Open Quantum Random Walks on Graphs

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Open quantum random walks (OQRW) are introduced as quantum Markov chains on graphs. It is shown that OQRWs contain as a limit classical random walks. A suggested physical realization procedure for OQRW can recover unitary quantum random walks. A straightforward unravelling of the OQRW allows for stochastic simulations in terms of quantum trajectories. Simple examples of OQRWs show a rich dynamical behavior. In particular, promising dissipative mechanisms of transport of excitations can be implemented in the formalism, which makes them interesting candidates for the investigation of quantum efficiency.

Introduction. Random walks [1, 2] are a useful mathematical concept, which found successful applications, e. g., in physics [2], computer science [3], economics [4] and biology [5]. Basically, the trajectory of a random walk consists of a sequence of random steps on some underlying set of connected vertices [2]. It is appealing to extend the concept of the classical random walk to the quantum domain. QRWs can be introduced in a discrete time [6] and in a continuous time [7] fashion. While for a classical random walk the probability distribution of the position of the walker depends only on the transition rates between the nodes of the graph, in the quantum case [8] the probability amplitude of the walker depends on the dynamics of his internal degrees of freedom. The appearance of interference effects makes these walks truly quantum.

Unitary quantum random walks found wide application in quantum computing [9]. Although, physical implementation of any quantum concept is usually difficult due to unavoidable dissipation and decoherence effects [10], experimental realizations of unitary quantum random walks have been reported. Implementations with negligible effect of decoherence and dissipation were realized in optical lattices [11], on photons in waveguide lattices [12], with trapped ions [13] and free single photons in space [14].

Recently, there has been interest in understanding the role of quantum transport in biological systems [15]. Naturally, this raises the question of finding a framework for quantum walks in an open environment, for which dissipation and decoherence will play a non negligible role. On the contrary, such open quantum random walks may even assist in the understanding of quantum efficiency.

During the last few years attempts were made to take into account decoherence and dissipation in the description of the quantum walks [16]. However, in these approaches decoherence is treated as an extra modification of the unitary quantum walk scheme, the effect of which needs to be minimized and eliminated. Recently, the general framework of quantum stochastic walks was proposed [17], which incorporates unitary and non-unitary effects of the quantum Markovian dynamics.

In this paper we introduce a formalism for discrete time open quantum walks, which is exclusively based on the non-unitary dynamics induced by the environment. The formalism suggested is similar to the formalism of quantum Markov chains [18] and rests upon the implementation of appropriate completely positive maps [10, 19]. As we will show below the formalism of the open quantum random walks includes the classical random walk and through a physical realization procedure a connection to the unitary quantum walk is established. Furthermore, the OQRW allows for an unravelling in terms of quantum trajectories. In general, the behavior of the walk can not be explained in terms of classical or unitary walks. The particular properties of the OQRW make it a promising candidate for modeling of quantum efficiency in biological systems and quantum computing.

General setup. We consider a random walk on a set of nodes or vertices $\mathcal{V}$ with oriented edges $\{(i,j)\,;\ i,j \in \mathcal{V}\}$. The number of nodes is considered to be finite or countable infinite. The space of states corresponding to the dynamics on the graph specified by the set of nodes $\mathcal{V}$ will be denoted by $\mathcal{K} = \mathbb{C}^{\mathcal{V}}$. If $\mathcal{V}$ is an infinite countable set, the space of states $\mathcal{K}$ will be any separable Hilbert space with an orthonormal basis $(|i\rangle)_{i\in\mathcal{V}}$ indexed by $\mathcal{V}$. The internal degrees of freedom of the quantum walker, e.g. the spin or n-energy levels, will be described by a separable Hilbert space $\mathcal{H}$ attached to each node of the graph. More concisely, any state of the quantum walker will be described on the direct product of the Hilbert spaces $\mathcal{H} \otimes \mathcal{K}$.

Let us now describe the dynamics of the quantum walker. To this end, for each edge (i,j) we introduce a bounded operator $B^i_j \in \mathcal{H}$. This operator describes the change in the internal degree of freedom of the walker due to the shift from node j to node i. By imposing for each j that,

$$\sum_i {B^i_j}^\dagger B^i_j = I, \tag{1}$$

we make sure, that for each vertex of the graph $j \in \mathcal{V}$ there is a corresponding completely positive map on the positive operators of $\mathcal{H}$:

$$\mathcal{M}_j(\tau) = \sum_i B^i_j \tau {B^i_j}^\dagger.$$

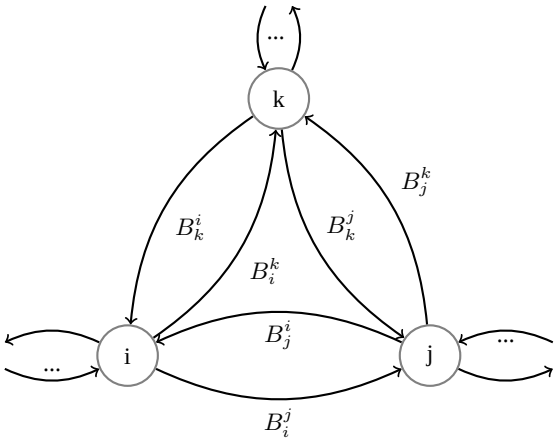

FIG. 1: Schematic illustration of the formalism of the Open Quantum Random Walk: The walk is realized on a graph with a set of vertices denoted by $i, j, k \in \mathcal{V}$. The operators B_i^j decribes transitions in the internal degree of freedom of the "walker" jumping from node (i) to node (j).

Since the operators B_j^i act only on $\mathcal{H}$ and do not perform transitions from node j to node i, an operator $M_j^i \in \mathcal{H} \otimes \mathcal{K}$ can be introduced in the following form

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

It is clear that, if the condition expressed in Eq. (1) is satisfied, then $\sum_{i,j} M_j^{i\dagger} M_j^i = 1$. This latter condition defines a completely positive map for density matrices on $\mathcal{H} \otimes \mathcal{K}$, i.e.,

$$\mathcal{M}(\rho) = \sum_i \sum_j M_j^i \, \rho \, M_j^{i\dagger}. \tag{2}$$

The above map defines the discrete time *open quantum random walk* (OQRW). It is easy to see that for an arbitrary initial state the density matrix $\sum_{i,j} \rho_{i,j} \otimes |i\rangle\langle j|$ will take a diagonal form after just one step of the open quantum random walk Eq. (2). Hence, in the following, we will assume that the initial state of the system has the form

$$\rho = \sum_i \rho_i \otimes |i\rangle\langle i|, \tag{3}$$

with

$$\sum_i \mathrm{Tr}\,(\rho_i) = 1. \tag{4}$$

It is straightforward to give an explicit formula for the iteration of the OQRW from step n to step $n+1$

$$\rho^{[n+1]} = \mathcal{M}(\rho^{[n]}) = \sum_i \rho_i^{[n+1]} \otimes |i\rangle\langle i|, \tag{5}$$

where

$$\rho_i^{[n+1]} = \sum_j B_j^i \rho_j^{[n]} B_j^{i\,\dagger}. \tag{6}$$

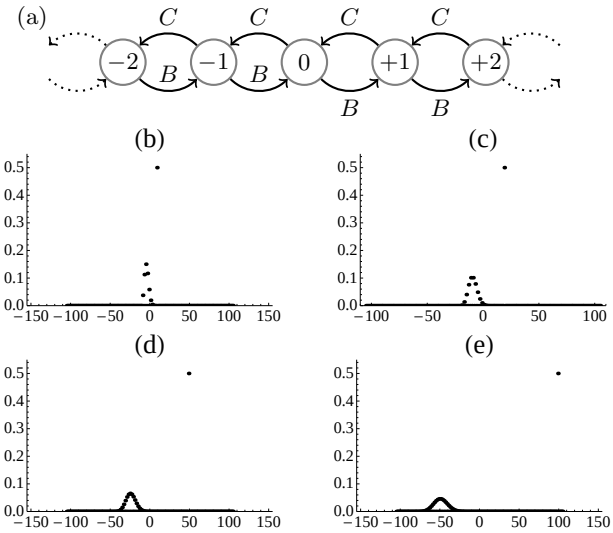

FIG. 2: OQRW on $\mathbb{Z}$. (a) A schematic representation of the OQRW on $\mathbb{Z}$: all transitions to the right are induced by the operator $B_i^{i+1} \equiv B$, while all transitions to the left are induced by the operator $B_i^{i-1} \equiv C$ (see Eq. (7)); Figures (b)-(e) show the occupation probability distribution for the "walker" with the initial state $I_2/2 \otimes |0\rangle\langle 0|$ and transition operators given by Eq. (7) after 10, 20, 50 and 100 steps, respectively.

The above iteration formula gives a clear physical meaning to the mapping that we introduced: the state of the system on site i is determined by the conditional shift from all connected sites j, which are defined by the explicit form of the operators B_j^i. Also, one can see that $\mathrm{Tr}[\rho^{[n+1]}] = \sum_i \mathrm{Tr}[\rho_i^{[n+1]}] = 1$.

Quantum trajectories. The above introduction of a OQRW allows for a very useful quantum trajectory interpretation. Assuming that at the start of the walk the system is prepared in a pure state $|\psi\rangle = |b_j\rangle \otimes |j\rangle$ on site j, it is easily recognized that after one step it will jump to one of the pure states

$$\frac{1}{\sqrt{p_j^i}} B_j^i |b_j\rangle \otimes |i\rangle,$$

with probability $p_j^i = \left\| B_j^i |b_j\rangle \right\|^2$. In other words, for pure states the OQRW describes a classical Markov chain on the space of stochastic wave functions. As is the case for the usual Quantum Trajectories methods for Markovian open quantum systems, by averaging over an ensemble of realizations of the stochastic wave function one recovers the OQRW.

A simple example: OQRW on $\mathbb{Z}$. Let us elucidate the formalism by considering the simple OQRW on a graph in which only adjacent sites are connected. The situation we describe is depicted in Fig. 2 (a). For this simple one-dimensional walk, the only non-zero transition out of cell i are given by operators of the form $B_i^{i+1} \equiv B$ and $B_i^{i-1} \equiv C$ (again, the notation is illustrated in Fig. 2(a)). Obviously, the operators B and C satisfy the condition $B^\dagger B + C^\dagger C = I$, as imposed in Eq. (1). Assuming the initial state of the system to be localized on site 0, i.e., $\rho_0 = \rho \otimes |0\rangle\langle 0|$, after one step the

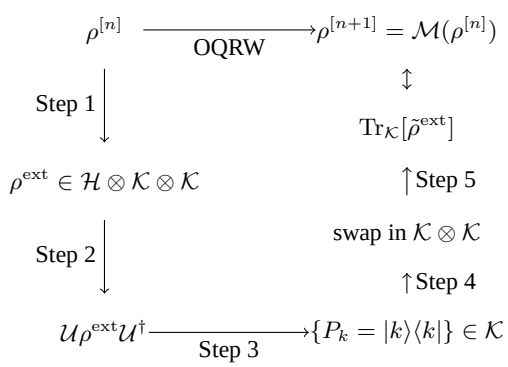

FIG. 3: Scheme of the various steps required for the physical realization of the Open Quantum Random Walk.

system will jump to sites ± 1 so that the new density matrix will be $\rho^{[1]} = B\rho B^\dagger \otimes |1\rangle\langle 1| + C\rho C^\dagger \otimes |-1\rangle\langle -1|$. The procedure can easily be iterated. In Figs. 2(b)-(e) we show the probability to find a "walker" on a particular lattice site for different numbers of steps. For this simulation we have chosen the transition matrices B and C as follows,

$$B = \begin{pmatrix} 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix}, \quad C = \begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{pmatrix}. \tag{7}$$

As we said, the system is initially localized on site 0. A remarkable non-Gaussian behavior is observed, which indicates the dynamical richness of OQRWs. Already after 10 steps, one can clearly see two distinctive behaviors of the "walker". The first is a Gaussian wave-packet moving slowly to the left and the second one is a completely deterministic trapped state propagating to the right at a speed of 1 in units of cells per time step. Other examples of the OQRW on $\mathbb{Z}$ can be found in [20].

Physical realization. It is natural to ask how to derive a OQRW by reduction of the unitary dynamics of an appropriately enlarged system. The situation is illustrated in Fig. 3 and will be described step by step. To achieve this goal we need to extend the Hilbert space of the system by an ancilla-graph identical to the graph described by the space $\mathcal{K}$ and define on this extended Hilbert space $\mathcal{H} \otimes \mathcal{K} \otimes \mathcal{K}$ a specially chosen unitary operator $\mathcal{U}$. It is alway possible for any given k to define a unitary operator $U(k) \in \mathcal{H} \otimes \mathcal{K}$, such that the first column of the operator is given by B_k^i and by filling the rest with corresponding elements to fulfill the unitary condition

$$U_1^i(k) = B_k^i, \qquad \sum_j U_j^{i'}(k)^\dagger U_j^i(k) = \delta_{i,i'} I.$$

The unitary operator $\mathcal{U}$ is a diagonal sum of the operators $U(k)$ with corresponding projector representation

$$\mathcal{U} = \sum_k U(k) \otimes |k\rangle\langle k|.$$

Again, we assume the initial state $\rho = \sum_i \rho_i \otimes |i\rangle\langle i| \in \mathcal{H} \otimes \mathcal{K}$.

The first step is to extend the state into a larger Hilbert space in the following way

$$\rho = \sum_i \rho_i \otimes |i\rangle\langle i| \to \rho^{\mathrm{ext}} = \sum_i \rho_i \otimes |1\rangle\langle 1| \otimes |i\rangle\langle i|,$$

so that the extended density matrix $\rho^{\mathrm{ext}} \in \mathcal{H} \otimes \mathcal{K} \otimes \mathcal{K}$.

Step 2 is the application of the unitary operator $\mathcal{U}$ to the extended density matrix ρ^{ext}, i.e.,

$$\mathcal{U}\rho^{\mathrm{ext}}\mathcal{U}^\dagger = \sum_{i,j,p} B_i^j \rho_i B_i^{p\dagger} \otimes |j\rangle\langle p| \otimes |i\rangle\langle i|.$$

In *Step 3* we perform a full set of measurements $P_k = I_{\mathcal{H}} \otimes |k\rangle\langle k| \otimes I_{\mathcal{K}}$ on the "extra" position space or we subject the system to decoherence in this "extra" position subspace. As result of Step 3 we obtain the following density matrix

$$\sum_{i,j} B_i^j \rho_i B_i^{j\dagger} \otimes |j\rangle\langle j| \otimes |i\rangle\langle i|.$$

In Step 4 we swap position subspaces. The result of this operation is the following density matrix

$$\sum_{i,j} B_i^j \rho_i B_i^{j\dagger} \otimes |i\rangle\langle i| \otimes |j\rangle\langle j|.$$

The last step (Step 5) is tracing out the "extra" position subspace and one obtains the OQRW as promised

$$\sum_{i,j} B_i^j \rho_i B_i^{j\dagger} \otimes |j\rangle\langle j|.$$

Connection to the unitary random walk. The *unitary quantum random walk* (UQRW) can be recovered from the OQRW realization procedure by a special choice of the transition operators B_i^j and by excluding from the physical realization procedure illustrated in Fig. 3 Step 3 (measurements). This is easily demonstrated for a UQRW on $\mathbb{Z}$. In this case of a UQRW on the line an additional condition needs to be imposed on the transition operators B and C: next to the normalization condition $B^\dagger B + C^\dagger C = I$ we need to request that $C^\dagger B = 0$. In this case the sum of B and C is a unitary operator. Explicitly, in order to recover the Hadamard UQRW on the line we may choose

$$B = \begin{pmatrix} \alpha & \beta \\ 0 & 0 \end{pmatrix}, \quad C = \pm \begin{pmatrix} 0 & 0 \\ -\beta^* & \alpha^* \end{pmatrix},$$

where $|\alpha|^2 + |\beta|^2 = 1$ and $\alpha, \beta \in \mathbb{C}$. Starting from the state $|\psi_0\rangle \otimes |0\rangle$ and following the physical realization procedure (Fig. 3) while skipping Step 3, the state of the system after one step is given by $B|\psi_0\rangle \otimes |+1\rangle + C|\psi_0\rangle \otimes |-1\rangle$. This is exactly a Hadamard UQRW on $\mathbb{Z}$. The general condition for obtaining UQRWs from OQRWs can be found in [20].

The classical random walk. It is interesting to note that the OQRW contains, as a special case, the classical random walk as well. To see this, we specialize $\mathcal{H} = \mathcal{K} = \mathbb{C}^{\mathcal{V}}$, introduce a matrix $P = \{P_{i,j}\}$ of classical transition probabilities on

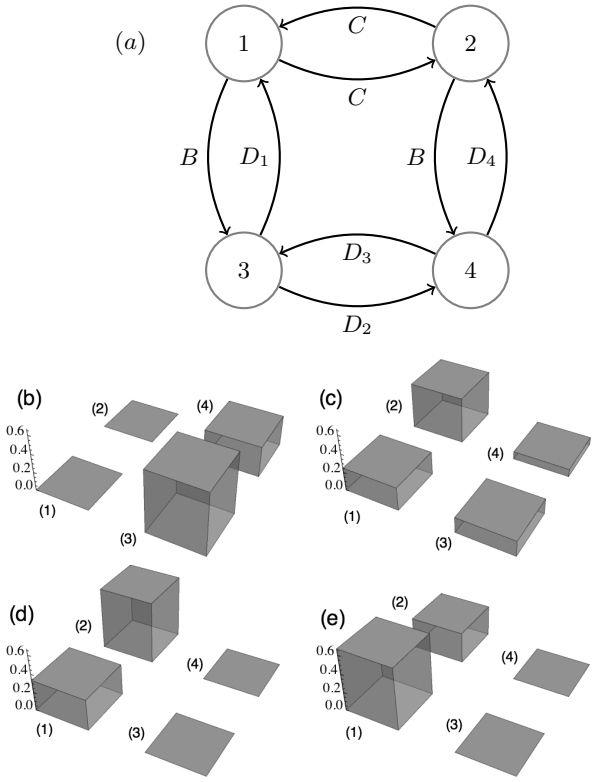

FIG. 4: Open Quantum Random Walk on a 4-node graph. Figure (a) shows the scheme for a OQRW on the 4-node graph; Fig. (b) shows the occupation probability distribution for the initial state of the walker $\rho_0 = \frac{1}{3} I_2 \otimes |3\rangle\langle 3| + \frac{1}{6} I_2 \otimes |4\rangle\langle 4|$; Figs. (c)-(e) show the occupation probability densities on the graph after 5, 25 and 40 steps, respectively.

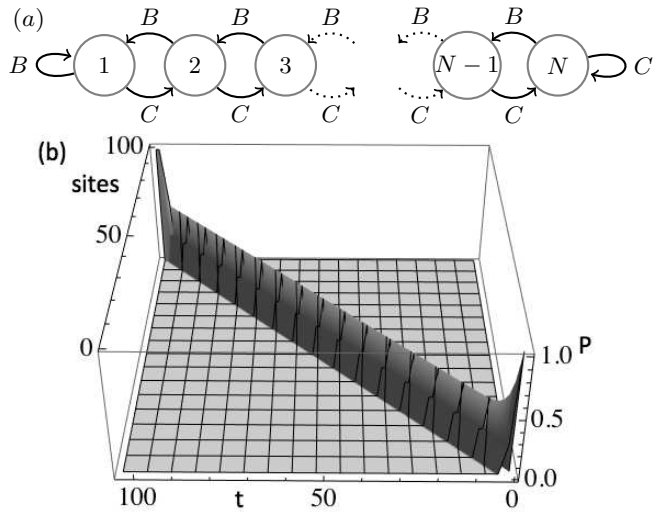

FIG. 5: Efficient transport with Open Quantum Random Walk. Fig. (a): a scheme of the chain of the N nodes with neighbor-neighbor interaction. The transition operators B and C are given by Eq. (8). Fig. (b): occupation probability distribution as a function of time and lattice sites. The initial state of the walker is localized in the first node and given by $\rho_0 = \frac{1}{2} I_2 \otimes |1\rangle\langle 1|$.

the graph $\mathcal{V}$ with normalization condition $\sum_i P_{j,i} = 1$, and consider an arbitrary family of unitary operators, $U_i^j \in \mathbb{C}^{\mathcal{V}}$. In this case, it seems natural to choose the transition operators B_i^j to have the form $B_i^j = \sqrt{P_{i,j}} U_i^j$. Then, for the initial state $\rho = \sum_k \rho_k \otimes |k\rangle\langle k|$ the probability to find a "walker" after one step on the site i reads $\sum_k p_{k,i} \mathrm{Tr}(\rho_k)$. After two steps the probability to find walker on the site i will be given by $\sum_{k,m} p_{m,k} p_{k,i} \mathrm{Tr}(\rho_m)$, and so on. Thus, the probability of transition does not depend on the internal degrees of freedom of the "walker". It only depends on the classical transition probability matrix P, as expected for a classical random walk.

OQRW on a 4-node graph. To motivate the potential of OQRW in the understanding of quantum transport we consider as a first example the 4-node graph illustrated in Fig. 4 (a) with initial population distributed between nodes (3) and (4), i.e., $\rho_0 = \frac{1}{3} I_2 \otimes |3\rangle\langle 3| + \frac{1}{6} I_2 \otimes |4\rangle\langle 4|$. The distribution of the occupation probabilities at the initial moment of time is shown in Fig 4. (b). The transitions in the system are induced by the operators B, C, D_1, D_2, D_3 and D_4 (see Fig. 4 (a)), which are explicitly given by

$$B = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad C = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 \\ 0 & 1 \end{pmatrix}, \qquad (8)$$

and $D_i = \frac{1}{\sqrt{2}} I_2$ for $i = 1, 2, 3, 4$. In Fig. 4 (c)-(e) the distribution of the occupation probability for different number of step is presented. As one can see the initial population is trapped in sites 3 and 4. Essentially, after 10 steps of the OQRW all populations are shifted to nodes 1 and 2, indicating a clear mechanism of transport.

Efficient quantum transport. As a last example we illustrate the importance role OQRW may play in the description of highly efficient transport of an excitation, as it is relevant for the understanding of transport properties in biological systems. To this end we consider a chain of nodes (see Fig. 5(a)). An initial excitation is in node (1), so that $\rho_0 = \frac{1}{2} I_2 \otimes |1\rangle\langle 1|$. To be specific, we chose transition operators B and C as in the previous example. It is very interesting to note that in this case the excitation propagates through the chain with velocity almost equal to 1 (in units of cells per time step): in other words, the initial excitation in node (1) is completely transferred to the last node (N) in N+3 steps. As an explicit example, in Fig. 5 (b) we consider a 100 node chain and show that the initial excitation reaches the final node (100) in 103 steps. The high performance of transport of excitations in the OQRW formalism opens up new avenues of research into the understanding of quantum efficiency in open systems.

In conclusion, we have introduced above a very flexible framework of open quantum random walks, which clearly shows a richness of different dynamical behaviors, and, at the same time, includes as special cases the classical random walk and through the realization procedure the unitary quantum random walks. The examples we have have considered show that the framework can be used to explain non-trivial highly efficient transport phenomena not only in linear but

also in more complex topologies of the underlying graphs. We expect the potential of this framework to be soon revealed in the realms of quantum biology and quantum computing.

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