QUANTUM MARKOV CHAINS

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Abstract

A new approach to quantum Markov chains is presented. We first define a transition operation matrix (TOM) as a matrix whose entries are completely positive maps whose column sums form a quantum operation. A quantum Markov chain is defined to be a pair $(G, \mathcal{E})$ where G is a directed graph and $\mathcal{E} = [\mathcal{E}_{ij}]$ is a TOM whose entry $\mathcal{E}_{ij}$ labels the edge from vertex j to vertex i. We think of the vertices of G as sites that a quantum system can occupy and $\mathcal{E}_{ij}$ is the transition operation from site j to site i in one time step. The discrete dynamics of the system is obtained by iterating the TOM $\mathcal{E}$. We next consider a special type of TOM called a transition effect matrix (TEM). In this case, there are two types of dynamics, a state dynamics and an operator dynamics. Although these two types are not identical, they are statistically equivalent. We next give examples that illustrate various properties of quantum markov chains. We conclude by showing that our formalism generalizes the usual framework for quantum random walks.

1 Introduction

Quantum Markov chains and the closely related concepts of quantum Markov processes and quantum random walks have been studied for many years [1, 2, 3, 9]. More recently, there have been important applications of quantum random walks to quantum computation and information theory [8, 10, 11, 12].

In this paper we present a different approach to quantum Markov chains. We think that this approach is closer to the classical theory of Markov chains and is easier to visualize than some of the other approaches. Although the formalism we present is different from previous frameworks, we do make some comparisons and point out some of the differences between our approach to quantum Markov chains and their classical counterparts.

We begin by defining a transition operation matrix (TOM). A TOM is a matrix whose entries are completely positive maps and whose column sums form a quantum operation. We show that there is a natural bijection between TOMs and discrete quantum Markov kernels. A quantum Markov chain is defined to be a pair $(G, \mathcal{E})$ where G is a directed graph and $\mathcal{E} = [\mathcal{E}_{ij}]$ is a TOM whose entry $\mathcal{E}_{ij}$ labels the edge from vertex j to vertex i. We think of the vertices of G as sites that a quantum system can occupy and $\mathcal{E}_{ij}$ is the transition operation from site j to site i in one time step. The distribution of the system is determined by a vector state $S = (S_1, S_2, \dots)$ where S_i are positive trace class operators such that $\sum_i \mathrm{tr}(S_i) = 1$. Then $\mathrm{tr}(S_j)$ is the probability that the system is initially at site j. We think of S as a column vector and define $\mathcal{E}(S)$ by the usual matrix multiplication. It is shown that $\mathcal{E}(S)$ is again a vector state.

If $\mathcal{E}$ and $\mathcal{F}$ are TOMs of the same size on the same Hilbert space and we define $\mathcal{E}\mathcal{F}$ by matrix multiplication, then $\mathcal{E}\mathcal{F}$ is again a TOM. In particular, we define $\mathcal{E}^{(n)}$ recursively by $\mathcal{E}^{(n)} = \mathcal{E}\mathcal{E}^{(n-1)}$, $n = 2, 3, \dots$, where $\mathcal{E}^{(1)} = \mathcal{E}$. If $(G, \mathcal{E})$ is a quantum markov chain, then the dynamics is determined by the maps $\mathcal{E}^{(n)}$, $n = 1, 2, \dots$. If $S = (S_1, S_2, \dots)$ is a vector state, we use the notation

$$\mathrm{tr}(S) = (\mathrm{tr}(S_1), \mathrm{tr}(S_2), \dots)$$

The distribution of the system at the nth time step is $\mathrm{tr}\left[\mathcal{E}^{(n)}(S)\right]$, $n = 0, 1, 2, \dots$. Section 2 concludes with a characterization of TOMs in terms of the operation elements of their column sums.

Section 3 considers a special type of TOM called a transition effect matrix (TEM). A TEM is a matrix $E = [E_{ij}]$ whose columns are discrete positive operator valued measures; that is, $E_{ij} \geq 0$ and $\sum_i E_{ij} = I$ for all j. If S is a vector state and E is a TEM we define $E \circ S$ in terms of matrix multiplication and sequential products [6, 7]. Again, $E \circ S$ is a vector state and the state dynamics is given by the maps

$$E_{(n)}(S) = E \circ (\cdots E \circ (E \circ S))$$

We also have an operator type dynamics which we denote by $E^{(n)}$. Although $E^{(n)}(S) \neq E_{(n)}(S)$ in general, we show that

$$\operatorname{tr}\left[E^{(n)}(S)\right] = \operatorname{tr}\left[E_{(n)}(S)\right]$$

for every vector state S so that the two types of dynamics are statistically equivalent.

Section 4 presents examples that illustrate various properties of quantum Markov chains. These examples are given in terms of TEMs because they are much simpler than the more general TOMs. Finally, Section 5 shows that our formalism generalizes the usual framework for quantum random walks [8, 10, 12].

2 Transition Operation Matrices

Let H be a complex Hilbert space and let $\mathcal{B}(H)$ be the set of bounded linear operators on H. We denote the set of positive operators on H by $\mathcal{B}^+(H)$ and the set of positive trace class operators on H by $\mathcal{T}^+(H)$. The following sets of operators are also useful:

$$\begin{aligned}
\mathcal{E}(H) &= \{A \in \mathcal{B}(H) \colon 0 \leq A \leq I\} \\
\mathcal{P}(H) &= \left\{P \in \mathcal{B}(H) \colon P = P^* = P^2\right\} \\
\mathcal{D}(H) &= \left\{D \in \mathcal{T}^+(H) \colon \operatorname{tr}(D) = 1\right\}
\end{aligned}$$

Of course, $\mathcal{D}(H), \mathcal{P}(H) \subseteq \mathcal{E}(H) \subseteq \mathcal{B}^+(H)$. We call the elements of $\mathcal{E}(H)$ **effects**, the elements of $\mathcal{P}(H)$ **projections** or **sharp effects** and the elements of $\mathcal{D}(H)$ **density operators** or **states**. A linear map $\phi \colon \mathcal{B}(H) \to \mathcal{B}(H)$ is **positive** if $\phi(A) \in \mathcal{B}^+(H)$ for all $A \in \mathcal{B}^+(H)$. A linear map $\phi \colon \mathcal{B}(H) \to \mathcal{B}(H)$ is **completely positive** [4, 11] if for any complex Hilbert space K, the map $\phi \otimes I$ is positive on $\mathcal{B}(H) \otimes \mathcal{B}(K)$. A **quantum operation** [4, 11] is a completely positive map ϕ on $\mathcal{B}(H)$ that satisfies $\operatorname{tr}[\phi(D)] = \operatorname{tr}(D)$ for all $D \in \mathcal{T}^+(H)$. Quantum operations are very important in the fields of quantum computation and information [11]. A **transition operation matrix** (TOM) is a finite or infinite matrix of the form $\mathcal{E} = [\mathcal{E}_{ij}]$ where $\mathcal{E}_{ij}$ is a completely positive map on $\mathcal{B}(H)$ such that $\sum_i \mathcal{E}_{ij}(D) \in \mathcal{D}(H)$ for every j and every $D \in \mathcal{D}(H)$ where the summation converges in the strong operator topology.

Lemma 2.1. *A matrix of completely positive maps* $\mathcal{E} = [\mathcal{E}_{ij}]$ *is a* TOM *if and only if* $\sum_i \mathcal{E}_{ij}$ *is a quantum operation for all* j.

Proof. If $\sum_i \mathcal{E}_{ij}$ is a quantum operation then for any $D \in \mathcal{D}(H)$ we have

$$\operatorname{tr}\left[\sum_i \mathcal{E}_{ij}(D)\right] = \operatorname{tr}(D) = 1$$

Hence, $\sum_i \mathcal{E}_{ij}(D) \in \mathcal{D}(H)$ for all j so $\mathcal{E}$ is a TOM. Conversely, let $\mathcal{E}$ be a TOM and suppose $D \in \mathcal{T}^+(H)$. If $D = 0$, then clearly the trace condition holds. If $D \neq 0$, then $D/\operatorname{tr}(D) \in \mathcal{D}(H)$ and for every j we have

$$\operatorname{tr}\left[\sum_i \mathcal{E}_{ij}(D)\right] = \operatorname{tr}(D)\operatorname{tr}\left[\sum_i \mathcal{E}_{ij}\left(D/\tau(D)\right)\right] = \operatorname{tr}(D)$$

Hence, $\sum_i \mathcal{E}_{ij}$ is a quantum operation for all j. □

We now give an alternative formulation for a TOM. Let $CP(H)$ be the set of completely positive maps on H, let J be a finite or countable index set and let $\mathcal{P}(J) = 2^J$ be the power set on J. A **discrete instrument** [4] on H is a normalized CP-valued measure $\mathcal{I}\colon \mathcal{P}(J) \to CP(H)$. That is, $\mathcal{I}$ satisfies the conditions:

(1) $\operatorname{tr}[\mathcal{I}(\Delta)D] \leq \operatorname{tr}(D)$ for all $D \in \mathcal{T}^+(H)$, $\Delta \in \mathcal{P}(J)$;

(2) $\operatorname{tr}[\mathcal{I}(J)D] = \operatorname{tr}(D)$ for all $D \in \mathcal{T}^+(H)$, that is, $\mathcal{I}(J)$ is a quantum operation;

(3) if $\Delta_i \in \mathcal{P}(J)$ with $\Delta_i \cap \Delta_j = \emptyset$, $i \neq j$, then $\mathcal{I}(\cup\Delta_i) = \sum \mathcal{I}(\Delta_i)$ where the summation converges in the strong operator topology.

A **discrete quantum Markov kernel** is a map $K\colon \mathcal{P}(J) \times J \to CP(H)$ where $\Delta \mapsto K(\Delta, j)$ is a discrete instrument for every $j \in J$. There is a natural bijection between TOMs and discrete quantum Markov kernels. Indeed, if $\mathcal{E} = [\mathcal{E}_{ij}]$, $i, j \in J$, is a TOM then

$$\mathcal{E}(\Delta, j) = \sum_{i \in \Delta} \mathcal{E}_{ij}$$

is a discrete quantum Markov kernel. Conversely, if $K\colon \mathcal{P}(J) \times J \to CP(H)$ is a discrete quantum Markov kernel, then $\mathcal{E}_{ij} = K(\{i\}, j)$ $i, j \in J$, are the entries of a TOM.

A **quantum Markov chain** is a finite or countable directed graph G in which the edge from vertex j to vertex i is labeled $\mathcal{E}_{ij}$ (if there is no edge from vertex j to vertex i, $\mathcal{E}_{ij}=0$) and $\mathcal{E}=[\mathcal{E}_{ij}]$ forms a TOM. We may think of the vertices of G as sites that a quantum system can occupy and $\mathcal{E}_{ij}$ is the transition operation from site j to site i in one time step. The reason for the reverse order of j and i is that $\mathcal{E}_{ij}$ can be interpreted as a conditional operation $\mathcal{E}_{i|j}$ that the system is at site i given that it was at site j one time step previously. Alternatively, the kernel $\mathcal{E}(\Delta,j)$ is the transition operation from site j to some site in Δ. Notice that a TOM is a generalization of a classical stochastic matrix. Indeed, if p_{ij} are nonnegative real numbers satisfying $\sum_i p_{ij}=1$ for all j then $[p_{ij}]$ is a stochastic matrix and $[p_{ij}I]$ is a TOM where I is the identity completely positive map. In this way, quantum Markov chains generalize classical Markov chains.

Let $(G,\mathcal{E})$ be a quantum Markov chain. Suppose the corresponding quantum system is initially at site j and is described by the state $D\in\mathcal{D}(H)$. After one time step the transition to site i is described by the partial state $\mathcal{E}_{ij}(D)$ and the total state of the system is given by $\sum_i\mathcal{E}_{ij}(D)$. This is the reason for the condition $\sum_i\mathcal{E}_{ij}(D)\in\mathcal{D}(H)$ in the definition of a TOM. The conditional probability that the system occupies site i after one time step becomes

$$P_D(i\mid j)=\operatorname{tr}\left[\mathcal{E}_{ij}(D)\right]$$

and the total probability that the system moves to some site in one time step is

$$\sum_i P_D(i\mid j)=\sum_i\operatorname{tr}\left[\mathcal{E}_{ij}(D)\right]=\operatorname{tr}\left[\sum_i\mathcal{E}_{ij}(D)\right]=1$$

In general, the quantum system is initially described by a **vector state** $A=(A_1,A_2,\dots)$ where $A_i\in\mathcal{T}^+(H)$, $i=1,2,\dots$, and $\sum_i\operatorname{tr}(A_i)=1$. Then $\operatorname{tr}(A_j)$ is the probability that the system is initially at site j. We think of A as a column vector and if $\mathcal{E}$ is a TOM, we define the column vector $\mathcal{E}(A)=(B_1,B_2,\dots)$ where $B_i=\sum_j\mathcal{E}_{ij}(A_j)$ is given by matrix multiplication. The following calculation shows that $\mathcal{E}(A)$ is again a vector state:

$$\begin{aligned}\sum_i\operatorname{tr}(B_i)&=\sum_i\operatorname{tr}\left[\sum_j\mathcal{E}_{ij}(A_j)\right]=\sum_{i,j}\operatorname{tr}\left[\mathcal{E}_{ij}(A_j)\right]\\&=\sum_j\operatorname{tr}\left[\sum_i\mathcal{E}_{ij}(A_j)\right]=\sum_j\operatorname{tr}(A_j)=1\end{aligned}$$

If A describes the initial vector state of the system, we interpret $\mathcal{E}(A)$ as the vector state after one time step.

If $\mathcal{A}, \mathcal{B} \in CP(H)$, we write $\mathcal{A}\mathcal{B}$ for the composition $\mathcal{A}\mathcal{B}(A) = \mathcal{A}\left(\mathcal{B}(A)\right)$ and $\mathcal{A} + \mathcal{B}$ for addition $(\mathcal{A} + \mathcal{B})(A) = \mathcal{A}(A) + \mathcal{B}(A)$. It is well known that $\mathcal{A}\mathcal{B}, \mathcal{A} + \mathcal{B} \in CP(H)$. For TOMs $\mathcal{E}$ and $\mathcal{F}$ on H that are the same size, we define their product by

$$\mathcal{E}\mathcal{F} = [\mathcal{E}_{ij}]\,[\mathcal{F}_{ij}] = [\mathcal{G}_{ij}]$$

where $\mathcal{G}_{ij} = \sum_k \mathcal{E}_{ik}\mathcal{F}_{kj}$ is given by matrix multiplication. In a similar way, if $\mathcal{E}(\Delta, j)$, $\mathcal{F}(\Delta, j)$ are quantum Markov kernels, we define their product $\mathcal{G} = \mathcal{E}\mathcal{F}$ by

$$\mathcal{G}(\Delta, j) = \sum_k \mathcal{E}(\Delta, k)\mathcal{F}(k, j)$$

This last definition can be written in the integral form

$$\mathcal{G}(\Delta, j) = \int \mathcal{E}(\Delta, \lambda)\mathcal{F}(d\lambda, j)$$

which is the usual equation for classical Markov kernels.

Lemma 2.2. (a) *If $\mathcal{E}$ and $\mathcal{F}$ are TOMs on H of the same size then $\mathcal{E}\mathcal{F}$ is a TOM.* (b) *If $\mathcal{E}(\Delta, j)$ and $\mathcal{F}(\Delta, j)$ are discrete quantum Markov kernels on the same index set, then $\mathcal{G} = \mathcal{E}\mathcal{F}$ is a discrete quantum Markov kernel.*

Proof. (a) We first show that the sum $\mathcal{G}_{ij} = \sum_k \mathcal{E}_{ik}\mathcal{F}_{kj}$ converges to a completely positive map. For $D \in \mathcal{D}(H)$ we have that $\sum_k \mathcal{F}_{kj}(D) = D_0 \in \mathcal{D}(H)$. Hence, for any $N, M \in \mathbb{N}$ we have

$$\sum_{k=1}^{N} \mathcal{E}_{ik}\left(\mathcal{F}_{kj}(D)\right) \le \sum_{k=1}^{N}\sum_{i=1}^{M} \mathcal{E}_{ik}\left(\mathcal{F}_{kj}(D)\right) \le \sum_{k=1}^{N} \mathcal{F}_{kj}(D) \le D_0$$

Hence,

$$N \mapsto \sum_{k=1}^{N} \mathcal{E}_{ik}\left(\mathcal{F}_{kj}(D)\right)$$

is an increasing sequence in $\mathcal{T}^+(H)$ that is bounded above by $D_0 \in \mathcal{T}^+(H)$. It follows that this sequence converges in the strong operator topology to an element in $\mathcal{T}^+(H)$. We conclude that $\mathcal{G}_{ij} \in CP(H)$. To show that $\mathcal{G} = \mathcal{E}\mathcal{F}$ is a TOM, let $D \in \mathcal{D}(H)$. By Lemma 2.1 we have

$$\begin{aligned}\operatorname{tr}\left[\sum_i \mathcal{G}_{ij}(D)\right] &= \operatorname{tr}\left[\sum_i \sum_k (\mathcal{E}_{ik}\mathcal{F}_{kj})(D)\right] = \sum_k \operatorname{tr}\left[\sum_i \mathcal{E}_{ik}\left(\mathcal{F}_{kj}(D)\right)\right] \\ &= \sum_k \operatorname{tr}\left[\mathcal{F}_{kj}(D)\right] = \operatorname{tr}\left[\sum_k \mathcal{F}_{kj}(D)\right] = 1\end{aligned}$$

Part (b) easily follows from (a). □

It is easy to verify that our defined products are associative; that is, $(\mathcal{E}\mathcal{F})\mathcal{G} = \mathcal{E}(\mathcal{F}\mathcal{G})$ and $(\mathcal{E}\mathcal{F})(A) = \mathcal{E}\left(\mathcal{F}(A)\right)$.

Suppose a quantum Markov chain is described by the TOM $\mathcal{E}$ and A is the initial vector state. Then it is natural to interpret

$$\mathcal{E}_{ij}^{(2)} = (\mathcal{E}\mathcal{E})_{ij} = \sum_k \mathcal{E}_{ik}\mathcal{E}_{kj}$$

as a two-step transition operation from site j to site i. By Lemma 2.2, $\mathcal{E}^{(2)}$ is a TOM and $\mathcal{E}^{(2)}(A)$ is the vector state after two time steps. In general, the vector state at the nth time step is $\mathcal{E}^{(n)}(A) = \mathcal{E}\mathcal{E}^{(n-1)}(A)$. By convention, we define $\mathcal{E}^{(0)}(A) = A$ for every vector state A. Notice that we can also write $\mathcal{E}^{(n)}(A)$ as $\mathcal{E}\left(\mathcal{E}\cdots\mathcal{E}(A)\right)$. If $A = (A_1, A_2, \dots)$ is a vector state, we use the notation

$$\operatorname{tr}(A) = \left(\operatorname{tr}(A_1), \operatorname{tr}(A_2), \dots\right)$$

The **distribution** of the system at the nth time step is

$$\operatorname{tr}\left[\mathcal{E}^{(n)}(A)\right] = \left(\operatorname{tr}\left(\mathcal{E}^{(n)}(A)_1\right), \operatorname{tr}\left(\mathcal{E}^{(n)}(A)_2\right), \dots\right)$$

$n = 0, 1, 2, \dots$. Of course, $\operatorname{tr}\left[\mathcal{E}^{(n)}(A)\right]$ gives a probability distribution.

A completely positive map $\mathcal{E}$ is **simple** if it has the form $\mathcal{E}(A) = EAE^*$, $E \in \mathcal{B}(H)$, and in this case we write $\mathcal{E} = \widehat{E}$. Notice that $\widehat{E}\widehat{F} = (EF)^\wedge$ and

$$\widehat{E}(\widehat{F} + \widehat{G}) = \widehat{E}\widehat{F} + \widehat{E}\widehat{G} = (EF)^\wedge + (EG)^\wedge$$

However, in general $(E+F)^\wedge \neq \widehat{E} + \widehat{F}$. Any normal completely positive map $\mathcal{E}$ can be written as a sum $\mathcal{E} = \sum \widehat{E}_i$ of simple maps where E_i, $i = 1, 2, \dots$, are called the **operation elements** of $\mathcal{E}$ [11]. We say that $\mathcal{E}$ is **trace preserving** if $\sum E_i^*E_i = I$ and in this case $\mathcal{E}$ is a quantum operation. A TOM $[T_{ij}]$ is **simple** if T_{ij} is simple for every i,j. We can then write $[T_{ij}] = [\widehat{T}_{ij}]$, $T_{ij} \in \mathcal{B}(H)$. For $x \in H$ with $\|x\| = 1$, we denote the one-dimensional projection onto the subspace spanned by x as P_x.

Theorem 2.3. *Let $\mathcal{E} = [\mathcal{E}_{ij}]$ where $\mathcal{E}_{ij} \in CP(H)$ has the form $\mathcal{E}_{ij} = \sum_k \widehat{E}_{ij}^k$. Then $\mathcal{E}$ is a TOM if and only if $\sum_{i,k} E_{ij}^{k*}E_{ij}^k = I$ for every j.*

Proof. Suppose $\sum_{i,k} E_{ij}^{k*}E_{ij}^k = I$ for every j and let $D \in \mathcal{D}(H)$. Then for every j we have

$$\begin{aligned}\operatorname{tr}\left[\sum_i \mathcal{E}_{ij}(D)\right] &= \operatorname{tr}\left[\sum_i\sum_k \widehat{E}_{ij}^k(D)\right] = \operatorname{tr}\left[\sum_{i,k} E_{ij}^k D E_{ij}^{k*}\right]\\ &= \sum_{i,k} \operatorname{tr}\left(E_{ij}^k D E_{ij}^{k*}\right) = \sum_{i,k} \operatorname{tr}\left(E_{ij}^{k*} E_{ij}^k D\right)\\ &= \operatorname{tr}\left[\left(\sum_{i,k} E_{ij}^{k*}E_{ij}^k\right) D\right] = \operatorname{tr}(D) = 1\end{aligned}$$

Hence, $\mathcal{E}$ is a TOM. Conversely, suppose $\mathcal{E}$ is a TOM. By the previous calculation, for an $D \in \mathcal{D}(H)$ we have

$$\operatorname{tr}\left[\left(\sum_{i,k} E_{ij}^{k*}E_{ij}^k\right) D\right] = \operatorname{tr}\left[\sum_i \mathcal{E}_{ij}(D)\right] = 1$$

In particular, if $D = P_x$ then $D \in \mathcal{D}(H)$ and we have

$$\left\langle \sum_{i,k} E_{ij}^{k*}E_{ij}^k x, x\right\rangle = 1 = \langle x, x\rangle$$

Hence, $\sum_{i,k} E_{ij}^{k*}E_{ij}^k = 1$ for every j, which proves the result. □

Let $T = [\widehat{T}_{ij}]$, $T_{ij} \in \mathcal{B}(H)$, be a simple TOM. It follows from Theorem 2.3 that $\sum_i T_{ij}^*T_{ij} = I$ for every j. We conclude that the column sums of a simple TOM constitute quantum operations. For a vector state $A = (A_1, A_2, \dots)$ we have for every i that

$$(TA)_i = \sum_j \widehat{T}_{ij}A_j = \sum_j T_{ij}A_jT_{ij}^*$$

If A is the initial vector state, then the probability that the system occupies site i after one time step is

$$\operatorname{tr}[(TA)_i] = \sum_j \operatorname{tr}(T_{ij}^* T_{ij} A)$$

If $S = [\widehat{S}_{ij}]$, $S_{ij} \in \mathcal{B}(H)$, is another simple TOM, then $U = ST$ is the TOM $U = [U_{ij}]$ given by

$$U_{ij} = \sum_k \widehat{S}_{ik} \widehat{T}_{kj} = \sum_k (S_{ik} T_{kj})^\wedge$$

We conclude that the product of two simple TOMs and a power of a simple TOM are not simple in general.

An example of a simple TOM is $T = \operatorname{diag}(\widehat{U}_{ii})$ where U_{ii} is an isometry ($U_{ii}^* U_{ii} = I$). This would result in a stationary dynamics. Another example is $T = [(\lambda_{ij} U_{ij})^\wedge]$ where U_{ij} are isometries and $\lambda_{ij} \in \mathbb{C}$ satisfy $\sum_i |\lambda_{ij}|^2 = 1$ for every j. In this case we have $\widehat{T}_{ij} = (\lambda_{ij} U_{ij})^\wedge$ and

$$\sum_i T_{ij}^* T_{ij} = \sum_i |\lambda_{ij}|^2 U_{ij}^* U_{ij} = \sum_i |\lambda_{ij}|^2 I = I$$

A slightly different example is $T = \left[p_{ij} \widehat{U}_{ij}\right]$ where U_{ij} are isometries and $p_{ij} \in \mathbb{R}$ are nonnegative with $\sum_i p_{ij} = 1$ for every j. Then $\widehat{T}_{ij} = \left(\sqrt{p_{ij}}\, U_{ij}\right)^\wedge$ and as before $\sum_i T_{ij}^* T_{ij} = I$.

3 Transition Effect Matrices

The **sequential product** of two effects $E, F \in \mathcal{E}(H)$ is defined by $E \circ F = E^{1/2} F E^{1/2}$ where $E^{1/2}$ is the unique positive square root of E [6, 7]. It is easy to check that $E \circ F \in \mathcal{E}(H)$. If $\mathcal{A} = \{A_1, A_2, \ldots\}$ is a sequence in $\mathcal{E}(H)$ satisfying $\sum_i A_i = I$, then $\mathcal{A}$ is a discrete POVM or a (**discrete**) **measurement**. For two measurements $\mathcal{A} = \{A_i\}$, $\mathcal{B} = \{B_i\}$ we define the **sequential product** of $\mathcal{A}$ and $\mathcal{B}$ by $\mathcal{A} \circ \mathcal{B} = \{A_i \circ B_j\}$ [5]. Again, it is easy to check that $\mathcal{A} \circ \mathcal{B}$ is a measurement. We shall show that the product of TOMs gives a generalization of the sequential product of measurements. In this way, measurements can be used to specify quantum Markov chains.

Let T be a simple TOM of the form $T=\left[(E_{ij}^{1/2})^\wedge\right]$ where $E_{ij}\geq 0$. In this case

$$\sum_i E_{ij}=\sum_i E_{ij}^{1/2}E_{ij}^{1/2}=I$$

so $\{E_{1j},E_{2j},\ldots\}$ is a measurement for every j. For a vector state $S=(S_1,S_2,\ldots)$ we have

$$(TS)_i=\sum_j\left(E_{ij}^{1/2}\right)^\wedge S_j=\sum_j E_{ij}^{1/2}S_jE_{ij}^{1/2}=\sum_j E_{ij}\circ S_j$$

Equivalently, we can think of T as a matrix $E=[E_{ij}]$ where $E_{ij}\in\mathcal{E}(H)$ and $\sum_i E_{ij}=I$ for every j. We then define

$$(E\circ S)_i=\sum_j E_{ij}\circ S_j$$

so that $E\circ S=TS$ for every vector state S.

A matrix of the form $E=[E_{ij}]$ where $E_{ij}\in\mathcal{E}(H)$ and $\sum_i E_{ij}=I$ for every j is called a **transition effect matrix** (TEM). We conclude that if E is a TEM and S is a vector state, then $E\circ S$ is a vector state. We interpret E_{ij} as the effect that the system performs a transition from site j to site i in one time step. If the initial vector state is S, then the vector state after one time step is $E\circ S$ and the distribution after one time step is

$$\operatorname{tr}(E\circ S)=(\operatorname{tr}(E\circ S)_1,\operatorname{tr}(E\circ S)_2,\ldots)$$

Moreover, the vector state after N time steps is

$$E_{(n)}(S)=E\circ(\cdots E\circ(E\circ S))$$

which is the same type of dynamics as in Section 2.

For a TEM E, we denote the set of vector states of the proper size for matrix multiplication by E as $\mathcal{S}_E(H)$. For simplicity we write $\mathcal{S}(H)=\mathcal{S}_E(H)$ and no confusion should result. The maps $E_{(n)}\colon\mathcal{S}(H)\to\mathcal{S}(H)$, $n=1,2,\ldots$, are called the **state dynamics**. The next result shows that if two TEMs are statistically equivalent, they coincide.

Lemma 3.1. *If $E=[E_{ij}]$ and $F=[F_{ij}]$ are TEMs of the same size that satisfy* $\operatorname{tr}(E\circ S)=\operatorname{tr}(F\circ S)$ *for all $S\in\mathcal{S}(H)$, then $E=F$.*

Proof. Let $S = \mathcal{S}(H)$ be defined by $S_i = \delta_{ij} P_x$. Then

$$(E \circ S)_i = E_{ij} \circ P_x$$

For every j and we have

$$\operatorname{tr}(E_{ij} \circ P_x) = \operatorname{tr}(E_{ij} P_x) = \langle E_{ij} x, x \rangle$$

Hence, $\langle E_{ij} x, x \rangle = \langle F_{ij} x, x \rangle$ for all $x \in H$ so $E_{ij} = F_{ij}$ for all i, j. $\square$

We now introduce a dual dynamics called the operator dynamics. For the state dynamics, the vector state S evolves and the TEM E is considered fixed. For the operator dynamics the TEM evolves and the vector state is considered fixed. Roughly speaking this is analogous to the Schrödinger picture and Heisenberg picture for quantum dynamics. In this framework the two types of dynamics are not identical, however as in the usual quantum dynamics they produce the same probability distributions; that is, they are statistically equivalent. More precisely, suppose the system is initially in the vector state S and the evolution is described by the TEM E. In the state dynamics, after n time steps, the system will be in the vector state $E_{(n)}(S)$. In the operator dynamics, the system will again be in the vector state $E_{(1)}(S) = E \circ S$ after one time step. However, after two time steps, the system will be in the state $E^{(2)} \circ S$ (that we shall define shortly) and after n time steps, the system will be in state $E^{(n)} \circ S$. As we shall see in examples, because of nonassociativity, $E_{(2)}(S) \neq E^{(2)} \circ S$ in general but we always have $\operatorname{tr}\left[E_{(2)}(S)\right] = \operatorname{tr}\left[E^{(2)} \circ S\right]$.

A **dual** TEM is a matrix $E = [E_{ij}]$ where $E_{ij} \in \mathcal{E}(H)$ and $\sum_j E_{ij} = I$ for all i. Thus E is a dual TEM if and only if E is the transpose F^T of a TEM F. If $E = [E_{ij}]$ and $F = [F_{ij}]$ are dual TEMs of the same size, we define $E \circ F = G = [G_{ij}]$ by the modified matrix multiplication $G_{ij} = \sum_k E_{ik} \circ F_{kj}$.

Lemma 3.2. *If E and F are dual TEMs of the same size on H, then $E \circ F$ is a dual TEM.*

Proof. We first show that the summation $G_{ij} = \sum_k E_{ik} \circ F_{kj}$ converges in the strong operator topology. Since

$$\sum_{k=1}^{N} E_{ik} \circ F_{kj} \leq \sum_{k=1}^{N} E_{ik} \leq I$$

we have that $N \mapsto \sum_{k=1}^{N} E_{ik} \circ F_{kj}$ is an increasing sequence of positive operators bounded above by I. Hence, the sequence converges to an element of $\mathcal{E}(H)$ in the strong operator topology. We then have that

$$\begin{aligned}\sum_j G_{ij} &= \sum_j \sum_k E_{ik} \circ F_{kj} = \sum_k E_{ik} \circ \left(\sum_j F_{kj} \right) \\ &= \sum_k E_{ik} \circ I = \sum_k E_{ik} = I\end{aligned}$$

for every i. □

Notice that the multiplication of dual TEMs gives a generalization of the sequential product of measurements. For example, using the notation $A' = I - A$ for $A \in \mathcal{E}(H)$, let $\mathcal{A} = \{A, A'\}$, $\mathcal{B} = \{B, B'\}$ be two-valued measurements. Form the dual TEMs

$$E = \begin{bmatrix} A & A' & 0 & 0 \\ 0 & I & 0 & 0 \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}, \qquad F = \begin{bmatrix} B & B' & 0 & 0 \\ 0 & 0 & B & B' \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}$$

Their product becomes

$$E \circ F = \begin{bmatrix} A \circ B & A \circ B' & A' \circ B & A' \circ B' \\ 0 & 0 & B & B' \\ 0 & 0 & I & 0 \\ 0 & 0 & 0 & I \end{bmatrix}$$

This matrix has $\mathcal{A} \circ \mathcal{B}$ in the first row and measurements in the other rows. Of course, this can be generalized to measurements with more values.

If $E_1, \ldots, E_n$ are dual TEMs of the same size, by Lemma 3.2 their product is again a dual TEM. However, the product $\circ$ is nonassociative in general and when we write

$$E_n \circ \cdots \circ E_2 \circ E_1$$

we mean

$$E_n \circ \cdots \circ \{E_4 \circ [E_3 \circ (E_2 \circ E_1)]\}$$

If E is a TEM and $n\in\mathbb{N}$, we define the n-**step** TEM $E^{(n)}$ by

$$E^{(n)}=\left(E^T\circ E^T\circ\cdots\circ E^T\right)^T\quad (n\text{ factors})$$

Notice that care must be taken with the nonassociative product because, for example $(E\circ E)^T\ne E^T\circ E^T$ in general. Of course, $E^{(n)}$ is indeed a TEM and we interpret $E_{ij}^{(n)}$ as the effect that the system evolves from site j to site i in n time steps. The maps $E^{(n)}\colon\mathcal{S}(H)\to\mathcal{S}(H)$, $n=1,2,\ldots$, given by $S\mapsto E^{(n)}\circ S$ are called the **operator dynamics**. As we already mentioned $E^{(n)}\ne E_{(n)}$ in general. One reason for introducing the operator dynamics is because the state dynamics $E_{(n)}(S)$ depends on $S\in\mathcal{S}(H)$ while $E^{(n)}$ is independent of the vector state. Thus, if a general form for $E^{(n)}$ can be derived, it can be applied to any $S\in\mathcal{S}(H)$.

Lemma 3.3. *If E and F are TEMs of the same size on H, then*

$$\operatorname{tr}\left[(E^T\circ F^T)^T\circ S\right]=\operatorname{tr}\left[F\circ(E\circ S)\right]$$

for every $S\in\mathcal{S}(H)$.

Proof. Since

$$\left[(E^T\circ F^T)^T\circ S\right]_i=\sum_j(E^T\circ F^T)_{ji}\circ S_j=\sum_j\left(\sum_k E_{kj}\circ F_{ik}\right)\circ S_j$$

we have that

$$\begin{aligned}\operatorname{tr}\left\{\left[(E^T\circ F^T)^T\circ S\right]_i\right\}&=\sum_j\operatorname{tr}\left[\left(\sum_k E_{kj}\circ F_{ik}\right)\circ S_j\right]\\&=\sum_j\operatorname{tr}\left[\left(\sum_k E_{kj}\circ F_{ik}\right)S_j\right]\\&=\sum_{j,k}\operatorname{tr}\left[(E_{kj}\circ F_{ik})S_j\right]\end{aligned}$$

Since

$$\begin{aligned}\left[F\circ(E\circ S)\right]_i&=\sum_k F_{ik}\circ(E\circ S)_k=\sum_k F_{ik}\circ\left(\sum_j E_{kj}\circ S_j\right)\\&=\sum_{j,k}F_{ik}\circ(E_{kj}\circ S_j)\end{aligned}$$

we have that

$$\begin{aligned}\operatorname{tr}\{[F\circ(E\circ S)]_i\} &= \sum_{j,k}\operatorname{tr}\left[F_{ik}\circ(E_{kj}\circ S_j)\right]\\ &= \sum_{j,k}\operatorname{tr}\left[(E_{kj}\circ F_{ik})S_j\right]\end{aligned}$$

and the result follows □

The next result shows that two types of dynamics are statistically equivalent.

Theorem 3.4. *If E is a TEM, then $\operatorname{tr}[E^{(n)}\circ S]=\operatorname{tr}[E_{(n)}(S)]$ for every $S\in\mathcal{S}(H)$.*

Proof. We prove the result by induction on n. The result clearly holds for $n=1$. Suppose the result holds for $n\in\mathbb{N}$. Applying Lemma 3.3 and the induction hypothesis gives

$$\begin{aligned}\operatorname{tr}\left[E^{(n+1)}\circ S\right] =&\operatorname{tr}\left[(E^T\circ E^{(n)T})^T\circ S\right]=\operatorname{tr}\left[E^{(n)}\circ(E\circ S)\right]\\ =&\operatorname{tr}\left[E_{(n)}\circ(E\circ S)\right]=\operatorname{tr}\left[E_{(n+1)}(S)\right]\end{aligned}$$

The result follows by induction. □

We close this section by showing that $(E\circ E)^T\neq E^T\circ E^T$ in general. Indeed,

$$(E\circ E)^T_{ij}=(E\circ E)_{ji}=\sum_k E_{jk}\circ E_{ki}$$

while

$$(E^T\circ E^T)_{ij}=\sum_k E^T_{ik}\circ E^T_{kj}=\sum_k E_{ki}\circ E_{jk}$$

For example, in the 2×2 case

$$(E\circ E)^T_{11}=E_{11}\circ E_{11}+E_{12}\circ E_{21}$$

and

$$(E^T\circ E^T)_{11}=E_{11}\circ E_{11}+E_{21}\circ E_{12}$$

These coincide if and only if $E_{12}E_{21}=E_{21}E_{12}$ [7].

4 Examples

This section presents examples that illustrate various properties of quantum Markov chains. These examples are given in terms of TEMs because they are much simpler than the more general TOMs.

Example 1. We first consider one of the simplest nontrivial examples. Let $P, Q \in \mathcal{P}(H)$ and form the TEM

$$E = \begin{bmatrix} P & Q \\ P' & Q' \end{bmatrix}$$

We then have

$$E^T \circ E^T = \begin{bmatrix} P & P' \\ Q & Q' \end{bmatrix} \circ \begin{bmatrix} P & P' \\ Q & Q' \end{bmatrix} = \begin{bmatrix} P + P' \circ Q & P' \circ Q' \\ Q \circ P & Q \circ P' + Q' \end{bmatrix}$$

so that

$$E^{(2)} = (E^T \circ E^T)^T = \begin{bmatrix} P + P' \circ Q & Q \circ P \\ P' \circ Q' & Q \circ P' + Q' \end{bmatrix}$$

If $S = (S_1, S_2)$ is the initial vector state, then in the operator dynamics, the vector state at two time steps is

$$\begin{aligned} E^{(2)} \circ S &= \begin{bmatrix} P + P' \circ Q & Q \circ P \\ P' \circ Q' & Q \circ P' + Q' \end{bmatrix} \circ \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} \\ &= \begin{bmatrix} (P + P' \circ Q) \circ S_1 + (Q \circ P) \circ S_2 \\ (P' \circ Q') \circ S_1 + (Q \circ P' + Q') \circ S_2 \end{bmatrix} \end{aligned}$$

To find the vector state at two time steps in the state dynamics, we first compute the vector state at one time step

$$E \circ S = \begin{bmatrix} P & Q \\ P' & Q' \end{bmatrix} \circ \begin{bmatrix} S_1 \\ S_2 \end{bmatrix} = \begin{bmatrix} P \circ S_1 + Q \circ S_2 \\ P' \circ S_1 + Q' \circ S_2 \end{bmatrix}$$

At two time steps, $E_{(2)}(S)$ becomes

$$E\circ(E\circ S)=\begin{bmatrix}P & Q\\ P' & Q'\end{bmatrix}\circ\begin{bmatrix}P\circ S_1+Q\circ S_2\\ P'\circ S_1+Q'\circ S_2\end{bmatrix}$$

$$=\begin{bmatrix}P\circ S_1+P\circ(Q\circ S_2)+Q\circ(P'\circ S_1)\\ P'\circ(Q\circ S_2)+Q'\circ(P'\circ S_1)+Q'\circ S_2\end{bmatrix}$$

The two expressions, $E^{(2)}\circ S$ and $E_{(2)}(S)$ are quite different. For example, if $\dim H=2$ and $S=(I/2,0)$ then

$$E^{(2)}\circ S=\frac{1}{2}\begin{bmatrix}P+P'\circ Q\\ P'\circ Q'\end{bmatrix},\quad E_{(2)}(S)=\frac{1}{2}\begin{bmatrix}P+Q\circ P'\\ Q'\circ P'\end{bmatrix}$$

These agree if and only if $P'\circ Q=Q\circ P'$ which is equivalent to $PQ=QP$ [7]. Of course, this latter condition does not hold in general.

This example also illustrates the fact that the state dynamics $E_{(n)}(S)$ cannot be given by any operator dynamics in general. For instance, there need not be a TEM F such that $F\circ S=E_{(2)}(S)$ for all $S\in\mathcal{S}(H)$. Indeed, applying Theorem 3.4 we have that $\operatorname{tr}\left[E^{(2)}\circ S\right]=\operatorname{tr}\left[E_{(2)}(S)\right]$ for all $S\in\mathcal{S}(H)$. Hence, if such an F exists, we would have that $\operatorname{tr}[F\circ S]=\operatorname{tr}\left[E^{(2)}\circ S\right]$ for all $S\in\mathcal{S}(H)$. Applying Lemma 3.1 gives $F=E^{(2)}$. Thus, $E^{(2)}\circ S=E_{(2)}(S)$ for all $S\in\mathcal{S}(H)$ which is a contradiction.

Example 2. We now study the long term behavior of the dynamics given by the TEM E of Example 1. By repeated matrix multiplication we obtain

$$\begin{aligned}
E_{11}^{(1)}&=P\\
E_{11}^{(2)}&=P+P'\circ Q\\
E_{11}^{(3)}&=P+P'\circ Q\circ P\\
E_{11}^{(4)}&=P+P'\circ Q\circ P+P'\circ Q\circ P'\circ Q\\
E_{11}^{(5)}&=P+P'\circ Q\circ P+P'\circ Q\circ P'\circ Q\circ P\\
E_{11}^{(6)}&=P+P'\circ Q\circ P+P'\circ Q\circ P'\circ Q\circ P+P'\circ Q\circ P'\circ Q\circ P'\circ Q\\
&\;\;\vdots
\end{aligned}$$

We now assume that $\|P' \circ Q\| < 1$. Then in the strong operator topology we have

$$\lim_{n\to\infty} E_{11}^{(n)} = P + P' \circ Q(I + P' \circ Q)^{-1}$$

Applying a similar analysis to the other entries of $E^{(n)}$ we obtain

$$\lim_{n\to\infty} E^{(n)} = \begin{bmatrix} P + P' \circ Q(I + P' \circ Q)^{-1} & Q - Q \circ P'(I + Q \circ P')^{-1} \\ P' - P' \circ Q(I + P' \circ Q)^{-1} & Q' + Q \circ P'(I + Q \circ P')^{-1} \end{bmatrix}$$

Let us consider the particular case where $\dim H = 2$ and $P = P_x$, $P' = P_{x'}$, $Q = P_y$, $Q' = P_{y'}$ are one-dimensional projectors onto subspaces spanned by the unit vectors x, x', y, y', respectively. In this case $\{x, x'\}$ and $\{y, y'\}$ are orthonormal bases for H. We then have

$$P' \circ Q = P_{x'} P_y P_{x'} = |\langle x', y\rangle|^2 P_{x'}$$

and

$$Q \circ P' = P_y P_{x'} P_y = |\langle x', y\rangle|^2 P_y$$

It follows that

$$(I + P' \circ Q)^{-1} = \left(I + |\langle x', y\rangle|^2\right) P_{x'})^{-1} = \frac{1}{1 + |\langle x', y\rangle|^2} P_{x'} + P_x$$

Hence,

$$\begin{aligned} P + P' \circ Q(I + P' \circ Q)^{-1} =& P_x + |\langle x', y\rangle|^2 P_{x'} \left[\frac{1}{1 + |\langle x', y\rangle|^2} P_{x'} + P_x\right] \\ =& \frac{1}{1 + |\langle x', y\rangle|^2} \left[P_x + |\langle x', y\rangle|^2 I\right] \end{aligned}$$

and

$$P' - P' \circ Q(I + P' \circ Q)^{-1} = \frac{1}{1 + |\langle x', y\rangle|^2} P_{x'}$$

The limiting matrix then becomes

$$A = \lim_{n\to\infty} E^{(n)} = \frac{1}{1 + |\langle x', y\rangle|^2} \begin{bmatrix} P_x + |\langle x', y\rangle|^2 I & P_y \\ P_{x'} & P_{y'} + |\langle x', y\rangle|^2 I \end{bmatrix}$$

Straightforward computations give the expected results that

$$(A^T \circ A^T)^T = A, \qquad (E^T \circ A^T)^T = A$$

If the initial vector state is $S = (S_1, S_2)$ then the limiting vector state becomes

$$A \circ S = \frac{1}{1 + |\langle x', y\rangle|^2} \begin{bmatrix} (P_x + |\langle x', y\rangle|^2 I) \circ S_1 + P_y \circ S_2 \\ P_{x'} \circ S_1 + (P_{y'} + |\langle x', y\rangle|^2 I) \circ S_2 \end{bmatrix}$$

Hence, the limiting distribution is

$$\mathrm{tr}(A \circ S) = \frac{1}{1 + |\langle x', y\rangle|^2} \begin{bmatrix} \langle S_1 x, x\rangle + \langle S_2 y, y\rangle + |\langle x', y\rangle|^2 \,\mathrm{tr}(S_1) \\ \langle S_1 x', x'\rangle + \langle S_2 y', y'\rangle + |\langle x', y\rangle|^2 \,\mathrm{tr}(S_2) \end{bmatrix}$$

Example 3. We now consider a quantum random walk with absorbing barriers. In this example, $P \in \mathcal{P}(H)$ and the sites are labeled by $-2, -1, 0, 1, 2$. Suppose the quantum random walk is governed by the TEM

$$E = \begin{bmatrix} I & P' & 0 & 0 & 0 \\ 0 & 0 & P' & 0 & 0 \\ 0 & P & 0 & P' & 0 \\ 0 & 0 & P & 0 & 0 \\ 0 & 0 & 0 & P & I \end{bmatrix}$$

We then have

$$E^{(2)} = \begin{bmatrix} I & P' & P' & 0 & 0 \\ 0 & 0 & 0 & P' & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & P & 0 & 0 & 0 \\ 0 & 0 & P & P & I \end{bmatrix}, \qquad E^{(3)} = \begin{bmatrix} I & P' & P' & P' & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & P & P & P & I \end{bmatrix}$$

and $E^{(3)} = E^{(4)} = E^{(5)} = \ldots$. Suppose the initial vector state is $S = (0, 0, P_x, 0, 0)$. Then

$$\begin{aligned} \mathrm{tr}(E \circ S) &= (0, \langle P'x, x\rangle, 0, \langle Px, x\rangle, 0) \\ \mathrm{tr}(E^{(2)} \circ S) &= (\langle P'x, x\rangle, 0, 0, 0, \langle Px, x\rangle) \end{aligned}$$

and $\text{tr}(E^{(2)} \circ S) = \text{tr}(E^{(3)} \circ S) = \ldots$. The dynamics shows that if the system is initially at the site 0, it moves directly to the right or to the left and is absorbed at the boundary sites ± 2 in two time steps. There is no classical random walk that would produce this type of dynamics.

Example 4. In this example, the sites are labeled by $1, 2, 3$. Let $P_1, P_2, P_3 \in \mathcal{P}(H)$ with $P_1 + P_2 + P_3 = I$ and $P_i \neq 0$, $i = 1, 2, 3$. It follows that $P_i P_j = 0$ for $i, j = 1, 2, 3$, $i \neq j$. Suppose the quantum Markov chain is governed by the TEM

$$E = \begin{bmatrix} P_2 + P_3 & P_1 & 0 \\ P_1 & P_2 & P_1 \\ 0 & P_3 & P_2 + P_3 \end{bmatrix}$$

We then have

$$E^{(2)} = \begin{bmatrix} I & 0 & P_1 \\ 0 & P_1 + P_2 & 0 \\ 0 & P_3 & P_2 + P_3 \end{bmatrix}$$

$E^{(2n+1)} = E^{(1)} = E$ for $n = 1, 2, \ldots$, and $E^{(2n)} = E^{(2)}$ for $n = 1, 2, \ldots$.

This example illustrates another important difference between general quantum Markov chains and classical Markov chains. An important property of classical Markov chains is that sites (which are called "states" in the classical case) can be decomposed into equivalence classes. This is important because sites in the same equivalence class have similar behaviors.

To be precise, let $M = [p_{ij}]$ be the transition matrix for a classical Markov chain. Then $p_{ij} \geq 0$, $\sum_i p_{ij} = 1$ for all j, and p_{ij} is the transition probability from site j to site i. We say that site i is **accessible** from site j and write $j \to i$ if $M_{ij}^n > 0$ for some $n \in \mathbb{N}$. It is easy to check that accessibility is transitive. Indeed, suppose $j \to i$ and $i \to k$. Then $M_{ij}^m > 0$ and $M_{ki}^n > 0$ for some $n, n \in \mathbb{N}$. We then have

$$M_{kj}^{m+n} = \sum_r M_{kr}^n M_{rj}^m \geq M_{ki}^n M_{ij}^m > 0$$

so that $j \to k$. If $i \to j$ and $j \to i$ we write $i \leftrightarrow j$ and it follows that $\leftrightarrow$ is an equivalence relation on the sites of a classical Markov chain.

We now extend this concept to a quantum Markov chain governed by a TEM $E = [E_{ij}]$. As before we write $j \to i$ if $E_{ij}^{(n)} \neq 0$ for some $n \in \mathbb{N}$ and we write $i \leftrightarrow j$ if $i \to j$ and $j \to i$. In Example 4 we have that $1 \to 2$ and $2 \to 3$ but $1 \not\to 3$ so $\to$ is not transitive. We also have the stronger result that $1 \leftrightarrow 2$ and $2 \leftrightarrow 3$ but $1 \not\leftrightarrow 3$ so $\leftrightarrow$ is not an equivalence relation.

Example 5. This is a simple example that again illustrates the unusual behavior that is possible for a quantum Markov chain. Label the three sites by $1, 2, 3$, let $P \in \mathcal{P}(H)$ and suppose the quantum Markov chain is governed by the TEM

$$E = \begin{bmatrix} P' & 0 & 0 \\ P & P & 0 \\ 0 & P' & I \end{bmatrix}$$

We then have $E^{(n)} = E$ for $n = 1, 2, \ldots$. Notice that $1 \to 2$ and $2 \to 3$ but $1 \not\to 3$ so accessibility is not transitive. If $S \in \mathcal{S}(H)$ then for $n = 1, 2, \ldots,$ we have that

$$E_{(n)}(S) = \begin{bmatrix} P' \circ S_1 \\ P \circ S_1 + P \circ S_2 \\ P' \circ S_2 + S_3 \end{bmatrix}$$

We conclude that for any $S \in \mathcal{S}(H)$, the vector state $E \circ S$ is stationary in the sense that $E_{(n)}(E \circ S) = E \circ S$ for all $n \in \mathbb{N}$. For example, if the system is initially at site 2 so the initial vector state is $(0, P_x, 0)$ with distribution $(0, 1, 0)$ then for all future times the vector state is $(0, P \circ P_x, P' \circ P_x)$ with distribution $(0, \langle Px, x\rangle, 1 - \langle Px, x\rangle)$.

5 Quantum Random Walks

This section briefly shows that our formalism generalizes the usual framework for quantum random walks [8, 10, 12]. For simplicity we consider a one-dimensional quantum random walk on the integers $\mathbb{Z}$ and this work can be easily generalized to higher dimensions. We adopt the usual Dirac notation for this framework. The Hilbert space for the system is $H = H_P \otimes H_C$ where H_P is the position Hilbert space for a particle and H_C is the coin Hilbert space. A basis for H_P is $\{|n\rangle : n \in \mathbb{Z}\}$ and a basis for the 2-dimensional coin space H_C is $\{|L\rangle, |R\rangle\}$. The basis vector $|n\rangle$ locates the particle at $n \in \mathbb{Z}$. We think of $\{|L\rangle, |R\rangle\}$ as the two sides of a "quantum coin" and after the coin is "flipped" if $|L\rangle$ appears the particle moves left one unit and if $|R\rangle$ appears the particle moves right one unit. Alternatively, we may think of the particle as having spin 1/2 and $|L\rangle$, $|R\rangle$ correspond to spin up or down in the z-direction.

The particle moves along the integers in discrete time steps in accordance with the coin state. The operator that induces a single displacement has the form

$$S = \sum_n |n-1\rangle\langle n| \otimes |L\rangle\langle L| + \sum_n |n+1\rangle\langle n| \otimes |R\rangle\langle R|$$

A single step of the particle consists of a "flip" or "rotation" of the coin state by an arbitrary, but fixed, unitary operator C and then the conditional displacement S. The time evolution describing one step of the quantum random walk is performed by the unitary operator $U = S(I \otimes C)$. If the initial state of the particle is $|\psi(0)\rangle$, then after t steps its state will be given by $|\psi(t)\rangle = U^t|\psi(0)\rangle$.

We now show that this framework is a special case of our formalism for quantum Markov chains. For the Hilbert space $H = H_P \otimes H_C$ form the TOM $T = [\widehat{T}_{ij}]$ where

$$T_{j+1,j} = I \otimes |R\rangle\langle R|C, \qquad T_{j-1,j} = I \otimes |L\rangle\langle L|C$$

and $T_{ij} = 0$ for $i \neq j \pm 1$, $i, j \in \mathbb{Z}$. This is a very simple matrix with only two nonzero entries in each row and column. Notice that T is indeed a TOM because

$$\begin{aligned}(I \otimes |R\rangle\langle R|C)^* \,(I\otimes\, |R\rangle\langle R|C) + (I \otimes |L\rangle\langle L|C)^* \\ (I \otimes |L\rangle\langle L|C) =& I \otimes C^*|R\rangle\langle R|C + I \otimes C^*|L\rangle\langle L|C \\ =& I \otimes C^*\left(|R\rangle\langle R| + |L\rangle\langle L|\right)C = I \otimes C^*C = I \otimes I\end{aligned}$$

Now T acting on the state $|n, L\rangle$ is given by

$$\begin{aligned}T(P_{|n,L\rangle}) =& (I \otimes |R\rangle\langle R|C)\, P_{|n+1,L\rangle}\, (I \otimes |R\rangle\langle R|C)^* \\ &+ (I \otimes |L\rangle\langle L|C)\, P_{|n-1,L\rangle}\, (I \otimes |L\rangle\langle L|C)^* \\ =& \langle R|C|L\rangle P_{|n+1,R\rangle} + \langle L|C|L\rangle P_{|n-1,L\rangle}\end{aligned}$$

and similarly, T acting on the state $|n, R\rangle$ is given by

$$T(P_{|n,R\rangle}) = \langle R|C|R\rangle P_{|n+1,R\rangle} + \langle L|C|R\rangle P_{|n-1,L\rangle}$$

Comparing this to U acting on $|n, L\rangle$ and $|n, R\rangle$ we have

$$U(|n, L\rangle) = S(|n, CL\rangle) = \langle L|C|L\rangle|n-1, L\rangle + \langle R|C|L\rangle|n+1, R\rangle$$

and

$$U(|n, R\rangle) = S(|n, CR\rangle) = \langle L|C|L\rangle|n-1, L\rangle + \langle R|C|R\rangle|n+1, R\rangle$$

We see that these results coincide.

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