

Limiting properties of stochastic quantum walks on directed graphs

Adam Glos^{1,2}, Jarosław Adam Miszczak¹
and Mateusz Ostaszewski^{1,2}

¹ Institute of Theoretical and Applied Informatics, Polish Academy of Sciences,
Bałtycka 5, 44-100 Gliwice, Poland

² Institute of Informatics, Silesian University of Technology, Akademicka 16,
44-100 Gliwice, Poland

E-mail: mostaszewski@iitis.pl

Received 8 March 2017, revised 8 November 2017

Accepted for publication 14 November 2017

Published 15 December 2017



Abstract

The main results of our work is determining the differences between limiting properties in various models of quantum stochastic walks. In particular, we prove that in the case of strongly connected and a class of weakly connected directed graphs, local environment interaction evolution is relaxing, and in the case of undirected graphs, global environment interaction evolution is convergent. For other classes of directed graphs we show, that the character of connectivity has a large influence on the limiting properties. We also study the limiting properties for the non-moralizing global interaction case. We demonstrate that the digraph observance is recovered in this case.

Keywords: quantum stochastic walks, stationary states, state convergence, relaxing

(Some figures may appear in colour only in the online journal)

1. Introduction and preliminaries

1.1. Motivation

Results from the past few decades show that the choice of the quantum analogue of classical random walk is highly non-unique. Some of the most popular models include the discrete coined quantum walk [1], continuous quantum walk [2], Szegedy walk [3], open walk [4], staggered quantum walk [5], and quantum stochastic walk [6]. They have found applications in the designing PageRank algorithm [7–9], search algorithms [10–13], solving triangle problem [14], and describing chemical reactions [15]. All of them outperform their classical counterpart at least for some large class of graphs. From the algorithmic perspective, it is

crucial to understand the limiting behaviour of the walks. This includes the propagation speed, which decides about efficiency of the search algorithm [16], mixing time and relaxing, which find applications in PageRank algorithm [8, 17], limit theorem [18, 19, 20], and trapping [21].

A special kind of continuous quantum evolution is the quantum stochastic walk, which generalizes both the classical and quantum walk [6]. The model has been investigated in the context of relaxing property [8, 17], propagation speed [22], and applications to various physics [15] and computer science [8] problems. The difference comparing to the original continuous-time quantum walk is the Lindblad operators appearance. The choice of Lindblad operators is highly nontrivial, and in the case where each one-dimensional subspace corresponds to different vertex, two models are of particular interest: local environment interaction and global environment interaction [6, 22].

The local environment interaction case has been extensively used and analysed. The model has been analysed in context of relaxation [17] and application in PageRank algorithm [8]. In particular, it was shown that in the case of undirected graphs, the QSW is always relaxing [17]. However, the evolution is decohering, and hence it destroys the ballistic propagation [23].

The ballistic propagation was one of the basic motivations for the analysis of quantum walk. Fortunately, the global environment interaction QSW is proved to have ballistic propagation [22]. However, the global environment interaction suffers from graph topology change [16], due to its character called *moralization*. Thanks to the correction scheme it is possible to bound the QSW with the global interaction to the digraph structure. Such evolution, called non-moralizing global environment QSW, is verified numerically to have at least superdiffusive propagation [16].

The main contribution of this paper is the description of the limiting properties of various models of quantum stochastic walks. We describe how the connectivity of the graph influences the convergence or the relaxation. Numerical analysis suggests, at least in some cases, that the convergence/relaxation appears on all graphs in the sense of Erdős–Renyi random graph model $\mathcal{G}(n, p)$. Furthermore, our results includes the directed graph preservation analysis for directed graphs in the case of non-moralizing evolution. The main results are collected in table 1

The paper is organized as follows. In the following part of this section we provide some basic definitions concerning graph theory and QSW. In section 2 we analyse the limiting properties of the local environment interaction case. In sections 3 and 4 we analyse the limiting properties of the global environment interaction case, the standard and the non-moralizing respectively. We conclude our results in section 5.

1.2. Graph theory terminology

Let $G = (V, E)$ be a digraph with vertex set V and arc set E . The underlying graph $G^u(V, E^u)$ is an undirected simple graph, for which every arc from G is replaced with an edge. We say that digraph is weakly connected if its underlying graph is connected. We say that digraph is strongly connected, if for arbitrary $v, w \in V$ there is a directed path from v to w . The strongly connected components are the maximal strongly connected subgraphs. We call v a sink vertex, if its outdegree (number of outgoing arcs) is zero. We denote $S(G)$ to be a set of sink vertices.

Let $\mathbb{G} = (\mathbb{V}, \mathbb{E})$ be condensation of $G = (V, E)$, i.e. a directed graph constructed as follows. We make a partition \mathbb{V} of vertex set V in such a way, that each block forms a maximal strongly connected component in G . Then $(\mathbf{v}, \mathbf{w}) \in \mathbb{E}$ iff there exists $v \in \mathbf{v}, w \in \mathbf{w}$ such that $(v, w) \in E$. In other words there is an arc from one maximal strongly connected component to the other, if there is at least one arc (in consistent direction) between their elements. Note that

Table 1. Main analytical results. Case $\omega \in (0, 1]$ is only considered here.

	Local interaction	Global interaction	Non-moralizing global interaction
Convergence	– Unknown in general case	– Undirected graphs – Counterexample for digraphs	– Counterexample for undirected graphs
Relaxing	– Strongly connected digraphs – Weakly connected digraphs with one sink in condensation graph	– Never for undirected graphs – Counterexample for digraphs	– Counterexample for undirected graphs

\mathbb{G} is directed acyclic graph, hence $S(\mathbb{G}) \neq \emptyset$. Furthermore, if G is weakly connected, then for each $\mathbf{w} \in \mathbb{V}$ there exists $\mathbf{s} \in \mathbf{S}(\mathbb{G})$ such that there exists directed path from \mathbf{w} to \mathbf{s} .

The directed moral graph $G_M = (V, E_M)$ of the directed graph $G = (V, E)$ is defined as follows. For each $v, v' \in V$ we have $(v, v') \in E_M$ iff $(v, v') \in E$ or there exists $w \in V$ such that $(v, w), (v', w) \in E$. In other words, directed moral graph is constructed by adding edge between the vertices which have common child. Note that original moral graph is defined as underlying graph of the directed moral graph [24, 25].

In this work we are using Erdős–Rényi model of random graphs. The Erdős–Rényi random graph $\mathcal{G}(n, p)$ is a graph with n vertices such that any pair of vertices is connected with probability p [26].

Throughout this paper we will assume that the graph is at least weakly connected.

1.3. GKSL master equation and quantum stochastic walks

To define quantum stochastic walks in general, let us start with the Gorini–Kossakowski–Sudarshan–Lindblad (GKSL) master equation [27–29]

$$\frac{d}{dt}\varrho = \mathcal{M}[\varrho] = -i[H, \varrho] + \sum_{L \in \mathcal{L}} \left(L\varrho L^\dagger - \frac{1}{2}\{L^\dagger L, \varrho\} \right), \quad (1)$$

where $\{A, B\}$ is the anticommutator and \mathcal{M} is the evolution superoperator. Here H is the Hamiltonian, which describes the evolution of the closed system, and \mathcal{L} is the collection of Lindblad operators, which describes the evolution of the open system. This master equation describes general Markov continuous evolution of mixed quantum states. Note, that in the case of $\mathcal{L} = \emptyset$ and H being an adjacency matrix of some graph we recover the original continuous quantum walk, however on mixed states.

The GKSL master equation was used for defining quantum stochastic walks (QSW), which are a generalization of both classical random walks and quantum walks [6]. Both H and \mathcal{L} correspond to the graph structure, however one may verify that at least a choice of Lindblad operators may be non-unique [6, 22]. Suppose we have a directed graph $G = (V, E)$. Since Hamiltonian H needs to be hermitian, we always choose adjacency matrix of the underlying graph. In the *local environment interaction case* each Lindblad operator corresponds to a single arc, $\mathcal{L} = \{c_{(v,w)}|w\rangle\langle v| : (v, w) \in E\}$ for $c_{(v,w)} \in \mathbb{C}_{\neq 0}$. In the *global environment interaction case* we choose a single Lindblad operator, which is adjacency matrix of directed graph.

To analyse the impact of Lindbladian part, we add the smoothing parameter $\omega \in [0, 1]$

$$\frac{d}{dt}\varrho = -i(1-\omega)[H, \varrho] + \omega \sum_{L \in \mathcal{L}} \left(L\varrho L^\dagger - \frac{1}{2}\{L^\dagger L, \varrho\} \right). \quad (2)$$

In [23] it was shown, by infinite path graph analysis, that the local interaction case leads to the classical propagation of the walk. Oppositely, in the case of the global interaction, the ballistic propagation is obtained for arbitrary middle value ω . Since for $\omega = 0$ we recover continuous quantum walk (CQW) on closed system, we are particularly interested in $\omega \in (0, 1]$ case.

In [16] it has been noted that the global interaction QSW suffers for the graph topology change and the resulting process fails to reproduce the structure of the original graph. The resulting graph, according to which the system is evolving, is the directed moral graph [24, 25], of the original one. This effect is called a spontaneous moralization and to prevent this a correction scheme based on the system enlargement has been proposed [16]. The scheme consist of following steps: first we combine with each vertex a subspace of the system of dimension equal to the indegree of the vertex (in the case of source vertices the subspace is onedimensional). Next, we choose a family of orthogonal matrices for new Lindblad operator \tilde{L} , which destroys the spontaneous moralization. The last step is to add a Hamiltonian \tilde{H}_{local} acting locally on the subspaces corresponding to different vertices. The Hamiltonian \tilde{H} corresponding to the graphs structure is a 0-1 matrix, for which zero values coincides with zero values of \tilde{L} . For details we refer the reader to the original paper. Since in this model we combine each vertex with some orthogonal subspaces, a natural measurement is the collection of operations which projects the state onto the subspaces corresponding to the vertices. We call this model of evolution as *non-moralizing global environment interaction QSW*, or simply non-moralizing QSW. Similar to equation (2) we add smoothing parameter ω and the evolution takes the form

$$\frac{d}{dt}\varrho = -i(1-\omega)[\tilde{H}, \varrho] + \omega \left(-i[\tilde{H}_{\text{local}}, \varrho] + \tilde{L}\varrho\tilde{L}^\dagger - \frac{1}{2}\{\tilde{L}^\dagger\tilde{L}, \varrho\} \right). \quad (3)$$

Numerical simulation of the QSW with non-moralizing global environment interaction is difficult because of enlarging of the system. With the increase of the input graph density, the size and density of output Lindblad operator \tilde{L} increases rapidly.

Throughout this paper we analyse the limit behaviour of QSW in all of three mentioned cases: local environment interaction, global environment interaction, and corrected non-moralizing environment interaction. We analyse the evolution in context of convergence and relaxation. We say that evolution is convergent, if for arbitrary initial state ϱ_0 there exists stationary state ϱ_∞ such that $\varrho_t \xrightarrow{t \rightarrow \infty} \varrho_\infty$. We say that evolution is relaxing, if there exists unique stationary state. In GKSL master equation uniqueness of stationary state is equivalent to relaxing property, see theorem 1 from [30]. Similarly one can define convergence and relaxing in the context of probability distribution of quantum measurement. Note that relaxation implies convergence, but the opposite does not hold in general.

In the case of QSW H and \mathcal{L} do not depend on time. Henceforth, we can solve the differential equation analytically: if we choose initial state ϱ_0 , then

$$|\varrho_t\rangle\rangle = \exp(tF)|\varrho_0\rangle\rangle, \quad (4)$$

where

$$F = -i(H \otimes \mathbb{1} - \mathbb{1} \otimes \tilde{H}) + \sum_{L \in \mathcal{L}} \left(L \otimes \tilde{L} - \frac{1}{2}(L^\dagger L \otimes \mathbb{1} + \mathbb{1} \otimes L^\dagger L) \right), \quad (5)$$

and $|\cdot\rangle\rangle$ denotes the vectorization of the matrix (see eg. [31]). Note that the eigenvalues of F implies the behaviour of the evolution. If there exists purely imaginary nonzero eigenvalues, the evolution is non-convergent for some initial state ϱ_0 , otherwise it is convergent. If the null-space is one-dimensional, then the evolution is relaxing. Hence our numerical analysis is mostly based on analysing the spectrum of F .

2. Convergence of local interaction case

The local environment interaction case is relaxing for undirected graphs [17] and arbitrary Hamiltonian. The proof is based on the Spohn theorem [32], which requires the self-adjointness of the set of Lindblad operators, hence its applications is limited to the undirected graphs case. Nevertheless we show, that the result can be extended to strongly connected digraphs and weakly connected graphs with single sink vertex in \mathbb{G} graph. Our proofs utilise the Condition 2. and Condition 3. from [30], recalled here as lemmas 1 and 2. By interior we mean collection of density matrices with full rank.

Lemma 1 ([30]). *Let \mathcal{H} be a Hilbert space. If there is no proper subspace $S \subsetneq \mathcal{H}$, that is invariant under all Lindblad generators $L \in \mathcal{L}$ then the system has a unique steady state in the interior.*

Lemma 2 ([30]). *If there do not exist two orthogonal proper subspaces of \mathcal{H} that are simultaneously invariant under all Lindblad generators $L \in \mathcal{L}$, then the system has unique fixed point, either at the boundary or in the interior.*

Using the above lemmas we can prove the following.

Theorem 1. *Let $G = (V, E)$ be a strongly connected digraph and let $\mathcal{L} = \{L_{vw} = c_{(v,w)}|w\rangle\langle v| : (v, w) \in E\}$ for some $c_{(v,w)} \in \mathbb{C}_{\neq 0}$. Then evolution described by equation (1) is relaxing for arbitrary Hamiltonian H with stationary state in the interior.*

Proof. Let \mathcal{H} be a Hilbert space spanned by $\{|v\rangle : v \in V\}$ and $S \neq \{0\}$ be arbitrary subspace of \mathcal{H} invariant under \mathcal{L} . Furthermore, suppose that $|\psi\rangle \in S$ is a nonzero vector and $v \in V$ is such that $\langle v|\psi\rangle \neq 0$. Since G is strongly connected, there is a directed path $(v_1 = v, v_2, \dots, v_k, w)$ for arbitrary $w \in V$. Then $c_w|w\rangle = L_{v_k w} L_{v_{k-1} v_k} \dots L_{v_2, v_1} |\psi\rangle \in S$ for some $c_w \in \mathbb{C}_{\neq 0}$. Since $\{|w\rangle : w \in V\}$ forms a basis of \mathcal{H} , we have $S = \mathcal{H}$. By lemma 1 the theorem is true. \square

Theorem 2. *Let $G = (V, E)$ be a weakly connected digraph such that $|S(\mathbb{G})| = |\{s\}| = 1$ and let $\mathcal{L} = \{c_{(v,w)}|w\rangle\langle v| : (v, w) \in E\}$ for some $c_{(v,w)} \in \mathbb{C}_{\neq 0}$. Then the evolution described by equation (1) is relaxing for arbitrary Hamiltonian H .*

Proof. Suppose $S_1 \neq \{0\}, S_2 \neq \{0\}$ are two subspaces of \mathcal{H} and let $|\psi_1\rangle \in S_1, |\psi_2\rangle \in S_2$. Similarly to method in theorem 1 one can show that there exist $L_1^1, \dots, L_k^1 \in \mathcal{L}$ and $L_1^2, \dots, L_{k'}^2 \in \mathcal{L}$ such that $c_w^1|w\rangle = L_k^1 L_{k-1}^1 \dots L_1^1 |\psi_1\rangle$ and $c_w^2|w\rangle = L_{k'}^2 L_{k'-1}^2 \dots L_1^2 |\psi_2\rangle$ for some $w \in s$ and $c_w^1, c_w^2 \in \mathbb{C}_{\neq 0}$. Hence S_1 and S_2 are not orthogonal and by lemma 2 the theorem holds. \square

Note that no information about the graph structure needs to be encoded in the Hamiltonian—the graph structure is encoded in the \mathcal{L} only.

The remaining class of weakly connected graphs is those for which $|S(\mathbb{G})| > 1$. However in this case one can show that the Hamiltonian has an impact on the limiting behaviour of the evolution. In the case of $\omega = 1$, one can show that the evolution is equivalent to the classical

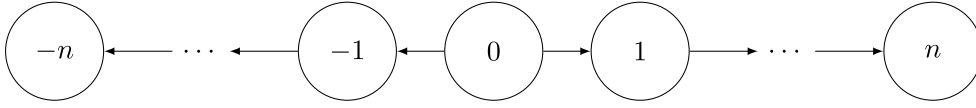


Figure 1. Bidirected path graph of size $2n + 1$.

one. Because of that, there are different stationary states in each of the sinks. Hence, the evolution is not relaxing. However, due to the de-cohering character of the evolution, it should be convergent to the state from the sinks subspace.

Similarly convergence is expected in the case of $\omega \in (0, 1)$. In this case, if the Hamiltonian impact is sufficiently large, one can observe the relaxation of the evolution. As an example, we analyse a bidirected path with vertex set $\{-n, -(n-1), \dots, n-1, n\}$, and edge set $E = \{(i, i+1) : i < 0\} \cup \{(i-1, i) : i > 0\}$ (see figure 1). The Hamiltonian is chosen to be the adjacency matrix of the underlying graph, i.e. the path graph. In figure 2 the values of ω for which the evolution is relaxing are presented. One can see that for each n there is ω_t such that for $\omega < \omega_t$ evolution is relaxing, and for $\omega > \omega_t$ is not. As the value of ω_t decreased with n , one can observe that for larger graphs the stronger influence of the coherent part is necessary to ensure the relaxing property.

We have analysed the graphs from Erdős–Rényi model $\mathcal{G}(n, \frac{1}{10})$ with $|S(\mathbb{G})| > 1$. For each size $n = 10, 15, \dots, 45$ we have tested 200 graphs with values $\omega \in \{0.05, 0.1, \dots, 1\}$. We have ignored the graphs for which $|S(\mathbb{G})| > 1$ was not satisfied or which were not weakly connected. We have not found any example of graph for which the evolution was non-convergent. All graphs yield convergent evolution for $\omega = 1$. Moreover, for all graphs it was possible to find such ω_t , that for all $\omega \in (0, \omega_t)$ the evolution is relaxing, while for $(\omega_t, 1]$ the evolution is convergent.

However, we were able to identify graphs which are non-relaxing for all $\omega \in (0, 1)$. Let us consider a star graph in figure 3. One can show, that for arbitrary $\omega \in (0, 1]$ the evolution operator F consists of at least 4 zero eigenvalues. Hence, the evolution for such graph is never relaxing. Star graphs of bigger size yield similar properties. On the other hand, we were not able to find any graph, which yields relaxing evolution for all $\omega \in (0, 1)$.

3. Convergence of global interaction case

3.1. Undirected graphs

We start this section with providing the general result for the commuting operators. The result generalizes the case of quantum stochastic walk with global interaction for all undirected graphs and for some directed graphs [22], including circulant matrices.

Proposition 3. *Let us consider equation (4) in the case of commuting Lindbladian operators \mathcal{L} and Hamiltonian H . Then the evolution operation is of the form*

$$(U \otimes \bar{U}) \exp(tD_{F_\omega})(U \otimes \bar{U})^\dagger, \quad (6)$$

where

$$D_{F_\omega} = -i(1 - \omega)(D_H \otimes \mathbb{1} - \mathbb{1} \otimes D_H) + \omega \sum_{L \in \mathcal{L}} (D_L \otimes \bar{D}_L - \frac{1}{2} \bar{D}_L D_L \otimes \mathbb{1} - \frac{1}{2} \mathbb{1} \otimes D_L \bar{D}_L) \quad (7)$$

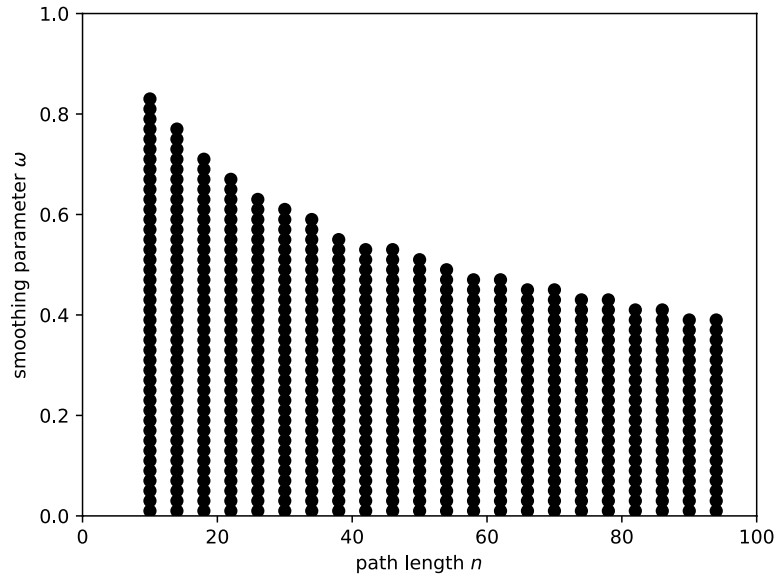


Figure 2. Values of ω for which the evolution on bidirected path graph is relaxing on local environment interaction evolution. Note that for each n there is a threshold ω_t , before which the evolution is relaxing. Numerical analysis was performed for $n = 10, 14, \dots, 94$ and for $\omega = 0.01, 0.03, \dots, 0.99$.

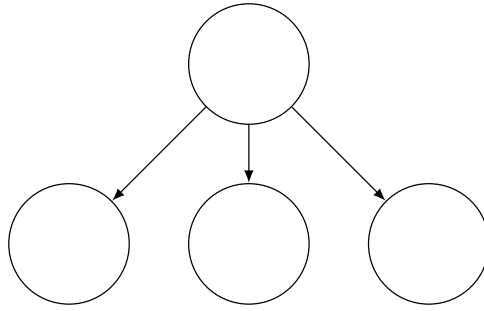


Figure 3. Star graph of size 4, which yields non-relaxing evolution for $\omega \in (0, 1]$.

is a diagonal matrix. Here we assume that U is a unitary operator and D_H, D_L are diagonal operators such that $H = UD_HU^\dagger$ and $L = UD_LU^\dagger$.

Proof. The proof comes directly from the eigendecompositions of the operators. Since all operators commute, it is possible to find common eigendecomposition with the same unitary matrix. By this we can easily find the result. \square

One can note the global interaction quantum stochastic walk on undirected graphs is a special case of the evolution described in the above theorem. In the walk model the difference comes from the size of \mathcal{L} , where we choose only single Lindbladian operator. Hence we prove a result concerning undirected graphs.

Theorem 4. *The stationary states in the GKSL master equation evolution for which $\mathcal{L} = \{H\}$ are precisely the stationary states of the pure continuous quantum evolution. The evolution is convergent for $\omega \in (0, 1]$, but not relaxing iff the system size is greater than one.*

Proof. By the model construction we have $\mathcal{L} = H$. Hence the formula equation (7) simplifies to

$$D_{F_\omega} = -i(1 - \omega)(D \otimes \mathbb{1} - \mathbb{1} \otimes D) + \omega(D \otimes D - \frac{1}{2}D^2 \otimes \mathbb{1} - \frac{1}{2}\mathbb{1} \otimes D^2). \quad (8)$$

Here we assume $H = UDU^\dagger$. Since H is Hermitian, operator D is a real-valued diagonal matrix. The diagonal entries of operator D_{F_ω} are eigenvalues which characterize the evolution. We have

$$\begin{aligned} \langle i, j | D_{F_\omega} | i, j \rangle &= -i(1 - \omega)(\langle i | D | i \rangle - \langle j | D | j \rangle) + \omega(\langle i | D | i \rangle \langle j | D | j \rangle - \frac{1}{2}(\langle i | D^2 | i \rangle + \langle j | D^2 | j \rangle)) \\ &= -i(1 - \omega)(\langle i | D | i \rangle - \langle j | D | j \rangle) - \frac{\omega}{2}(\langle i | D | i \rangle - \langle j | D | j \rangle)^2. \end{aligned} \quad (9)$$

Note $-i(1 - \omega)(\langle i | D | i \rangle - \langle j | D | j \rangle)$ corresponds to purely Hamiltonian evolution, and hence to continuous quantum walk. Since 0-eigenvalues of F_ω correspond to 0-eigenvalues of H Hamiltonian part of the system, which furthermore correspond to the stationary states of the continuous-time quantum walk, we obtained the first part of the theorem.

Note that there are no purely imaginary eigenvalues of F_ω . Hence, we have that the evolution is convergent. Since the set of stationary states of continuous-time quantum walk of size n has at least n elements, we obtain that QSW with global interaction is never relaxing. \square

Note that the result from the above theorem implies that we can generate the stationary states from the continuous quantum walk by adding the same Lindbladian operator.

Remark 5. Global interaction case QSW is convergent, but not relaxing for arbitrary undirected graph with number of vertices greater than one 1 and for arbitrary $\omega \in (0, 1]$. Furthermore, the stationary states are precisely those from CQW.

In the next section we show that theorem 4 cannot be generalized for directed graphs.

3.2. Directed graphs

In this section we provide an example of a directed graph for which we do not necessary obtain a stationary state. It has been proven that the evolution converges for arbitrary initial state iff all nonzero eigenvalues of F_ω have a negative real part [33, theorem 5.4]. We found an example of a digraph which does not satisfy the condition, and provide an exemplary initial state which results in non-convergent evolution. One should note, that it is possible (and more probable) to find non-convergent states.

Theorem 6. *Let us take the evolution for which the only Lindbladian operator is an adjacency matrix of the directed graph and the Hamiltonian is an adjacency matrix of the underlying graph. Then there exists a directed graph G and an initial state ϱ_0 for which the evolution is non-convergent for an arbitrary value of the smoothing parameter $\omega \in (0, 1]$.*

Proof. As an example we choose a circulant graph of size $4k$ for $k > 1$ and with extra jump every two vertices. An example for $k = 2$ is presented in figure 4. The graph and its underlying graph are circulant matrices. Therefore, we can use equation (7) to find out that there exists one eigenvalue of the form $2(1 - \omega)i$ with corresponding eigenvector $|C_k\rangle\overline{|C_{2k}\rangle}$, where $\overline{(\cdot)}$ denotes the element-wise conjugation and $|C_i\rangle$ is the i -th eigenvector of a circulant matrix of

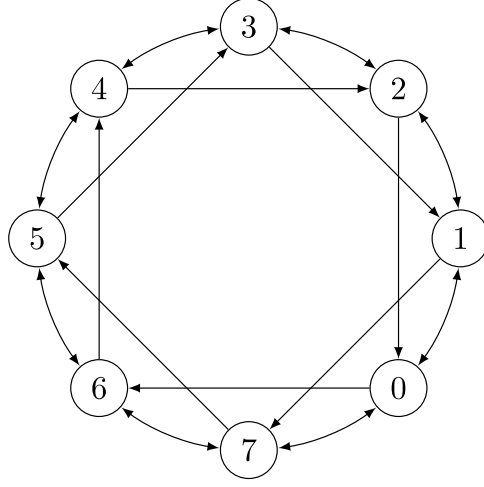


Figure 4. An example of strongly connected directed graph, for which the global interaction case evolution is not convergent.

the form

$$|C_i\rangle = \frac{1}{2\sqrt{k}} \sum_{j=0}^{4k} \exp\left(\frac{2\pi i j}{4k-1}\right) |i\rangle. \quad (10)$$

We need to find a matrix which is not orthogonal to $|C_k\rangle\langle C_{2k}|$. Our exemplary initial state is

$$\varrho_0 = \frac{1}{2}(|C_k\rangle + |C_{2k}\rangle)(\langle C_k| + \langle C_{2k}|). \quad (11)$$

The ϱ_t takes the form

$$\varrho_t = \frac{1}{2}(|C_k\rangle\langle C_k| + |C_{2k}\rangle\langle C_{2k}| + e^{2i(1-\omega)t}|C_k\rangle\langle C_{2k}| + e^{-2i(1-\omega)t}|C_{2k}\rangle\langle C_k|). \quad (12)$$

Since ϱ_t is periodic with period $\frac{\pi}{(1-\omega)}$, we obtain the result. \square

Note, that for different t we can obtain different states in the sense of possible measurement output. For example we have $\langle 0|\varrho_0|0\rangle = \frac{1}{2k}$, but at the same time we have $\langle 0|\varrho(\frac{\pi}{2(1-\omega)})|0\rangle = 0$.

Remark 7. The evolution for which the only Lindbladian operator is an adjacency matrix of the directed graph and the Hamiltonian is an adjacency matrix of the underlying graph, does not converge in general, even in the sense of the canonical measurement probability distribution.

Circulant graphs provide an infinite collection of directed graphs for which the convergence does not hold. Note that the example used in the proof is strongly connected directed graph. This shows, that the convergence in the local interaction case does not imply the convergence in the global interaction case.

Contrary, it is very difficult to find a directed graph for which the convergence does not hold. We have made numerical analysis for Erdős–Rényi model $\mathcal{G}(n, 0.5)$ for $n = 10, 15, \dots, 45$ and

for $\omega = 0.05, 0.1, \dots, 1$. We have guaranteed that the graph is weakly connected by ignoring such cases if they appear. For each n we chose 200 graphs and we have not found any graph which is not convergent. At the same time it is possible to find the relaxing evolution. We were not able to identify graph properties causing such behaviour. From all 1600 graphs, 1599 were relaxing for all value of ω , and there was one graph of size 10 which was relaxing for $\omega \in \{0.05, \dots, 0.95\}$ and convergent for $\omega = 1$. Therefore, relaxing property is statistically common for directed graphs in the global environment interaction case.

4. Convergence of non-moralizing global interaction case

4.1. Non-convergent in the space state

The non-moralizing model has been introduced in [16] and provides a similar example of a graph and initial state such that it does not converge. Similarly we found a digraph, for which an evolution operator $S_{t,\omega}$ has an imaginary part. Again, it is easy to find a state for which the evolution is non-convergent.

Theorem 8. *Let us take the non-moralizing evolution described in [16]. Then there exists a directed graph G and initial state q_0 for which the evolution is periodic in time for an arbitrary value of the smoothing parameter $\omega \in (0, 1]$.*

Proof. Let us take a graph presented in figure 5. Using the scheme presented in [16], new graph will consist of five copies of vertex v_0 , two copies of vertices v_4 and v_5 , and a single copy of other vertices. As the orthogonal matrices we choose the Fourier matrices and in order to remove the premature localization we choose the rotating Hamiltonian \tilde{H}_{rot} constructed from the Hamiltonians of the form

$$\begin{bmatrix} 0 & i & & & \\ -i & \ddots & \ddots & & \\ & \ddots & \ddots & i & \\ & & & -i & 0 \end{bmatrix}. \quad (13)$$

Let us choose two eigenvectors of the rotating Hamiltonian

$$|\lambda_{\tilde{H}_{\text{rot}}}^1\rangle = \frac{1}{2\sqrt{3}}|v_0^0\rangle - \frac{i}{2}|v_0^1\rangle - \frac{1}{\sqrt{3}}|v_0^2\rangle + \frac{i}{2}|v_0^3\rangle + \frac{1}{2\sqrt{3}}|v_0^4\rangle, \quad (14)$$

$$|\lambda_{\tilde{H}_{\text{rot}}}^2\rangle = \frac{1}{2\sqrt{3}}|v_0^0\rangle - \frac{i}{2}|v_0^1\rangle - \frac{1}{\sqrt{3}}|v_0^2\rangle + \frac{i}{2}|v_0^3\rangle + \frac{1}{2\sqrt{3}}|v_0^4\rangle. \quad (15)$$

One can show that the vectors $|\lambda_{\tilde{H}_{\text{rot}}}^1\rangle, \bar{\lambda}_{\tilde{H}_{\text{rot}}}^1\rangle, |\lambda_{\tilde{H}_{\text{rot}}}^2\rangle, \bar{\lambda}_{\tilde{H}_{\text{rot}}}^2\rangle, |\lambda_{\tilde{H}_{\text{rot}}}^3\rangle, \bar{\lambda}_{\tilde{H}_{\text{rot}}}^3\rangle, |\lambda_{\tilde{H}_{\text{rot}}}^4\rangle, \bar{\lambda}_{\tilde{H}_{\text{rot}}}^4\rangle$ are the eigenvectors of the increased evolution operator $S_{t,\omega}$ for arbitrary $\omega \in (0, 1]$. Corresponding eigenvalues are respectively $0, -2i\sqrt{3}\omega, 2i\sqrt{3}\omega, 0$. Similarly to the example presented in the previous section, the state

$$\tilde{q}_0 = \frac{1}{2}(|\lambda_{\tilde{H}_{\text{rot}}}^1\rangle + |\lambda_{\tilde{H}_{\text{rot}}}^2\rangle)(\langle\lambda_{\tilde{H}_{\text{rot}}}^1| + \langle\lambda_{\tilde{H}_{\text{rot}}}^2|) \quad (16)$$

is the required initial state. The state after time t takes the form

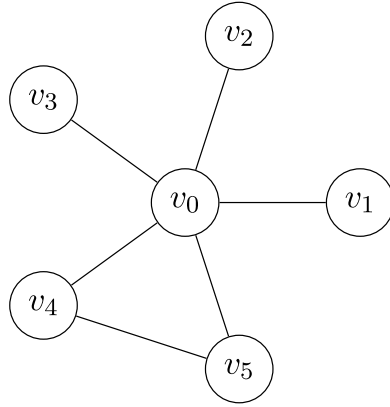


Figure 5. An example of graph for which non-moralizing global interaction evolution is not convergent.

$$\tilde{\varrho}_t = \frac{1}{2}(|\lambda_{\tilde{H}_{\text{rot}}}^1\rangle\langle\lambda_{\tilde{H}_{\text{rot}}}^1| + e^{-2it\sqrt{3}\omega}|\lambda_{\tilde{H}_{\text{rot}}}^1\rangle\langle\lambda_{\tilde{H}_{\text{rot}}}^2| + e^{2it\sqrt{3}\omega}|\lambda_{\tilde{H}_{\text{rot}}}^2\rangle\langle\lambda_{\tilde{H}_{\text{rot}}}^1| + |\lambda_{\tilde{H}_{\text{rot}}}^2\rangle\langle\lambda_{\tilde{H}_{\text{rot}}}^2|). \quad (17)$$

The function $\tilde{\varrho}_t$ is periodic with period $\frac{\pi}{\sqrt{3}\omega}$, hence we obtained the result. \square

4.2. Convergence in the sense of the measurement

The example from theorem 8, the probability distribution obtained from the measurement in the canonical basis of the system changes in time. However, when we analyse the canonical measurement from [16], where as the measurement operators we choose the projections onto the subspaces corresponding to different vertices, we can observe that the probability does not change—in this case the probability of measuring vertex v_0 for each time point is one.

We have performed numerical analysis for graphs of size $n = 9$ from Erdős–Rényi $\mathcal{G}(n, 0.5)$ model for $\omega \in \{0, 0.1, \dots, 1\}$. We have checked 200 random graphs and the non-moralizing QSW on each of them was convergent.

Conjecture. Let us choose the non-moralizing evolution model. Let $\Pi(\varrho_0, t)$ denotes the probability distribution of canonical measurement onto the subspaces of vertices in time t with the initial state ϱ_0 . Then for arbitrary ϱ_0 there exists probability distribution Π_∞ such that

$$\lim_{t \rightarrow \infty} \Pi(\varrho_0, t) = \Pi_\infty. \quad (18)$$

Note, that the probability distribution may be nonunique. To see that let us analyse the graph presented in figure 6. We choose $\omega = \frac{1}{2}$ and two initial states $\tilde{\varrho}_0 = |v_6^0\rangle\langle v_6^0|$ and $\tilde{\varrho}_1 = |v_7^0\rangle\langle v_7^0|$. We have found the limiting probability distribution

$$\Pi_0 := \lim_{t \rightarrow \infty} \Pi(\varrho_0, t), \quad (19)$$

$$\Pi_1 := \lim_{t \rightarrow \infty} \Pi(\varrho_1, t). \quad (20)$$

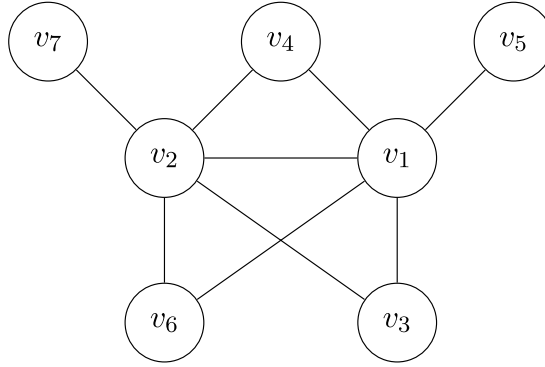


Figure 6. Graph for which there exists two different stationary states in the sense of the natural measurement. The states can be obtained by starting in vertices v_7 and v_6 .

The probability distributions differs, for example $\Pi_0(v_0) = 0.666\,616$ and $\Pi_1(v_0) = 0.118\,97$.

4.3. The digraph structure observance

In [16] it was suggested, that the non-moralizing global environment interaction QSW can be applied for modelling the walk on directed graphs. Moreover, an example suggesting that the original global interaction evolution, where Lindbladian operator is an adjacency matrix of the directed graph, does not preserve the digraph structure have been provided. Let us take the graph from figure 7(a) and let us analyse the graph without the Hamiltonian. One can find that

$$\frac{1}{4}(|v_1\rangle - |v_2\rangle)(\langle v_1| - \langle v_2|) + \frac{1}{2}|v_3\rangle\langle v_3| \quad (21)$$

is in proper stationary state. There is a nonzero probability of measuring the state in vertex v_1 and v_2 . Thus, one can see that the superoperator constructed using a directed graphs can lead to the evolution on some other structure, namely the directed moral graph. This behaviour, expected in the case when the Hamiltonian part is present, is surprising in the pure Lindbladian case.

For the purpose of quantifying this behaviour we introduce the following property of the evolution on directed graphs.

Property (Digraph structure observance). Let us assume that for an arbitrary vertex there is a path to some sink vertex. We say that the evolution on a directed graph has the *digraph structure observance* property if an arbitrary initial state converges to the state spanned by vectors corresponding to the sink vertices from the condensation of the graph.

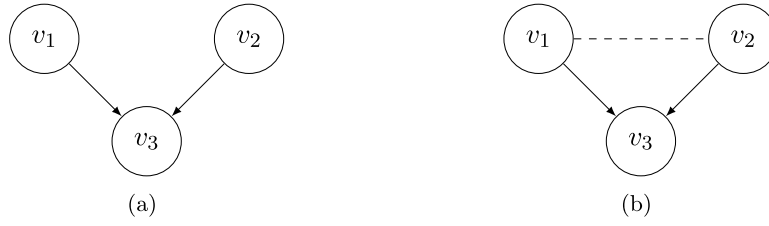
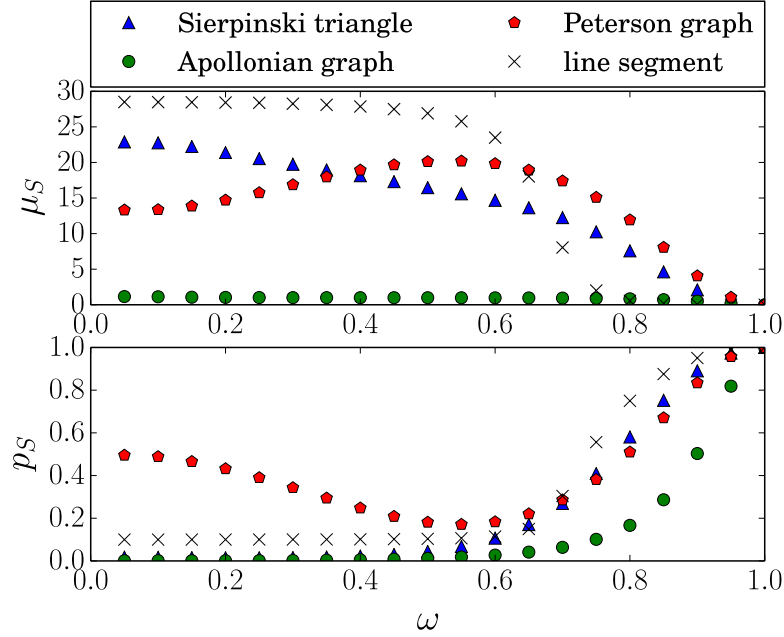
We require that the evolution on the directed graph, at least for the Lindbladian part, should have the digraph structure observance property.

One should note that digraph structure observance can be quantified for any directed graph using additional sink vertices attached to the original vertices.

In the case of the example in figure 7 the arbitrary state should converge to the state $|v_3\rangle\langle v_3|$.

The unintuitive stationary state in equation (21) comes from the spontaneous moralization of the graph [16]. Since the moralization of the graph was corrected, it is necessary to check whether the improper stationary state still occurs in the non-moralizing evolution. This can be achieved by analysing the stationary states.

The numerical analysis was performed as follows. Let S be a set of all sink vertices. We start in some vertex with nonzero outdegree. We determine the state ϱ_∞ for large time value

**Figure 7.** Visualisation of a directed graph and (a) its spontaneous moralization (b).**Figure 8.** Top plot shows the second moment of the distance from the vertex to the closest sink vertex. Bottom plot shows the probability of measuring the only single sink vertex for large time graphs. Sierpinski triangle has 15 vertices, Apollonian graph has 12 vertices and length of path graph equals 10.

and we verified numerically, whether it is close to the stationary state in the sense of probability distribution of measurement. Then we compute the cumulated probability of measuring the state in the sink vertices

$$p_S(\varrho_\infty) = \sum_{v \in \bigcup S(G)} \langle v | \varrho_\infty | v \rangle \quad (22)$$

and the second moment of the distance from the sink vertices

$$\mu_S(\varrho_\infty) = \sum_{v \in V} d^2(v, S) \langle v | \varrho_\infty | v \rangle, \quad (23)$$

where $d(v, S)$ is the length of the shortest path from v to closest sink vertex, i.e. $d(v, S) = \min_{s \in \bigcup S(G)} d(v, s)$. We say, that the greater the value of p_S and the lower the value of μ_S are, the more the evolution preserves the graph.

We have analysed the evolution for $\omega \in (0, 1]$. For the purpose of our analysis we have selected four types of graphs, namely: a path graph, the Petersen graph, the Apollonian graph,

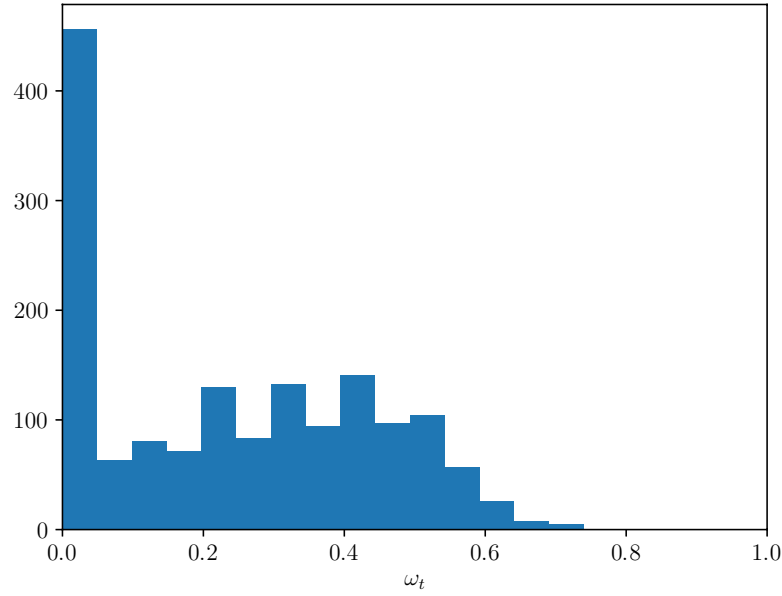


Figure 9. Histogram presents amount of graphs $\mathcal{G}(n, 0.2)$ with $n = 9, 11, 12$ having particular ω_0 .

and the Sierpinski triangle. We choose the orientation of the graphs such that each vertex is either a sink vertex, or there is a path from it to some sink vertex.

The obtained results are presented in figure 8. One can see that the larger the value of ω is, the more probability cumulates in the close neighbourhood of the sink vertices. In these examples for $\omega \in [0.7, 1]$, μ_S and p_S respectively decreases and grows with ω . One can also notice that in the $\omega \rightarrow 1$ limit the p_S converge to one and μ_S vanishes. The above analysis suggests that when $\omega = 1$, the directed graph structure is fully preserved.

We have completed further analysis for Erdős–Rényi graphs $\mathcal{G}(n, 0.2)$ with $n = 9, 11, 12$, for each size 500 samples. In all of these graphs for $\omega = 1$ we have $p_S = 1$ and $\mu_S = 0$, which suggests that at least for this extreme value of ω the digraph structure is observed.

Furthermore, we have searched for the ω_0 , for which for all $\omega > \omega_0$ both measures p_S and μ_S were monotonic in ω . We were selecting random graphs $\mathcal{G}(n, 0.2)$ with $n = 9, 11, 12$ and next we were calculating p_S and μ_S for ω from 1 to 0 with step -0.02 . When p_S started increasing or μ_S started decreasing we stopped the calculations and save ω_0 . The statistics of the threshold ω_0 is presented in figure 9. We have found no graph, for which $\omega_0 > 0.7$. This may suggest that for $\omega > 0.7$ structure of the directed graph is preserved at least for given sizes of the digraphs. However, to provide more information about this behaviour more detailed analysis is necessary.

5. Concluding remarks

In this article we analysed three cases of QSW: with local interaction, with global interaction and with non-moralizing global interaction. As for local interaction case our results generalize the results from [17]. We prove that the evolution is relaxing in the case of undirected graphs. We also show that the result can be extended to arbitrary strongly connected digraph and for weakly connected digraphs with one sink in the condensation graph. Furthermore, we show

that for strongly connected digraphs the stationary state is located in the interior. At the same time we provide a counterexample demonstrating that the result cannot be extended to all directed graphs.

Global interaction case QSW is convergent, but never relaxing for arbitrary undirected graph with number of vertices greater than one 1 and for arbitrary $\omega \in (0, 1]$. Furthermore the stationary states are precisely those from CQW. We show by example, that the result cannot be extended into arbitrary directed graphs. Surprisingly, applying the Hamiltonian may help relax the evolution.

In the non-moralizing global interaction case we provide examples demonstrating that the evolution does not need to be relaxing, or even convergent, even for undirected graphs. We also give an example of evolution, for which the evolution is not relaxing, even in the sense of canonical measurement. However, we conjecture by numerical analysis, that the evolution is convergent in the sense of the canonical measurement.

For the purpose of analysing digraph structure observance we have introduced a sink observance property. This property can be quantified by analysing the probability of measuring the state in the sink vertex and its neighbourhood. We argue that the bigger the probability of measuring the state in sink vertex or its closes neighbourhood, the better the structure observance. Since the Lindblad operators corresponds to the directed graph structure, we expect, that for ω close to 1 the probability of measuring the sink vertex is one. For the global interaction case the digraph structure is not preserved, even for a very simple example. Fortunately, the digraph observance is recovered in the non-moralizing global interaction case.

Acknowledgments

This work has been supported by the Polish National Science Centre under project number 2011/03/D/ST6/00413.

ORCID iDs

Adam Glos  <https://orcid.org/0000-0001-6320-7699>

Jarosław Adam Miszczak  <https://orcid.org/0000-0001-8790-101X>

Mateusz Ostaszewski  <https://orcid.org/0000-0001-7915-6662>

References

- [1] Aharonov D, Ambainis A, Kempe J and Vazirani U 2001 Quantum walks on graphs *Proc. Thirty-Third Annual ACM Symp. on Theory of Computing (ACM)* pp 50–9
- [2] Childs A M, Farhi E and Gutmann S 2002 An example of the difference between quantum and classical random walks *Quantum Inf. Process.* **1** 35–43
- [3] Szegedy M 2004 Quantum speed-up of markov chain based algorithms *Proc.: 45th Annual IEEE Symp. on Foundations of Computer Science (IEEE)* pp 32–41
- [4] Attal S, Petruccione F, Sabot C and Sinayskiy I 2012 Open quantum random walks *J. Stat. Phys.* **147** 832–52
- [5] Portugal R, Santos R A, Fernandes T D and Gonçalves D N 2016 The staggered quantum walk model *Quantum Inf. Process.* **15** 85–101
- [6] Whitfield J D, Rodríguez-Rosario C A and Aspuru-Guzik A 2010 Quantum stochastic walks: a generalization of classical random walks and quantum walks *Phys. Rev. A* **81** 022323
- [7] Loke T, Tang J, Rodriguez J, Small M and Wang J 2017 Comparing classical and quantum pageranks *Quantum Inf. Process.* **16** 25

- [8] Sánchez-Burillo E, Duch J, Gómez-Gardenes J and Zueco D 2011 Quantum navigation and ranking in complex networks *Sci. Rep.* **2** 605–5
- [9] Paparo G D, Müller M, Comellas F and Martin-Delgado M 2014 Quantum google algorithm *Eur. Phys. J. Plus* **129** 150
- [10] Childs A M and Goldstone J 2004 Spatial search by quantum walk *Phys. Rev. A* **70** 022314
- [11] Childs A M, Cleve R, Deotto E, Farhi E, Gutmann S and Spielman D A 2003 Exponential algorithmic speedup by a quantum walk *Proc. Thirty-Fifth Annual ACM Symposium on Theory of Computing* (ACM) pp 59–68
- [12] Shenvi N, Kempe J and Whaley K B 2003 Quantum random-walk search algorithm *Phys. Rev. A* **67** 052307
- [13] Glos A, Kukulski R, Krawiec A and Puchała Z 2017 Vertices cannot be hidden from quantum spatial search for almost all random graphs (arXiv:1709.06829)
- [14] Magniez F, Santha M and Szegedy M 2007 Quantum algorithms for the triangle problem *SIAM J. Comput.* **37** 413–24
- [15] Chia A, Górecka A, Tan K C, Paweł Ł, Kurzyński P, Paterek T and Kaszlikowski D 2016 Coherent chemical kinetics as quantum walks i: reaction operators for radical pairs *Phys. Rev. E* **93** 032407
- [16] Domino K, Glos A and Ostaszewski M 2017 Superdiffusive quantum stochastic walk definable on arbitrary directed graph *Quantum Inf. Comput.* **17** 973–86
- [17] Liu C and Balu R 2017 Steady states of continuous-time open quantum walks *Quantum Inf. Process.* **16** 173
- [18] Nayak A and Vishwanath A 2000 Quantum walk on the line (arXiv:quant-ph/0010117)
- [19] Konno N 2005 A new type of limit theorems for the one-dimensional quantum random walk *J. Math. Soc. Japan* **57** 1179–95
- [20] Sadowski P and Paweł Ł 2016 Central limit theorem for reducible and irreducible open quantum walks *Quantum Inf. Process.* **15** 2725–43
- [21] Sadowski P, Miszcza J A and Ostaszewski M 2016 Lively quantum walks on cycles *J. Phys. A: Math. Theor.* **49** 375302
- [22] Domino K, Glos A, Ostaszewski M, Paweł Ł and Sadowski P 2016 Properties of quantum stochastic walks from the asymptotic scaling exponent (arXiv:1611.01349)
- [23] Bringuier H 2017 Central limit theorem and large deviation principle for continuous time open quantum walks *Ann. Henri Poincaré* **18** 3167
- [24] Cowell R G, Dawid A P, Lauritzen S L and Spiegelhalter D J 1999 *Building, Using Probabilistic Networks* (New York: Springer) pp 25–41
- [25] Studeny M 2001 On mathematical description of probabilistic conditional independence structures *PhD Thesis* Institute of Information Theory and Automation, Academy of Sciences of the Czech Republic
- [26] Erdős P and Rényi A 1960 On the evolution of random graphs *Publ. Math. Inst. Hung. Acad. Sci.* **5** 17–60
- [27] Kossakowski A 1972 On quantum statistical mechanics of non-hamiltonian systems *Rep. Math. Phys.* **3** 247–74
- [28] Lindblad G 1976 On the generators of quantum dynamical semigroups *Commun. Math. Phys.* **48** 119–30
- [29] Gorini V, Kossakowski A and Sudarshan E C G 1976 Completely positive dynamical semigroups of n-level systems *J. Math. Phys.* **17** 821–5
- [30] Schirmer S G and Wang X 2010 Stabilizing open quantum systems by Markovian reservoir engineering *Phys. Rev. A* **81** 062306
- [31] Miszcza J A 2011 Singular value decomposition and matrix reorderings in quantum information theory *Int. J. Mod. Phys. C* **22** 897–918
- [32] Spohn H 1977 An algebraic condition for the approach to equilibrium of an open n-level system *Lett. Math. Phys.* **2** 33–8
- [33] Rivas A and Huelga S F 2012 *Open Quantum Systems* (Berlin: Springer)