

# Open Quantum Random Walks\*

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## Abstract

A new model of quantum random walks is introduced, on lattices as well as on finite graphs. These quantum random walks take into account the behavior of open quantum systems. They are the exact quantum analogue of classical Markov chains. We explore the “quantum trajectory” point of view on these quantum random walks, that is, we show that measuring the position of the particle after each time-step gives rise to a classical Markov chain, on the lattice times the state space of the particle. This quantum trajectory is a simulation of the master equation of the quantum random walk. The physical pertinence of such quantum random walks and the way they can be concretely realized is discussed. Connections and differences with the already well-known quantum random walks, such as the Hadamard random walk, are established. We explore several examples and compute their limit behavior. We show that the typical behavior of Open Quantum Random Walks seems to be very different from Hadamard-type quantum random walks. Indeed, while being very quantum in their behavior, Open Quantum Random Walks tend to become more and more classical as time goes.

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# 1 Introduction

Nowadays quantum random walks, such as the Hadamard quantum random walk, are quite a successful domain of research, with important applications in Quantum Information Theory (see [Kem] for a survey). These quantum random walks are particular discrete-time quantum dynamics on a state space of the form  $\mathcal{H} \otimes \mathbb{C}^{\mathbb{Z}^d}$ . The space  $\mathbb{C}^{\mathbb{Z}^d}$  stands for a state space labelled by a net  $\mathbb{Z}^d$ , while the space  $\mathcal{H}$  stands for the degrees of freedom given on each point of the net. The quantum evolution concerns pure states of the system which are of the form

$$|\Psi\rangle = \sum_{i \in \mathbb{Z}^d} |\varphi_i\rangle \otimes |i\rangle.$$

After one step of the dynamics, this state is transformed into another pure state,

$$|\Psi'\rangle = \sum_{i \in \mathbb{Z}^d} |\varphi'_i\rangle \otimes |i\rangle.$$

Each of these two states gives rise to a probability distribution on  $\mathbb{Z}^d$ , the one we would obtain by measuring the position on  $\mathbb{C}^{\mathbb{Z}^d}$ :

$$\text{Prob}(\{i\}) = \|\varphi_i\|^2.$$

The point is that the probability distribution associated to  $|\Psi'\rangle$  cannot be deduced from the distribution associated to  $|\Psi\rangle$  by “classical rules”, that is, there is no classical probabilistic model (such as a Markov transition kernel, or else) which gives the distribution of  $|\Psi'\rangle$  in terms of the one of  $|\Psi\rangle$ . One needs to know the whole state  $|\Psi\rangle$  in order to compute the distribution of  $|\Psi'\rangle$ .

These quantum random walks, that we shall call Unitary Quantum Random Walks (for a reason which will appear clear in Section 10) have been successful for they give rise to strange behaviors of the probability distribution as time goes to infinity. In particular one can prove that they satisfy a rather surprising Central Limit Theorem whose speed is  $n$ , instead of  $\sqrt{n}$  as usually, and the limit distribution is not Gaussian, but more like functions of the form (see [Kon])

$$x \mapsto \frac{\sqrt{1-a^2}(1-\lambda x)}{\pi(1-x^2)\sqrt{a^2-x^2}},$$

where  $a$  is a constant.

The purpose of this article is to introduce a new type of quantum random walks, that we suggest to call *Open Quantum Random Walks* (O.Q.R.W.).

These quantum random walks also deal with a quantum dynamics on a state space  $\mathcal{H} \otimes \mathbb{C}^{\mathbb{Z}^d}$ , but they consider the evolution of density matrices

$$\rho = \sum_{i \in \mathbb{Z}^d} \rho_i \otimes |i\rangle\langle i|.$$

More or less, the principle is the same as above, and the dynamics leads to a new density matrix

$$\rho' = \sum_{i \in \mathbb{Z}^d} \rho'_i \otimes |i\rangle\langle i|.$$

To each of them is associated the probability distribution obtained when measuring the position

$$\text{Prob}(\{i\}) = \text{Tr}(\rho_i), i \in \mathbb{Z}^d.$$

This new type of quantum random walks is very different from the Unitary Quantum Random Walks. It seems that there is no inclusion whatsoever, though we prove in Section 10 a very strong link between the two walks, in the way they can be physically implemented.

Actually, the limit behavior of Open Quantum Random Walks shows up a dissipative character, it tends to converge to a classical behavior, that is, it seems to give rise to classical Central Limit Theorems: one can see the distribution converging to Gaussian limits, or to mixtures of Gaussian limits.

The point to be stressed is the generality of our setup. It allows to consider a very wide class of quantum random walks on nets as well as on graphs. Our setup is the exact quantum generalization of the construction of a classical Markov chain on a net, or on a graph. By the way, we shall show that Open Quantum Random Walks contain all the classical Markov chains as particular cases.

Our conviction is that this type of quantum random walks gives rise to a vast field of exploration for the behavior of open quantum systems. It may be as rich as the one of classical Markov chains and it shall give rise to the same type of questions: existence of invariant states, ergodic behavior, Central Limit Theorems, Large Deviation Principle, recurrence and transience, etc.

Many of the examples that we have explored lead us to think that these quantum random walks may apply in many realistic physical situations. Their dissipative behavior makes them physically more realistic, while keeping a very quantum behavior. For example, some of the examples that we shall explore in this article make us think of possible applications, such as heat conduction and quantum Fourier's law for a one dimensional model

(such as the quantum version of the “Simple Exclusion Process”, see [Bod]) and realistic model for excitation transport on a chain of quantum systems.

Note that the main physical implications of this article have already been announced and summarized in a letter [APSS].

Also, it has to be said that the idea of considering matrices of completely positive maps such that the lines (or columns, depending on the point of view) form a so-called quantum operation, appeared earlier in [Gud]. This approach is presented as a “quantum Markov chain”. These objects present clearly several common points in their structure with our Open Quantum Random Walks, but they are not studied as giving rise to quantum random walks. Except at the end of the article where an incorrect parallel with Unitary Quantum Random Walk is claimed.

## 2 General Setup

We now introduce the general mathematical and physical setup of the Open Quantum Random Walks. For sake of completeness we recall in this section several technical lemmas which ensure that our definitions are consistent. The proofs of these lemmas are postponed to Section 13.

We are given a set  $\mathcal{V}$  of vertices, which might be finite or countable infinite. We consider all the oriented edges  $\{(i, j); i, j \in \mathcal{V}\}$ . We wish to give a quantum analogue of a random walk on the associated graph (or lattice).

We consider the space  $\mathcal{K} = \mathbb{C}^{\mathcal{V}}$ , that is, the state space of a quantum system with as many degrees of freedom as the number of vertices; when  $\mathcal{V}$  is infinite countable we put  $\mathcal{K}$  to be any separable Hilbert space with an orthonormal basis indexed by  $\mathcal{V}$ . We fix an orthonormal basis of  $\mathcal{K}$  which we shall denote by  $(|i\rangle)_{i \in \mathcal{V}}$ .

Let  $\mathcal{H}$  be a separable Hilbert space; it stands for the space of degrees of freedom (or *chirality* as they call it in Quantum Information Theory) given at each point of  $\mathcal{V}$ . Consider the space  $\mathcal{H} \otimes \mathcal{K}$ .

For each edge  $(i, j)$  we are given a bounded operator  $B_j^i$  on  $\mathcal{H}$ . This operator stands for the effect of passing from  $j$  to  $i$ . We assume that, for each  $j$

$$\sum_i B_j^{i*} B_j^i = I, \quad (1)$$

where the above series is strongly convergent (if infinite). This constraint has to be understood as follows: “the sum of all the effects leaving the site

$j$  is  $I$ ". It is the same idea as the one for transition matrices associated to Markov chains: "the sum of the probabilities leaving a site  $j$  is 1".

By Lemma 2.1 which follows, to each  $j \in \mathcal{V}$  is associated a completely positive map on the density matrices of  $\mathcal{H}$ :

$$\mathcal{M}_j(\rho) = \sum_i B_j^i \rho B_j^{i*}.$$

**Lemma 2.1** *Let  $(B_i)$  be a sequence of bounded operators on a separable Hilbert space  $\mathcal{H}$  such that the series  $\sum_i B_i^* B_i$  converges strongly to a bounded operator  $T$ . If  $\rho$  is a positive trace-class operator on  $\mathcal{H}$  then the series*

$$\sum_i B_i \rho B_i^*$$

*is trace-norm convergent and*

$$\mathrm{Tr} \left( \sum_i B_i \rho B_i^* \right) = \mathrm{Tr}(\rho T).$$

The operators  $B_j^i$  act on  $\mathcal{H}$  only, we dilate them as operators on  $\mathcal{H} \otimes \mathcal{K}$  by putting

$$M_j^i = B_j^i \otimes |i\rangle\langle j|.$$

The operator  $M_j^i$  encodes exactly the idea that while passing from  $|j\rangle$  to  $|i\rangle$  on the lattice, the effect is the operator  $B_j^i$  on  $\mathcal{H}$ .

By Lemma 2.2, which follows, the series  $\sum_{i,j} M_j^{i*} M_j^i$  converges strongly to the operator  $I$ .

**Lemma 2.2** *Let  $\mathcal{K}$  and  $\mathcal{H}$  be separable Hilbert spaces. Consider an orthonormal basis  $(|i\rangle)$  of  $\mathcal{K}$ . Assume that  $B_j^i$  are bounded operators on  $\mathcal{H}$  such that, for all  $j$ , the series  $\sum_i B_j^{i*} B_j^i$  is strongly convergent to  $I$ . Define the bounded operators*

$$M_j^i = B_j^i \otimes |i\rangle\langle j|$$

*on  $\mathcal{H} \otimes \mathcal{K}$ . Then the series  $\sum_{i,j} M_j^{i*} M_j^i$  converges strongly to  $I$ .*

As a consequence we can apply Lemma 2.1 to the set of operators  $(M_j^i)_{i,j}$  and the mapping

$$\mathcal{M}(\rho) = \sum_i \sum_j M_j^i \rho M_j^{i*} \quad (2)$$

defines a completely positive map on  $\mathcal{H} \otimes \mathcal{K}$ .

We shall especially be interested in density matrices on  $\mathcal{H} \otimes \mathcal{K}$  with the particular form

$$\rho = \sum_i \rho_i \otimes |i\rangle\langle i|, \quad (3)$$

where each  $\rho_i$  is not exactly a density matrix on  $\mathcal{H}$ : it is a positive and trace-class operator but its trace is not 1. Indeed the condition that  $\rho$  is a state aims to

$$\sum_i \text{Tr}(\rho_i) = 1. \quad (4)$$

The importance of those density matrices is justified by the following.

**Proposition 2.3** *Whatever is the initial state  $\rho$  on  $\mathcal{H} \otimes \mathcal{K}$ , the density matrix  $\mathcal{M}(\rho)$  is of the form (3).*

Before proving this proposition, let us recall a basic result on partial traces.

**Lemma 2.4** *Let  $\rho$  be a trace-class operator on  $\mathcal{H} \otimes \mathcal{K}$  and  $(|j\rangle)$  be an orthonormal basis of  $\mathcal{K}$ . The operator*

$$(I \otimes |i\rangle\langle j|) \rho (I \otimes |j\rangle\langle i|)$$

*can be written as*

$$\rho_j \otimes |i\rangle\langle i|$$

*for some trace-class operator  $\rho_j$  on  $\mathcal{H}$ , which we shall denote by  $\langle j| \rho |j\rangle$ . Furthermore we have*

$$\text{Tr}(\langle j| \rho |j\rangle) = \text{Tr}(\rho(I \otimes |j\rangle\langle j|)).$$

We can now come back to the proof of the proposition.

**Proof** [of Proposition 2.3] We have

$$\begin{aligned} \mathcal{M}(\rho) &= \sum_{i,j} (B_j^i \otimes |i\rangle\langle j|) \rho (B_j^{i*} \otimes |j\rangle\langle i|) \\ &= \sum_{i,j} (B_j^i \otimes I)(I \otimes |i\rangle\langle j|) \rho (I \otimes |j\rangle\langle i|)(B_j^{i*} \otimes I). \end{aligned}$$

If we put  $\rho_j = \langle j| \rho |j\rangle$  (as in Lemma 2.4), we get

$$\begin{aligned} \mathcal{M}(\rho) &= \sum_{i,j} (B_j^i \otimes I)(\rho_j \otimes |i\rangle\langle i|)(B_j^{i*} \otimes I) \\ &= \sum_{i,j} B_j^i \rho_j B_j^{i*} \otimes |i\rangle\langle i|. \end{aligned}$$

Each of the operators  $B_j^i \rho_j B_j^{i*}$  is positive and trace-class, hence so is the operator  $\sum_{j \leq M} B_j^i \rho_j B_j^{i*}$ . But we have

$$\mathrm{Tr} \left( \sum_{j \leq M} B_j^i \rho_j B_j^{i*} \right) = \sum_{j \leq M} \mathrm{Tr} (\rho_j B_j^{i*} B_j^i).$$

As  $\sum_i B_j^{i*} B_j^i = I$ , each of the operators  $B_j^{i*} B_j^i$  is smaller than  $I$  (in the sense that  $I - B_j^{i*} B_j^i$  is a positive operator). Hence,  $\mathrm{Tr} (\rho_j B_j^{i*} B_j^i) \leq \mathrm{Tr} (\rho_j)$ , as can be easily checked. This shows that

$$\sum_j \mathrm{Tr} (B_j^i \rho_j B_j^{i*}) < \infty$$

and that  $\sum_{j \leq M} B_j^i \rho_j B_j^{i*}$  converges in trace-norm to a positive trace-class operator  $\sum_j B_j^i \rho_j B_j^{i*}$  which satisfies

$$\mathrm{Tr} \left( \sum_j B_j^i \rho_j B_j^{i*} \right) = \sum_j \mathrm{Tr} (\rho_j B_j^{i*} B_j^i).$$

In particular by Lemma 2.1 we have,

$$\begin{aligned} \sum_i \mathrm{Tr} \left( \sum_j B_j^i \rho_j B_j^{i*} \right) &= \sum_i \sum_j \mathrm{Tr} (\rho_j B_j^{i*} B_j^i) \\ &= \sum_j \mathrm{Tr} \left( \rho_j \left( \sum_i B_j^{i*} B_j^i \right) \right) \\ &= \sum_j \mathrm{Tr} (\rho_j) \\ &= 1. \end{aligned}$$

This means that the series (in the variable  $i$ )

$$\sum_i \left( \sum_j B_j^i \rho_j B_j^{i*} \right) \otimes |i\rangle\langle i|$$

is trace-norm convergent. We now immediately have the relation

$$\sum_{i,j} B_j^i \rho_j B_j^{i*} \otimes |i\rangle\langle i| = \sum_i \left( \sum_j B_j^i \rho_j B_j^{i*} \right) \otimes |i\rangle\langle i|.$$



This proves that  $\mathcal{M}(\rho)$  is of the form (3). □

The states of the form (3) are mixtures of initial states  $\rho_i$  on each site  $i$ , but they express no mixing between the sites. An immediate consequence of the proof of Proposition 2.3 is the following important formula.

**Corollary 2.5** *If  $\rho$  is a state on  $\mathcal{H} \otimes \mathcal{K}$  of the form*

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

then

$$\mathcal{M}(\rho) = \sum_i \left( \sum_j B_j^i \rho_j B_j^{i*} \right) \otimes |i\rangle\langle i|. \quad (5)$$

This is exactly the quantum analogue of a usual random walk: after one step, on the site  $i$  we have all the contributions from those pieces of the state which have travelled from  $j$  to  $i$ .

### 3 Open Quantum Random Walks

If the state of the system  $\mathcal{H} \otimes \mathcal{K}$  is of the form

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

then a measurement of the “position” in  $\mathcal{K}$ , that is, a measurement along the orthonormal basis  $(|i\rangle)_{i \in \mathcal{V}}$ , gives the value  $|i\rangle$  with probability

$$\text{Tr}(\rho_i).$$

As proved in Corollary 2.5, after applying the completely positive map  $\mathcal{M}$  the state of the system  $\mathcal{H} \otimes \mathcal{K}$  is

$$\mathcal{M}(\rho) = \sum_i \sum_j B_j^i \rho_j B_j^{i*} \otimes |i\rangle\langle i|.$$

Hence a measurement of the position in  $\mathcal{K}$  would give that each site  $i$  is occupied with probability

$$\sum_j \text{Tr}(B_j^i \rho_j B_j^{i*}). \quad (6)$$

For each fixed choice of the initial states  $\rho_i$ , the probability to find the particle on the site  $i$  after one step is the usual one for the usual random walk where the probabilities to go from  $j$  to  $i$  are  $\text{Tr} (B_j^i \rho_j B_j^{i*})$ .

Now, let us see what would have happened if the measurement happens after two steps only. The state of the system is

$$\mathcal{M}^2(\rho) = \sum_i \sum_j \sum_k B_j^i B_k^j \rho_k B_k^{j*} B_j^{i*} \otimes |i\rangle\langle i|.$$

Hence measuring the position, we get the site  $|i\rangle$  with probability

$$\sum_j \sum_k \text{Tr} (B_j^i B_k^j \rho_k B_k^{j*} B_j^{i*}). \quad (7)$$

Had we repeated the rule for the first step, as for a classical random walk, we would have found

$$\sum_j \sum_k \text{Tr} (B_j^i \rho_j B_j^{i*}) \text{Tr} (B_k^j \rho_k B_k^{j*}),$$

which is clearly different from (7), in general. Actually there is no way to understand the probability measure given in (7) for two steps with the help of only the probability measure on one step (6).

The random walk which is described this way by the iteration of the completely positive map  $\mathcal{M}$  is not a classical random walk, it is a quantum random walk. The rules for jumping from a site to another are dictated by the sites, but also by the chirality. This is what we call an ‘‘Open Quantum Random Walk’’.

Let us resume these remarks in the following proposition, which follows easily from the previous results and remarks.

**Proposition 3.1** *Given any initial state  $\rho^{(0)}$  on  $\mathcal{H} \otimes \mathcal{K}$ , then for all  $n \geq 1$  the states  $\rho^{(n)} = \mathcal{M}^n(\rho^{(0)})$  are all of the form*

$$\rho^{(n)} = \sum_i \rho_i^{(n)} \otimes |i\rangle\langle i|.$$

*They are given inductively by the following relation:*

$$\rho_i^{(n+1)} = \sum_j B_j^i \rho_j^{(n)} B_j^{i*}.$$

*For each  $n \geq 1$ , the quantities*

$$p_i^{(n)} = \text{Tr} (\rho_i^{(n)}), \quad i \in \mathcal{V}$$

*define a probability distribution  $p^{(n)}$  on  $\mathcal{V}$ , it is called the ‘‘probability distribution of the open quantum random walk at time  $n$ ’’.*

## 4 Examples

Before going ahead with the properties of the Open Quantum Random Walks, let us introduce a few examples that we shall discuss in more detail in Sections 11 and 12.

### 4.1 An Example on $\mathbb{Z}$

First of all, it is very easy to define a stationary open quantum random walk on  $\mathbb{Z}$ . Let  $\mathcal{H}$  be any Hilbert space and  $B, C$  be two bounded operators on  $\mathcal{H}$  such that

$$B^*B + C^*C = I.$$

Then we can define an open quantum random walk on  $\mathbb{Z}$  by saying that one can only jump to nearest neighbors: a jump to the left is given by  $B$  and a jump to the right is given by  $C$ .

In other words, we put

$$B_i^{i-1} = B \quad \text{and} \quad B_i^{i+1} = C$$

for all  $i \in \mathbb{Z}$ , all the others  $B_j^i$  being equal to 0.

Starting with an initial state  $\rho^{(0)} = \rho_0 \otimes |0\rangle\langle 0|$ , after one step we have the state

$$\rho^{(1)} = B\rho_0 B^* \otimes |-1\rangle\langle -1| + C\rho_0 C^* \otimes |1\rangle\langle 1|.$$

The probability of presence in  $|-1\rangle$  is  $\text{Tr}(B\rho_0 B^*)$  and the probability of presence in  $|1\rangle$  is  $\text{Tr}(C\rho_0 C^*)$ .

After the second step, the state of the system is

$$\begin{aligned} \rho^{(2)} = & B^2\rho_0 B^{2*} \otimes |-2\rangle\langle -2| + C^2\rho_0 C^{2*} \otimes |2\rangle\langle 2| + \\ & + (CB\rho_0 B^* C^* + BC\rho_0 C^* B^*) \otimes |0\rangle\langle 0|. \end{aligned}$$

The associated probabilities for the presence in  $|-2\rangle$ ,  $|0\rangle$ ,  $|2\rangle$  are then

$$\text{Tr}(B^2\rho_0 B^{2*}), \quad \text{Tr}(CB\rho_0 B^* C^* + BC\rho_0 C^* B^*) \quad \text{and} \quad \text{Tr}(C^2\rho_0 C^{2*}),$$

respectively.

One can iterate the above procedure and generate our open quantum random walk on  $\mathbb{Z}$ .

As further example, that we shall discuss more later, take

$$B = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

and

$$C = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}.$$

The operators  $B$  and  $C$  do satisfy  $B^*B + C^*C = I$ . Let us consider the associated open quantum random walk on  $\mathbb{Z}$ . Starting with the state

$$\rho^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |0\rangle\langle 0|,$$

we find the following probabilities for the 4 first steps:

	$ -4\rangle$	$ -3\rangle$	$ -2\rangle$	$ -1\rangle$	$ 0\rangle$	$ +1\rangle$	$ +2\rangle$	$ +3\rangle$	$ +4\rangle$
$n = 0$					1				
$n = 1$				$\frac{1}{3}$		$\frac{2}{3}$			
$n = 2$			$\frac{1}{9}$		$\frac{3}{9}$		$\frac{5}{9}$		
$n = 3$		$\frac{1}{27}$		$\frac{5}{27}$		$\frac{11}{27}$		$\frac{10}{27}$	
$n = 4$	$\frac{1}{81}$		$\frac{10}{81}$		$\frac{27}{81}$		$\frac{26}{81}$		$\frac{17}{81}$

## 4.2 An Example on a Graph

In order to give an example on finite graphs it is useful to fix a notation. We shall denote the operators involved in the dissipative quantum random walk in a way similar to the notation of stochastic matrices for Markov chains. If the set of vertices is  $\mathcal{V} = \{1, \dots, V\}$ , we shall denote the operators  $B_j^i$  inside a  $V \times V$ -matrix as follows:

$$\begin{pmatrix} B_1^1 & B_1^2 & \dots & B_1^V \\ B_2^1 & B_2^2 & \dots & B_2^V \\ \vdots & \vdots & \vdots & \vdots \\ B_V^1 & B_V^2 & \dots & B_V^V \end{pmatrix}.$$

That is, on line  $j$  are all the operators for the contributions  $B_j^i$  which start from  $j$  and go to another site  $i$ . The usual property for stochastic matrices that the sum of each line is 1, is replaced by

$$\sum_i B_j^{i*} B_j^i = I$$

for each line.

With this notation one can easily describe examples. On the graph with two vertices we consider the transition operators of the form

$$\begin{pmatrix} D_1 & D_2 \\ B & C \end{pmatrix}$$

where  $D_1$  and  $D_2$  are any diagonal matrices such that  $D_1^* D_1 + D_2^* D_2 = I$  and where

$$B = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix},$$

for some  $p \in (0, 1)$ .

For example, with

$$D_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{pmatrix} \quad \text{and} \quad D_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \sqrt{\frac{2}{3}} \end{pmatrix}$$

and  $p = 1/4$ , with the initial state

$$\frac{1}{2} I \otimes |1\rangle\langle 1|,$$

we find the following probabilities for the first steps

site:	$ 1\rangle$	$ 2\rangle$
$n = 0$	1	0
$n = 1$	0.42	0.58
$n = 2$	0.22	0.78
$n = 3$	0.16	0.84
$n = 4$	0.13	0.87

In Section 12 we shall study this example in more details.

## 5 Inhomogeneous Case

Note that our presentation of Open Quantum Random Walks is based on a behavior which is “homogeneous” in time. This is to say that our assumption is that the operators  $B_j^i$  for passing from site  $|j\rangle$  to site  $|i\rangle$  are always the same, step after step. This is the analogue of an homogenous Markov chain.

Of course one may be interested in even more complicated situations, such as non-homogeneous Markov chains. This would correspond here to choosing time-dependent operators  $B_j^i(n)$  for the transitions. For each  $n$  the constraint

$$\sum_i B_j^i(n)^* B_j^i(n) = I$$

has to be respected for all  $j$ . This allows to define the time-dependent completely positive maps  $\mathcal{M}(n)$  by

$$\mathcal{M}(n)(\rho) = \sum_{i,j} (B_j^i(n) \otimes |i\rangle\langle j|) \rho (B_j^i(n) \otimes |i\rangle\langle j|)^* .$$

The quantum random walk is then the one given by the products of these completely positive maps  $\mathcal{L}(n)$ :

$$\rho^{(n+1)} = \mathcal{M}(n+1)(\rho^{(n)}).$$

## 6 Recovering Classical Markov Chains

It is very interesting to notice that all the classical Markov chains can be recovered as particular cases of Open Quantum Random Walks. We only treat here the homogenous case, the discussion would be similar in the non-homogeneous case.

Consider  $P = (P(j, i))$  a stochastic matrix, that is  $P(j, i)$  are classical probability transitions on  $\mathcal{V}$ . They express the transition probabilities of a Markov chain  $(X_n)$  on  $\mathcal{V}$ , that is,

$$P(j, i) = \mathbb{P}(X_{n+1} = i | X_n = j).$$

In particular, recall that

$$\sum_{i \in \mathcal{V}} P(j, i) = 1$$

for all  $j$ .

**Proposition 6.1** *Put  $\mathcal{H} = \mathcal{K} = \mathbb{C}^{\mathcal{V}}$  and consider any family of unitary operators  $U_j^i$  on  $\mathbb{C}^N$ ,  $i, j \in \mathcal{V}$ . Consider the operators*

$$B_j^i = \sqrt{P(j, i)} U_j^i.$$

*They satisfy*

$$\sum_i B_j^{i*} B_j^i = I$$

*for all  $j$ . Furthermore, given any initial state  $\rho^{(0)}$ , the associated open quantum random walk  $(\mathcal{M}^n)$  has the same probability distributions  $(p^{(n)})$  as the classical Markov chain  $(X_n)$  with transition probability matrix  $P$  and initial measure*

$$p_i^{(0)} = \text{Tr}(\langle i | \rho^{(0)} | i \rangle).$$

**Proof** The relation on the operators  $B_j^i$  is obvious for

$$\sum_i B_j^{i*} B_j^i = \sum_i P(j, i) U_j^{i*} U_j^i = \sum_i P(j, i) I = I.$$

Whatever is the initial state  $\rho$ , if we put  $\rho_i = \langle i | \rho | i \rangle$ , we get by Proposition 2.3 and its proof

$$\mathcal{M}(\rho) = \sum_i \left( \sum_k P(k, i) U_k^i \rho_k U_k^{i*} \right) \otimes |i\rangle\langle i|.$$

The probability to be located on site  $i$  is then

$$\sum_k P(k, i) \text{Tr} (U_k^i \rho_k U_k^{i*}) = \sum_k P(k, i) \text{Tr} (\rho_k).$$

That is, we get the classical transition probabilities for a classical Markov chain on the set  $\mathcal{V}$ , driven by the transition probabilities  $P(i, j)$  and with initial measure  $p_i^{(0)} = \text{Tr} (\rho_i)$ .

After two steps, the probability to be located at site  $i$  is

$$\sum_k \sum_l P(l, k) P(k, i) \text{Tr} (U_k^i U_l^k \rho_l U_l^{k*} U_k^{i*}) = \sum_k \sum_l P(l, k) P(k, i) \text{Tr} (\rho_l).$$

That is, once again the usual transition probabilities for two steps of the above Markov chain. It is not difficult to get convinced, by induction, that this works for any number of steps.  $\square$

## 7 Quantum Trajectories

Coming back to general Open Quantum Random Walks, we shall now describe a very interesting way to simulate them by means of *Quantum Trajectories*. This property seems very important when one wants to study the limit behavior of these quantum random walks.

The principle of the quantum trajectories associated to an open quantum random walk is the following. Starting from any initial state  $\rho$  on  $\mathcal{H} \otimes \mathcal{K}$  we apply the mapping  $\mathcal{M}$  and then a measurement of the position in  $\mathcal{K}$ . We end up with a random result for the measurement and a reduction of the wave-packet gives rise to a random state on  $\mathcal{H} \otimes \mathcal{K}$  of the form

$$\rho_i \otimes |i\rangle\langle i|.$$

We then apply the procedure again: an action of the mapping  $\mathcal{M}$  and a measurement of the position in  $\mathcal{K}$ .

**Theorem 7.1** *By repeatedly applying the completely positive map  $\mathcal{M}$  and a measurement of the position on  $\mathcal{K}$ , one obtains a sequence of random states*

on  $\mathcal{H} \otimes \mathcal{K}$ . This sequence is a non-homogenous Markov chain with law being described as follows. If the state of the chain at time  $n$  is  $\rho \otimes |j\rangle\langle j|$ , then at time  $n + 1$  it jumps to one of the values

$$\frac{1}{p(i)} B_j^i \rho B_j^{i*} \otimes |i\rangle\langle i|, \quad i \in \mathcal{V},$$

with probability

$$p(i) = \text{Tr} (B_j^i \rho B_j^{i*}) .$$

This Markov chain  $(\rho^{(n)})$  is a simulation of the master equation driven by  $\mathcal{M}$ , that is,

$$\mathbb{E} [\rho^{(n+1)} | \rho^{(n)} = \rho] = \mathcal{M}(\rho) .$$

Furthermore, if the initial state is a pure state, then the quantum trajectory stays valued in pure states and the Markov chain is described as follows. If the state of the chain at time  $n$  is the pure state  $|\varphi\rangle \otimes |j\rangle$ , then at time  $n + 1$  it jumps to one of the values

$$\frac{1}{\sqrt{p(i)}} B_j^i |\varphi\rangle \otimes |i\rangle, \quad i \in \mathcal{V},$$

with probability

$$p(i) = \|B_j^i |\varphi\rangle\|^2 .$$

**Proof** Let  $\rho \otimes |j\rangle\langle j|$  be the initial state. After acting by  $\mathcal{M}$  the state is

$$\sum_i (B_i^j \rho B_i^{j*}) \otimes |i\rangle\langle i| .$$

Measuring the vertices, gives the site  $i$  with probability

$$p(i) = \text{Tr} (B_i^j \rho B_i^{j*}) .$$

By the usual wave-packet reduction postulate, the state after having been measured with this value is

$$\frac{1}{p(i)} (B_i^j \rho B_i^{j*}) \otimes |i\rangle\langle i| .$$

This state being given, if we repeat the procedure, then clearly the next step depends only on the new state of the system. We end up with a (non-homogenous) Markov chain structure.



On average, the values of this Markov chain after one step is

$$\begin{aligned}\mathbb{E} [\rho^{(n+1)} | \rho^{(n)} = \rho \otimes |j\rangle\langle j|] &= \sum_i p(i) \frac{1}{p(i)} (B_i^j \rho B_i^{j*}) \otimes |i\rangle\langle i| \\ &= \sum_i (B_i^j \rho B_i^{j*}) \otimes |i\rangle\langle i| \\ &= \mathcal{M}(\rho^{(n)}).\end{aligned}$$

If  $\rho$  is a pure state  $|\phi\rangle\langle\phi| \otimes |i\rangle\langle i|$ , then it stays a pure state at each step. Indeed, any initial pure state  $|\phi\rangle\langle\phi| \otimes |i\rangle\langle i|$  will jump randomly to one of the states

$$\frac{1}{p_i^j} B_i^j |\phi\rangle\langle\phi| B_i^{j*} \otimes |j\rangle\langle j|$$

with probability

$$p(i) = \text{Tr} (B_i^j |\phi\rangle\langle\phi| B_i^{j*}).$$

In other words, it jumps from the pure state  $|\phi\rangle \otimes |i\rangle$  to any of the pure states

$$\frac{1}{\sqrt{p(i)}} B_i^j |\phi\rangle \otimes |j\rangle$$

with probability

$$p(i) = \|B_i^j |\phi\rangle\|^2.$$

We have a classical Markov chain valued in the space of wave functions of the form  $|\phi\rangle \otimes |i\rangle$ . On average, this random walk simulates the master equation driven by  $\mathcal{M}$ .  $\square$

## 8 Physical Implementation

It is natural to wonder how such Open Quantum Random Walks can actually be realized physically. We shall here discuss a way to achieve it.

For the sake of a simple discussion, we restrict ourselves in this section to the case where either  $\mathcal{V}$  is finite, or the number of non-vanishing  $B_j^i$ 's is finite for every fixed  $j$ . This is the case in all our examples and makes all the sums finite in the following.

Consider an open quantum random walk on  $\mathcal{V}$  with chirality space  $\mathcal{H}$  and with associated transition operators  $B_j^i$ . Recall that we have supposed that

$$\sum_{i \in \mathcal{V}} B_j^{i*} B_j^i = I$$

for all  $j \in \mathcal{V}$ . Hence, for all  $j \in \mathcal{V}$  there exists a unitary operator  $U(j)$  on  $\mathcal{H} \otimes \mathcal{K}$  whose first column (we choose  $|1\rangle$  to be the first vector) is given by

$$U_1^i(j) = B_j^i.$$

This unitary operator is a unitary operator that dilates the completely positive map

$$\mathcal{M}_j(\rho) = \sum_i B_j^i \rho B_j^{i*}.$$

In other words, the completely positive map  $\mathcal{M}_j$  on  $\mathcal{H}$  is the partial trace of some unitary interaction between  $\mathcal{H}$  and some environment  $\mathcal{E}$ . It is well-known that the dimension of the environment can be chosen to be the same as the number of Krauss operators appearing in the decomposition of  $\mathcal{M}_j$ , that is, in our case they are indexed by  $\mathcal{V}$ . Hence the environment can be chosen to be  $\mathcal{E} = \mathcal{K}$ .

The state space on which one performs the physical implementation is  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2$  where  $\mathcal{K}_1$  and  $\mathcal{K}_2$  are two copies of  $\mathcal{K}$ . Let us present the main ingredients which shall appear in the physical implementation.

Each unitary operator  $U(j)$  defined above acts on  $\mathcal{H} \otimes \mathcal{K}_1$ . We construct the unitary operator

$$U = \sum_j U(j) \otimes |j\rangle\langle j|$$

which acts now on  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2$ .

We shall also need the so-called *swap operator*  $S$  on  $\mathcal{K}_1 \otimes \mathcal{K}_2$  defined by

$$S(|j\rangle \otimes |k\rangle) = |k\rangle \otimes |j\rangle.$$

It is a unitary operator on  $\mathcal{K}_1 \otimes \mathcal{K}_2$  which simply expresses the fact of exchanging the two systems  $\mathcal{K}_1$  and  $\mathcal{K}_2$ .

We shall also use a *decoherence procedure* on the space  $\mathcal{K}_1$ , along the basis ( $|i\rangle$ ). By this we mean the following: if the system is in a superposition of pure states

$$|\varphi\rangle = \sum_i \lambda_i |i\rangle,$$

then this system is coupled to an environment in such a way and in a sufficiently long time, for the state of  $\mathcal{K}_1$  to become

$$\sum_i |\lambda_i|^2 |i\rangle\langle i|.$$

This is to say that we have chosen a coupling of  $\mathcal{K}_1$  with some environment which makes the off-diagonal terms of the density matrix  $|\varphi\rangle\langle\varphi|$  converge exponentially fast to 0. This kind of decoherence is now well-known in physics. It is rather easy to describe an environment and an explicit Hamiltonian which will produce such a result. For example, by performing a coupling to an environment which gives rise on  $\mathcal{K}$  to a Lindblad semigroup evolution with generator

$$L(\rho) = -\frac{1}{2}[Q, [Q, \rho]]$$

where  $Q$  is the operator

$$Q = \sum_i i |i\rangle\langle i|,$$

for example. In that case it is easy to see that any initial state  $\rho_0$  has its off-diagonal terms decaying like  $\exp(-(i-j)^2 t/2)$  and the diagonal terms remaining constant. One can give an Hamiltonian description of such a decoherence procedure by using the continuous-time limit of repeated quantum interactions as developed in [A-P].

Finally, we shall need a *refreshing procedure*, that is, if  $\mathcal{K}_1$  is in any state  $\rho$  then we put it back to the state  $|1\rangle\langle 1|$ .

**Proposition 8.1** *Consider the quantum system  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2$ , together with some initial state*

$$\rho^{(0)} = \sum_k \rho_k \otimes |1\rangle\langle 1| \otimes |k\rangle\langle k|.$$

*If we perform successively*

- 1) *an action of the unitary operator  $U$ ,*
- 2) *a decoherence on the basis  $(|i\rangle)$  of the system  $\mathcal{K}_1$ ,*
- 3) *an action of the swap operator  $I \otimes S$*
- 4) *a refreshing of the system  $\mathcal{K}_1$  to the state  $|1\rangle\langle 1|$*

*then the state of the system becomes*

$$\sum_k \left( \sum_l B_l^k \rho_l B_l^{k*} \right) \otimes |1\rangle\langle 1| \otimes |k\rangle\langle k|.$$

*That is, one reads the first step of the dissipative quantum random walk on  $\mathcal{H} \otimes \mathcal{K}_2$ .*

*By iterating this whole procedure one produces the dissipative quantum random walk on  $\mathcal{H} \otimes \mathcal{K}_2$ .*

**Proof** The unitary operator  $U(k)$  admits a decomposition

$$U(k) = \sum_{i,j} U_j^i(k) \otimes |j\rangle\langle i|.$$

In particular we have

$$\sum_j U_j^{i'}(k)^* U_j^i(k) = \delta_{i,i'} I.$$

On the space  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2$  the operator  $U$  as defined above is then decomposed into

$$U = \sum_{i,j,k} U_j^i(k) \otimes |j\rangle\langle i| \otimes |k\rangle\langle k|.$$

Now starting in a pure state  $|\phi\rangle \otimes |1\rangle \otimes |k\rangle$ , we get

$$U(|\phi\rangle \otimes |1\rangle \otimes |k\rangle) = \sum_j U_1^j(k) |\phi\rangle \otimes |j\rangle \otimes |k\rangle = \sum_j B_k^j |\phi\rangle \otimes |j\rangle \otimes |k\rangle.$$

This is the first step of the procedure.

The second step consists in performing a decoherence on the first space  $\mathcal{K}$ . The pure state

$$\sum_j B_k^j |\phi\rangle \otimes |j\rangle \otimes |k\rangle$$

is then mapped to the density matrix

$$\sum_j B_k^j |\phi\rangle\langle\phi| B_k^{j*} \otimes |j\rangle\langle j| \otimes |k\rangle\langle k|. \quad (8)$$

Applying  $I \otimes S$  to the state (8) we get the state

$$\sum_j B_k^j |\phi\rangle\langle\phi| B_k^{j*} \otimes |k\rangle\langle k| \otimes |j\rangle\langle j|. \quad (9)$$

On the space  $\mathcal{H}$  and the second space  $\mathcal{K}$  one can now read the first step of our quantum random walk.

Finally, *refresh* the first space  $\mathcal{K}$  into the state  $|1\rangle$ , we then end up with the state

$$\sum_j B_k^j |\phi\rangle\langle\phi| B_k^{j*} \otimes |1\rangle\langle 1| \otimes |j\rangle\langle j|,$$

on which one can apply our procedure again.

If the initial state is not a pure state but a density matrix, a mixture of pure states, it is not difficult to see that the procedure described above gives the right combination and the right final state.  $\square$

To summarize, the quantum random walk is obtained in the following way. Dilate each of the maps  $\mathcal{L}_k$  into a unitary operator  $U(k)$  on  $\mathcal{H} \otimes \mathcal{K}_1$ , start in the desired initial state on  $\mathcal{H}$  and the second space  $\mathcal{K}_2$ , with the first space  $\mathcal{K}_1$  being in the state  $|1\rangle$ , then iterate the following procedure on  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2$ :

- apply the unitary operator  $\sum_k U(k) \otimes |k\rangle\langle k|$ ,
- perform a decoherence on  $\mathcal{K}_1$
- apply the unitary shift  $I \otimes S$
- refresh the first space  $\mathcal{K}_1$  into the state  $|1\rangle$ .

The dissipative quantum random walk now appears on  $\mathcal{H} \otimes \mathcal{K}_2$ .

## 9 Coming Back to Examples

Let us illustrate this physical implementation on the two physical examples developed in Section 4.

### 9.1 The Example on $\mathbb{Z}$

In the case of stationary walks on  $\mathbb{Z}$  the procedure can be considerably simplified, as follows. The procedure we describe below is slightly different from the one presented in Proposition 8.1, but it is actually the same one, presented in a different way, taking into account several simplifications offered by the model.

Consider an open quantum random walk on  $\mathbb{Z}$  driven by two operators  $B$  and  $C$  on  $\mathcal{H}$ . Consider a unitary operator  $U$  on  $\mathcal{H} \otimes \mathbb{C}^2$  of the form

$$U = \begin{pmatrix} B & X \\ C & Y \end{pmatrix},$$

that is, a dilation of the completely positive map driven by  $B$  and  $C$ . Let  $\mathcal{K} = \mathbb{C}^{\mathbb{Z}}$  and consider the space  $\mathcal{H} \otimes \mathbb{C}^2 \otimes \mathcal{K}$ . On the space  $\mathbb{C}^2 \otimes \mathcal{K}$  we consider the *shift* operator given by

$$S(|0\rangle\langle 0| \otimes |k\rangle\langle k|) = |0\rangle\langle 0| \otimes |k-1\rangle\langle k-1|$$

and

$$S(|1\rangle\langle 1| \otimes |k\rangle\langle k|) = |0\rangle\langle 0| \otimes |k+1\rangle\langle k+1|.$$

Now, let us detail the procedure. Starting with a state  $|\varphi\rangle \otimes |0\rangle \otimes |k\rangle$  we apply the operator  $U \otimes I$  and end up with the state

$$B|\varphi\rangle \otimes |0\rangle \otimes |k\rangle + C|\varphi\rangle \otimes |1\rangle \otimes |k\rangle.$$

Applying the decoherence on  $\mathbb{C}^2$  we get the state

$$B|\varphi\rangle\langle\varphi|B^* \otimes |0\rangle\langle 0| \otimes |k\rangle\langle k| + C|\varphi\rangle\langle\varphi|C^* \otimes |1\rangle\langle 1| \otimes |k\rangle\langle k|.$$

Applying the shift operator, the state becomes

$$B|\varphi\rangle\langle\varphi|B^* \otimes |0\rangle\langle 0| \otimes |k-1\rangle\langle k-1| + C|\varphi\rangle\langle\varphi|C^* \otimes |1\rangle\langle 1| \otimes |k+1\rangle\langle k+1|.$$

Refreshing the space  $\mathbb{C}^2$  we end up with

$$B|\varphi\rangle\langle\varphi|B^* \otimes |0\rangle\langle 0| \otimes |k-1\rangle\langle k-1| + C|\varphi\rangle\langle\varphi|C^* \otimes |0\rangle\langle 0| \otimes |k+1\rangle\langle k+1|.$$

One can read the first step of the dissipative quantum random walk on  $\mathcal{H} \otimes \mathcal{K}$ :

$$B|\varphi\rangle\langle\varphi|B^* \otimes |k-1\rangle\langle k-1| + C|\varphi\rangle\langle\varphi|C^* \otimes |k+1\rangle\langle k+1|.$$

## 9.2 The Example on a Graph

Let us now detail the second example of Section 4, the open quantum random walk on the 2-vertices graph.

Consider a two-level quantum system  $\mathcal{H}$  coupled to another two-level quantum system  $\mathcal{K}_1$  via the Hamiltonian

$$H = i\gamma(a \otimes a^* - a^* \otimes a)$$

where

$$a = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

Then the unitary evolution associated to this Hamiltonian, for a time length  $t = 1$  is given by

$$U = e^{-iH} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\gamma) & -\sin(\gamma) & 0 \\ 0 & \sin(\gamma) & \cos(\gamma) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Hence, for a good choice of  $\gamma$ , that is, for  $\sin(\gamma) = \sqrt{p}$  we have

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \sqrt{1-p} & -\sqrt{p} & 0 \\ 0 & \sqrt{p} & \sqrt{1-p} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

In other words  $U$  is of the form

$$U = \begin{pmatrix} C & X \\ B & Y \end{pmatrix}$$

as a block matrix on  $\mathcal{K}_1$ , where  $B$  and  $C$  are those matrices associated to our example. This is to say that we have given here an explicit dilation of the completely positive map associated to the matrices  $B$  and  $C$ .

If  $D_1$  and  $D_2$  are two diagonal matrices satisfying  $D_1^*D_1 + D_2^*D_2 = I$  then assume, for simplicity only, that they have real entries

$$D_1 = \begin{pmatrix} a & 0 \\ 0 & \alpha \end{pmatrix}, \quad D_2 = \begin{pmatrix} b & 0 \\ 0 & \beta \end{pmatrix},$$

with  $a^2 + b^2 = \alpha^2 + \beta^2 = 1$ . Then, one can write  $a = \cos(\lambda)$  and  $\alpha = \cos(\mu)$ . Considering the Hamiltonian

$$K = \begin{pmatrix} \lambda & 0 \\ 0 & \mu \end{pmatrix} \otimes \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},$$

we get that  $e^{-iK}$  is of the form

$$V = \begin{pmatrix} D_1 & X' \\ D_2 & Y' \end{pmatrix}.$$

We have realized a concrete physical dilation of the completely positive map associated to  $D_1$  and  $D_2$ .

Following Proposition 8.1, consider on  $\mathcal{H} \otimes \mathcal{K}_1 \otimes \mathcal{K}_2 = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$  the unitary evolution

$$\begin{pmatrix} V & 0 \\ 0 & U \end{pmatrix},$$

written as a block matrix on  $\mathcal{K}_2$ . This is to say that  $\mathcal{H}$  is coupled to  $\mathcal{K}_1$  with the Hamiltonian  $K$  when  $\mathcal{K}_2$  is in the state  $|1\rangle\langle 1|$  and  $\mathcal{H}$  is coupled to  $\mathcal{K}_1$  with the Hamiltonian  $H$  when  $\mathcal{K}_2$  is in the state  $|2\rangle\langle 2|$ .

In this context, the swap operator  $S$  takes the following simple form on  $\mathcal{K}_1 \otimes \mathcal{K}_2$

$$S = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Then, following the four steps of Proposition 8.1 gives a realization of the associated quantum random walk on  $\mathcal{H} \otimes \mathcal{K}_2$ .

## 10 Unitary Quantum Random Walks

The Open Quantum Random Walks we have been describing up to now are actually very different from the well-known Unitary Quantum Random Walks, such as the Hadamard random walk (see Introduction for some references). This is to say that they produce probability distributions which are not of the same type as the ones usually observed with the Hadamard quantum random walks.

It seems to us that there is no way to produce limit distributions such as the one observed in the Hadamard quantum random walk central limit theorem, with open quantum random walks. The limit behaviors of Open Quantum Random Walks seems to be all Gaussian or mixtures of Gaussians. The dissipative character of our quantum random walks makes them very different from the unitary evolution describing the usual type of quantum random walks. In fact there is quite a surprising and strong link between the two types of quantum random walks. Let us develop it here.

Let  $\mathcal{V}$  be a set of vertices, let  $\mathcal{H}$  be a Hilbert space representing the chirality. For each pair  $(i, j)$  in  $\mathcal{V}^2$  we have a bounded operator  $B_j^i$  on  $\mathcal{H}$ . Instead of the usual condition

$$\sum_i B_j^{i*} B_j^i = I$$

for all  $j$ , we shall ask here a much stronger condition, namely for all  $j, j' \in \mathcal{V}$

$$\sum_i B_j^{i*} B_{j'}^i = \delta_{jj'} I. \quad (10)$$

In other words, being given two starting points  $j$  and  $j'$ , the sum of the “contributions” which go to the same points  $i \in \mathcal{V}$  vanish, unless  $j = j'$  in which case we recover the usual condition.

Note that there is no classical analogue of this condition for classical Markov matrices.

Let us illustrate this condition with an example. For a stationary quantum random walk on  $\mathbb{Z}$  we are given two operators  $B$  and  $C$  on  $\mathcal{H}$  which represent the effect of making one step to the left or one step to the right. The usual condition, obtained by taking  $j = j'$  gives

$$B^*B + C^*C = I.$$

Now, taking  $j' = j + 1$ , we get a supplementary condition:

$$C^*B = 0.$$



This is the only new condition added to the usual one in that case. Note that these two conditions together imply in particular that  $B + C$  is unitary.

These two conditions are typically satisfied by the following family of examples. Let

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

be a unitary matrix on  $\mathbb{C}^2$ . Put

$$B = \begin{pmatrix} a & b \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 0 & 0 \\ c & d \end{pmatrix}.$$

Then,  $B$  and  $C$  satisfy

$$B^*B + C^*C = I \quad \text{and} \quad C^*B = 0.$$

This is typically the case with Hadamard random walk where

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

Let us see what happens, in the general context, with this additional condition. The point is the following, if we are given a pure state on  $\mathcal{H} \otimes \mathcal{K}$  of the form

$$|\psi\rangle = \sum_i |\varphi_i\rangle \otimes |i\rangle$$

with the condition

$$\|\psi\|^2 = \sum_i \|\varphi_i\|^2 = 1$$

then the state

$$|\psi'\rangle = \sum_i \left( \sum_j B_j^i |\varphi_j\rangle \right) \otimes |i\rangle$$

is of the same form and satisfies

$$\begin{aligned} \|\psi'\|^2 &= \sum_i \sum_{j,j'} \langle \varphi_j, B_j^{i*} B_{j'}^i \varphi_{j'} \rangle \\ &= \sum_{j,j'} \langle \varphi_j, \delta_{jj'} I \varphi_{j'} \rangle \\ &= \sum_j \|\varphi_j\|^2 \\ &= 1. \end{aligned}$$

Hence, at each step we get a state of the form

$$|\psi\rangle = \sum_i |\varphi_i\rangle \otimes |i\rangle$$

with the condition

$$\|\psi\|^2 = \sum_i \|\varphi_i\|^2 = 1.$$

In particular it determines, at each step, a probability distribution on  $\mathcal{V}$  by putting

$$P(i) = \|\varphi_i\|^2.$$

This is exactly the picture for the Unitary Quantum Random Walks, such as the Hadamard quantum random walk.

Now the interesting point is the way one can physically realize such Unitary Quantum Random Walks and the way this construction is similar to the one of Open Quantum Random Walks.

**Proposition 10.1** *If the transition operators  $B_j^i$  satisfy the more restrictive condition (10), then applying the same physical procedure as in Proposition 8.1 without the decoherence step (step 2) gives rise to a unitary quantum random walk.*

**Proof** Let us follow again the steps of the construction in Proposition 8.1. Starting in a pure state  $|\phi\rangle \otimes |1\rangle \otimes |k\rangle$ , we get

$$U(|\phi\rangle \otimes |1\rangle \otimes |k\rangle) = \sum_j U_1^j(k) |\phi\rangle \otimes |j\rangle \otimes |k\rangle = \sum_j B_k^j |\phi\rangle \otimes |j\rangle \otimes |k\rangle.$$

This is the first step of the procedure.

We now skip the decoherence part and apply  $I \otimes S$  to the state. We get the state

$$\sum_j B_k^j |\phi\rangle \otimes |k\rangle \otimes |j\rangle. \quad (11)$$

On the space  $\mathcal{H}$  and the second space  $\mathcal{K}$  one can now read the first step of the quantum random walk.

Finally, *refresh* the first space  $\mathcal{K}$  into the state  $|1\rangle$ , we then end up with the state

$$\sum_j B_k^j |\phi\rangle \otimes |1\rangle \otimes |j\rangle,$$

on which one can apply our procedure again. We recognize the action of the type of quantum random walks we announced.  $\square$

## 11 Examples on $\mathbb{Z}$

We are now back to Open Quantum Random Walks. In this section and the following one, we shall review several concrete examples. We shall show up their limit behaviors, based on simulations.

### 11.1 A Walk With Only One Step to the Left

Recall the way one constructs dissipative quantum random walks on  $\mathbb{Z}$  with the help of two operators  $B$  and  $C$  on  $\mathcal{H}$  (Section 4). We start with a rather simple example. Take

$$B = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{1-p} \end{pmatrix},$$

for some  $p \in [0, 1]$ . Put  $q = 1 - p$ . Consider the initial state

$$\rho_0 = \begin{pmatrix} \alpha & z \\ \bar{z} & \beta \end{pmatrix} \otimes |0\rangle\langle 0|.$$

After the first step, the state on the site  $|-1\rangle$  is

$$\begin{pmatrix} p\beta & 0 \\ 0 & 0 \end{pmatrix}$$

and the state on the site  $|+1\rangle$  is

$$\begin{pmatrix} \alpha & 0 \\ 0 & q\beta \end{pmatrix}.$$

This means that the value  $|-1\rangle$  is reached with probability  $p\beta$  and the value  $|+1\rangle$  with probability  $\alpha + q\beta$ .

Let us compute the second step. As  $B^2 = 0$  then  $|-2\rangle$  is not reached. Only the sites  $|0\rangle$  and  $|+2\rangle$  are reached, with respective states

$$\begin{pmatrix} (p + pq)\beta & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} (1 - q^2)\beta & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\begin{pmatrix} \alpha & 0 \\ 0 & q^2\beta \end{pmatrix}.$$

The probability to reach  $|+2\rangle$  is  $\alpha + q^2\beta$  and the probability to reach  $|0\rangle$  is  $(1 - q^2)\beta$ .

By an easy induction we get that the state at time  $n$  is supported by  $|n-2\rangle$  and  $|n\rangle$  only, with respective states

$$\begin{pmatrix} (1-q^n)\beta & 0 \\ 0 & 0 \end{pmatrix}$$

and

$$\begin{pmatrix} \alpha & 0 \\ 0 & q^n\beta \end{pmatrix},$$

with probability  $(1-q^n)\beta$  and  $\alpha+q^n\beta$ , respectively.

Hence, computing for example the quantum trajectories associated to this open quantum random walk, we have the behavior of a random walk which goes straight to the right, with only one possible jump to the left. Before the first step to the left, the probability to go to the right, at step  $n$ , is

$$\frac{\alpha+q^{n+1}\beta}{\alpha+q^n\beta}$$

and the probability to jump to the left is

$$\frac{(q^n-q^{n+1})\beta}{\alpha+q^n\beta}.$$

After the first step to the left, the walk will only go to the right with probability one.

As  $n$  goes to  $+\infty$  the states on  $|n-2\rangle$  and  $|n\rangle$  converge respectively to

$$\begin{pmatrix} \beta & 0 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \alpha & 0 \\ 0 & 0 \end{pmatrix}.$$

## 11.2 A More Quantum Example

Take the same structure of quantum random walk on  $\mathbb{Z}$ , but with

$$B = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad C = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}.$$

We have given in Section 4 the first few probability distributions associated to this quantum random walk. It appears immediately rather wild, asymmetric and uncentered.

The point is that, on numerical simulations, one can see these quantum distributions tend to a centered Gaussian. We start with the density matrix

$$\rho^{(0)} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |0\rangle\langle 0|.$$

Figure 1 then shows the distribution obtained at times  $n=4$ ,  $n=8$  and  $n=20$ .

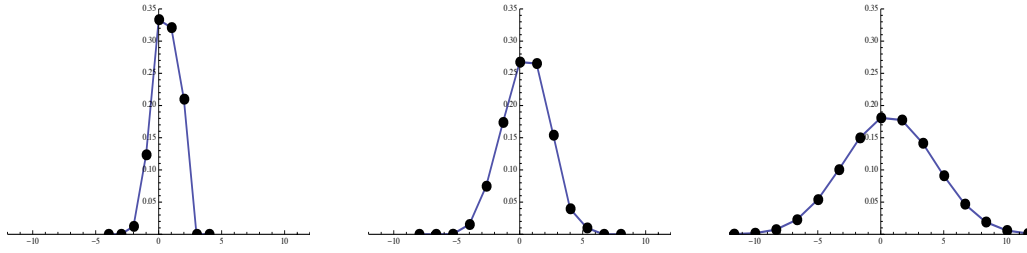


Figure 1: An O.Q.R.W. on  $\mathbb{Z}$  which gives rise to a centered Gaussian at the limit, while starting clearly uncentered (at time  $n = 4$ ,  $n = 8$ ,  $n = 20$ )

### 11.3 Examples with Several Gaussians

One can produce examples where several Gaussians are appearing, including the case where Gaussians are reduced to Dirac masses. For example, taking

$$B = \begin{pmatrix} 0 & 0 \\ 0 & \frac{2}{\sqrt{5}} \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{\sqrt{5}} \end{pmatrix},$$

gives the following shapes (Figure 2), when starting with the initial state

$$\rho^{(0)} = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \otimes |0\rangle\langle 0|.$$

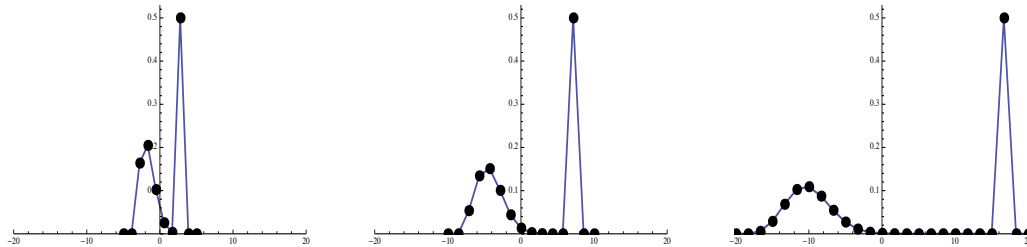


Figure 2: An O.Q.R.W. on  $\mathbb{Z}$  which gives rise to a Gaussian travelling to the left and a Dirac mass travelling to the right (at times  $n = 5$ ,  $n = 10$ ,  $n = 20$ )

When  $n$  tends to  $+\infty$  then both the “Dirac soliton” on the right hand side and the Gaussian on the left hand side survive.

One can produce a perturbation of the above model, it will then converge to a different limit. Put

$$B = \begin{pmatrix} 0 & \beta \\ 0 & \sqrt{\frac{4}{5} - \frac{\beta^2}{2}} \end{pmatrix}$$

and

$$C = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{\frac{1}{5} - \frac{\beta^2}{2}} \end{pmatrix}.$$

We get the following shapes (Figures 3,4 and 5), where the Gaussian does not survive anymore at  $+\infty$ .

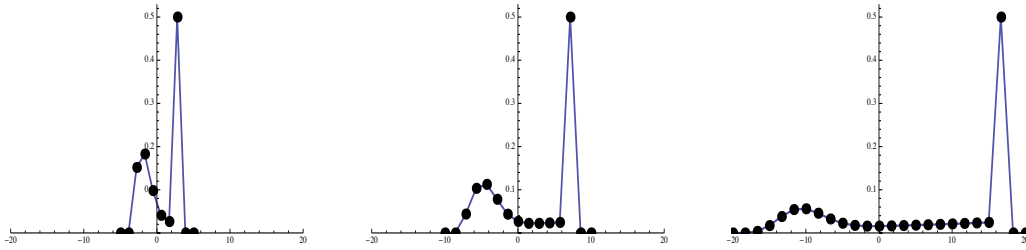


Figure 3: With a small perturbation ( $\beta = 1/5$ ) of the model of Fig. 2, one can see the walk starting with almost the same shape, but the Gaussian moving towards left does not survive (at times  $n = 5$ ,  $n = 10$ ,  $n = 20$ )

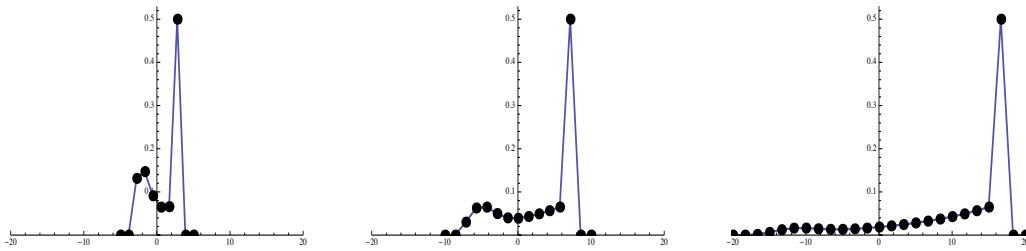


Figure 4: With a larger perturbation ( $\beta = 1/3$ ) the Gaussian appears for a little while and disappears quickly (at times  $n = 5$ ,  $n = 10$ ,  $n = 20$ )

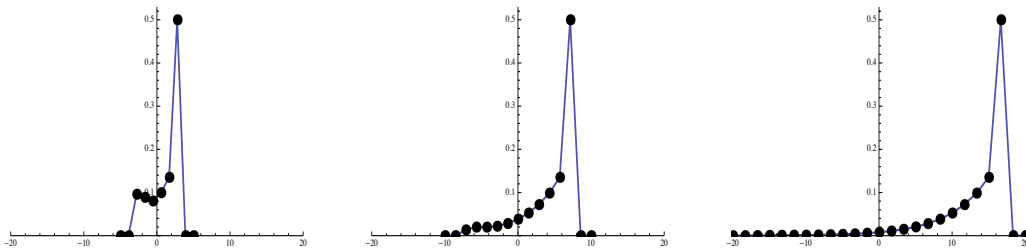


Figure 5: With  $\beta = 1/2$  the Gaussian part has completely disappeared and the behavior is really different from Fig. 2 (at times  $n = 5$ ,  $n = 10$ ,  $n = 20$ )

## 11.4 An Example in Dimension 5

Another interesting family of behaviors is obtained with the following choice of  $B$  and  $C$ . For the sake of a compact notation, we put  $C_2 = \cos(2t)$ ,  $C_4 = \cos(4t)$ ,  $S_2 = \sin(2t)$  and  $S_4 = \sin(4t)$ . Consider the matrices

$$B = \frac{1}{4} \begin{pmatrix} 0 & -2S_2 - S_4 & 0 & 2S_2 - S_4 & 0 \\ -2S_2 - S_4 & 0 & -2\sqrt{\frac{3}{2}}S_4 & 0 & 2S_2 - S_4 \\ 0 & -2\sqrt{\frac{3}{2}}S_4 & 0 & -2\sqrt{\frac{3}{2}}S_4 & 0 \\ 2S_2 - S_4 & 0 & -2\sqrt{\frac{3}{2}}S_4 & 0 & -2S_2 - S_4 \\ 0 & 2S_2 - S_4 & 0 & -2S_2 - S_4 & 0 \end{pmatrix}$$

and

$$C = \frac{1}{8} \begin{pmatrix} L & 0 & C & 0 & L' \\ 0 & 4(C_2 + C_4) & 0 & 4(-C_2 + C_4) & 0 \\ C & 0 & 2(1 + 3C_4) & 0 & C \\ 0 & 4(-C_2 + C_4) & 0 & 4(C_2 + C_4) & 0 \\ L' & 0 & C & 0 & L \end{pmatrix},$$

where

$$L = 3 + 4C_2 + C_4, \quad L' = 3 - 4C_2 + C_4, \quad C = -\sqrt{6}(1 - C_4).$$

Simulations of this open quantum random walk indicates that the limit behavior exhibits two Gaussians plus a Dirac soliton. The two Gaussians get slowly constructed, point by point, as the soliton loses its mass. In Figure 6 we show the time evolution when the parameter  $t$  is equal to  $t = \pi/40$ , the initial state being  $\rho^{(0)} = \frac{1}{5}I \otimes |0\rangle\langle 0|$ .

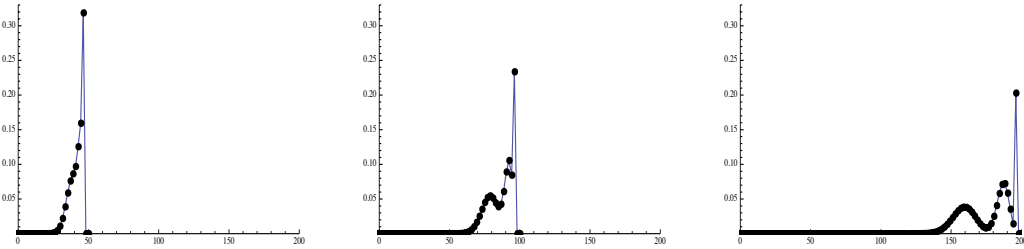


Figure 6: Two Gaussians moving towards right are constructed point by point while the soliton loses its mass (parameter  $t = \pi/40$ , times  $n = 50$ ,  $n = 100$ ,  $n = 200$ )

Changing the parameter  $t$  makes the Gaussians moving at different speeds and even change their direction (Figures 7 and 8).

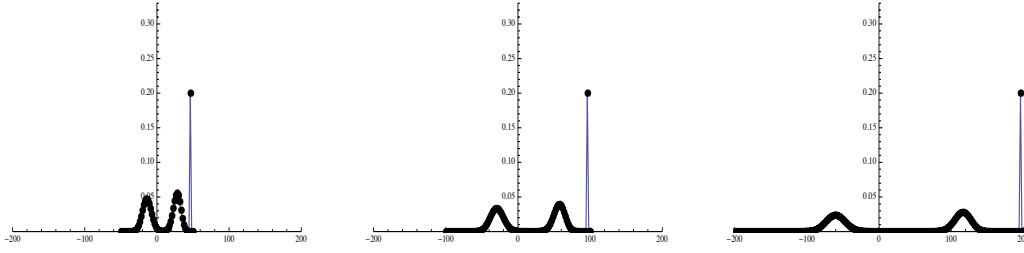


Figure 7: With the parameter  $t = 3\pi/40$ , one Gaussian is now moving towards left (at times  $n = 50$ ,  $n = 100$ ,  $n = 200$ )

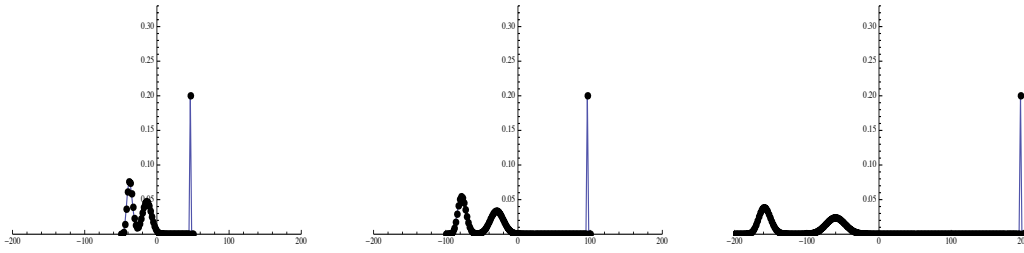


Figure 8: With the parameter  $t = 6\pi/40$ , both Gaussians are now travelling towards left (at times  $n = 50$ ,  $n = 100$ ,  $n = 200$ )

## 11.5 Examples on $\mathbb{Z}^2$

It is easy to produce Open Quantum Random Walks on  $\mathbb{Z}^2$  by specifying 4 matrices  $N, W, S, E$  on  $\mathcal{H}$  which satisfy

$$N^*N + W^*W + S^*S + E^*E = I. \quad (12)$$

Then, we ask the random walk to jump from any site to the four nearest neighbors, following  $N, W, S$  or  $E$ , respectively.

One can for example combine two 1-dimensional Open Quantum Random Walks by asking them to act on the different coordinate axis. For example, take

$$N = \sqrt{\lambda} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad S = \sqrt{\lambda} \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$$

together with

$$W = \sqrt{(1-\lambda)} \begin{pmatrix} 0 & \cos(\theta) \cos(\phi) \\ 0 & \sin(\theta) \end{pmatrix} \quad \text{and} \quad E = \sqrt{(1-\lambda)} \begin{pmatrix} 1 & 0 \\ 0 & \cos(\theta) \sin(\phi) \end{pmatrix},$$

for some  $\lambda \in [0, 1]$ .

One can obtain behaviors with a single Gaussian, as below (Figure 9), with  $\lambda = 1/6$ ,  $\theta = \pi/3$ ,  $\phi = \pi/7$ .



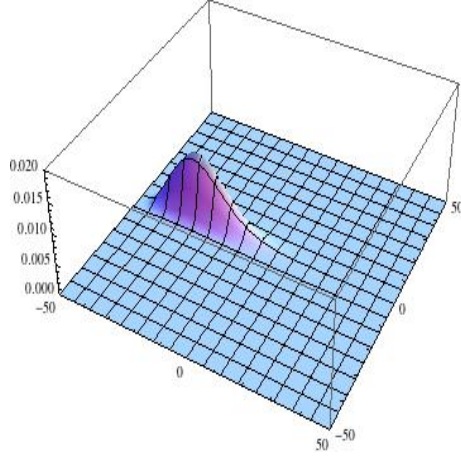


Figure 9: An O.Q.R.W. on  $\mathbb{Z}^2$  which exhibits a single Gaussian asymptotically (at time  $n = 50$ )

With some different parameters we obtain two Gaussians, as below (Figure 10), with  $\lambda = 1/50$ ,  $\theta = 5\pi/11$ ,  $\phi = 7\pi/15$ .

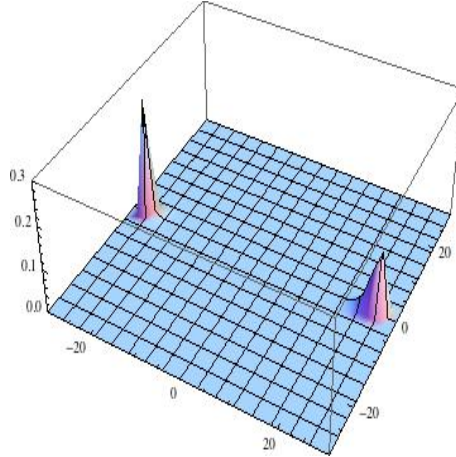


Figure 10: With different parameters, the O.Q.R.W. on  $\mathbb{Z}^2$  gives rise to two Gaussian pics (at time  $n = 30$ )

It is remarkable to notice that one can construct a two-dimensional Open Quantum Random Walk with the help of two one-dimensional Open Quantum Random Walks as follows. If  $B^*B + C^*C = I$  and  $A^*A + D^*D = I$  then putting

$$N = AB, \quad W = DB, \quad S = AC, \quad E = DC,$$

one gets the relation (12). But it does not seem obvious to us that the properties of the two-dimensional walk constructed this way can be directly related to the properties of the two one-dimensional walks which helped its construction.

As an example, take

$$B = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad C = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$$

together with

$$A = \begin{pmatrix} 0 & \beta \\ 0 & \sqrt{\frac{4}{5} - \frac{\beta^2}{2}} \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{\frac{1}{5} - \frac{\beta^2}{2}} \end{pmatrix},$$

which are two Open Quantum Random Walks on  $\mathbb{Z}$  that we have already considered above. Even when  $\beta = 0$  one does not see anymore any sign of the Dirac soliton behavior in the corresponding 2-dimensional random walk. In the following picture (Figure 11), the initial state is

$$\frac{1}{2}I \otimes |(0,0)\rangle\langle(0,0)|.$$

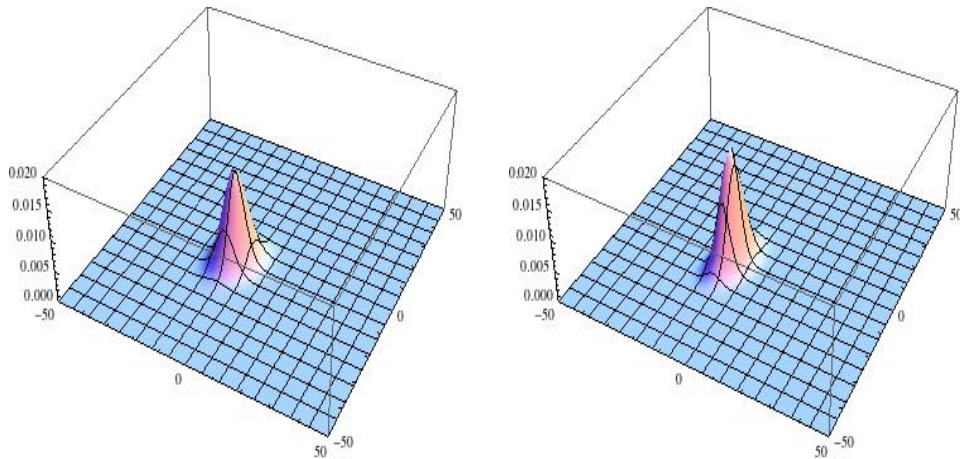


Figure 11: In this combination of two one-dimensional O.Q.R.W. the soliton travelling to the right of Fig.2 and Fig.5 has now disappeared (at time  $n = 50$ , for  $\beta = 0$  and  $\beta = 1/2$ )

## 12 Examples on Graphs

### 12.1 O.Q.R.W. on the 2-Graph

Let us come back to our example of an open quantum random walk on 2 sites, driven by the transition matrix

$$\begin{pmatrix} D_1 & D_2 \\ B & C \end{pmatrix},$$

with

$$B = \begin{pmatrix} 0 & \sqrt{p} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad C = \begin{pmatrix} 1 & 0 \\ 0 & \sqrt{q} \end{pmatrix},$$

for some  $p \in (0, 1)$ ,  $q = 1 - p$  and

$$D_1 = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \quad \text{and} \quad D_2 = \begin{pmatrix} c & 0 \\ 0 & d \end{pmatrix}$$

where we assume for simplicity that  $a, b, c, d$  are reals such that  $a^2 + c^2 = 1$ ,  $b^2 + d^2 = 1$ ,  $0 < a^2 < 1$ ,  $0 < b^2 < 1$ ,  $a \neq b$ ,  $c \neq d$ ,  $ab \neq \sqrt{q}$ ,  $a^2 \neq q$ ,  $b^2 \neq q$ . All the cases can be considered and easily solved, but it is not worth developing them here. The cases that we consider here are the nontrivial ones.

**Proposition 12.1** *Whatever is the initial state, the state of the open quantum random walk defined above converges to*

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |2\rangle\langle 2|.$$

*The speed of convergence is  $v^n$  where  $v = \min\{a^2, b^2, |ab|, \sqrt{q}\}$ .*

**Proof** Let

$$\rho^{(n)} = \rho_1^{(n)} \otimes |1\rangle\langle 1| + \rho_2^{(n)} \otimes |2\rangle\langle 2|$$

be the state at time  $n$ , where we put

$$\rho_i^{(n)} = \begin{pmatrix} \alpha_i^{(n)} & z_i^{(n)} \\ \bar{z}_i^{(n)} & \beta_i^{(n)} \end{pmatrix}.$$

The induction formula is then

$$\begin{cases} \rho_1^{(n+1)} = D_1 \rho_1^{(n)} D_1^* + B \rho_2^{(n)} B^* \\ \rho_2^{(n+1)} = D_2 \rho_1^{(n)} D_2^* + C \rho_2^{(n)} C^* \end{cases},$$

which gives

$$\begin{cases} \alpha_1^{(n+1)} = a^2 \alpha_1^{(n)} + p \beta_2^{(n)} \\ z_1^{(n+1)} = ab z_1^{(n)} \\ \beta_1^{(n+1)} = b^2 \beta_1^{(n)} \\ \alpha_2^{(n+1)} = c^2 \alpha_1^{(n)} + \alpha_2^{(n)} \\ z_2^{(n+1)} = cd z_1^{(n)} + \sqrt{q} z_2^{(n)} \\ \beta_2^{(n+1)} = d^2 \beta_1^{(n)} + q \beta_2^{(n)}. \end{cases}$$

This can be easily solved explicitly, giving

$$\begin{aligned} z_1^{(n)} &= z_1^{(0)} (ab)^n \\ \beta_1^{(n)} &= \beta_1^{(0)} b^{2n} \\ z_2^{(n)} &= z_2^{(0)} q^{n/2} + cd z_1^{(0)} \frac{q^{n/2} - (ab)^n}{\sqrt{q} - ab} \\ \beta_2^{(n)} &= \beta_2^{(0)} q^n + d^2 \beta_1^{(0)} \frac{q^n - b^{2n}}{q - b^2} \\ \alpha_1^{(n)} &= \alpha_1^{(0)} a^{2n} + p \left( \beta_2^{(0)} + \frac{d^2 \beta_1^{(0)}}{q - b^2} \right) \frac{a^{2n} - q^n}{a^2 - q} - p \frac{d^2 \beta_1^{(0)}}{q - b^2} \frac{a^{2n} - b^{2n}}{a^2 - b^2} \\ \alpha_2^{(n)} &= \alpha_2^{(0)} + c^2 \alpha_1^{(0)} \frac{1 - a^{2n}}{1 - a^2} + \frac{c^2 p \beta_2^{(0)}}{a^2 - q} \left( \frac{1 - a^{2n}}{1 - a^2} - \frac{1 - q^n}{1 - q} \right) + \\ &\quad + \frac{c^2 d^2 \beta_1^{(0)}}{(q - b^2)(a^2 - q)} \left( \frac{1 - a^{2n}}{1 - a^2} - \frac{1 - q^n}{1 - q} \right) - \\ &\quad - \frac{c^2 p d^2 \beta_1^{(0)}}{(q - b^2)(a^2 - b^2)} \left( \frac{1 - a^{2n}}{1 - a^2} - \frac{1 - b^{2n}}{1 - b^2} \right). \end{aligned}$$

One can see easily that all the terms are then converging to 0, with speed at least  $v^n$ , except the term  $\alpha_2^{(n)}$  which tends to  $\alpha_2^{(0)} + \alpha_1^{(0)} + \beta_1^{(0)} + \beta_2^{(0)}$  (after a few lines of computations), that is, it tends to 1.  $\square$

## 12.2 Excitation Transport

The above idea can be generalized to a chain of  $N$  sites connected as follows

$$\begin{pmatrix} D_1 & D_2 & 0 & 0 & \dots & 0 & 0 & 0 \\ D_3 & 0 & D_4 & 0 & \dots & 0 & 0 & 0 \\ 0 & D_5 & 0 & D_6 & \dots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & D_{2N-3} & 0 & D_{2N-2} \\ 0 & 0 & 0 & 0 & \dots & 0 & B & C \end{pmatrix}.$$

Then any initial state, for example any state of the form  $\rho_0 \otimes |1\rangle\langle 1|$ , will converge to the state

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |N\rangle\langle N|.$$

Though this example is rather classical in its behavior, it is interesting for it gives a model of a sort of “excitation transport”: giving any initial state on the site 1 only, the state will then be, more or less quickly, transported along the chain and will end up into the excited state on the site  $|N\rangle$ .

The model can be very much sped up by replacing the transition matrix with

$$\begin{pmatrix} B & C & 0 & 0 & \dots & 0 & 0 & 0 \\ B & 0 & C & 0 & \dots & 0 & 0 & 0 \\ 0 & B & 0 & C & \dots & 0 & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \dots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & B & 0 & C \\ 0 & 0 & 0 & 0 & \dots & 0 & B & C \end{pmatrix}.$$

In this case the probability distribution can be easily seen (and proved) to be a soliton of probability, supported by three sites only, traveling along the chain at speed 1 and ending up into the excited state on  $|N\rangle$ .

### 12.3 An Example on a 4-Graph

Take a graph made of 4 vertices  $|1\rangle, |2\rangle, |3\rangle$  and  $|4\rangle$ . They are connected as follows.

$$\begin{pmatrix} 0 & C & B & 0 \\ C & 0 & 0 & B \\ D_1 & 0 & 0 & D_2 \\ 0 & D_3 & D_4 & 0 \end{pmatrix},$$

where  $B$  and  $C$  are as in the first example and where  $D_1, D_2, D_3, D_4$  are diagonal matrices such that

$$D_1^* D_1 + D_2^* D_2 = D_3^* D_3 + D_4^* D_4 = I.$$

The invariant state of this quantum random walk is

$$\rho = \sum_{i=1}^4 \rho_i \otimes |i\rangle\langle i|$$

with

$$\begin{cases} \rho_1 = C\rho_2C^* + D_1\rho_3D_1^* \\ \rho_2 = C\rho_1C^* + D_3\rho_4D_3^* \\ \rho_3 = B\rho_1B^* + D_4\rho_4D_4^* \\ \rho_4 = B\rho_2B^* + D_2\rho_3D_2^*. \end{cases}$$

It is not very difficult to check that the unique invariant state for this random walk is

$$\frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |1\rangle\langle 1| + \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes |2\rangle\langle 2|.$$

For any initial state, for example

$$\frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes |3\rangle\langle 3| + \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes |4\rangle\langle 4|,$$

all the “mass” of the states will get transferred to the sites 1 and 2 and end up in the ground state.

## 13 Appendix: Proofs of the Lemmas

As promised we end up with the complete proofs of the lemmas given in Section 2.

**Proof** [of Lemma 2.1]

Each of the operators  $B_i\rho B_i^*$  is positive and trace-class. Put  $Y_N = \sum_{n \leq N} B_i\rho B_i^*$ , for all  $N \in \mathbb{N}$ . For all  $N < M$  the operator  $Y_M - Y_N$  is positive and trace-class. Put  $T_N = \sum_{n \leq N} B_i^* B_i$ . Then, for all  $N < M$  we have

$$\begin{aligned} \|Y_M - Y_N\|_1 &= \text{Tr}(Y_M - Y_N) \\ &= \sum_{N < n \leq M} \text{Tr}(B_i\rho B_i^*) \\ &= \text{Tr}(\rho(T_M - T_N)). \end{aligned}$$

As  $\rho$  can be decomposed into

$$\sum_n \lambda_n |e_n\rangle\langle e_n|,$$

with  $\sum_n \lambda_n < \infty$ , the last term above is equal to

$$\sum_n \lambda_n \langle e_n, (T_M - T_N)e_n \rangle.$$

As the operators  $T_N$  converge strongly to  $T$ , each of the terms  $\langle e_n, (T_M - T_N)e_n \rangle$  converge to 0 as  $N$  and  $M$  go to  $+\infty$ . Furthermore, they are all bounded independently of  $N$  and  $M$ , for the sequence  $(T_N e_n)_{N \in \mathbb{N}}$  is bounded. By Lebesgue's theorem  $\|Y_M - Y_N\|_1$  tends to 0, that is,  $(Y_N)_{N \in \mathbb{N}}$  is a Cauchy sequence in trace-norm. Hence it converges to a trace-class operator  $Y$ . The identity  $\text{Tr}(Y) = \text{Tr}(\rho T)$  is now obvious.  $\square$

**Proof** [of Lemma 2.2]

Put  $T_N = \sum_{n \leq N} B_n^* B_n$ . We have

$$\begin{aligned} \sum_{i \leq M} \sum_{j \leq N} M_j^{i*} M_j^i &= \sum_{i \leq M} \sum_{j \leq N} B_j^{i*} B_j^i \otimes |j\rangle\langle i| |i\rangle\langle j| \\ &= \sum_{i \leq M} \sum_{j \leq N} B_j^{i*} B_j^i \otimes |j\rangle\langle j| \\ &= \sum_{j \leq N} T_M \otimes |j\rangle\langle j|. \end{aligned}$$

Then for all  $\phi \in \mathcal{H} \otimes \mathcal{K}$  we have

$$\begin{aligned} \left\| \sum_{j \leq N} (T_M \otimes |j\rangle\langle j|) \phi - \phi \right\| &\leq \left\| \sum_{j \leq N} (T_M \otimes |j\rangle\langle j|) \phi - \sum_{j \leq N} (I \otimes |j\rangle\langle j|) \phi \right\| + \\ &\quad + \left\| \sum_{j \leq N} (I \otimes |j\rangle\langle j|) \phi - \phi \right\| \\ &\leq \sum_{j \leq N} \left\| (T_M \otimes |j\rangle\langle j|) \phi - (I \otimes |j\rangle\langle j|) \phi \right\| + \left\| \sum_{j \leq N} (I \otimes |j\rangle\langle j|) \phi - \phi \right\|. \end{aligned}$$

The last term converges to 0 with  $N$ , for the sum  $\sum_j I \otimes |j\rangle\langle j|$  converges strongly to  $I$ . Hence choose a  $N$  such that this term is smaller than  $\varepsilon/2$ . The first term of the right hand side converges to 0 with  $M$ , for the operators  $T_M \otimes |j\rangle\langle j|$  converge strongly to  $I \otimes |j\rangle\langle j|$ . Choose a  $M$  such that this term is smaller than  $\varepsilon/2$ . We have proved the announced strong convergence.  $\square$

**Proof** [of Lemma 2.4]

Consider the following sesquilinear form on  $\mathcal{H}^2$

$$(\phi, \psi) \mapsto \langle \phi \otimes j, \rho(\psi \otimes j) \rangle.$$

Since

$$|\langle \phi \otimes j, \rho(\psi \otimes j) \rangle| \leq \|\phi\| \|\psi\| \|\rho\|$$

this sesquilinear form is obviously of the form

$$\langle \phi, \rho_j \psi \rangle$$

for some bounded operator  $\rho_j$  on  $\mathcal{H}$ .

For any orthonormal basis  $(e_n)$  of  $\mathcal{H}$  we have

$$\sum_n |\langle e_n, \rho_j e_n \rangle| = \sum_n |\langle e_n \otimes j, \rho(e_n \otimes j) \rangle|.$$

As  $\rho$  is trace-class, the right hand side above is finite. This means that the left hand side is finite for every orthonormal basis  $(e_n)$ , hence  $\rho_j$  is trace-class.

In particular we have

$$\begin{aligned} \text{Tr}(\rho_j) &= \sum_n \langle e_n \otimes j, \rho(e_n \otimes j) \rangle \\ &= \sum_n \sum_i \langle e_n \otimes i, \rho(I \otimes |j\rangle\langle j|)(e_n \otimes i) \rangle \\ &= \text{Tr}(\rho(I \otimes |j\rangle\langle j|)). \end{aligned}$$

Now, for any  $\phi, \psi \in \mathcal{H}$  and any  $x, y \in \mathcal{K}$  we have

$$\begin{aligned} \langle \phi \otimes x, (I \otimes |i\rangle\langle j|) \rho(I \otimes |j\rangle\langle i|)(\psi \otimes y) \rangle &= \langle x, i \rangle \langle i, y \rangle \langle \phi \otimes j, \rho(\psi \otimes j) \rangle \\ &= \langle x, i \rangle \langle i, y \rangle \langle \phi, \rho_j \psi \rangle \\ &= \langle \phi \otimes x, (\rho \otimes |i\rangle\langle i|)(\psi \otimes y) \rangle. \end{aligned}$$

This proves that

$$(I \otimes |i\rangle\langle j|) \rho(I \otimes |j\rangle\langle i|) = \rho_j \otimes |i\rangle\langle i|.$$

We have proved all the assertions of the lemma. □



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