 & 3 & 0 & 0 & 0 & 0 \\ 1 & -2 & -2 & 5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 5 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & -1 & 4 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 4 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 3 \end{bmatrix}.$$

The last ingredient we needed for Theorem 1.20 is the matrix E, which in our case is

$$E = \begin{bmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Finally, by Theorem 1.20, and with the specific form used for G, we fall under the hypothesis of item (b) of that theorem, so we can use formula (1.5.5). It gives us

$$\begin{aligned} \tau(\phi \to V) &= \operatorname{Tr}\left(\left[D(I - G + G_d E)\right]_{12}\rho_\phi\right) \\ &= \operatorname{Tr}\left(\frac{1}{6}\begin{bmatrix} -51 & 24 & 24 & -9 \\ 18 & -4 & -8 & 6 \\ 18 & -8 & -4 & 6 \\ 87 & -36 & -36 & 21 \end{bmatrix} \cdot \begin{bmatrix} 1/2 \\ -1/2 \\ -1/2 \\ 1/2 \end{bmatrix}\right) \\ &= \operatorname{Tr}\left(\begin{bmatrix} -9 \\ 3 \\ 3 \\ 15 \end{bmatrix}\right) = -9 + 15 = 6. \end{aligned}$$

And that is in fact the same result we obtained above in (1.5.6), as expected.

1.6 Beyond the irreducible case

First, we take a brief detour on randomizations of quantum channels. This discussion will motivate certain questions which, on their turn, will lead us to hitting time results concerning non-irreducible channels.

1.6.1 A digression: randomizations

Let us recall an interesting result due to Burgarth et al. [9]. We recall the notion of ergodicity used by them, which is slightly different from the one used in this thesis. Nevertheless, we will consider their result under the assumption that the channel is irreducible, so that the result below can be immediately employed.

Definition 1.21. *A channel $\mathcal{M}$ is said to be* **ergodic** *(following [9]) if there exists a unique state $\rho_* \in \mathcal{S}(\mathcal{H})$ such that $\mathcal{M}\rho_* = \rho_*$.*

Theorem 1.22. *Let $\mathcal{M}$ and $\mathcal{M}'$ two channels, and let $\mathcal{M}$ be ergodic. Then for all $p \in (0,1]$ the channel*

$$\mathcal{M}_p := p\mathcal{M} + (1-p)\mathcal{M}'$$

is also ergodic. Moreover, denoting by ρ_* and $\rho_{*,p}$ the fixed states of $\mathcal{M}$ and $\mathcal{M}_p$, respectively, then

$$\rho_{*,p} = \pi_p \rho_* + (1-\pi_p)\sigma_p$$

for some probability $\pi_p \in (0,1]$ and some state $\sigma_p \in \mathcal{S}(\mathcal{H})$.

With this fact in mind, let us examine some examples, having in mind some of the previous results of hitting times and generalized inverses.

Example 1.23. *As an example, consider the matrices*

$$J_1 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad J_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad J_3 = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}$$

and the unitary matrix

$$U = \begin{bmatrix} 1/2 & \sqrt{3}/6 & \sqrt{6}/3 \\ \sqrt{3}/2 & -1/6 & -\sqrt{2}/3 \\ 0 & 2\sqrt{2}/3 & -1/3 \end{bmatrix}.$$

With these matrices we can define two different quantum channels,

$$\lceil \Phi \rceil = \sum_{i=1}^{3} J_i \otimes \bar{J}_i, \quad \text{and} \quad \lceil \mathcal{M}' \rceil = U \otimes \bar{U}.$$

With these definitions, we have that $\mathcal{M}'$ is unitary, and we can also verify that Φ is irreducible. Now let us define the randomization

$$\lceil \mathcal{M}_p \rceil = p\lceil \Phi \rceil + (1-p)\lceil \mathcal{M}' \rceil, \quad p \in (0,1].$$

By what was discussed above, $\lceil \mathcal{M}_p \rceil$ is an irreducible channel for every p in the prescribed range. Moreover, we have that

$$\pi = \frac{1}{3}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

is the unique invariant faithful state of the quantum channel Φ*, and it happens in this case to be the unique faithful state of* $\mathcal{M}_p$ *for every* $p \in (0,1]$*, since being* π *a multiple of the identity, it is invariant under* $\mathcal{M}'$ *because* $\mathcal{M}'\pi = U\pi U^* = \pi UU^* = \pi$*. So* $\mathcal{M}_p\pi = p\Phi\pi + (1-p)\mathcal{M}'\pi = p\pi + (1-p)\pi = \pi$*.*

We choose two orthogonal states,

$$|\phi\rangle = \begin{bmatrix} 0 & 0 & 1 \end{bmatrix}^T, \quad |\psi\rangle = \begin{bmatrix} 1 & 0 & 0 \end{bmatrix}^T,$$

and consider ϕ *as initial state and* $V = \operatorname{span}\{\psi\}$ *as the arrival subspace. The calculations of the mean hitting times will be with respect to these states. We have that the limit matrix for* $\mathcal{M}_p$ *is* $\Omega = |\pi\rangle\langle e_{I_3}|$*, with which we can calculate the* **fundamental matrix** *for* $\mathcal{M}_p$*, defined by*

$$Z_p := \left(I - \lceil \mathcal{M}_p \rceil + \Omega\right)^{-1}.$$

Defining the projectors $\lceil \mathbb{P} \rceil = P \otimes P$*, where* $P := |\psi\rangle\langle\psi|$ *and* $\lceil \mathbb{Q} \rceil = Q \otimes Q$ *where* $Q := I - P$*, we can calculate the mean hitting time operator* K_p *of the channel* $\mathcal{M}_p$*,*

$$\lceil K_p \rceil = \lceil \mathcal{M}_p \rceil (I - \lceil \mathbb{Q} \rceil \lceil \mathcal{M}_p \rceil)^{-2},$$

and from it obtain

$$\lceil (K_p)_{11} \rceil = (I - \lceil \mathbb{Q} \rceil) \lceil K_p \rceil (I - \lceil \mathbb{Q} \rceil).$$

We also calculate

$$\lceil (Z_p)_{11} \rceil = (I - \lceil \mathbb{Q} \rceil) \lceil Z_p \rceil (I - \lceil \mathbb{Q} \rceil) \quad \textit{and} \quad \lceil (Z_p)_{12} \rceil = (I - \lceil \mathbb{Q} \rceil) \lceil Z_p \rceil \lceil \mathbb{Q} \rceil.$$

Now we can then apply [Thm. 4.3, [25]] to obtain

$$\begin{aligned} \tau(\phi \to V) &= \operatorname{Tr}\left(\lceil (K_p)_{11} \rceil \left(\lceil (Z_p)_{11} \rceil |\rho_\psi\rangle - \lceil (Z_p)_{12} \rceil |\rho_\phi\rangle \right) \right) \\ &= \frac{1}{3} \left(\frac{2p^2 + 11p + 41}{2p^2 - p + 8} \right). \end{aligned}$$

If we take the limit to $p \to 0$*, we obtain*

$$\lim_{p \to 0} \tau(\phi \to V) = \frac{41}{24}.$$

This should be interpreted as the limit of the expected time of first visit to the subspace V *when starting at* ϕ *of the channel* $\mathcal{M}_p$ *when* p *goes to zero. Note that when* p *goes to zero, then* $\mathcal{M}_p \to \mathcal{M}'$*, a unitary channel, and hence not irreducible.*

It can be verified that this result in fact agrees with the one obtained when we calculate $\tau(\phi \to V)$ *directly for the quantum channel* $\mathcal{M}'$*. We can simply calculate the mean hitting time map*

$$K = \mathcal{M}'(I - \mathbb{Q}\mathcal{M}')^{-2},$$

and then use the fact that $\tau(\phi \to V) = \operatorname{Tr}(\mathbb{P} K \rho_\phi)$ *and this expression indeed gives* $41/24$*.*

However, if we try to take the limit of Z_p *as* $p \to 0$*, we will find that the fundamental matrix does not behave well. For example the first entry of the matrix* $\lceil Z_p \rceil$ *is*

$$\frac{1}{9} \left(\frac{3p^3 - 5p^2 + 19p + 4}{(p^2 - 2p + 4)p} \right),$$

which goes to infinity when p *goes to zero. In fact in this example all the entries of the fundamental matrix diverge in the limit* $p \to 0$*.*

Next, instead of using the fundamental matrix, we can define a QMC $\Lambda_p = \Lambda_{\mathcal{M}_p,V}$ dependent on the randomization $\mathcal{M}_p$ and the arrival subspace V and find a generalized inverse for this QMC and then use Theorem 1.20. This is a different way of calculating the mean hitting time in our example, and we can subsequently see how it behaves on the limit when the randomization tends to the unitary case.

So let

$$\lceil\Lambda_p\rceil = \begin{bmatrix} (I-\lceil\mathbb{Q}\rceil)\lceil\mathcal{M}_p\rceil & (I-\lceil\mathbb{Q}\rceil)\lceil\mathcal{M}_p\rceil \\ \lceil\mathbb{Q}\rceil\lceil\mathcal{M}_p\rceil & \lceil\mathbb{Q}\rceil\lceil\mathcal{M}_p\rceil \end{bmatrix}.$$

Let $|u\rangle \in \mathbb{C}^{18}$ be the vector with first component equal to 1 and the remaining equal to zero. We have that $\langle u|\pi\rangle = 1/3 \neq 0$, a condition that will have to be verified next. Also define $|f\rangle \in \mathbb{C}^{18}$ as the vector with only the 2^{nd} and 18^{th} entries equal to 1, say, and the remaining ones zero.

Now let the g-inverse for $I - \lceil\Lambda\rceil_p$ be

$$G = \big(I - \lceil\Lambda\rceil_p + |u\rangle\langle e_{I_3^2}|\big)^{-1} + |f\rangle\langle e_{I_3^2}|,$$

and let G_d be its block diagonal version. Note here that $G = G_p$ is dependent on the parameter p because Λ depends on p. We have that G_p exists for every $p > 0$ because the randomization $\mathcal{M}_p$ is irreducible for $p > 0$, thus, for these values of p, Λ_p is irreducible, which is a sufficient condition for the existence of the g-inverse as defined above. However, in this example, G_p does not exist for $p = 0$. For example, we have that the entry $(2,2)$ of $G = G_p$ is

$$\frac{1}{27}\left(\frac{p^4 + 49p^3 - 74p^2 - 204p + 336}{(p^2 - 2p + 4)(7p^2 - 18p + 12)p}\right)$$

which goes to infinity as $p \to 0$.

Define

$$E := \begin{bmatrix} I_9 & I_9 \\ I_9 & I_9 \end{bmatrix},$$

and let $\lceil K\rceil$ be the matrix of the mean hitting time operator for the QMC Λ, and let $D := \lceil K\rceil_d$ be the block diagonal of this matrix. By Theorem 1.20, item (b), we have

$$\tau(\phi \to V) = \mathrm{Tr}\left(\Big[D\big(I - G + G_d E\big)\Big]_{12}\rho_\phi\right),$$

and by a routine calculation, this expression gives

$$\frac{1}{3}\left(\frac{2p^2 + 11p + 41}{2p^2 - p + 8}\right),$$

which is the same expression found before using the fundamental matrix of the randomization, and therefore it will obviously result in the same limit $\frac{41}{24}$ when $p \to 0$.

However, let us consider the matrix expression in the formula above for $\tau(\phi \to V)$ and call it the Hunter Kernel, or H, i.e.,

$$H := \Big[D\big(I - G + G_d E\big)\Big].$$

As it happens with G, $H = H_p$ is also a function of p. A perhaps remarkable fact is that, although $\lim_{p\to 0} G_p$ does not exist, the limit $H_0 := \lim_{p\to 0} H_p$ exists.

If we now use this limit to calculate $\tau(\phi \to V)$, we obtain

$$\mathrm{Tr}((H_0)_{12}\rho_\phi) = \frac{41}{24}$$

as expected. We can verify that the matrix $A := I - \lceil\Lambda\rceil$ has index 1, therefore by [Thm. 7.6.1, [12]], we can *calculate the Drazin Inverse of* A *via the limit*

$$A^D = \lim_{z\to 0}(A^{l+1} + zI)^{-1}A^l,$$

for every integer $l \geq \operatorname{Ind}(A) = 1$*. In particular, we can calculate it by taking* $l = 1$ *and obtain*

$$A^D = \lim_{z\to 0}(A^2 + zI)^{-1}A.$$

Because the index of A *is* 1*, [Thm. 7.2.4, [12]] tells us that* A^D *is a g-inverse of* $A = I - \lceil\Lambda\rceil_p$*. Therefore we can use* A^D *in place of* G *to calculate Hunter's kernel:*

$$\tilde{H} := D\big(I - A^D - (A^D)_d E\big).$$

Despite A^D *being different from* G*, we have that* $\tilde{H} = H$*. The Hunter kernels using these two different generalized inverses are the same.*

As happened with G*,* A^D *does not have a limit at* $p \to 0$*. In fact, the entry* $(1,1)$ *of* A^D *is*

$$\frac{p^2 + 7p + 4}{9p\,(p^2 - 2p + 4)},$$

which diverges when p *goes to zero.*

Instead of working with the limit $p \to 0$*, we could set directly* $p = 0$ *and consider* Λ_0*, the QMC obtained from the unitary quantum channel* $\mathcal{M}'$*. This QMC is not irreducible anymore, but the index of* $I - \lceil\Lambda_0\rceil$ *is 1, so there is a group inverse* B *for* $I - \lceil\Lambda_0\rceil$ *that we can calculate algebraically.*

If we now apply Hunter's formula and calculate

$$\operatorname{Tr}\left(\Big[D\big(I - B + B_d E\big)\Big]_{12}\rho_\phi\right),$$

we obtain the expected result $41/24$*.*

$\Diamond$

Example 1.24. *Consider the matrices*

$$A_1 = \sqrt{1 - \frac{3s}{4}}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}, \quad A_2 = \frac{\sqrt{s}}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}, \quad A_3 = \frac{\sqrt{s}}{2}\begin{bmatrix}0 & -i\\ i & 0\end{bmatrix}, \quad A_3 = \frac{\sqrt{s}}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix},$$

with $0 < s < 1$*, and the unitary matrix*

$$U = \frac{1}{2}\begin{bmatrix}\sqrt{3} & -1\\ 1 & \sqrt{3}\end{bmatrix}.$$

Let the quantum channels $\lceil\Phi\rceil$ *and* $\lceil\mathcal{M}'\rceil$ *be defined by*

$$\lceil\Phi\rceil = \sum_{i=1}^{4} A_i \otimes \overline{A_i} \quad \textit{and} \quad \lceil\mathcal{M}'\rceil = U \otimes \overline{U}.$$

Now we define the randomization

$$\lceil\mathcal{M}_p\rceil = p\lceil\Phi\rceil + (1-p)\lceil\mathcal{M}'\rceil, \quad 0 < p \leq 1.$$

The channel Φ *is irreducible and has as only fixed state*

$$\pi = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}.$$

It is easy to see that this state is also the fixed state of $\mathcal{M}_p$ *for all* $p \in (0,1]$ *by direct calculation:* $\mathcal{M}_p\pi = p\Phi\pi + (1-p)\mathcal{M}'\pi = p\pi + (1-p)U\pi U^* = p\pi + (1-p)\pi UU^* = p\pi + (1-p)\pi = \pi$*. And by*

Theorem 1.22, $\mathcal{M}_p$ is ergodic for $0 < p \leq 1$, so π is the only fixed point of $\mathcal{M}_p$.

Let us choose two orthogonal states in $\mathscr{H} = \mathbb{C}^2$, $\psi = \begin{bmatrix} 1 & 0 \end{bmatrix}^T$ and $\phi = \begin{bmatrix} 0 & 1 \end{bmatrix}^T$. We will consider the mean hitting times with ϕ as initial state and $V = \operatorname{span}\{\psi\}$ as the arrival subspace. We define the projectors $\lceil \mathbb{P} \rceil = P \otimes \bar{P}$ and $\lceil \mathbb{Q} \rceil = Q \otimes \bar{Q}$ where $P := |\psi\rangle\langle\psi|$ and $Q = I - P$. With that, we can define an OQW dependent on the randomized quantum channel $\mathcal{M}_p$ and the arrival subspace V,

$$\lceil \Lambda_p \rceil = \begin{bmatrix} (I - \lceil \mathbb{Q} \rceil)\lceil \mathcal{M}_p \rceil & (I - \lceil \mathbb{Q} \rceil)\lceil \mathcal{M}_p \rceil \\ \mathbb{Q}\lceil \mathcal{M}_p \rceil & \mathbb{Q}\lceil \mathcal{M}_p \rceil. \end{bmatrix}$$

Consider the vectors from $\mathbb{C}^8$

$$\begin{aligned} |t\rangle &= \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}^T, \\ |f\rangle &= \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}^T, \\ |e_{I_2^2}\rangle &= \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}^T, \end{aligned}$$

where $|u\rangle$ and $|f\rangle$ are chosen arbitrarily. With these, we can define the matrix

$$G = \left(I - \lceil \Lambda_p \rceil + |t\rangle\langle e_{I_2^2}|\right)^{-1} + |f\rangle\langle e_{I_2^2}|,$$

noted that $\langle e_I|t\rangle$ and $\langle u|\pi\rangle$ are not zero and Λ_p is irreducible. These conditions, by Corollary 1.16, guarantee that the matrix $G = G_p$ defined above exists and is a g-inverse for $I - \lceil \Lambda_p \rceil$. The matrix $G = G_p$ will exist for $0 < p \leq 1$, however its limit when $p \to 0$ will not exist. For instance, the entry $(2,2)$ of G is

$$\frac{2p^2 - 3p^2 s - 4p + 4p^2 s^2 + 3ps + 2}{4\left(p^2 s^2 - p^2 s + p^2 - 2p + ps + 1\right) ps},$$

which diverges when p goes to zero.

Now we define the matrix

$$E = \begin{bmatrix} I_4 & I_4 \\ I_4 & I_4 \end{bmatrix},$$

and the block diagonal matrix $D = D_p$ of the mean hitting time operator for $\lceil \Lambda_p \rceil$. So we can define the p-dependent Hunter Kernel

$$H := \left[D\left(I - G + G_d E\right)\right].$$

By Theorem 1.20, equation (1.5.5), we have that the time to reach subspace V starting in state ϕ with our randomization channel $\mathcal{M}_p$ is

$$\begin{aligned} \tau(\phi \to V) &= \operatorname{Tr}\left(H_{12}\rho_\phi\right) \\ &= \frac{4}{-p + 2ps + 1} \end{aligned} \tag{1.6.1}$$

where $\rho_\phi = |\phi\rangle\langle\phi|$. We can see by the expression above that the mean hitting time exists and so does its limit when $p \to 0$. This is consistent with direct calculation for the unitary channel $\mathcal{M}'$: if we compute

$$\begin{aligned} K_U :&= \lceil \mathcal{M}' \rceil \left(I - \lceil \mathbb{Q} \rceil \lceil \mathcal{M}' \rceil\right)^{-2} \\ &= \begin{bmatrix} 2 & \sqrt{3} & \sqrt{3} & 4 \\ -\sqrt{3} & -3 & -4 & -4\sqrt{3} \\ -\sqrt{3} & -4 & -3 & -4\sqrt{3} \\ 4 & 4\sqrt{3} & 4\sqrt{3} & 12 \end{bmatrix}, \end{aligned}$$

then $\tau(\phi \to V) = \operatorname{Tr}\left(K_U \rho_\phi\right) = 4$. And this is the same when we take the limit $p \to 0$ of (1.6.1).

Despite the limit G_p not existing when p goes to zero, we find that the Hunter Kernel has a limit $H_0 = \lim_{p\to 0} H_p$, and in this case it is

$$H_0 = \begin{bmatrix} 2 & \sqrt{3} & \sqrt{3} & 4 & 2 & \sqrt{3} & \sqrt{3} & 4 \\ -\sqrt{3} & -3 & -4 & -4\sqrt{3} & -\sqrt{3} & -3 & -4 & -4\sqrt{3} \\ -\sqrt{3} & -4 & -3 & -4\sqrt{3} & -\sqrt{3} & -4 & -3 & -4\sqrt{3} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\sqrt{3} & 2 & 1 & -\frac{1}{2}\sqrt{3} & -\frac{1}{2}\sqrt{3} & 2 \end{bmatrix},$$

and it will give us $\tau(\phi \to V) = \mathrm{Tr}\left((H_0)_{12}\rho_\phi\right) = 4$.

Now we consider $A = I - \lceil \Lambda_p \rceil$, and calculate its Drazin inverse A^D, which we know by Theorem 1.26 that it is also a group inverse, and hence a g-inverse.

We can calculate the Hunter Kernel with it

$$\tilde{H} = D\big(I - A^D + (A^D)_d E\big),$$

and although we can verify that A^D is different from G calculated previously, we have that $\tilde{H} = H$, the Hunter Kernels are equal. So of course we will have the same $\tau(\phi \to V)$ found in (1.6.1) if we use $\tilde{H}$. And as happened with G_p, A^D also diverges when $p \to 0$. In fact, the entry $(2,2)$ of A^D is the same as that of G, which we have shown to be divergent.

We finish this example by setting $p = 0$ on Λ_p, and by calculating $\tau(\phi \to V)$ for the unitary channel $\mathcal{M}'$ with the OQW Λ_0 via the Drazin Inverse. Let $B = I - \lceil \Lambda_0 \rceil$. We then obtain

$$B^D = \frac{1}{4}\begin{bmatrix} 1 & -\sqrt{3} & -\sqrt{3} & -1 & -3 & -\sqrt{3} & -\sqrt{3} & -1 \\ \sqrt{3} & 1 & 1 & -\sqrt{3} & \sqrt{3} & -3 & 1 & -\sqrt{3} \\ \sqrt{3} & 1 & 1 & -\sqrt{3} & \sqrt{3} & 1 & -3 & -\sqrt{3} \\ 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\ -1 & \sqrt{3} & \sqrt{3} & -3 & -1 & \sqrt{3} & \sqrt{3} & 1 \end{bmatrix}.$$

We also calculate D for Λ_0, and with it we can obtain the Hunter Kernel with $\hat{H} := D\big(I - B^D + (B^D)_d E\big)$. It turns out that $\hat{H} = H_0$, i.e., it is the same as the limit $p \to 0$ of the p-dependent Hunter Kernel we found previously. So clearly it gives us $\tau(\phi \to V) = \mathrm{Tr}\left((\hat{H})_{12}\rho_\phi\right) = 4$.

$\Diamond$

1.6.2 Another hitting time formula: extending the irreducible case

Our brief look at randomizations of quantum channels in the previous section, together with the examples, suggest a natural direction regarding hitting time formulae for unitary maps. Briefly, we have the following: given a randomization of an irreducible channel, we have that generalized inverses for the dynamics always exist. Then, by taking $p \to 0$ we obtain the correct values for the hitting times. The proper (Hunter) kernel is obtained and the limit of the trace calculation behaves as expected. On the other hand, the generalized inverses themselves cannot be obtained via such limit in general, as the examples have clearly shown. Moreover, we have also seen that by setting $p = 0$ directly, one obtains the proper hitting times by choosing the group inverse, but that such inverse is not the limit of g-inverses of randomizations in general.

With all this in consideration, we ask the following natural question: is there a g-inverse that could be obtained regardless of randomizations, and such that its existence is guaranteed even in the reducible case? We will present a positive answer to this, which is in fact given by the group inverse. Let us discuss this in more general terms, also clarifying how the irreducibility assumption can be replaced by a weaker notion.

We state without proof a result that will be used next.

Theorem 1.25 (Trivial Jordan blocks for peripheral spectrum). *Let $T : M_d(\mathbb{C}) \to M_d(\mathbb{C})$ be a trace-preserving (or unital) positive linear map. If λ is an eigenvalue of T with $|\lambda| = 1$, then its geometric multiplicity equals its algebraic multiplicity, i.e., all Jordan blocks for λ are one-dimensional.*

For a proof, we refer to [Proposition 6.2, [31]].

Theorem 1.26. *For every positive, trace preserving map T on a finite dimensional Hilbert space, matrix $A^{\#}$ exists, where $A = I - T$.*

Proof. By Theorem 1.25, the matrix $\lceil T \rceil$ has only one-dimensional Jordan blocks relative to the eigenvalue 1, so its Jordan decomposition will have the form

$$\lceil T \rceil = X \begin{bmatrix} I & \\ & B \end{bmatrix} X^{-1},$$

where I is an identity matrix of some dimension and B is a matrix with no eigenvalue equal to 1. It follows that

$$A = I - \lceil T \rceil = X \begin{bmatrix} O & \\ & I - B \end{bmatrix} X^{-1} \quad \Longrightarrow \quad A^2 = X \begin{bmatrix} O & \\ & (I - B)^2 \end{bmatrix} X^{-1}.$$

Because B has no eigenvalues equal to 1, it follows that $I - B$ is nonsingular, and hence so is $(I - B)^2$. By Lemma A.5, both A and A^2 have the same rank as $I - B$ and $(I - B)^2$, so $\mathrm{Ind}(A) \leq 1$. Therefore, by Theorem 1.7, the group inverse $A^{\#}$ exists.

□

Now we state an important lemma, regarding a conditioning on the first step reasoning. The conditioning reasoning below, in terms of the operator L, has been introduced in [23] in the context of OQWs.

Lemma 1.27. *Let Φ be a finite ergodic QMC, let K be its Hitting Time operator and $D = \mathrm{diag}(K_{11}, \ldots, K_{nn})$, and define $L := K - (K - D)\Phi$. Then for ρ_j a density concentrated at site j, for all i, and $c \in \mathbb{R}$, it holds that $\mathrm{Tr}\left(L_{ij}(c\rho_j)\right) = \mathrm{Tr}(c\rho_j) = c$.*

Proof. By a first-step conditioning reasoning, we can define

$$k_{ij}(\rho_j \mid X_1 = l) := 1 + k_{il}\left(\frac{\Phi_{lj}(\rho_j)}{\mathrm{Tr}(\Phi_{lj}(\rho_j))}\right).$$

Then for $i \neq j$,

$$\begin{aligned}
k_{ij}(\rho_j) &= \sum_{l=1}^{n} k_{ij}(\rho_j \mid X_1 = l)\mathbb{P}_{j,\rho_j}(X_1 = l) = \sum_{l=1}^{n} k_{ij}(\rho_j \mid X_1 = l)\,\mathrm{Tr}\left(\Phi_{lj}(\rho_j)\right) \\
&= \sum_{l=1}^{n}\left[1 + k_{il}\left(\frac{\Phi_{lj}(\rho_j)}{\mathrm{Tr}(\Phi_{lj}(\rho_j))}\right)\right]\mathrm{Tr}\left(\Phi_{lj}(\rho_j)\right) \\
&= 1 + k_{ii}\left(\frac{\Phi_{ij}(\rho_j)}{\mathrm{Tr}(\Phi_{ij}(\rho_j))}\right)\mathrm{Tr}\left(\Phi_{ij}(\rho_j)\right) + \sum_{\substack{l=1 \\ l \neq i}}^{n} k_{lj}\left(\frac{\Phi_{lj}(\rho_j)}{\mathrm{Tr}(\Phi_{lj}(\rho_j))}\right)\mathrm{Tr}\left(\Phi_{lj}(\rho_j)\right).
\end{aligned}$$

If we rewrite the above without the trace terms, we are left with

$$k_{ij}(\rho_j) = 1 + \sum_{l \neq i} k_{il}(\Phi_{lj}(\rho_j)),$$

which can be rearranged, and by multiplication of a constant $c \in \mathbb{R}$, by linearity of the operators, it becomes

$$c = k_{ij}(\rho_j) - \sum_{l \neq i} k_{il}(\Phi_{lj}(\rho_j)).$$

Defining $L := K - (K - D)\Phi$, where $D = \operatorname{diag}(K_{11}, \ldots, K_{nn})$, then by taking the block (i, j) of the operator L and applying it on $c\rho_j$, for a density ρ_j, and taking the trace:

$$\operatorname{Tr}\left(L_{ij}(c\rho_j)\right) = \operatorname{Tr}\left[K_{ij}(c\rho_j) - [(K - D)\Phi]_{ij}(c\rho_j)\right] = k_{ij}(c\rho_j) - \sum_{l \neq i} k_{lj}(c\rho_j) = c.$$

□

Finally, we are ready to state our main result. For the following, we consider a QMC Φ as defined in (1.5.2), a V-dependent QMC induced by a quantum channel T, without assuming T irreducible.

Theorem 1.28. *Let $\Phi = \Lambda_{T,V}$ be a QMC acting on two vertices, let $\mathbb{P}$ be the orthogonal projection onto the first vertex, and let $\mathbb{Q} = I - \mathbb{P}$. Suppose that 1 does not belong to the spectrum of $\mathbb{Q}\Phi$ and let ρ denote state in the second vertex. Let $A = I - \Phi$ and let $A^{\#}$ denote its group inverse. Then,*

$$\tau(\rho \to V) = \operatorname{Tr}\left(\left[D(I - A^{\#} + A_d^{\#}E)\right]_{12}\rho\right).$$

Remark 1.29. *In [16], it is proven that if the dynamics is irreducible, then 1 does not belong to the spectrum of $\mathbb{Q}\Phi$. This basic fact ensures the analyticity of the generating function $\mathbb{G}(z) = z(I - z\mathbb{Q}\Phi)^{-1}$ at $z = 1$ (recall Section 1.4 for this notion), and so implies the finiteness of the mean hitting times for any initial state. This provides a global condition that allows us to write hitting time formulae in terms of a kernel which is well-defined for the entire space. As it becomes clear in the examples, there are reducible examples which also satisfy this spectral condition, thus extending the previous results seen in the literature.*

Proof. We start with the definition $L := K - (K - D)\Phi$, where $D = K_d$, and rearrange it to obtain

$$K(I - \Phi) = L - D\Phi. \tag{1.6.2}$$

Operator L is well-defined, due to the assumption that 1 does not belong to the spectrum of $\mathbb{Q}\Phi$, also see Remark 1.29. Now define $A := I - \Phi$ and solve equation (1.6.2) for K using the group inverse $A^{\#}$ of A, which we know exists, by Theorem 1.26. We use Proposition 1.2, which affirms that equation (1.6.2) is consistent if and only if

$$(L - D\Phi)(I - A^{\#}A) = 0 \quad \Longleftrightarrow \quad KA(I - A^{\#}A) = 0.$$

But it is clear that the equation on the right is satisfied by the properties of $A^{\#}$, namely $AA^{\#}A = A$. So, we have that the solution to (1.6.2) is given by

$$K = (L - D\Phi)A^{\#} + V(I - AA^{\#}), \tag{1.6.3}$$

where V is an arbitrary matrix.

Note that the i-th row of the matrix $I - AA^{\#}$ is $\langle e_i|(I - AA^{\#})$, where $|e_i\rangle$ is the i-th standard basis vector of $\mathbb{C}^{2k^2}$. And the row vector $\langle e_i|(I - AA^{\#})$ is a fixed point of Φ to the left, because $\langle e_i|(I - AA^{\#})(I - \Phi) = \langle e_i|(I - AA^{\#})A = \langle e_i|(A - AA^{\#}A) = 0$, since $AA^{\#}A = A$. However, our matrix for Φ has the form

$$\begin{bmatrix} X & X \\ Y & Y \end{bmatrix}, \tag{1.6.4}$$

where X and Y are $k^2 \times k^2$ blocks. So if $\left[\langle v_1| \quad \langle v_2|\right]$ is a row vector where each $\langle v_i|$ is row vector of length k^2, we have, supposing it is a fixed point of Φ to the right, that

$$\left[\langle v_1| \quad \langle v_2|\right] = \left[\langle v_1| \quad \langle v_2|\right] \begin{bmatrix} X & X \\ Y & Y \end{bmatrix} = \left[\langle v_1|X + \langle v_2|Y \quad \langle v_1|X + \langle v_2|Y\right],$$

in conclusion, $\langle v_1| = \langle v_2|$. So every row of $I - AA^{\#}$ will have the form $\begin{bmatrix}\langle v| & \langle v|\end{bmatrix}$, and $I - AA^{\#}$ will have the same form as in (1.6.4). And it is easy to see that the same will apply to $V(I - AA^{\#})$, for any matrix V. Because of these facts, if we define

$$E := \begin{bmatrix} I_{k^2} & I_{k^2} \\ I_{k^2} & I_{k^2}, \end{bmatrix},$$

we will have $(I - AA^{\#})_d E = (I - AA^{\#})$ and $\big(V(I - AA^{\#})\big)_d E = V(I - AA^{\#})$.

We can define $B := \big(V(I - AA^{\#})\big)_d$ and substitute $V(I - AA^{\#}) = BE$ in (1.6.3) to get:

$$K = (L - D\Phi)A^{\#} + BE. \tag{1.6.5}$$

We take the diagonal and obtain

$$D = K_d = (LA^{\#})_d - D(\Phi A^{\#})_d + B \quad \Longrightarrow \quad B = D + D(\Phi A^{\#})_d - (LA^{\#})_d.$$

Now we define $W := L - D(I - AA^{\#})$ and use it to eliminate L in the equation for B above, so we get:

$$\begin{aligned} B &= D + D(\Phi A^{\#})_d - (WA^{\#})_d + \big(D(I - AA^{\#})A^{\#}\big)_d \\ &= D + D(\Phi A^{\#})_d - (WA^{\#})_d. \end{aligned} \tag{1.6.6}$$

where one term was canceled because $(I - AA^{\#})A^{\#} = (I - A^{\#}A)A^{\#} = A^{\#} - A^{\#}AA^{\#} = 0$. Substituting B from (1.6.6) in (1.6.5), and eliminating L using W, we have

$$\begin{aligned} K &= \Big(W + D(I - AA^{\#}) - D\Phi\Big)A^{\#} + DE + D(\Phi A^{\#})_d E - (WA^{\#})_d E \\ &= D\Big[-\Phi A^{\#} + E + (\Phi A^{\#})_d E\Big] + WA^{\#} - (WA^{\#})_d E, \end{aligned} \tag{1.6.7}$$

where again a term has vanished because $(I - AA^{\#})A^{\#} = 0$.

Now consider $H := (I - AA^{\#})_d$. We know $HE = I - AA^{\#}$, so

$$I - AA^{\#} = I - A^{\#} + \Phi A^{\#} = HE,$$

and hence, taking the diagonal we obtain

$$\begin{aligned} & I - (A^{\#})_d + (\Phi A^{\#}) = H \\ \Longrightarrow & E - (A^{\#})_d E + (\Phi A^{\#})_d E = HE = I - A^{\#} + \Phi A^{\#} \\ \Longrightarrow & -\Phi A^{\#} + E + (\Phi A^{\#})_d E = I - A^{\#} + A^{\#}_d E. \end{aligned} \tag{1.6.8}$$

Subsituting (1.6.8) into (1.6.7), we obtain

$$K = D\Big[I - A^{\#} + A^{\#}_d E\Big] + WA^{\#} - (WA^{\#})_d E. \tag{1.6.9}$$

It remains to show that the $\mathrm{Tr}\Big((WA^{\#})_{12}\rho\Big)$ and $\mathrm{Tr}\Big(\big[(WA^{\#})_d E\big]_{12}\rho\Big)$ are zero for any ρ.

Note that by multiplying (1.6.2) on the right by any Φ-invriant vector $|\rho\rangle$, we obtain $L|\rho\rangle = D|\rho\rangle$, whence

$$\mathrm{Tr}\left(K_{11}|\rho_1\rangle\right) = \mathrm{Tr}\left((L|\rho\rangle)_1\right) = \sum_j \mathrm{Tr}\left(L_{1j}|\rho_j\rangle\right) = \sum_j \mathrm{Tr}(\rho_j) \tag{1.6.10}$$

where in the third equality the property of Lemma 1.27 was used. Also, note that for any vector $|\rho\rangle$, the new vector $(I - AA^{\#})|\rho\rangle$ will be invariant by Φ, with

$$\begin{aligned} \sum_j \mathrm{Tr}\Big(\big((I - AA^{\#})|\rho\rangle\big)_j\Big) &= \mathrm{Tr}\Big((I - AA^{\#})|\rho\rangle\Big) \\ &= \langle e_{I^2_{k^2}}|(I - AA^{\#})|\rho\rangle = \langle e_{I^2_{k^2}}|\rho\rangle \\ &= \sum_j \langle e_{I_{k^2}}|\rho_j\rangle = \sum_j \mathrm{Tr}(\rho_j). \end{aligned} \tag{1.6.11}$$

If $|\rho\rangle$ is a vector concentrated at site m, i.e., if it is of the form

$$|\rho\rangle = \begin{bmatrix}\rho\\0\end{bmatrix} \text{ or } \begin{bmatrix}0\\\rho\end{bmatrix},$$

then equation (1.6.11) reduces to

$$\sum_j \mathrm{Tr}\left(\left((I - AA^{\#})|\rho\rangle\right)_j\right) = \mathrm{Tr}\left(\rho\right) \tag{1.6.12}$$

Now we proceed to show that the terms involving W in (1.6.9) will have trace zero.

$$\begin{aligned}
\mathrm{Tr}\left((WA^{\#})_{1r}\rho\right) &= \mathrm{Tr}\left((LA^{\#})_{1r}\rho\right) - \mathrm{Tr}\left(\left(D(I - AA^{\#})A^{\#}\right)_{1r}\rho\right) \\
&= \sum_m \left[\mathrm{Tr}\left(L_{1m}A^{\#}_{mr}\rho\right) - \mathrm{Tr}\left(K_{11}(I - AA^{\#})_{1m}A^{\#}_{mr}\rho\right)\right] \\
&= \sum_m \left[\mathrm{Tr}\left(A^{\#}_{mr}\rho\right) - \mathrm{Tr}\left(K_{11}(I - AA^{\#})_{1m}A^{\#}_{mr}\rho\right)\right]
\end{aligned} \tag{1.6.13}$$

where again the property of the operator L was used, and the index r can be either 1 or 2. Note that

$$(I - AA^{\#})_{1m}A^{\#}_{mr}\rho = \left[(I - AA^{\#})|\rho\rangle\right]_1,$$

where $|\rho\rangle$ is the vector with $A^{\#}_{mr}\rho$ concentrated at site m. So, for this choice of $|\rho\rangle$,

$$\begin{aligned}
\mathrm{Tr}\left(K_{11}(I - AA^{\#})_{1m}A^{\#}_{mr}\rho\right) &= \mathrm{Tr}\left(K_{11}\left[(I - AA^{\#})|\rho\rangle\right]_1\right) \\
&= \sum_j \mathrm{Tr}\left(\left[(I - AA^{\#})|\rho\rangle\right]_j\right) \\
&= \mathrm{Tr}\left(A^{\#}_{mr}\rho\right),
\end{aligned} \tag{1.6.14}$$

where in the second equality we used equation (1.6.10), and in the last equality we used (1.6.12). Inserting (1.6.14) back into (1.6.13) we get

$$\mathrm{Tr}\left((WA^{\#})_{1r}\rho\right) = \sum_m \left[\mathrm{Tr}\left(A^{\#}_{mr}\rho\right) - \mathrm{Tr}\left(A^{\#}_{mr}\rho\right)\right] = 0.$$

It is immediate from the above with $r = 2$ that $\mathrm{Tr}\left((WA^{\#})_{12}\rho\right) = 0$. But also for $r = 1$ it gives us

$$\mathrm{Tr}\left(\left((WA^{\#})_d E\right)_{12}\rho\right) = \mathrm{Tr}\left((WA^{\#})_{11}\rho\right) = 0.$$

Therefore, when we calculate $\mathrm{Tr}\left(K_{12}\rho\right)$ using (1.6.9), the terms involving W vanish and the result follows.

□

Consider the general form of a g-inverse for an irreducible QMC Φ with invariant state $|\pi\rangle$,

$$G = \left(I - \Phi + |t\rangle\langle u|\right)^{-1} + |\pi\rangle\langle f| + |g\rangle\langle e_I| \tag{1.6.15}$$

with $\langle u|\pi\rangle \neq 0$ and $\langle e_I|t\rangle \neq 0$. We could not use this method to find the group inverse for an irreducible Φ. But if Φ is irreducible, we know that by varying the parameters $|f\rangle$ and $|g\rangle$, and possibly $|u\rangle$ and $|t\rangle$, we can produce every g-inverse of $I - \Phi$, in particular, we can produce the g-inverse. So we can ask, for $A := I - \Phi$, what choices of parameters will give us $G = A^{\#}$.

Corollary 2.7 suggests the choice $|u\rangle = |e_I\rangle$ and $|f\rangle = 0$ in (1.6.15) in order to get $G = A^{\#}$, because with this choice we could derive the same conclusion of Theorem 1.28. So, with

$$G = \left(I - \Phi + |t\rangle\langle e_I|\right)^{-1} + |g\rangle\langle e_I|,$$

we can try to adjust the other paramenters to obtain the properties $AA^{\#} = A^{\#}A$ and $A^{\#}AA^{\#} = A^{\#}$.

For the first one, the commutative property, we have $G(I-\Phi) = (I-\Phi)G$ if and only if

$$I - |\pi\rangle\langle e_I| = I - \frac{|t\rangle\langle e_I|}{\langle e_I|t\rangle} + (I-\Phi)|g\rangle\langle e_I|,$$

which will be verified if we choose, for example, $|t\rangle = |\pi\rangle$ and $|g\rangle = c \cdot |\pi\rangle$, for some scalar c.

For the other property, we will have $G(I-\Phi)G = G$ if and only if

$$\frac{|\pi\rangle\langle e_I|}{\langle e_I|t\rangle} + \big(\langle e_I|g\rangle\big) \cdot |\pi\rangle\langle e_I| = 0$$

which will be verified if $|t\rangle = |\pi\rangle$ and $\langle e_I|g\rangle = -1$.

It is easy to see that if we choose $|t\rangle = |\pi\rangle$ and $|g\rangle = -|\pi\rangle$, then these conditions will be fulfilled, and we will have G written as

$$G = \Big(I - \Phi + |\pi\rangle\langle e_I|\Big)^{-1} - |\pi\rangle\langle e_I|,$$

where we can recognize $\Omega = |\pi\rangle\langle e_I|$ and the fundamental matrix $Z = \big(I - \Phi + \Omega\big)^{-1}$.

In conclusion, we have that if Φ is an irreducible QMC, then the group inverse for $A := I - \Phi$ is given by $Z - \Omega$, a result analogous to what is known in the classical setting (see for example, Theorem 3.1, [28]). In addition, because of Corollary 2.7 with $G = A^{\#}$, we will have that if a walk starts with density ρ_j concentrated at site j, then the mean hitting time to hit site i will be given by

$$\tau(\rho_j \otimes |j\rangle \to |i\rangle) = \mathrm{Tr}\Big(\big[D(I - A^{\#} + A^{\#}_d E\big]_{ij}\rho_j\Big),$$

where E and D are as defined in the statement of that corollary.

Chapter 2

Continuous-time QMCs

2.1 Continuous-time QMCs

This chapter serves as a complement to the theory discussed in Chapter 1. Here we illustrate how some of the constructions translate naturally to the context of continuous semigroups, in analogy with what one has in the classical theory of Markov chains. There is no intention of being comprehensive regarding the collection of results presented here, as the main reasonings for the theorems are similar to the ones seen in the discrete-time case.

2.1.1 Review on semigroups

We refer the reader to [31] for more on this setting. An operator **semigroup** $\mathcal{T}$ on a Banach space $\mathcal{B}$ is a family of bounded linear operators (T_t), $t \geq 0$ acting on $\mathcal{B}$, such that

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

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

Theorem 2.1. *The following assertions are equivalent for a semigroup $\mathcal{T}$ on $\mathcal{B}$:*

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

$$T_t = e^{t\mathcal{L}}, \textit{ for all } t \in \mathbb{R}^+.$$

Further, if these conditions are satisfied, then

$$\mathcal{L} = \lim_{t\to\infty} \frac{1}{t}(T_t - I_{\mathcal{B}}).$$

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

Definition 2.2. *Let $\mathcal{K}$ be a Hilbert space. A* **Quantum Markov Semigroup** *(QMS) on the set of trace-class operators $\mathcal{I}_1(\mathcal{K})$ is a semigroup $\mathcal{T} := (T_t)$, $t \geq 0$ of completely positive trace-preserving maps acting on $\mathcal{I}_1(\mathcal{K})$.*

When $\lim_{t\to 0} \|T_t - \mathrm{Id}\| = 0$, then $\mathcal{T}$ has a **generator** $\mathcal{L} = \lim_{t\to\infty}(T_t - \mathrm{Id})/t$, which is a bounded operator on $\mathcal{I}_1(\mathcal{K})$, called a **Lindblad operator**.

Regarding generators of completely positive semigroups, we recall the fundamental result due to Gorini, Kossakowski, Sudarshan and Lindblad [14, 27]:

Theorem 2.3. *A linear operator $L : M_n \to M_n$ is the generator of a completely positive dynamical semigroup on M_n if, and only if it can be written in the form*

$$L\rho = -i[H,\rho] + \frac{1}{2}\sum_{i,j=1}^{N^2-1} c_{ij}\left([F_i, \rho F_j^*] + [F_i\rho, F_j^*]\right),$$

where $H = H^*$, $\mathrm{tr}(H) = 0$, $\mathrm{tr}(F_i) = 0$ e $\mathrm{tr}(F_i^* F_j) = \delta_{i,j}$.

Remark 2.4. *Regarding Lindblad generators, we remark the important useful fact that, given any quantum channel Φ the map $\Phi - I$ is a valid generator, that is, $e^{t(\Phi-I)}$, $t \geq 0$, is a completely positive semigroup [Lemma 1.1, [31]]. Motivated by this, in this work we will consider generators of the form*

$$\mathcal{L} = \lambda(\Phi - I),$$

where Φ is a quantum channel and $\lambda > 0$ is the **transition rate** *of the walk.*

2.1.2 Continuous-time QMCs

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

$$\mathcal{H} = \bigoplus_{i\in V} \mathfrak{h}_i, \tag{2.1.1}$$

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

To define precisely the CTOQW, we recall that the set of density operators on $\mathcal{K}$ is denoted

$$\mathcal{S}(\mathcal{K}) := \{\rho \in \mathcal{I}_1(\mathcal{K}), \rho \geq 0, \mathrm{Tr}(\rho) = 1\}.$$

The set of block-diagonal density operators on $\mathcal{H}$ is denoted by

$$\mathcal{D} := \left\{\rho \in \mathcal{S}(\mathcal{H}) \;:\; \rho = \sum_{i\in V} \rho_i \otimes |i\rangle\langle i|\right\}.$$

This means that if $\rho \in \mathcal{D}$, then $\rho_i \in \mathcal{I}_1(\mathfrak{h}_i)$, $\rho_i \geq 0$ and $\sum_{i\in V} \mathrm{Tr}(\rho_i) = 1$.

Definition 2.5. *Let V be a finite or countably infinite set and $\mathcal{H}$ be a Hilbert space of the form (2.1.1). A* **Continuous-Time QMC** *(CTQMC) is an uniformly continuous QMS on $\mathcal{I}_1(\mathcal{H})$ with Lindblad operator of the form*

$$\begin{aligned}\mathcal{L} : \mathcal{I}_1(\mathcal{H}) &\to \mathcal{I}_1(\mathcal{H})\\ \rho &\mapsto -i[H,\rho] + \sum_{i,j\in V}\left(S_i^j \rho S_i^{j^*} - \frac{1}{2}\left\{S_i^{j*} S_i^j, \rho\right\}\right),\end{aligned} \tag{2.1.2}$$

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

Sometimes (2.1.2) is called **Lindblad Master Equation** *of the semigroup.*

2.2 Hunter's hitting time formula for CTQMCs

A useful identity follows from the fact that $(I - \Phi + |t\rangle\langle u|)^{-1}|t\rangle\langle u| = I - (I - \Phi + |t\rangle\langle u|)^{-1}(I - \Phi)$. If we multiply both sides on the right by $|\pi\rangle$ and noticing that $(I - \Phi)|\pi\rangle = 0$, we then have

$$(I - \Phi + |t\rangle\langle u|)^{-1}|t\rangle\langle u|\pi\rangle = |\pi\rangle \quad \Longleftrightarrow \quad (I - \Phi + |t\rangle\langle u|)^{-1}|t\rangle\langle u| = \frac{|\pi\rangle\langle u|}{\langle u|\pi\rangle}. \tag{2.2.1}$$

Similarly, if we multiply both sides of the equation $|t\rangle\langle u|(I-\Phi+|t\rangle\langle u\rangle)^{-1} = I-(I-\Phi)(I-\Phi|t\rangle\langle u|)^{-1}$ on the left by $\langle e_I|$, seeing that $\langle e_I|(I-\Phi)=0$, we have

$$\langle e_I|t\rangle\langle u|(I-\Phi+|t\rangle\langle u|)^{-1} = \langle e_I| \quad\iff\quad |t\rangle\langle u|(I-\Phi+|t\rangle\langle u|)^{-1} = \frac{|t\rangle\langle e_I|}{\langle e_I|t\rangle}. \tag{2.2.2}$$

Theorem 2.6. *Let Φ an irreducible QMC acting on a finite graph with $n \geq 2$ vertices and internal degree $k \geq 2$, and let T be the semigroup given by*

$$T = e^{\lambda(\Phi-I)t}, \quad t \geq 0, \quad \lambda > 0.$$

Let π be its stationary density and Ω its limit map. Let $K=(k_{ij})$ denote the matrix of mean hitting time operators to vertices $i=1,...,n$, $D=K_d=diag(k_{11},...,k_{nn})$, G be any g-inverse of $I-\Phi$, and let E denote the block matrix for which each block equals the identity of order k^2. (a) The mean hitting time for the walk to reach vertex i, beginning at vertex j with initial density ρ_j, is given by

$$\mathrm{Tr}(k_{ij}\rho_j) = \mathrm{Tr}\left(\big[D\big(\Omega G-(\Omega G)_d E + I - G + G_d E\big)\big]_{ij}\rho_j\right)$$

Proof. We begin with the definition $L := K-(K-D)\Phi$ so we can write K as

$$K(I-\Phi) = L - D\Phi.$$

By Corollary 1.3 the above equation for K is consistent if, and only if, the following holds

$$(L-D\Phi)G(I-\Phi) = L-D\Phi \quad\iff\quad (L-D\Phi)\big[I-G(I-\Phi)\big]=0.$$

Looking at the term in square brackets, and using the general form of G given by 1.16, we have

$$\begin{aligned}
I-G(I-\Phi) &= I-\big(I-\Phi+|t\rangle\langle u|\big)^{-1}(I-\Phi) - |\pi\rangle\langle f|(I-\Phi) - |g\rangle\langle e_I|(I-\Phi)\\
&= \frac{|\pi\rangle\langle u|}{\langle u|\pi\rangle} - |\pi\rangle\langle f|(I-\Phi)\\
&= |\pi\rangle\left(\frac{\langle u|}{\langle u|\pi\rangle} - \langle f|(I-\Phi)\right)
\end{aligned}$$

where we have used equation 2.2.1 and the fact that $\langle e_I|(I-\Phi)=0$. We thus have that $I-G(I-\Phi)$ is of the form $|\pi\rangle\langle v|$ for some vector $|v\rangle$. So the consistency condition is equivalent to

$$(L-D\Phi)|\pi\rangle\langle v| = 0$$

which is satisfied because $L-D\Phi = K(I-\Phi)$ and $(I-\Phi)|\pi\rangle = 0$.

Therefore the solution, by corollary 1.3 is

$$K = (L-D\Phi)G + V(I-(I-\Phi)G).$$

The term $I-(I-\Phi)G$ can be simplified using the expression for general G in 1.16

$$\begin{aligned}
I-(I-\Phi)G &= I-(I-\Phi)\big(I-\Phi+|t\rangle\langle u|\big)^{-1} - (I-\Phi)|\pi\rangle\langle f| - (I-\Phi)|g\rangle\langle e_I|\\
&= \frac{|t\rangle\langle e_I|}{\langle e_I|t\rangle} - (I-\Phi)|g\rangle\langle e_I|\\
&= \left(\frac{|t\rangle}{\langle e_I|t\rangle} - (I-\Phi)|g\rangle\right)\langle e_I|\\
&= |h\rangle\langle e_I|
\end{aligned} \tag{2.2.3}$$

where we used the fact that $(I-\Phi)|\pi\rangle=0$ and the identity (2.2.2), and $|h\rangle$ is some vector. Now we are left with

$$\begin{aligned}
K &= (L-D\Phi)G + V|h\rangle\langle e_I|\\
&= (L-D\Phi)G + |b\rangle\langle e_I|.
\end{aligned}$$

Define

$$B := (|b\rangle\langle e_I|)_d$$

where $(A)_d$, with A being a square matrix of order nk^2, denotes maintaining only the diagonal $k^2 \times k^2$ blocks of the matrix A and making all other blocks equal to the null matrix. With this definition it follows that $BE = |b\rangle\langle e_I|$. With this, we then have

$$K = (L - D\Phi)G + BE. \tag{2.2.4}$$

Taking the diagonal blocks on the equation for K, we are left with

$$\begin{aligned} D = K_d &= [(L - D\Phi)G]_d + (|b\rangle\langle e_I|)_d \\ &= (LG)_d - (D\Phi G)_d + B \\ &= (LG)_d - D(\Phi G)_d + B, \end{aligned}$$

where we note that for any square matrices of order nk^2 A and D, where D is block diagonal, it is true that $(AD)_d = A_d D$ and $(DA)_d = DA_d$. We can now solve the above equation for B to obtain

$$B = D + D(\Phi G)_d - (LG)_d. \tag{2.2.5}$$

Now define

$$W := L - D\Omega.$$

Substituting this in equation 2.2.5 to eliminate L, we get

$$\begin{aligned} B &= D + D(\Phi G)_d - D(\Omega G)_d - (WG)_d \\ &= D\big[I + (\Phi G)_d - (\Omega G)_d\big] - (WG)_d. \end{aligned}$$

Now if we substitute the above expression for B in equation 2.2.4, as well substitute L by $W + D\Omega$ in 2.2.4, then

$$\begin{aligned} K &= (L - D\Phi)G + BE \\ &= (W + D\Omega - D\Phi)G + \big(D\big[I + (\Phi G)_d - (\Omega G)_d\big] - (WG)_d\big)E \\ &= D\big[\Omega G - \Phi G + E + (\Phi G)_d E - (\Omega G)_d E\big] + WG - (WG)_d E \end{aligned} \tag{2.2.6}$$

For a simplification of this formula, we define, in the same manner we have defined B, the matrix H as $H := (|h\rangle\langle e_I|)_d$, and we have as a consequence that $HE = |h\rangle\langle e_I|$.

By equation 2.2.3 we have that

$$I - G + \Phi G = HE,$$

and then, taking the block diagonal of the above, it follows that

$$\begin{aligned} &I - G_d + (\Phi G)_d = HE_d = HI = H \\ \implies &E - G_d E + (\Phi G)_d E = HE = I - G + \Phi G. \end{aligned}$$

By rearranging terms we have

$$E + (\Phi G)_d E - \Phi G = I - G + G_d E,$$

and all the terms on the left-hand side of the above appear in the square brackets of 2.2.6. Therefore substituting it in 2.2.6 we obtain

$$K = D\big[\Omega G - (\Omega G)_d E + I - G + G_d E\big] + WG - (WG)_d E.$$

The theorem is proven if we can show that for an arbitrary density ρ_j concentrated at a site j we have $\mathrm{Tr}\left([WG-(WG)_dE]_{ij}\rho_j\right)=0$. Indeed,

$$\begin{aligned}
\langle e_{I_k}|(WG)_{ij}|\rho_j\rangle &= \langle e_{I_k}|[(L-D\Omega)G]_{ij}|\rho_j\rangle \\
&= \langle e_{I_k}|(LG)_{ij}|\rho_j\rangle - \langle e_{I_k}|(D\Omega G)_{ij}|\rho_j\rangle \\
&= \sum_{l=1}^{n}\langle e_{I_k}|L_{il}G_{lj}|\rho_j\rangle - \sum_{l=1}^{n}\langle e_{I_k}|k_{ii}|\pi_i\rangle\langle e_{I_k}|G_{lj}|\rho_j\rangle \\
&= \sum_{l=1}^{n}\langle e_{I_k}|G_{lj}|\rho_j\rangle - \sum_{l=1}^{n}\langle e_{I_k}|G_{lj}|\rho_j\rangle \\
&= 0,
\end{aligned}$$

where we used the fact that $\langle e_{I_k}|k_{ii}|\pi_i\rangle = 1$ due to 1.14, and that $\mathrm{Tr}(L_{ij}\rho_j)=\mathrm{Tr}(\rho_j)$ for all $i,j=1,\ldots,n$ and all $\rho_j\in M_k(\mathbb{C})$, by Lemma 1.27. The same calculation for the second term with W gives us

$$\begin{aligned}
\langle e_{I_k}|\big((WG)_dE\big)_{ij}|\rho_j\rangle &= \langle e_{I_k}|\big((LG-D\Omega G)_dE\big)_{ij}|\rho_j\rangle \\
&= \langle e_{I_k}|((LG)_dE)_{ij}|\rho_j\rangle - \langle e_{I_k}|(D(\Omega G)_dE)_{ij}|\rho_j\rangle \\
&= \langle e_{I_k}|(LG)_{ii}E_{ij}|\rho_j\rangle - \langle e_{I_k}|k_{ii}(\Omega G)_{ii}E_{ij}|\rho_j\rangle \\
&= \sum_{l=1}^{n}\langle e_{I_k}|L_{il}G_{lj}|\rho_j\rangle - \sum_{l=1}^{n}\langle e_{I}k|k_{ii}|\pi_i\rangle\langle e_{I_k}|G_{lj}|\rho_j\rangle \\
&= \sum_{l=1}^{n}\langle e_{I_k}|G_{lj}|\rho_j\rangle - \sum_{l=1}^{n}\langle e_{I_k}|G_{lj}|\rho_j\rangle \\
&= 0,
\end{aligned}$$

where we used the same results as before and the fact that $E_{ij}\in M_{k^2}(\mathbb{C})$ is the identity matrix. Therefore, we see that the terms $WG-(WG)_dE$ are irrelevant when we apply it to a density and take the trace. This completes the proof.

□

An immediate corollary of this Theorem is a shorter and simplified version of the Mean Hitting Time Formula that can be obtained by selecting the g-inverse in some particular way.

Corollary 2.7. *Under the conditions of Theorem 2.6, by setting $G=(I-\Phi+|t\rangle\langle e_I|)^{-1}+|g\rangle\langle e_I|$, where $|g\rangle$ is an arbitrary vector and $|t\rangle$ is a vector such that $\langle e_I|t\rangle\neq 0$, then we have that the mean hitting time for the walk to reach vertex i, beginning at vertex j with initial density ρ_j is given by*

$$\mathrm{Tr}\left(K_{ij}\rho_j\right)=\mathrm{Tr}\left(\big[D\big(I-G+G_dE\big)\big]_{ij}\rho_j\right).$$

Proof. By the general form of the generalized inverse for $I-\Phi$,

$$G=(I-\Phi+|t\rangle\langle u|)^{-1}+|\pi\rangle\langle f|+|g\rangle\langle e_I|,$$

we choose $|f\rangle=0$ and $|u\rangle=|e_I\rangle$, so

$$\Omega G=\Omega\big((I-\Phi+|t\rangle\langle e_I|)^{-1}+|g\rangle\langle e_I|\big)=|\pi\rangle\langle e_I|(I-\Phi+|t\rangle\langle e_I|)^{-1}+|\pi\rangle\langle e_I|g\rangle\langle e_I|.$$

Note that from 2.2.1, we have

$$\begin{aligned}
&|t\rangle\langle u|(I-\Phi+|t\rangle\langle u|)^{-1}=\frac{|t\rangle\langle e_I|}{\langle e_I|t\rangle} \quad \overset{\langle t|\cdot}{\Longrightarrow} \quad \cancel{\langle t|t\rangle}\langle u|(I-\Phi+|t\rangle\langle u|)^{-1}=\frac{\cancel{\langle t|t\rangle}\langle e_I|}{\langle e_I|t\rangle} \\
\overset{|\pi\rangle\cdot}{\Longrightarrow}\ &|\pi\rangle\langle u|(I-\Phi+|t\rangle\langle u|)^{-1}=\frac{|\pi\rangle\langle e_I|}{\langle e_I|t\rangle} \quad \overset{\langle u|=\langle e_I|}{\Longrightarrow} \quad |\pi\rangle\langle e_I|(I-\Phi+|t\rangle\langle e_I|)^{-1}=\frac{|\pi\rangle\langle e_I|}{\langle e_I|t\rangle},
\end{aligned}$$

and substituting this last equation in the expression for ΩG we have

$$\Omega G = \frac{|\pi\rangle\langle e_I|}{\langle e_I|t\rangle} + \langle e_I|g\rangle \cdot |\pi\rangle\langle e_I| = \left(\frac{1}{\langle e_I|t\rangle} + \langle e_I|g\rangle\right) \cdot |\pi\rangle\langle e_I| = \beta\Omega,$$

where $\beta = (1/\langle e_I|t\rangle + \langle e_I|g\rangle)$ is some complex number. Therefore,

$$(\Omega G)_d E = \beta\Omega_d E = \beta\Omega = \Omega G,$$

where the second equality follows because all the block columns of Ω are equal, therefore when we take only the diagonal terms with $(\cdot)_d$ and multiply on the right by E, we restore the terms outside the diagonal that we deleted. This can be made more precise if we take $\{|e_i\rangle\}$ as the standard basis for $\mathbb{C}^n$, so we can express Ω and E as

$$\begin{aligned} \Omega &= \sum_{i,j=1}^{n} |e_i\rangle\langle e_j| \otimes |\pi_i\rangle\langle e_{I_k}| \\ \Omega_d &= \sum_{l=1}^{n} |e_l\rangle\langle e_l| \otimes |\pi_l\rangle\langle e_{I_k}| \end{aligned} \qquad \text{and} \qquad E = \sum_{i,j}^{n} |e_i\rangle\langle e_j| \otimes I_{k^2},$$

so

$$\Omega_d E = \sum_{i,j,l=1}^{n} |e_l\rangle\langle e_l|e_i\rangle\langle e_j| \otimes |\pi_l\rangle\langle e_{I_k}|I_{k^2} = \sum_{i,j=1}^{n} |e_i\rangle\langle e_j| \otimes |\pi_i\rangle\langle e_{I_k}| = \Omega.$$

This establishes that the first terms $\Omega G - (\Omega G)_d E$ in the expression of Theorem 2.6 cancel each other because they are equal, and the proof is complete.

□

2.2.1 Example

We define an OQW on 3 sites and 2 degrees of freedom: let R and L be given by

$$R = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad L = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix},$$

and let $\lceil R \rceil = R \otimes \overline{R}$ and $\lceil L \rceil = L \otimes \overline{L}$. Let

$$\Phi = \begin{bmatrix} \mathbf{0} & \lceil L \rceil & \mathbf{I}/2 \\ \mathbf{I}/2 & \mathbf{0} & \mathbf{I}/2 \\ \mathbf{I}/2 & \lceil R \rceil & \mathbf{0} \end{bmatrix},$$

where $\mathbf{I}$ and $\mathbf{0}$ are respectively the 4×4 identity matrix and zero matrix. To this OQW we can associate a CTOQW by defining a Lindbladian generator $\mathcal{L}$ as

$$\mathcal{L} = \begin{bmatrix} -\lambda\mathbf{I} & \lambda\lceil L \rceil & \lambda\mathbf{I}/2 \\ \lambda\mathbf{I}/2 & -\lambda\mathbf{I} & \lambda\mathbf{I}/2 \\ \lambda\mathbf{I}/2 & \lambda\lceil R \rceil & -\lambda\mathbf{I} \end{bmatrix}$$

with $\lambda > 0$ a real constant.

In order to calculate the mean hitting time $\tau_{ij}(\rho)$ to go from a site j to another site i ($i \neq j$), starting with initial density ρ concentrated at site j, we consider the modified generator L_i that turns the state i into an absorbing state. In this example, we get

$$L_1 = \begin{bmatrix} \mathbf{0} & \lambda\lceil L \rceil & \lambda\mathbf{I}/2 \\ \mathbf{0} & -\lambda\mathbf{I} & \lambda\mathbf{I}/2 \\ \mathbf{0} & \lambda\lceil R \rceil & -\lambda\mathbf{I} \end{bmatrix}, \quad L_2 = \begin{bmatrix} -\lambda\mathbf{I} & \mathbf{0} & \lambda\mathbf{I}/2 \\ \lambda\mathbf{I}/2 & \mathbf{0} & \lambda\mathbf{I}/2 \\ \lambda\mathbf{I}/2 & \mathbf{0} & -\lambda\mathbf{I} \end{bmatrix}, \quad L_3 = \begin{bmatrix} -\lambda\mathbf{I} & \lambda\lceil L \rceil & \mathbf{0} \\ \lambda\mathbf{I}/2 & -\lambda\mathbf{I} & \mathbf{0} \\ \lambda\mathbf{I}/2 & \lambda\lceil R \rceil & \mathbf{0} \end{bmatrix}$$

by simply substituting the i-th block column of L by zeroes.

Let us calculate in particular the mean hitting time on state 1, given that we start in state 2 with density ρ_2. The time of occupation in state 2 given that it starts in state 2 with density ρ_2, until it reaches state 1 is given by:

$$\mathbb{E}_{2,\rho_2}(n_2) = \int_0^\infty \mathbb{P}_{2,\rho_2}(X_t = 2)dt = \int_0^\infty \text{Tr}\left[\mathbb{P}_2 e^{tL_1}\mathbb{P}_2\rho\right]dt$$

where n_j is the time spent in state j:

$$n_j = \int_0^\infty \mathbf{1}_{X_t=j}dt$$

and ρ is used to denote

$$\rho = \begin{bmatrix} 0 \\ \rho_2 \\ 0 \end{bmatrix}.$$

The $\mathbb{P}_i$ are the projectors on site i:

$$\mathbb{P}_1 = \begin{bmatrix} \mathbf{I} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}, \quad \mathbb{P}_2 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}, \quad \mathbb{P}_3 = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{I} \end{bmatrix}.$$

In this case, it is easy to see that $\mathbb{P}_2\rho = \rho$ because ρ is already concentrated at site 2.

Similarly, the time of occupation in state 3 given that the system starts in state 2 with density ρ_2, until it is absorbed in state 1 is

$$\mathbb{E}_{2,\rho_2}(n_3) = \int_0^\infty \text{Tr}\left[\mathbb{P}_3 e^{tL_1}\mathbb{P}_2\rho\right]dt.$$

If we sum these two quantities, we obtain the mean hitting time $\tau_{12}(\rho)$:

$$\tau_{12}(\rho) = \mathbb{E}_{2,\rho_2}(n_2) + \mathbb{E}_{2,\rho_2}(n_3) = \int_0^\infty \text{Tr}\left[(\mathbb{P}_2 + \mathbb{P}_3)e^{tL_1}\mathbb{P}_2\rho\right]dt = \int_0^\infty \text{Tr}\left[\mathbb{Q}_1 e^{tL_1}\mathbb{P}_2\rho\right]dt \tag{2.2.7}$$

where $\mathbb{Q}_i := I - \mathbb{P}_i$.

Doing the computation with

$$\rho_2 = \begin{bmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ 1 - \rho_{11} \end{bmatrix} \tag{2.2.8}$$

we obtain

$$\tau_{12}(\rho) = \frac{2 - \rho_{12} - \rho_{21}}{\lambda}. \tag{2.2.9}$$

Now we proceed to compute this same quantity but using Theorem 2.6. In order to do this, we first need to find the diagonal blocks of the mean hitting time operator.

Define

$$\tau_{ij}(\rho_j \mid Y_1 = l) := \lambda + \tau_{il}\left(\frac{\Phi_{lj}(\rho_j)}{\text{Tr}\left[\Phi_{lj}(\rho_j)\right]}\right),$$

which can be interpreted as: the average time to reach a state i starting from j with ρ_j, given that the next step of the system will be to state l, all this equals $1/\lambda$ (the time taken to jump out of j) plus the average time to reach i given that we start at l with density $\rho_l = \Phi_{lj}(\rho_j)/\operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]$. And let us denote $\tau_i(\rho_i)$ the time of first return to site i given that we start at this site with state ρ_i concentrated at it. Then we have

$$\begin{aligned}\tau_j(\rho_j) &= \sum_{\substack{l\\ l\neq j}} \tau_{jj}(\rho_j \mid Y_1 = l)\cdot \operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]\\ &= \sum_{\substack{l\\ l\neq j}} \left(\frac{1}{\lambda} + \tau_{jl}\left(\frac{\Phi_{lj}(\rho_j)}{\operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]}\right)\right)\operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]\\ &= \frac{1}{\lambda} + \sum_{\substack{l\\ l\neq j}} \tau_{jl}\left(\frac{\Phi_{lj}(\rho_j)}{\operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]}\right)\operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right]. \end{aligned} \tag{2.2.10}$$

Note that $\sum_{l\neq j} \operatorname{Tr}\left[\Phi_{lj}(\rho_j)\right] = 1$ because we have $\Phi_{jj} = 0$ for all j.

To calculate the τ_{jl}, recall that we deduced in this example (equation 2.2.7) that $\tau_{12} = \int_0^\infty \operatorname{Tr}\left[\mathbb{Q}_1 e^{tL_1}\mathbb{P}_2\right] dt$. This result can be generalized as

$$\tau_{ij}(\rho_j) = \int_0^\infty \operatorname{Tr}\left[\mathbb{Q}_i e^{tL_i}\mathbb{P}_j\rho\right] dt.$$

With this in hand we thus have

$$\tau_{jl}\big(\Phi_{lj}(\rho_j)\big) = \int_0^\infty \operatorname{Tr}\left[\mathbb{Q}_j e^{tL_j}\mathbb{P}_l\Phi(\rho)\right] dt.$$

plugging this back into equation 2.2.10 it gives us

$$\begin{aligned}\tau_j(\rho_j) &= \frac{1}{\lambda} + \sum_{l\neq j}\int_0^\infty \operatorname{Tr}\left[\mathbb{Q}_j e^{tL_j}\mathbb{P}_l\Phi(\rho)\right] dt\\ &= \frac{1}{\lambda} + \int_0^\infty \operatorname{Tr}\left[\mathbb{Q}_j e^{tL_j}\mathbb{Q}_j\Phi(\rho)\right] dt.\end{aligned}$$

We wish to find and operator K_{ii} represented by a 4×4 matrix such that when you apply it to a state ρ_j concentrated at site j and take the trace, it returns us the value $\tau_j(\rho_j)$. For this purpose, we can rearrange the above expression of τ_j as

$$\tau_j(\rho_j) = \operatorname{Tr}\left[\left(\frac{1}{\lambda}\mathbb{P}_j + \int_0^\infty \mathbb{Q}_j e^{tL_j}\mathbb{Q}_j\Phi\ \mathbb{P}_j\ dt\right)\rho\right]$$

where we note that multiplying ρ on the left by $\mathbb{P}_j$ leaves it unaltered since ρ is already concentrated at site j. Now the integrand, due to its rightmost term being $\mathbb{P}_j$, will have only the j-th block column not null. Also, its j-th block row will be null due to multiplication on the left by $\mathbb{Q}_j$. Consequently, the same will be true to the integral. A schematic representation of what the matrix inside the paranthesis above will look like, for example if $j = 2$, is

$$\begin{bmatrix}\mathbf{0} & \times & \mathbf{0}\\ \mathbf{0} & \times & \mathbf{0}\\ \mathbf{0} & \times & \mathbf{0}\end{bmatrix}$$

where each entry here represents a 4×4 block, and only the blocks in the 2-nd column are not necessarily null. In order to concentrate all the information of the matrices whose only j-th block column is not null, we introduce the matrices

$$\mathbb{S}_1 = \begin{bmatrix}\mathbf{I} & \mathbf{I} & \mathbf{I}\\ \mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{0}\end{bmatrix},\quad \mathbb{S}_2 = \begin{bmatrix}\mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{I} & \mathbf{I} & \mathbf{I}\\ \mathbf{0} & \mathbf{0} & \mathbf{0}\end{bmatrix},\quad \mathbb{S}_3 = \begin{bmatrix}\mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{0} & \mathbf{0} & \mathbf{0}\\ \mathbf{I} & \mathbf{I} & \mathbf{I}\end{bmatrix}.$$

If we take our matrix that has only the second block column not null and multiply it on the left by $\mathbb{S}_2$, we obtain a matrix whose only non zero block will be the block with coordinates $(2, 2)$. Additionally, when we apply this resulting matrix on ρ, the trace remains unaltered. So we can write

$$\tau_j(\rho_j) = \text{Tr}\left[\left(\frac{1}{\lambda}\mathbb{P}_j + \int_0^\infty \mathbb{Q}_j e^{tL_j}\mathbb{Q}_j\Phi\mathbb{P}_j \, dt\right)\rho\right] = \text{Tr}\left[\left(\mathbb{S}_j\left(\frac{1}{\lambda}\mathbb{P}_j + \int_0^\infty \mathbb{Q}_j e^{tL_j}\mathbb{Q}_j\Phi\mathbb{P}_j \, dt\right)\right)_{jj}\rho_j\right].$$

Therefore, by looking at the last part of this equation, we define

$$K_{jj} := \left(\mathbb{S}_j\left(\frac{1}{\lambda} + \int_0^\infty \mathbb{Q}_j e^{tL_j}\mathbb{Q}_j\Phi\mathbb{P}_j \, dt\right)\right)_{jj},$$

and these are the desired diagonal blocks of the mean hitting time operator we were looking for, i.e., such that $\tau_j(\rho_j) = \text{Tr}\left[K_{jj}\rho_j\right]$. The block diagonal of the mean hitting time operator is then

$$D = K_d = \begin{bmatrix} K_{11} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & K_{22} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & K_{33} \end{bmatrix}.$$

The concrete calculations in this example can be shown to be

$$K_{11} = \begin{bmatrix} \frac{9}{4\lambda} & 0 & 0 & 0 \\ 0 & \frac{9}{4\lambda} & 0 & 0 \\ 0 & 0 & \frac{9}{4\lambda} & 0 \\ \frac{3}{4\lambda} & -\frac{3}{4\lambda} & -\frac{3}{4\lambda} & \frac{3}{\lambda} \end{bmatrix}, \quad K_{22} = \begin{bmatrix} \frac{2}{\lambda} & \frac{1}{\lambda} & \frac{1}{\lambda} & \frac{1}{\lambda} \\ 0 & \frac{1}{\lambda} & 0 & 0 \\ 0 & 0 & \frac{1}{\lambda} & 0 \\ \frac{1}{\lambda} & -\frac{1}{\lambda} & -\frac{1}{\lambda} & \frac{2}{\lambda} \end{bmatrix}, \quad K_{33} = \begin{bmatrix} \frac{3}{\lambda} & \frac{3}{4\lambda} & \frac{3}{4\lambda} & \frac{3}{4\lambda} \\ 0 & \frac{9}{4\lambda} & 0 & 0 \\ 0 & 0 & \frac{9}{4\lambda} & 0 \\ 0 & 0 & 0 & \frac{9}{4\lambda} \end{bmatrix} \tag{2.2.11}$$

Next, we define

$$|t\rangle = \begin{bmatrix} 1 & 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}^T$$

and

$$\langle u| = \begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 & 1 \end{bmatrix}.$$

These are two arbitrary vectors $|t\rangle$, $|u\rangle$ obeying the constraint that $\langle e_I|t\rangle \neq 0$ and $\langle u|\pi\rangle \neq 0$, required by [Prop. 6.3, [24]] in order for

$$G = (I - \Phi + |t\rangle\langle u|)^{-1}$$

to exist. We thus have that G will be a generalized inverse for $I - \Phi$.

We now have in hands all the inputs necessary to use Theorem 2.6. Using ρ_j in the form as 2.2.8, we calculate the Mean Hitting Time Formula and obtain

$$\text{Tr}\left(\left[D\big(\Omega G - (\Omega G)_d E + I - G + G_d E\big)\right]_{12}\rho_2\right) = \frac{2 - \rho_{12} - \rho_{21}}{\lambda},$$

showing that we obtain the same result as in 2.2.9.

2.3 Hitting time formula for CTQMCs in terms of the fundamental matrix

We consider in this section another formula for mean hitting times. The results and definitions given here can be found in [23].

Let us consider finite QMCs from the following set:

$$\mathcal{E} := \left\{\Phi \text{ QMC } \mid \Phi^r \longrightarrow \Omega \text{ as } r \longrightarrow \infty\right\}$$

where $\Omega = |\pi\rangle\langle e_I|$, with $|\pi\rangle$ being the stationary state of of Φ, which is assumed to exist. We call the QMCs belonging to the set $\mathcal{E}$ **ergodic**. In other words, Φ is said to be ergodic if its matrix converges to the limit Ω.

Note that it is immediate from the definition of Ω that

$$\Phi\Omega = \Omega\Phi = \Omega \quad \text{and} \quad \Omega^2 = \Omega.$$

So consider the following calculation:

$$\begin{aligned}(\Phi-\Omega)^r &= \sum_{p=0}^{r}\binom{r}{p}\Phi^p(-\Omega)^{r-p} = \Phi^r + \sum_{p=0}^{r-1}\binom{r}{p}\Phi^p(-\Omega)^{r-p} \\ &= \Phi^r + \Omega\sum_{p=0}^{r-1}\binom{r}{k}(-1)^{r-p} = \Phi^r - \Omega.\end{aligned}$$

where in the last equality the Binomial Theorem was applied. Let us denote $A := \Phi - \Omega$. Then,

$$(I-A)(I+A+A^2+\cdots+A^{r-1}) = I - A^r = I - (\Phi-\Omega)^r = I - \Phi^r + \Omega.$$

We can see by letting $r \to \infty$, that

$$(I-A)\cdot\left(I+\sum_{r=1}^{\infty}A^r\right) = I,$$

so $I - A = I - \Phi + \Omega$ is invertible and its inverse is given by

$$(I-\Phi+\Omega)^{-1} = I + \sum_{r=1}^{\infty}(\Phi-\Omega)^r = I + \sum_{r=1}^{\infty}(\Phi^r-\Omega).$$

With this we can now state the following

Definition 2.8. *Let $\Phi \in \mathcal{E}$ be a finite QMC. The Matrix Z given by*

$$Z := I + \sum_{r=1}^{\infty}(\Phi^r - \Omega) = (I-\Phi+\Omega)^{-1}$$

is called the **Fundamental Matrix** *of the QMC Φ.*

A few properties follow from the definition of fundamental matrix. Note that

$$I = Z(I-\Phi+\Omega) = Z(I-\Phi) + Z\Omega$$

and multiplying both sides on the right by Ω, we obtain

$$\Omega = Z\overbrace{(I-\Phi)\Omega}^{=0} + Z\Omega^2 = Z\Omega.$$

Similarly, we can deduce that $\Omega = \Omega Z$. From the previous equation, we then have that

$$Z(I-\Phi) = I - Z\Omega = I - \Omega.$$

In like manner, we have also that $(I-\Phi)Z = I - \Omega$. We can summarize these properties as follows:

Lemma 2.9. *Let $\Phi \in \mathcal{E}$ be a finite QMC. Then its fundamental matrix Z satisfies:*

a) $Z\Omega = \Omega Z = \Omega$

b) $Z(I-\Phi) = (I-\Phi)Z = I - \Omega$.

Note that $\Omega \in M_{nk^2}(\mathbb{C})$ can be written in blocks as $\Omega = \left[|\pi_i\rangle\langle e_{I_k}|\right]_{ij}$. If we apply it on a certain density $\rho = \left[|\rho_i\rangle\right]_i$, and take the trace, we have

$$\mathrm{Tr}(\Omega\rho) = \sum_{j=1}^{n}\mathrm{Tr}\left((\Omega\rho)_j\right) = \sum_{j,l=1}^{n}\mathrm{Tr}\left(\Omega_{jl}\rho_l\right) = \sum_{j,l=1}^{n}\mathrm{Tr}\left(|\pi_j\rangle\langle e_{I_k}|\rho_l\rangle\right) = \mathrm{Tr}(\rho)\cdot\mathrm{Tr}(\pi) = \mathrm{Tr}(\rho),$$

showing us that Ω preserves the trace. This could also have been seen if Ω is a limit of an ergodic QMC, then we could simply take the limit:

$$\Omega = \lim_{r\to\infty}\Phi^r \quad\Longrightarrow\quad \mathrm{Tr}(\Omega\rho) = \lim_{r\to\infty}\mathrm{Tr}(\Phi^r\rho) = \mathrm{Tr}(\rho).$$

Another important property of Z that follows from its definition as a limit is that it is trace preserving, as a consequence of Φ and Ω being trace preserving: for any density $\rho = \sum_{i\in V} \rho_i \otimes |i\rangle\langle i|$,

$$\mathrm{Tr}(Z\rho) = \mathrm{Tr}\left(\left[I + \sum_{r=1}^{\infty}(\Phi^r - \Omega)\right]\rho\right) = \mathrm{Tr}(\rho) + \sum_{r=1}^{\infty}\left[\,\mathrm{Tr}(\Phi^r\rho) - \mathrm{Tr}(\Omega\rho)\right] = \mathrm{Tr}(\rho). \tag{2.3.1}$$

Recall the operator $L := K - (K-D)\Phi$ defined in Lemma 1.27 and define $N := K - D$, the matrix of the non-diagonal block terms of the mean hitting time matrix. We have

Lemma 2.10. *Let $\Phi \in \mathcal{E}$ be a finite, irreducible QMC and let Z denote its fundamental matrix. Let $K = (K_i j)$ be its mean hitting time operator and $D = \mathrm{diag}(K_{11}, \dots, K_{nn})$, $L := K - (K-D)\Phi$, $N := K - D$. Then*

$$N_{ij} = (DZ)_{ii} - (DZ)_{ij} + \Big[(LZ)_{ij} - (LZ)_{ii}\Big].$$

Proof. Rearrange the definition $L = K - (K-D)\Phi = N + D - N\Phi$ to obtain

$$N(I - \Phi) = L - D,$$

and multiply both sides on the right by Z so we obtain

$$N(I-\Phi)Z = LZ - DZ.$$

Apply the second item of Lemma 2.9, $(I-\Phi)Z = I - \Omega$, so our equation becomes

$$N(I-\Omega) = LZ - DZ \quad \Longrightarrow \quad N = LZ - DZ + N\Omega.$$

Note that the (i,j)-th block of $N\Omega$ is

$$(N\Omega)_{ij} = \sum_{l=1}^{n} N_{il}\Omega_{lj} = \sum_{l=1}^{n} N_{il}|\pi_l\rangle\langle e_{I_k}|,$$

i.e., it does not depend on j. So we have $(N\Omega)_{ij} = (N\Omega)_{ii}$ for all i,j. So if we take any diagonal term of N in the expression obtained above, together with the fact that the diagonal blocks of N are zero, we have

$$0 = N_{ii} = (LZ)_{ii} - (DZ)_{ii} + (N\Omega)_{ii} \quad \Longrightarrow \quad (N\Omega)_{ii} = (DZ)_{ii} - (LZ)_{ii}.$$

Finally, for $i \neq j$, with the observation about the blocks of $N\Omega$, we obtain

$$\begin{aligned} N_{ij} &= (LZ)_{ij} - (DZ)_{ij} + (N\Omega)_{ii} = (LZ)_{ij} - (DZ)_{ij} + (DZ)_{ii} - (LZ)_{ii} \\ &= (DZ)_{ii} - (DZ)_{ij} + \Big[(LZ)_{ij} - (LZ)_{ii}\Big]. \end{aligned}$$

∎

In Theorem 2.6, we considered a particular form of Lindbladian generator giving us a semigroup of the form $T = e^{\lambda(\Phi - I)}$, $\lambda > 0$, where Φ is an irreducible QMC, and we used generalized inverses of $I - \Phi$ to calculate the mean hitting times for that semigroup. We can do something similar using the fundamental matrix of the QMC Φ. This is expressed in the following result that is presented in [23] in the context of OQWs.

Theorem 2.11. *Let $\Phi \in \mathcal{E}$ be a finite irreducible QMC acting on $n \geq 2$ sites and $k \geq 2$ degrees of freedom, and let Z be its fundamental matrix. Let T be the semigroup given by*

$$T = e^{\lambda(\Phi - I)t}, \;\; t \geq 0, \;\; \lambda > 0.$$

Let K be the mean hitting time operator matrix, let $D = \mathrm{diag}(K_{11}, \dots, K_{nn})$ be its block diagonal and $N := K - D$. Then for every ρ density concentrated in one site and for all $i, j = 1, 2, \dots, n$,

$$\mathrm{Tr}(N_{ij}\rho) = \mathrm{Tr}\left(\left[(DZ)_{ii} - (DZ)_{ij}\right]\rho\right).$$

Proof. We have that for all $i, j = 1, \ldots, n$,

$$\begin{aligned}\operatorname{Tr}\left((LZ)_{ij}\rho\right) &= \sum_{l=1}^{n} \operatorname{Tr}\left(L_{il} Z_{lj}\rho\right) = \sum_{l=1}^{n} \operatorname{Tr}\left(Z_{lj}\rho\right) \\ &= \operatorname{Tr}\left(\begin{bmatrix} Z_{1j}\rho \\ Z_{2j}\rho \\ \vdots \\ Z_{nj}\rho \end{bmatrix}\right) = \operatorname{Tr}\left(Z \cdot \begin{bmatrix} 0 \\ \vdots \\ \rho \\ \vdots \\ 0 \end{bmatrix}\right) = \operatorname{Tr}\left(\begin{bmatrix} 0 \\ \vdots \\ \rho \\ \vdots \\ 0 \end{bmatrix}\right) = \operatorname{Tr}(\rho)\end{aligned}$$

where we have used in the second equality the property of the operator L given by Lemma 1.27, and in the second line we considered a vector that is zero except for the j-th position where it has density ρ, or in the tensor product notation, $\rho \otimes |j\rangle\langle j|$. Then we have used the trace preserving property of Z, equation 2.3.1.

Therefore the trace of $(LZ)_{ij}\rho$ is the same for all i, j, and hence by Lemma 2.10

$$\operatorname{Tr}\left(N_{ij}\rho\right) = \operatorname{Tr}\left(\left[(DZ)_{ii} - (DZ)_{ij} + \left[(LZ)_{ij} - (LZ)_{ii}\right]\right]\rho\right) = \operatorname{Tr}\left(\left[(DZ)_{ii} - (DZ)_{ij}\right]\rho\right).$$

□

2.3.1 Discussion: link between Theorems 2.6 and 2.11

We can see that the fundamental matrix $Z = (I - \Phi + \Omega)^{-1}$ is a particular case of a generalized inverse of $I - \Phi$ given by $G = (I - \Phi + |t\rangle\langle u|)^{-1}$ with $|t\rangle = |\pi\rangle$ and $\langle u| = \langle e_I|$. So we can ask how are the two theorems connected. This can be answered looking at Corollary 2.7, which is stated in the context of QMCs (see also [Thm. 6.1, [24]]).

The fundamental matrix Z is a particular generalized inverse that falls under the conditions specified in Corollary 2.7, therefore we must have that the mean hitting time to reach vertex i from j with initial density ρ_j is as given by that corollary:

$$\begin{aligned}\operatorname{Tr}\left(K_{ij}\rho_j\right) &= \operatorname{Tr}\left(\left[D\left(I - G + G_d E\right)\right]_{ij}\rho_j\right) \\ &= \operatorname{Tr}\left(D_{ij}\rho_j\right) - \operatorname{Tr}\left((DZ)_{ij}\rho_j\right) + \operatorname{Tr}\left(\left(D(Z_d E)\right)_{ij}\rho_j\right). \end{aligned} \tag{2.3.2}$$

Note that

$$\begin{aligned}\left(D(Z_d E)\right)_{ij} &= \sum_{l=1}^{n}\sum_{m=1}^{n} D_{il}(Z_d)_{lm}E_{mj} = \sum_{l=1}^{n} D_{il} Z_{ll} \\ &= K_{ii} Z_{ii} = (DZ)_{ii},\end{aligned}$$

so we can substitute this on equation 2.3.2 and rearrange terms to obtain

$$\begin{aligned}&\operatorname{Tr}\left(K_{ij}\rho_j\right) - \operatorname{Tr}\left(D_{ij}\rho_j\right) = -\operatorname{Tr}\left((DZ)_{ij}\rho_j\right) + \operatorname{Tr}\left((DZ)_{ii}\rho_j\right) \\ \Longrightarrow &\operatorname{Tr}\left((K-D)_{ij}\rho_j\right) = \operatorname{Tr}\left(N_{ij}\rho_j\right) = \operatorname{Tr}\left([(DZ)_{ii} - (DZ)_{ij}]\rho_j\right),\end{aligned}$$

which is exactly the formula given by Theorem 2.11.

In conclusion, Theorem 2.11 can be seen as a particular case of Theorem 2.6, even though their proofs are different in that the former uses special properties of the fundamental matrix whereas the latter uses only general properties of generalized inverses.

2.3.2 Example

We consider as in the example from Section 2.2.1 the matrices R and L,

$$R = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad L = \frac{1}{\sqrt{2}}\begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix},$$

and the QMC Φ in 3 sites and 2 degrees of freedom given by

$$\Phi = \begin{bmatrix} \mathbf{0} & \lceil L \rceil & \mathbf{I}/2 \\ \mathbf{I}/2 & \mathbf{0} & \mathbf{I}/2 \\ \mathbf{I}/2 & \lceil R \rceil & \mathbf{0} \end{bmatrix},$$

with $\lceil R \rceil = R \otimes \overline{R}$ and $\lceil L \rceil = L \otimes \overline{L}$. The Lindbladian generator of the one parameter semigroup will be $\mathcal{L} = \lambda(\Phi - I)$, $\lambda > 0$. The matrices L_i will be $\mathcal{L}$ with its i-th block column substituted by zeroes, for $i = 1, 2, 3$.

We have show in that example that if ρ_2 is given by

$$\rho_2 = \begin{bmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ 1 - \rho_{11} \end{bmatrix},$$

then the mean hitting time to visit site 1 given that we start at site 2 with density ρ_2 is (2.2.9), that is,

$$\tau_{12}(\rho) = \frac{2 - \rho_{12} - \rho_{21}}{\lambda}.$$

Now we proceed to calculate $\tau_{12}(\rho_2)$ using Theorem 2.11. It can be shown that the stationary vector of Φ in this example is

$$|\pi\rangle = \begin{bmatrix} |\pi_1\rangle \\ |\pi_2\rangle \\ |\pi_3\rangle \end{bmatrix} \quad \text{where} \quad \begin{matrix} |\pi_1\rangle = \begin{bmatrix} \frac{2}{9} & 0 & 0 & \frac{1}{9} \end{bmatrix}^T \\ |\pi_2\rangle = \begin{bmatrix} \frac{1}{6} & 0 & 0 & \frac{1}{6} \end{bmatrix}^T \\ |\pi_3\rangle = \begin{bmatrix} \frac{1}{9} & 0 & 0 & \frac{2}{9} \end{bmatrix}^T \end{matrix},$$

with which we define the limit matrix $\Omega = |\pi\rangle\langle e_{I_k^n}|$. Then the fundamental matrix is given by

$$Z = (I - \Phi + \Omega)^{-1},$$

and together with the diagonal blocks of the operator K, which we showed in 2.2.11, we can compute the terms in the formula of Theorem 2.11 and we obtain in this case

$$(DZ)_{11} - (DZ)_{12} = \begin{bmatrix} \frac{2}{\lambda} & 0 & 0 & -\frac{1}{\lambda} \\ 0 & \frac{3}{\lambda} & 0 & 0 \\ 0 & 0 & \frac{3}{\lambda} & 0 \\ 0 & -\frac{1}{\lambda} & -\frac{1}{\lambda} & \frac{3}{\lambda} \end{bmatrix},$$

so

$$\begin{aligned} \tau_{12}(\rho) &= \mathrm{Tr}\left(N_{ij}\rho\right) = \mathrm{Tr}\left(\left[(DZ)_{11} - (DZ)_{12}\right]\rho\right) \\ &= \mathrm{Tr}\left(\begin{bmatrix} \frac{2}{\lambda} & 0 & 0 & -\frac{1}{\lambda} \\ 0 & \frac{3}{\lambda} & 0 & 0 \\ 0 & 0 & \frac{3}{\lambda} & 0 \\ 0 & -\frac{1}{\lambda} & -\frac{1}{\lambda} & \frac{3}{\lambda} \end{bmatrix} \begin{bmatrix} \rho_{11} \\ \rho_{12} \\ \rho_{21} \\ 1 - \rho_{11} \end{bmatrix}\right) = \mathrm{Tr}\left(\begin{bmatrix} \frac{2\rho_{11}}{\lambda} - \frac{1-\rho_{11}}{\lambda} \\ \frac{3\rho_{12}}{\lambda} \\ \frac{3\rho_{21}}{\lambda} \\ -\frac{\rho_{12}}{\lambda} - \frac{\rho_{21}}{\lambda} + \frac{3(1-\rho_{11})}{\lambda} \end{bmatrix}\right) \\ &= \frac{2 - \rho_{12} - \rho_{21}}{\lambda}, \end{aligned}$$

and that is the result we expected.

Chapter 3

Concluding Remarks and Further Questions

We have seen in Section 1.5 how we can define a positive trace-preserving map Λ from a quantum channel and with it we deduced an analogous to Hunter's Formula for any irreducible quantum channel.

Then, investigating what happens to irreducible quantum channels in the limit when they become reducible, in the sense laid out in Subsection 1.6.1 via randomizations, we have found that we can use the group inverse to calculate mean hitting times for some examples of unitary channels, which are reducible. Finally, under the assumption that $1 \notin \sigma(\mathbb{Q}\Phi)$ (see Remark 1.29), we were able to state and prove Theorem 1.28, which is a new result that allows us to use generalized inverses to calculate mean hitting times of quantum channels without the hypothesis of irreducibility. This is the main result of this work.

In this work, we were concerned mainly with mean hitting times, motivated by the classical reference of Hunter [20]. However, Hunter has also examined the problem of higher moments of hitting times [21]. One could ask if it is possible to apply generalized inverses to obtain higher moments of hitting times in the quantum setting. We have not investigated this question.

In Chapter 2 we have found an analogous to Hunter's Formula for CTQMCs, presented in Theorem 2.6, where we have considered a particular form of Lindbladian generator. Can we find a similar formula for a more general kind of semigroup generator in that context? This is a question we did investigate, but we did not find a general answer so far. We believe this is an interesting research direction worth pursuing.

Appendix A

Appendix

Here we prove some matrix identities that are used in the text. These identities are highlighted with boxes. Let us start by fixing some notations.

We denote the space of $m \times n$ matrices with entries in the field $\mathbb{F}$ by $\mathbb{F}^{m\times n}$, or equivalently by $M_{m,n}(\mathbb{C})$. If $m = n$, we write $M_{n,n}(\mathbb{C})$ simply as $M_n(\mathbb{C})$ If A is a matrix, then A^T denotes its transpose. Given a matrix $A \in \mathbb{F}^{m\times n}$ and subsets $\mathcal{S}_1 \subset \{1, 2, \ldots, m\}$ and $\mathcal{S}_2 \subset \{1, 2, \ldots, n\}$, we denote by $A_{(\mathcal{S}_1,\mathcal{S}_2)}$ the $|\mathcal{S}_1| \times |\mathcal{S}_2|$ matrix obtained by deleting from A its rows which are not listed in $\mathcal{S}_1$ and deleting the columns of A which are not listed in $\mathcal{S}_2$. Here, $|\mathcal{S}|$ denotes the cardinality of the set $\mathcal{S}$. We call $A_{\mathcal{S}_1,\mathcal{S}_2)}$ a **submatrix** of A. By convention, A is a submatrix of itself. In the case of one element subsets, we write simply $A_{(\{i\},\{j\})} = A_{(i,j)}$, the (i, j)-entry of A.

Similarly, we denote by $A_{(\tilde{\mathcal{S}}_1,\tilde{\mathcal{S}}_2)}$ the $(m - |\mathcal{S}_1|) \times (n - |\mathcal{S}_2|)$ matrix obtained from A by deleting the rows listed in $\mathcal{S}_1$ and the columns listed in $\mathcal{S}_2$. In this way, given a matrix $A \in M_n(\mathbb{F})$, we define by $A_{[i,j]}$ as the matrix in $M_{n-1}(\mathbb{F})$ given by $A_{[i,j]} := A_{(\{\tilde{i}\},\{\tilde{j}\})}$, i.e., the matrix obtained from A by deleting row i and column j.

With these notations, given $A \in M_n(\mathbb{F})$ we define the **adjugate** matrix of A, denoted by $\operatorname{adj} A$, or A^A, as the $n \times n$ matrix with entries given by

$$(A^A)_{(i,j)} := (-1)^{i+j} \det A_{[j,i]}. \tag{A.0.1}$$

We want to demonstrate the following:

Lemma A.1. *For any matrix $X \in M_n(\mathbb{F})$ and column vectors $x, y \in \mathbb{F}$, we have:*

$$\boxed{\det(X + xy^T) = \det X + y^T X^A x}$$

Most of the notations used above are found in [5]. Consider the following:

Fact A.2. *Let $A \in M_n(\mathbb{F})$, $x, y \in \mathbb{F}^n$ be column vectors and $a \in \mathbb{F}$, with $a \neq 0$. Then,*

$$\det \begin{bmatrix} A & x \\ y^T & a \end{bmatrix} = a \det(A - a^{-1}xy^T).$$

Proof. The identity below [Fact 2.16.2,[5]] is an immediate consequence of block matrix multiplication:

$$\begin{bmatrix} A & x \\ y^T & a \end{bmatrix} = \begin{bmatrix} I_n & a^{-1}x \\ \mathbf{0}_{1\times n} & 1 \end{bmatrix} \cdot \begin{bmatrix} A - a^{-1}xy^T & \mathbf{0}_{n\times 1} \\ \mathbf{0}_{1\times n} & a \end{bmatrix} \cdot \begin{bmatrix} I_n & \mathbf{0}_{n\times 1} \\ a^{-1}y^T & 1 \end{bmatrix},$$

where the dimensions of the zero blocks and identities are indicated by subscripts. Therefore, the result follows by the multiplicative property of the determinant, and the fact that matrices of the form $\begin{bmatrix} A & C \\ \mathbf{0} & B \end{bmatrix}$, where A and B are square matrices, have determinant equal to $\det A \cdot \det B$ (see for example, [equation (5-19), [19]] or [equation (2.7.6), [5]]).

□

We now calculate the determinant of $\begin{bmatrix} A & x \\ y^T & a \end{bmatrix}$ in a different way, this time in terms of A^A, proceeding directly by Laplace's Expansion Theorem [29], or cofactor expansion, given in the next fact.

Fact A.3. *Let $A \in M_n(\mathbb{F})$, $x, y \in \mathbb{F}^n$ be column vectors and $a \in \mathbb{F}$. Then,*

$$\det \begin{bmatrix} A & x \\ y^T & a \end{bmatrix} = a \det A - y^T A^A x.$$

Proof. Denote by $A[i]$ the $n \times (n-1)$ matrix obtained by deleting column i from A and let $\begin{bmatrix} [A[i] & x \end{bmatrix}$ be the $n \times n$ matrix obtained by juxtaposing the column x to the right of $A[i]$. By computing the cofactor expansion over the last row of the matrix, we have

$$\det \begin{bmatrix} A & x \\ y^T & a \end{bmatrix} = \sum_{i=1}^{n} (-1)^{n+1+i} y_i \det \begin{bmatrix} [A[i] & x \end{bmatrix} + a \det A. \tag{A.0.2}$$

Noticing that $\begin{bmatrix} [A[i] & x \end{bmatrix}$ can also be calculated using the cofactor expansion over the rightmost column, we obtain:

$$\begin{aligned} \det \begin{bmatrix} [A[i] & x \end{bmatrix} &= \sum_{j=1}^{n} (-1)^{j+n} x_j A_{[j,i]} \\ &= \sum_{j=1}^{n} (-1)^{j+n} (-1)^{i+j} (A^A)_{(i,j)} \\ &= \sum_{j=1}^{n} (-1)^{i+n} (A^A)_{(i,j)}, \end{aligned}$$

where we have used definition (A.0.1) in the second equality. So substituting this into equation (A.0.2), we have:

$$\begin{aligned} \det \begin{bmatrix} A & x \\ y^T & a \end{bmatrix} &= \sum_{i=1}^{n} (-1)^{n+1+i} \sum_{j=1}^{n} (-1)^{i+n} y_i (A^A)_{(i,j)} x_j + a \det A \\ &= \sum_{i,j=1}^{n} (-1)^{2n+2i+1} y_i (A^A)_{(i,j)} x_j + a \det A \\ &= - \sum_{i,j=1}^{n} y_i (A^A)_{(i,j)} x_j + a \det A \\ &= -y^T A^A x + a \det A. \end{aligned}$$

□

With these two identities at hand, it now becomes trivial to prove what we wanted.

Proof of Lemma A.1. Using facts A.2 and A.3, with scalar $a = -1$, we have

$$-\det(X + xy^T) = -\det X - y^T X^A x$$

because both sides are equal to $\det \begin{bmatrix} X & x \\ y^T & -1 \end{bmatrix}$, and the result follows.

□

Another result to be proven is that if a matrix $A \in M_n(\mathbb{C})$ has eigenvalues $\lambda_1, \ldots, \lambda_n$ of which only $\lambda_1 = 0$, then

$$\boxed{\operatorname{Tr}(\operatorname{adj} A) = \prod_{i=2}^{n} \lambda_i} \tag{A.0.3}$$

This comes from a relation between the symmetric functions of the eigenvalues of A,

$$\begin{aligned} s_1 &= \lambda_1 + \lambda_2 + \lambda_3 + \cdots + \lambda_n \\ s_2 &= \lambda_1\lambda_2 + \lambda_1\lambda_3 + \cdots + \lambda_{n-1}\lambda_n \\ &\vdots \\ s_n &= \lambda_1\lambda_2\lambda_3 \cdots \lambda_n \end{aligned} \tag{A.0.4}$$

and its **principal subdeterminants**, which are, by definition, the determinants of submatrices of A of the form $A_{(\mathcal{S},\mathcal{S})}$, $\mathcal{S} \subset \{1, 2, \dots, n\}$ obtained by selecting the same set of rows and columns of A. In this case, if $|\mathcal{S}| = k$, we say that $\det A_{(\mathcal{S},\mathcal{S})}$ is a $k \times k$ principal subdeterminant of A.

To establish relation (A.0.3), we start from the characteristic polynomial of A:

$$p(\lambda) = \det(A - \lambda I) = (-1)^n \lambda^n + a_1 \lambda^{n-1} + \cdots + a_{n-1}\lambda + a_n \tag{A.0.5}$$

and obtain the coefficients a_j through successive derivation with respect to λ:

$$a_{n-k} = \frac{p^{(k)}(0)}{k!} = \frac{1}{k!} \frac{d^k \det(A - \lambda I)}{d\lambda^k}\bigg|_{\lambda=0}, \quad 0 \le k \le n-1 \tag{A.0.6}$$

On the other hand, if we derive a general determinant, supposing that the entries of a matrix $B \in M_n(\mathbb{C})$ are functions of a variable t, say, $B = \big(b_{ij}(t)\big)_{ij}$ we obtain:

$$\begin{aligned} \frac{d \det B}{dt} &= \frac{d}{dt}\left(\sum_{\sigma} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} b_{i,\sigma(i)} \right) \\ &= \sum_{\sigma} \operatorname{sgn}(\sigma) \frac{d}{dt} \prod_{i=1}^{n} b_{i,\sigma(i)} \\ &= \sum_{\sigma} \operatorname{sgn}(\sigma) \sum_{j=1}^{n} (b_{j,\sigma(j)})' \prod_{\substack{i=1 \\ i \ne j}}^{n} b_{i,\sigma(i)} \\ &= \sum_{j=1}^{n} \left[\sum_{\sigma} \operatorname{sgn}(\sigma) (b_{j,\sigma(j)})' \prod_{\substack{i=1 \\ i \ne j}}^{n} b_{i,\sigma(i)} \right] \\ &= \sum_{j=1}^{n} \det(B_j) \end{aligned}$$

where B_j denotes the matrix B, except its j^{th} row is replaced by its derivative with respect to t.

Using the same reasoning as above, by successive derivation we obtain

$$\frac{d^m \det B}{dt^m} = \sum_{i_1=1}^{n} \cdots \sum_{i_m=1}^{n} \det(B_{i_1,i_2,\dots,i_m}), \tag{A.0.7}$$

where $B_{i_1,i_2,\dots,i_m}$ denotes the matrix B with its row i_j derived each time the index i_j appears, possibly more than once.

Now using this formula to calculate the derivatives of $\det(A - \lambda I)$ with respect to λ, notice first that the derivative of the j-th row of $A - \lambda I$ with respect to λ is $-\mathbf{e}_j^T$ (-1 in the j-th component and zero otherwise). So if $n = 4$ for example, we have

$$(A - \lambda I)_2 = \begin{bmatrix} a_{11} - \lambda & a_{12} & a_{13} & a_{14} \\ 0 & -1 & 0 & 0 \\ a_{31} & a_{32} & a_{33} - \lambda & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} - \lambda \end{bmatrix}$$

It is immediate from the cofactor expansion using the second row, that $\det((A-\lambda I)_2) = (-1)\det(A-\lambda I)_{[2,2]}$, which, except for the minus sign, is one of the $(n-1)\times(n-1)$ principal subdeterminants of $A-\lambda I$. If we set $\lambda = 0$, then we have:

$$\left.\frac{d\det(A-\lambda I)}{d\lambda}\right|_{\lambda=0} = \sum_{j=1}^{n}(-1)\det A_{[j,j]} = \sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=1}} (-1)\det A_{(\tilde{\mathcal{S}},\tilde{\mathcal{S}})}.$$

We can see that $(A-\lambda I)_{i_1,i_2,\ldots,i_k}$ will be the matrix obtained by substituting row $i_1,\ldots,i_k$ of $A-\lambda I$ by $-e_{i_1}^T,\ldots,-e_{i_k}^T$, respectively. Note that if there are any repeated indexes, then $(A-\lambda I)_{i_1,i_2,\ldots,i_k}$ will have a zero row, and therefore its determinant will be zero. By cofactor expansion, it is easy to see that $\det(A-\lambda I)_{i_1,i_2,\ldots,i_k} = (-1)^k\det(A-\lambda I)_{(\widetilde{\{i_1,\ldots,i_k\}},\widetilde{\{i_1,\ldots,i_k\}})}$, if there are no repeated indexes. Thus we have, by applying relation (A.0.7) with $A-\lambda I$ in place of B, that:

$$\begin{aligned}
\frac{d^k\det(A-\lambda I)}{d\lambda^k} &= \sum_{i_1,\ldots,i_k}\det(A-\lambda I)_{i_1,i_2,\ldots,i_k}\\
&= \sum_{\substack{i_1,\ldots,i_k\\ i_j\neq i_l}}\det(A-\lambda I)_{i_1,i_2,\ldots,i_k}\\
&= (-1)^k\sum_{\substack{i_1,\ldots,i_k\\ i_j\neq i_l}}\det(A-\lambda I)_{(\widetilde{\{i_1,\ldots,i_k\}},\widetilde{\{i_1,\ldots,i_k\}})}\\
&= (-1)^k k!\sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=k}}\det(A-\lambda I)_{(\tilde{\mathcal{S}},\tilde{\mathcal{S}})},
\end{aligned}$$

where, in the last step, k factorial appears to account for the $k!$ possible permutations of the different indexes $i_1,\ldots,i_k$.

If we now evaluate the above expression with $\lambda = 0$, we will obtain

$$\left.\frac{d^k\det(A-\lambda I)}{d\lambda^k}\right|_{\lambda=0} = (-1)^k k!\sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=k}}\det(A)_{(\tilde{\mathcal{S}},\tilde{\mathcal{S}})}. \tag{A.0.8}$$

So, by comparing relations (A.0.6) and (A.0.8), we can conclude that the coefficients of the characteristic polynomial $p(\lambda)$ of A and the principal subdeterminants of A are related by

$$a_{n-k} = (-1)^k\sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=k}}\det(A)_{(\tilde{\mathcal{S}},\tilde{\mathcal{S}})} = (-1)^k\sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=n-k}}\det(A)_{(\mathcal{S},\mathcal{S})}. \tag{A.0.9}$$

But we also know that the polynomial $p(\lambda)$ can be written as

$$\begin{aligned}
p(\lambda) &= (\lambda_1-\lambda)(\lambda_2-\lambda)(\lambda_3-\lambda)\cdots(\lambda_n-\lambda)\\
&= (-1)^n\lambda^n + (-1)^{n-1}s_1\lambda^{n-1} + \cdots - s_{n-1}\lambda + s_n
\end{aligned} \tag{A.0.10}$$

where the s_i are the symmetric functions given by equations (A.0.4). We can compare expressions (A.0.5) and (A.0.10) to conclude that λ_i by $a_i = (-1)^{n-i}s_i$, for $1\le i\le n$, or equivalently,

$$a_{n-k} = (-1)^k s_{n-k}.$$

Finally, by comparing the above equality with (A.0.9) we conclude that

$$s_k = \sum_{\substack{\mathcal{S}\subset\{1,2,\ldots,n\}\\ \mathrm{card}(\mathcal{S})=k}}\det(A)_{(\mathcal{S},\mathcal{S})},$$

or, put in words, the k-th symmetric function of the roots of $A-\lambda I$, i.e., the eigenvalues of A, is equal to the sum of all $k\times k$ principal subdeterminants of A.

Now it is easy to reach the aimed result: the trace of the adjugate of A is by definition

$$\operatorname{Tr}(\operatorname{adj} A) = \sum_i \det A_{[i,i]} = \sum_{\substack{\mathcal{S} \subset \{1,2,\dots,n\} \\ \operatorname{card}(\mathcal{S}) = n-1}} \det(A)_{(\mathcal{S},\mathcal{S})},$$

the sum of the $(n-1)\times(n-1)$ principal subdeterminants of A, which as we have just deduced, is the same as the symmetric function

$$s_{n-1} = \sum_{1 \le i_1 < \cdots < i_{n-1} \le n} \lambda_{i_1} \cdots \lambda_{i_{n-1}}.$$

If all eigenvalues but λ_1 are different than zero, then s_{n-1} reduces to

$$s_{n-1} = \prod_{i=2}^{n} \lambda_i$$

which proves (A.0.3).

In what follows, we make some considerations about the rank of certain kinds of matrices. The next lemma [Theorem 2.4.4, [13]] is an elementary fact about matrices.

Lemma A.4. *Given a matrix $A \in \mathbb{F}^{m\times n}$ of rank r, there are nonsingular matrices $X \in \mathbb{F}^{m\times m}$ and $Y \in \mathbb{F}^{n\times n}$ such that*

$$A = X \begin{bmatrix} I_r & O \\ O & O \end{bmatrix} Y,$$

where I_r is the $r\times r$ identity matrix.

Proof. As we have seen in (1.1.2), any $m\times n$ matrix A can be turned into its reduced row-echelon form by multiplying it on the left by a nonsingular $m\times m$ matrix E, which is equivalent to performing elementary row operations on A. And then we can multiply EA on the right by an $n\times n$ permutation matrix P and obtain the form

$$EAP = \begin{bmatrix} I_r & K \\ O & O \end{bmatrix},$$

where K is unspecified matrix and the O's represent zero matrices. Now, in the same way that each elementary row operation can be obtained by a suitable multiplication on the left by a nonsingular matrix, we can analogously define elementary column operations, which can also be performed by multiplication on the right by nonsingular matrices. So if we multiply EAP on the right by a nonsingular $n\times n$ matrix F, we can cancel out the terms of the block K. Then we have

$$EAPF = \begin{bmatrix} I_r & O \\ O & O \end{bmatrix}.$$

If we define $X^{-1} := E$ and $Y^{-1} = PF$, the result follows.

With this lemma, we can now prove the following

Lemma A.5. *Let M be a block diagonal matrix of the form*

$$M = \begin{bmatrix} A & \\ & B \end{bmatrix},$$

where $A \in \mathbb{F}^{m\times m}$ and $B \in \mathbb{F}^{n\times n}$. Then the rank of the matrix M is the sum of the ranks of A and B.

Proof. Let r and s be the ranks of A and B, respectively. Then, by Lemma A.4, there are nonsingular matrices $X, Y \in F^{m\times m}$ and $X', Y' \in F^{n\times n}$ such that

$$A = X \begin{bmatrix} I_r & O \\ O & O \end{bmatrix} Y, \quad \text{and} \quad B = X' \begin{bmatrix} I_s & O \\ O & O \end{bmatrix} Y',$$

and thus we have

$$M = \begin{bmatrix} X \begin{bmatrix} I_r & O \\ O & O \end{bmatrix} Y & \\ & X' \begin{bmatrix} I_s & O \\ O & O \end{bmatrix} Y' \end{bmatrix} = \begin{bmatrix} X & \\ & X' \end{bmatrix} \begin{bmatrix} \begin{bmatrix} I_r & O \\ O & O \end{bmatrix} & \\ & \begin{bmatrix} I_s & O \\ O & O \end{bmatrix} \end{bmatrix} \begin{bmatrix} Y & \\ & Y' \end{bmatrix}.$$

The matrix in the middle of the right-hand side of the equation above has rank $r+s$ because it is diagonal and there are exactly $r+s$ 1's in the diagonal and the remaining terms are zero. As for the matrices multiplying it on each side, they are nonsingular, with inverses given by

$$\begin{bmatrix} X & \\ & X' \end{bmatrix}^{-1} = \begin{bmatrix} X^{-1} & \\ & X'^{-1} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} Y & \\ & Y' \end{bmatrix}^{-1} = \begin{bmatrix} Y^{-1} & \\ & Y'^{-1} \end{bmatrix}.$$

Because the rank of a matrix remains unaltered under multiplication by nonsingular matrices, the rank of M is also $r+s$, and this completes the proof.

□

Remark. The result of Lemma A.5 is stated for a block diagonal matrix with only 2 blocks. It can, however, be easily extended for a block diagonal matrix with any number of blocks.

In Section 1.3 we defined the Kronecker product between any two matrices (1.4.2) and we defined the function $\mathrm{vec} : M_{m,n}(\mathbb{C}) \to \mathbb{C}^{mn}$ by the map (1.4.1). We want to prove

Theorem A.6. *Let $A \in M_{m,n}(\mathbb{C})$, $X \in M_{n,p}(\mathbb{C})$ and $B \in M_{p,q}(\mathbb{C})$. Then*

$$\boxed{\mathrm{vec}\,(AXB) = A \otimes B^T \,\mathrm{vec}\,(X)}$$

Before we prove this, let us make a few considerations. Denote by $\ell_i(A)$ the i-th row of matrix A.

Then for any two matrices A and B,

$$\ell_k(AB) = \ell_k(A)B. \tag{A.0.11}$$

If we take $\begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix}$ to be a $1\times n$ matrix and $B \in M_{n,p}(\mathbb{C})$, then

$$\begin{bmatrix} x_1 & x_2 & \cdots & x_n \end{bmatrix} \cdot B = \begin{bmatrix} \sum_i x_i b_{i1} & \dots & \sum_i x_i b_{ip} \end{bmatrix} = \sum_{i=1}^{n} x_i \ell_i(B), \tag{A.0.12}$$

where b_{ij} are the entries of B.

If in a product AB of two matrices, we partition only the one on the left in a particular way, then the product can be expressed of that partition

Proof of Theorem A.6. We calculate the k-th row of AXB:

$$\begin{aligned} \ell_k(AXB) &= \ell_k(A)XB \\ &= \left(\sum_{h=1}^{n} a_{kh}\ell_h(X) \right) B \\ &= \sum_{h=1}^{n} \ell_h(X)(a_{kh}B), \end{aligned}$$

where the first equality follows from (A.0.11) and the second equality follows by (A.0.12). We can rewrite this sum as a product of two block-matrices to obtain

$$\ell_k(AXB) = \begin{bmatrix} \ell_1(X) & \ell_2(X) & \cdots & \ell_n(X) \end{bmatrix} \begin{bmatrix} a_{k1}B \\ a_{k2}B \\ \vdots \\ a_{kn}B \end{bmatrix}.$$

Note that the matrix on the left in the product above is $\mathrm{vec}\,(X)^T$ and the matrix multiplying on the right is $\ell_k(A)^T \otimes B$. Therefore

$$\ell_k(AXB) = \mathrm{vec}(X)^T(\ell_k(A)^T \otimes B),$$

or equivalently, taking the transpose,

$$\ell_k(AXB)^T = (\ell_k(A) \otimes B^T)\,\mathrm{vec}\,(X).$$

To obtain $\mathrm{vec}\,(AXB)$, we take each row of AXB transposed and stack them vertically in a column vector:

$$\begin{aligned} \mathrm{vec}(AXB) &= \begin{bmatrix} \ell_1(AXB)^T \\ \vdots \\ \ell_m(AXB)^T \end{bmatrix} \\ &= \begin{bmatrix} \ell_1(A) \otimes B^T \mathrm{vec}(X) \\ \vdots \\ \ell_m(A) \otimes B^T \mathrm{vec}(X) \end{bmatrix} \\ &= \begin{bmatrix} \ell_1(A) \otimes B^T \\ \vdots \\ \ell_m(A) \otimes B^T \end{bmatrix} \mathrm{vec}(X) \\ &= A \otimes B^T \mathrm{vec}(X). \end{aligned}$$

□

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