

See discussions, stats, and author profiles for this publication at: <https://www.researchgate.net/publication/322306042>

QSWALK.JL: Julia package for quantum stochastic walks analysis

Article in Computer Physics Communications · January 2018

DOI: 10.1016/j.cpc.2018.09.001

CITATIONS

7

READS

229

3 authors:



Adam Glos

Polish Academy of Sciences

46 PUBLICATIONS 195 CITATIONS

SEE PROFILE



Jarosław Adam Miszczak

Institute of Theoretical and Applied Informatics, Polish Academy of Sciences

92 PUBLICATIONS 979 CITATIONS

SEE PROFILE



Mateusz Ostaszewski

Polish Academy of Sciences

21 PUBLICATIONS 512 CITATIONS

SEE PROFILE

Some of the authors of this publication are also working on these related projects:



Analysis of patent activity in the field of quantum information processing [View project](#)



Spectral analysis of random complex networks [View project](#)

QSWALK.JL: Julia package for quantum stochastic walks analysis

Adam Glos^{a,b,*}, Jarosław Adam Miszczak^a, Mateusz Ostaszewski^{a,b}

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

^b*Institute of Informatics, Silesian University of Technology
Akademicka 16, 44-100 Gliwice, Poland*

Abstract

The presented paper describes QSWALK.JL package for Julia programming language, developed for the purpose of simulating the evolution of open quantum systems. The package enables the study of quantum procedures developed using stochastic quantum walks on arbitrary directed graphs. We provide a detailed description of the implemented functions, along with a number of usage examples. The package is compared with the existing software offering a similar functionality.

Keywords: directed graph, moral graph, quantum walk, open quantum system.

PROGRAM SUMMARY

Program Title: QSWALK.JL

Licensing provisions: MIT

Distribution format: Source code available at <https://github.com/QuantumWalks/QSWalk.jl>

Programming language: Julia

Nature of problem: The package implements functions for simulating quantum stochastic walks, including local regime, global regime, and nonmoralizing global regime [1]. It can be used for arbitrary quantum continuous evolution based on GKSL master equation on arbitrary graphs.

Solution method: We utilize Expokit routines for fast sparse matrix exponentials on vectors. For dense matrices exponentiation is computed separately, which is faster for small matrices.

Restrictions: Currently package requires Julia v0.6.

1. Introduction

During the last few years JULIA programming language [2, 3, 4] became highly popular in the scientific computing community because of its dynamical style of programming, combined

*Corresponding author.

E-mail address: aglos@iitis.pl

with strong typing and high efficiency. As such it provides a very attractive platform for simulating models used in quantum information processing.

In this paper we focus on the particular model used to study the dynamics of quantum systems, namely quantum stochastic walks. The model is used to study quantum-to-classical transition and to probe the influence of quantum evolution on the efficiency of information processing [5]. Quantum stochastic walks have been widely analysed in context of propagation [6, 7, 5, 1, 8], application in computer science [9, 10, 11] and physics [12, 13, 14]. In particular, new model of fast-propagating quantum walk on arbitrary directed graph was developed [1, 6]. To this end, we describe a package for JULIA programming language developed for the purpose of simulating and analyzing quantum stochastic walks [15] and we compare its efficiency with the existing software.

The main goal of the report is to describe a package QSWALK.JL for JULIA programming language which enables high-performance analysis of quantum stochastic walks. There are three main advantages of the presented package over the existing software. First, it enables the simulation of quantum stochastic walks analysis in both local and global regimes [6]. Second, it is the first package providing the implementation of the nonmoralizing evolution. Thus, it enables the simulation of fast continuous-time quantum walk model on arbitrary directed graph [1]. Finally, the presented package can be used to perform numerical experiments for very large graphs thanks to sparse matrices implementation used. This is especially important for investigating the statistical properties of complex graphs.

Comparison with the existing software. Many software packages for simulating quantum computing [16], including some focused on various models of quantum walks [17, 18, 19, 10] are available. Most of them are focused on the discrete-time evolution, restricted to the unitary operations and undirected graphs. The first exception is QSWALK.M package [10] for *Wolfram Mathematica*, which provides implementation of a quantum stochastic walk model. Package QSWALK.M utilizes `MatrixExp` function and sparse representation of superoperators for simulating the evolution of quantum stochastic walks. It provides the basic functionality required to simulate quantum stochastic walks. However, it has limitations related to the performance of simulation of high dimensional systems, see Sec. 4.5. In contrast, the package described in this paper enables the simulation of much larger systems. This is crucial for the analysis of complex networks and the analysis of the convergence on large graphs. Moreover, the presented package facilitates the analysis of the quantum stochastic walks by providing access to the functions for constructing generators of the dynamical subgroup and the superoperators. Moreover, it provides the implementation of non-moralizing evolution [1]. Additionally, JULIA is an open-source programming language and can be used for free for academic as well as commercial purposes.

2. Theoretical background

Before describing the functions provided by QSWALK.JL package, we review essential theoretical concepts used to define *quantum stochastic walks*. This model of quantum evolution defines the family of quantum processes in the discrete state space and with the continuous time parameter.

First, we recall the definition of the GKSL master equation, which describes the continuous evolution of the open quantum system. Next, we introduce quantum stochastic walks and briefly describe the local and global interaction regimes. Finally, we describe spontaneous moralization which is a side-effect of using global interaction model on directed graphs.

2.1. GKSL master equation

The starting point for introducing quantum stochastic walks is the Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation [20, 21, 22]

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

where 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. Operator ϱ is the density matrix representing the state of the system. While the Hamiltonian operator needs to be Hermitian, there is no general requirement on Lindblad operators $L \in \mathcal{L}$. This master equation describes the general continuous evolution of mixed quantum states.

In the case where H and \mathcal{L} do not depend on time, we say that Eq. (1) describes the Markovian evolution of the system. Henceforth, we can solve the differential equation analytically. If we choose initial state $\varrho(0)$, then

$$|\varrho(t)\rangle\rangle = \exp(tF)|\varrho(0)\rangle\rangle, \quad (2)$$

where

$$F = (H \otimes \mathbf{I} - \mathbf{I} \otimes \bar{H}) + \sum_{L \in \mathcal{L}} \left(L \otimes \bar{L} - \frac{1}{2} (L^\dagger L \otimes \mathbf{I} + \mathbf{I} \otimes L^\dagger L) \right) \quad (3)$$

and $|\cdot\rangle\rangle$ denotes the vectorization of the matrix [23]. We call F the *evolution generator* and corresponding $\exp(tF)$ a *superoperator*.

Since H and \mathcal{L} describe closed and open system evolution respectively, it is interesting how the change of impact of these parts affects the evolution. Hence we add smoothing parameter $\omega \in [0, 1]$ and change Eq. (1) into

$$\frac{d}{dt}\varrho = -i(1 - \omega)[H, \varrho] + \frac{1}{2}\omega \sum_{L \in \mathcal{L}} (2L\varrho L^\dagger - L^\dagger L\varrho - \varrho L^\dagger L). \quad (4)$$

The evolution generator F and the superoperator $\exp(tF)$ changes analogically. Note that for $\omega = 0$ we recovered the closed system evolution and for $\omega = 1$ we have the purely open evolution.

2.2. Quantum stochastic walks

The GKSL master equation describes the general form of the evolution of the open quantum system. If one introduces the Hamiltonian and the Lindblad operators using graphs as the underlying structure, the resulting process can be understood as the walk evolution.

In this manner, GKSL master equation was used for defining quantum stochastic walks. This model of evolution provides the generalization of both classical random walks and quantum walks [15]. In this case H and \mathcal{L} in Eq. (1) are constructed using the graph structure. However, one may verify that the choice of Lindblad operators may be non-unique [15, 5].

Let us suppose a directed graph $G = (V, A)$ is given, with $V = \{v_1, \dots, v_n\}$. By $\bar{G} = (V, E)$ we denote the underlying undirected graph of G . Two main variants of quantum stochastic walks can be distinguished. In the *local environment interaction case* each Lindblad operator corresponds to a single edge, $\mathcal{L}^l = \{|w\rangle\langle v| : (v, w) \in A\}$. On the other hand, in the *global environment interaction case* we choose a single Lindblad operator $\mathcal{L}^g = \{\sum_{(v,w) \in A} |w\rangle\langle v|\}$. In both models we choose the Hamiltonian H to be the adjacency matrix of the underlying graph \bar{G} . Both models were analyzed in context of propagation [8, 5] and convergence [7, 6, 1].

Furthermore, the global interaction was analyzed in the context of graph preservation. Let us fix global interaction evolution with Hamiltonian H and a single Lindblad operator L . It can be demonstrated [1] that if two nodes have a common child, then other amplitude transitions appear between them. This effect is presented in Fig. 1. To remove such undesirable effect, the following correction scheme has been proposed.

1. For each vertex v_i create $\text{outdeg}(v_i)$ copies, denoted as $\tilde{v}_i^0, \dots, \tilde{v}_i^{\text{outdeg}(v_i)-1}$. If $\text{outdeg}(v_i) = 0$, we create single copy \tilde{v}_i^0 .
2. Construct Hamiltonian \tilde{H} as

$$\langle \tilde{v}_i^k | \tilde{H} | \tilde{v}_j^l \rangle = \begin{cases} \langle v_i | H | v_j \rangle, & \{v_i, v_j\} \in E, \\ 0, & \text{otherwise.} \end{cases} \quad (5)$$

Note that for $\{v_i, v_j\} \in E$ other values may be chosen, but other elements should be essentially equal to zero in order to preserve the underlying graph structure.

3. Construct Lindblad operator \tilde{L} as

$$\langle \tilde{v}_i^k | \tilde{L} | \tilde{v}_j^l \rangle = \langle v_i | L | v_j \rangle \langle k | A_i | j \rangle. \quad (6)$$

Here A_i is a matrix which columns are pairwise orthogonal. Such definition captures the digraph structure.

4. Construct an additional, acting locally, Hamiltonian \tilde{H}_{loc} for which $\langle \tilde{v}_i^k | \tilde{H}_{\text{loc}} | \tilde{v}_j^l \rangle = 0$ for $i \neq j$.

The non-moralizing evolution obtained as the result of the above construction takes the form

$$\frac{d}{dt} \tilde{\rho} = -i(1 - \omega)[\tilde{H}, \tilde{\rho}] + \frac{1}{2}\omega \left(-i2[\tilde{H}_{\text{loc}}, \tilde{\rho}] + 2\tilde{L}\tilde{\rho}\tilde{L}^\dagger - \tilde{L}^\dagger\tilde{L}\tilde{\rho} - \tilde{\rho}\tilde{L}^\dagger\tilde{L} \right). \quad (7)$$

Note that the system enlarges, hence we need to adjust the representation of the initial state. For this reason, the canonical measurement corresponding to the vertices of original G graph takes the form

$$p(v_i) = \sum_k \langle \tilde{v}_i^k | \tilde{\rho}_t | \tilde{v}_i^k \rangle, \quad (8)$$

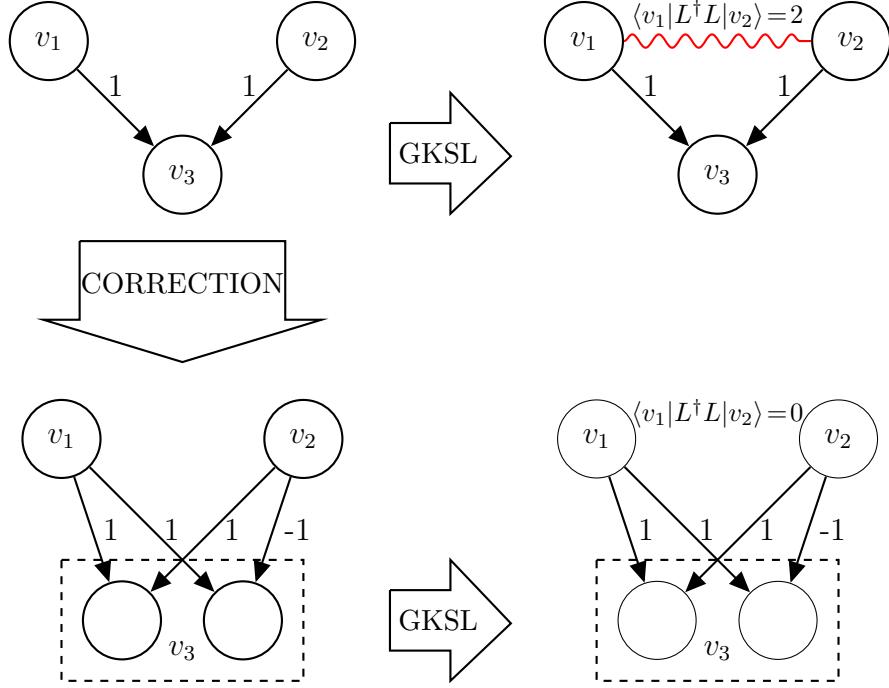


Figure 1: In the global interaction case the direct application of adjacency matrices results in an additional coherent transition. In the example above, another connection between v_1 and v_2 appears. The application of the correction procedure described in [1] enables the removal of such connections. Note that the correction creates additional nodes, which in turn result in the system enlargement.

where k goes over all copies of v_i . This is equivalent to the probability of measuring any of the copy of the vertex.

Note that for $\mathcal{L} = \emptyset$ case one can recover the original continuous quantum walk on mixed states. Hence, the model of quantum stochastic walk provides a generalization of the quantum walks in closed systems. In this case another numerical method based on formula

$$\varrho(t) = \exp(-iHt)\varrho(0)\exp(iHt) \quad (9)$$

can be applied. Here the exponentiation is computed for $n \times n$ matrix instead of $n^2 \times n^2$ matrix as in Eq. (2).

3. Package description

In this section we provided the description of QSWALK.JL package and the dependences required to run simulations created using it. We provide a detailed description of all its functions present a typical work-flow required to utilize the package.

3.1. Installation and recommended packages

QSWALK.JL package can be installed by issuing

```
julia> Pkg.clone("git://github.com/ZKSI/QSWalk.jl.git")
```

within the interpreter. Package QSWALK.JL requires EXPOKIT.JL package [24], which implements the method for calculating matrix exponent described in [25]. Package EXPOKIT.JL will be installed automatically during QSWALK.JL installation.

It is recommended to install IJULIA.JL package, which facilitates interactive development. This package can be installed using

```
julia> Pkg.add("IJulia")
```

command. Package IJULIA.JL provides browser-based development environment. In order to start IJULIA.JL session one has to execute commands

```
julia> using IJulia
julia> notebook(detached=true)
```

issued in the interactive JULIA console environment. Directory examples in QSWALK.JL distribution contains files with .ipynb extensions, which can be loaded using a web browser with running IJULIA.JL session. The directory contains standard JULIA files with .jl extension as well.

Additionally, we recommend LIGHTGRAPHS.JL package [26], which provides rich graph related functionality. In particular, it provides the methods for generating random graphs and their adjacency matrices. The examples distributed with the package utilize PYPLOT.JL module [27] for creating plots. The packages are necessary for running the provided exemplary scripts. One should note that both LIGHTGRAPHS.JL and PYPLOT.JL modules can be installed using Pkg.add function. Examples in .ipynb extensions need GRAPHPLOT.JL and TIKZGRAPHS.JL modules additionally.

3.2. Provided functions

Below we provide the description of the functionality implemented by QSWALK.JL package. The package introduces 4 data types and defines 22 functions. All names exported from the package can be inspected using names(QSWalk) command. They are grouped into five categories, based on their purpose.

JULIA interpreter provides access to the function documentation. In order to show description of the function some_function one should type

```
julia> ?some_function
```

One should note that ? mark disappears and the prompt is changed from julia> to help?>.

3.2.1. Data types

Package QSWALK.JL takes advantage of the strong typing capabilities of JULIA language. Data types defined in the package are used to represent internal data utilised during the calculations and enable the proper utilization of the functionality based on sparse matrices.

- SparseDenseMatrix – type representing matrices which can be dense or sparse.
- SparseDenseVector – type representing vectors which can be dense or sparse.

Types `Vertex` and `VertexSet` are used for the nonmoralizing evolution. In this case, the standard basis is partitioned for vertices. These two types are used to store partition description.

- `Vertex` – type describing the labels of vectors from the canonical basis corresponding to given `Vertex`. Function `subspace(Vertex)` returns the list of labels, while `Vertex[i]` return a unique label.
- `VertexSet` – type consisting of a list of `Vertex` objects. It describes the partition of the linear subspace. Objects of this type should be constructed with `make_vertex_set` or `nm_lind` functions. In order to get a list of the vertices one should use `vertices` function, or `vertexset[i]` for a i -th `Vertex`.

3.2.2. Construction of generators

This group of functions provides the methods for construction of generators of the dynamical subgroups from the graph representation.

- `local_lind(A[, epsilon])` splits the elements of the matrix `A` into a collection of sparse matrices with exactly one non-zero element. Matrices are added if the absolute value of the nonzero element is at least `epsilon`, which defaults to `eps()`.
- `evolve_generator(H, L[, localH][, omg])` creates the generator for the evolution as in Eq. (3), calculated according to Eq. (1), (4) or (7), given Hamiltonian `H`, collection of Lindblad operators `L`, local Hamiltonian `localH` and scaling parameter `omg`. Parameters `localH` and `omg` are optional. If `omg` is not provided, $(1 - \omega)$ and ω parts in Eq. (7) are set to 1.

3.2.3. Evolution

Functions in this group provide the interface for simulating quantum stochastic walks in the local and the global regimes. The functions use different approach if the evolution generator is sparse or dense. For a dense matrix its exponentiation is calculated, which is efficient for small matrices. For a sparse matrix `expmv` provided by `QSWALK.JLExpokit` package is used [24]. Note that sparsity is checked by the type of the evolution generator.

- `evolve(evo_gen, init_state, time)` is the simplest case where the function accepts evolution generator `evo_gen`, see Eq. (3), `init_state` describing the initial state of the evolution, and `time` specifying the time of the evolution. Argument `time` has to be non-negative.
- `evolve(evo_gen, init_state, tpoints)` is similar to the previous one, but a list of points of time `tpoints` is given. In this case, a list of the resulting states is returned. This results in speedup where `evo_gen` is a dense matrix.

If the evolution is applied to several initial states and the evolution generator operator is dense, it is more efficient to calculate the superoperator first, and next to apply it to the initial states. For this scenario the package provides two functions.

- `evolve_operator(evo_gen, time)` returns an exponent of $\text{time} \times \text{evo_gen}$ called superoperator. The function works for dense matrices only.
- `evolve(evo_super, init_state)` returns a state based on superoperator generated by `evolve_operator`. The function works for dense matrices only.

It is important to note that the user must provide input arguments fulfilling the appropriate conditions. For the procedure `evolve` to work correctly, `evo_gen` should be generated by `evolve_generator` function and `init_state` should be a proper density matrix.

3.2.4. Demoralization

The functions in this group provides functionality required to construct nonmoralizing evolution on directed graphs. This is necessary to reproduce the structure of directed graphs using quantum stochastic walks. In this case, one needs to provide an extended initial state, perform the evolution using a special Hamiltonian, and perform the measurement which interprets the enlarged space (see. Fig. 2).

- `default_nm_loc_ham(size)` returns a default part of a local Hamiltonian of size $\text{size} \times \text{size}$ for vertex subspace of given order. The Hamiltonian is sparse with nonzero elements on the first upper diagonal equal to $1im$ and the lower diagonal equal to $-1im$.
- `nm_loc_ham(vertexset, hams)` returns a Hamiltonian acting locally on each vertex from `vertexset` partition. Optional argument `hams` is a dictionary which, for a given dimension of vertex linear subspace, yields a hermitian operator. It can be `Dict{Int, SparseDenseMatrix}`, which returns the matrix by the indegree, or `Dict{Vertex, SparseDenseMatrix}` which, for different vertices, may return different matrices.
- `nm_lind(A[, linds][, epsilon])` returns a single Lindbladian operator and a vertex set describing how vertices are bound to subspaces. The operator is constructed according to the correction scheme presented in [1]. Parameter `A` is a square matrix, describing the connection between the canonical subspaces in a similar manner as the adjacency matrix. Parameter `epsilon`, with the default value `eps()`, determines the relevant values by `abs(A[i, j]) >= epsilon` formula. List `linds` describes the elementary matrices. It can be `Dict{Int, SparseDenseMatrix}`, which returns the matrix by the indegree, or `Dict{Vertex, SparseDenseMatrix}` which, for different vertices, may return different matrices. The matrix should have orthogonal columns and be of the size outdegree of the vertex. As the default, the function uses Fourier matrices (see. Sec. 3.2.5).
- `nm_glob_ham(A[, hams][, epsilon])` returns a global Hamiltonian for the moralization procedure. Matrix `A` should be a symmetric matrix, for which one aims to construct the nonmoralizing dynamics. Here, `hams` is an optional argument which is a dictionary with keys of type `Tuple{Int, Int}` or `Tuple{Vertex, Vertex}`. The

first one collects the submatrices according to their shape, while the second one collects them according to each pair of vertices. As the default, all-one submatrices are chosen. The last argument states that only the elements for which $\text{abs}(A[i, j]) > \text{epsilon}$ are considered.

- `nm_measurement(probability, vertexset)` returns the joint probability of probability, which is real-valued probability vector according to partition `vertexset`.
- `nm_measurement(state, vertexset)` returns the joint probability of canonical measurement of density matrix `state`, according to partition `vertexset`.
- `nm_init(init_vertices, vertexset)` returns the initial state in the case of the nonmoralizing evolution. The result is a block diagonal matrix, where each block corresponds to vertex from `vertexset`. If the first argument is of type `Vector{Vertex}`, then default block matrix `eye` is used. Note that in this case the initial density state is normalized in a uniform distribution way, ie. different vertices have the same probability.

`nm_init(init_states, vertexset)` – similar to the function above, the first argument is of type `Dict{Vertex, SparseDenseMatrix}`. For each given vertex a block from dictionary is used, otherwise zero matrix is chosen. Each matrix from dictionary should be nonnegative and sum of all traces should equal one. The keys of `init_vertices` should be a subset of `vertices(vertexset)`. Note that the matrix from `init_states` corresponding to vertex `v` should be of size `length(v) × length(v)`.

3.2.5. Dirac notation and matrix utilities

The last category of functions contains procedures used to manipulate matrices and vectors [23]. These functions can be used independently from the rest of the package. Note that JULIA package indexes list from 1, and similarly all relevant functions require a positive index.

- `ket(index, size)` returns `index`-th column vector from standard basis in the `size`-dimensional vector space.
- `bra(index, size)` returns `index`-th row vector from standard basis in the `size`-dimensional vector space.
- `ketbra(irow, icol, size)` return a matrix acting on `size`-dimensional vector space. The matrix consists of a single non-zero element equal to one, located at `(irow, icol)`.
- `proj(index, size)` returns a projector onto `index`-th base vector in `size`-dimensional vector space. This is equivalent to `ketbra(index, index, size)`.
- `proj(vector)` returns a projector onto the subspace spanned by vector `vector`.

- `res(mtx)` returns the vectorization of the matrix `mtx` in the row order. This is equivalent to `Base.vec(transpose(mtx))`.
- `unres(vector)` – inverse of `res` function.
- `fourier_matrix(dim)` returns Fourier matrix of size `dim`×`dim`.

3.3. Typical work-flow

Typical work-flow is presented in Fig. 2. For local and global regimes, all operators should be generated by the user. This includes the Hamiltonian, Lindblad operators and the initial state. In the local regime case, the QSWALK.JL package provides matrix splitting function, which generates local operations of the form $|v\rangle\langle w|$.

Nonmoralizing interaction requires additional steps. We start with the global regime Hamiltonian and a single Lindblad operator. Based on them, we construct nonmoralizing operators through `nm_glob_ham` and `nm_lind` functions. The user is encouraged to construct the local Hamiltonian by `nm_loc_ham` function. Function `nm_init` should be used to construct block-diagonally mixed state, where each block corresponds to a vertex.

Independently of the chosen regime, the Hamiltonian, the Lindblad operators and optional local Hamiltonian should be passed to `evolve_generator`, which constructs evolution generator according to the appropriate formula, and then pass it to `evolve`. At this point, we have a density matrix. In order to measure it, for local and global regimes `diag` function refers to canonic measurement. For nonmoralizing global interaction we provide a separate function `nm_measurement`.

4. Usage examples

In this section we provide some basic examples, which present functionalities of QSWALK.JL module. In particular, we demonstrate the examples with all described evolution regimes for quantum stochastic walk, namely local environment interaction, global environment interaction, and nonmoralizing global environment interaction. The examples are based on the results presented in [5, 1, 6, 7, 8].

Code snippets in this section can be found in the form of full examples in the `examples` subdirectory, contained in the package distribution. For convenience we provide the examples in the form of JULIA scripts (files with `.jl` extension), as well as JUPYTER notebooks (corresponding files with `.ipynb` extension). Some of the examples require LIGHTGRAPHS.JL and PYPLOT.JL modules. We use `#` (hash), denoting a comment in JULIA, to provide the result of the command.

4.1. Propagation on the line segment

The first example demonstrates the evolution on the line segment using different regimes. Code snippets from this section can be found in the `ex01_path_propagation.jl` file. The plots resulting from the above examples are presented in Fig. 3. One can note that the second moment for the global interaction case grows ballistically.

We would like to recover the results from [5] corresponding to the analysis of the second moment of the walker position. In the first step we prepare the essential data.

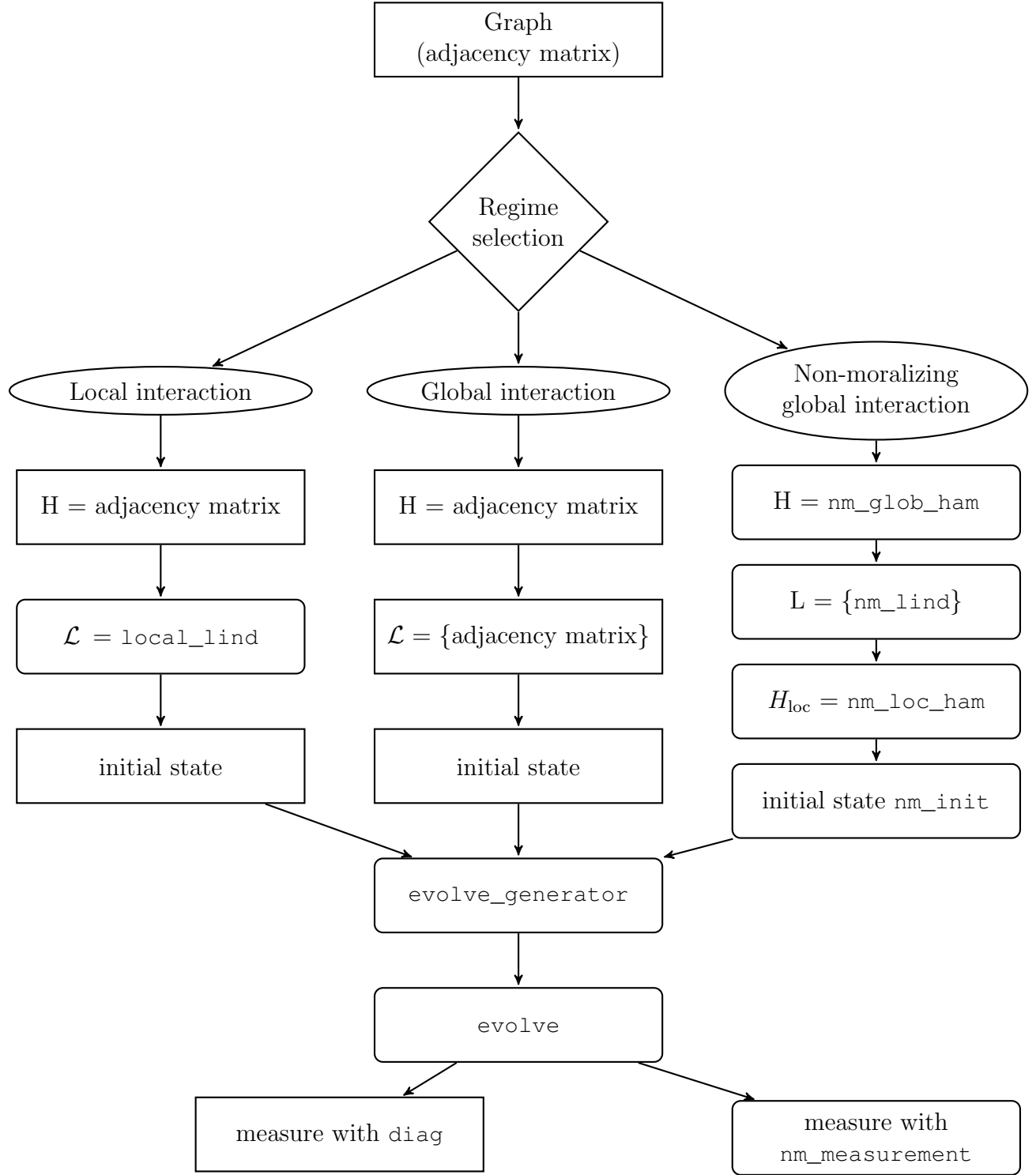


Figure 2: Typical steps required during the preparation of the simulation utilizing QSWALK.JL package. The rounded rectangles refer to the functions implemented in QSWALK.JL, while the standard rectangles require user input which should be provided by some external functions, eg. for `adjacency_matrix` from LIGHTGRAPHS.JL.

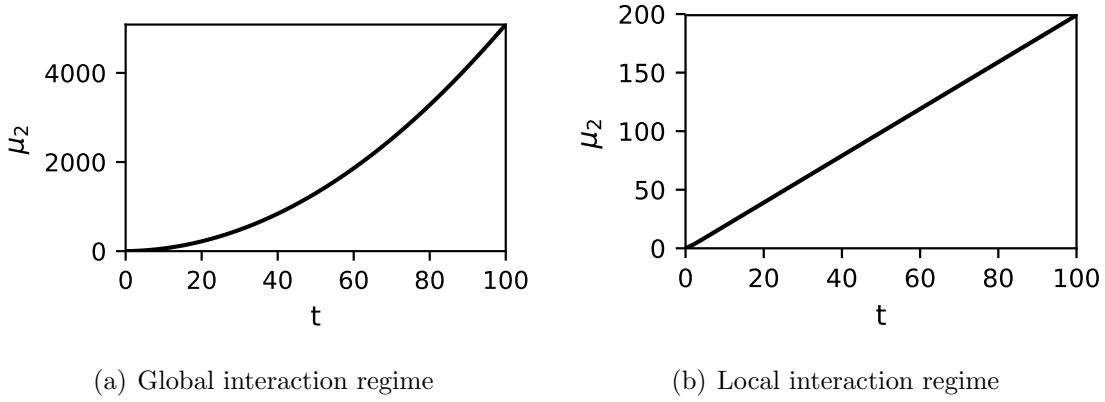


Figure 3: Second central moment as the function of time for the global (a) and the local (b) interaction regime. The value of the second moment grows ballistically for the global interaction case.

```
dim = 251
w = 0.5
timepoints = collect(0:2:100)
adjacency = adjacency_matrix(PathGraph(dim))
```

We consider both global and local interaction cases. Hence we need to prepare the evolution generators corresponding to both types of evolution.

```
lind_local = local_lind(adjacency)
midpoint = ceil(Int, dim/2)
op_global = evolve_generator(adjacency, [adjacency], w)
op_local = evolve_generator(adjacency, lind_local, w)
```

Note that `evolve_generator` accepts a list of matrices as the second argument and one needs to put extra square bracket for adjacency parameter in `op_global` case. Next, using the created operators, we simulate the evolution using `evolve` function.

```
rho_global = evolve(op_global, proj(midpoint, dim), timepoints)
rho_local = evolve(op_local, proj(midpoint, dim), timepoints)
```

Note that in both cases the second argument refers to the initial state of the evolution, which is at the middle-point of the path graph. Finally, we can calculate the second central moment of the distribution for the standard measurement of the position as

```
secmoment_global = Float64[]
secmoment_local = Float64[]
positions = (collect(1:dim)-midpoint)
for i=1:length(timepoints)
    push!(secmoment_global, sum(positions.^2 .* diag(rhoglobal[i])))
    push!(secmoment_local, sum(positions.^2 .* diag(rholocal[i])))
end
```

and prepare the plots

```
plot(timepoints, secmoment_global)
plot(timepoints, secmoment_local)
```

4.2. Convergence on random graphs

In this example we demonstrate the use of `evolve_operator` function for the purpose of analysing the convergence of the quantum stochastic walks. In this situation we are interested in the behaviour of the process, represented by the evolve generator, on different initial states. The code described here can be found in supplementary materials in `ex02_convergence.jl`.

Quantum stochastic walks have convergence properties different from typical quantum walk models. In particular, for the local environment interaction regime, for arbitrary strongly connected directed graph the evolution is relaxing, ie. there exists a unique density matrix which is the limiting state for the evolution for an arbitrary initial state [7, 6].

Let us consider a random directed graph generated according to Erdős-Rényi model.

```
dim = 10
digraph = erdos_renyi(dim, 0.5, is_directed=true)
graph = Graph(digraph)
adj_digraph = full(adjacency_matrix(digraph, :in))
adj_graph = full(adjacency_matrix(graph))
time = 100.
```

The Lindbladian and the subgroup generator corresponding to the above graph are constructed using `local_lind` and `evolve_generator` functions, respectively

```
lind = local_lind(adj_digraph)
evo_gen = evolve_generator(adj_graph, lind)
```

In this case, due to the small size of the analysed graph, it is better to choose the dense matrix type instead of the sparse one. In order to show the uniqueness of stationary state, it is enough to compute the dimensionality of the null-space of global operator matrix.

```
println(count(x->abs(x)<1e-5, eigvals(evo_gen)))
# 1
```

One can see that dimensionality equals one, and hence there is a unique stationary state. The existence of at least one stationary state is guaranteed by quantum Perron-Frobenius theorem [28].

To check that this is indeed the case we can choose different initial states to show that the stationary state is unique.

```
rhoinit1 = proj(1, dim)
rhoinit2 = proj(3, dim)
rhoinit3 = eye(dim)/dim
```

Since we simulate a single evolution for all of the above states, for dense matrices it is better to compute the exponential once, and then use it for all of the states.

```

U = evolve_operator(evo_gen, time)
rho1 = evolve(U, rhoinit1)
rho2 = evolve(U, rhoinit2)
rho3 = evolve(U, rhoinit3)

println(norm(rho1-rho2))
println(norm(rho2-rho3))
# 7.001526329112005e-17
# 4.1919257307409924e-17

```

One should note that, since the graph is chosen randomly from Erdős-Rényi distribution, the resulting number will be different for each execution of the above code.

4.3. Spontaneous moralization

In this section we present the basics of the spontaneous moralization [1]. The code described here can be found in supplementary materials in `ex03_moralization_simple.jl`. Here we plan to analyse the graph presented in Fig. 1. Let us analyse the case where the global Lindblad operator equal to adjacency matrix is the only operator used. Again we start with preparing the global operator

```

adjacency = [0 0 0;
              0 0 0;
              1 1 0]
opmoral = evolve_generator(zero(adjacency), [adjacency])
time = 100.

```

In the evolution we start in the top-left vertex. One could expect that for large time the state will converge to sink (bottom) vertex. However running the following commands shows, that it is not the case.

```

rho = evolve(opmoral, proj(1,3), time)
println(diag(rho))
# Complex{Float64}[0.25+0.0im, 0.25+0.0im, 0.5+0.0im]

```

We have a non-zero probability of measuring top vertices. Whats more, the amplitude transited from vertex top-left to top-right, although there is no path between them.

The key is to choose nonmoralizing procedure. We need to create new operators, called nonmoralizing Lindbladian operator and local Hamiltonian.

```

lnonmoral, vset = nm_lind(adjacency)
hlocal = nm_loc_ham(vset)
opnonmoral = evolve_generator(zero(lnonmoral), [lnonmoral], hlocal)

```

Note that new parameter `vset` appears. The nonmoralizing procedure needs description how the linear space is divided into subspaces corresponding to vertices. Usually, `vset` should be treated as the parametrization of the evolution, which should be passed for all of the functions without change. It can be generated by `nm_lind`, as in the example above, or simply by `make_vertex_set`.

Now, the operators have bigger size than the original ones. The size can be calculated with `vertexsetsize` function.

```
println(vertexsetsize(vset))
# 4
println(vset)
# QSWalk.VertexSet(QSWalk.Vertex[QSWalk.Vertex([1]), QSWalk.Vertex([2]),
# QSWalk.Vertex([3, 4])])
```

Here `vset` describes the partition of linear space, in this example $\text{span}(|1\rangle)$ corresponds to the first vertex, $\text{span}(|2\rangle)$ to the second vertex and $\text{span}(|3\rangle, |4\rangle)$ to the third vertex. While it is possible to write own density states, for states being block diagonal, where each block corresponds to a different vertex, simpler function can be chosen.

```
rho0 = nm_init(vset[[1]], vset)
```

Note that as the first argument we choose a list of vertices. The state is an identity matrix on a subspace corresponding to `rho0`. In this case after the evolution we obtain

```
rho = evolve(opnonmoral, rhoinit, time)
println(nm_measurement(rho, vset))
# [5.02465e-33, -5.74849e-33, 1.0]
```

Now we have the expected result, ie. all of the amplitudes are transfered into the sink (bottom vertex).

4.4. Spontaneous moralization on path graph

In this section we recover the results presented in [1]. The code described here can be found in supplementary materials in `ex04_moralization_path.jl`. Demoralizing procedure results in non-symmetric evolution. Let us again consider the code below.

```
dim = 101 #odd for unique middle point
w = 0.5
time = 40.
adjacency = adjacency_matrix(PathGraph(dim))

midpoint = ceil(Int, dim/2)
lind, vset = nm_lind(adjacency)
hglocal = nm_glob_ham(adjacency)
hlocal = nm_loc_ham(vset)
opnonsymmetric = evolve_generator(hglocal, [lind], hlocal, w)
rhoinit = nm_init(vset[[midpoint]], vset)
```

```
rho_nonsymmetric = evolve(opnonsymmetric, rhoinit, time)
```

For the canonical measurement, the distribution should be symmetric with respect to midpoint, and hence the commands

```
positions = (collect(1:dim)-midpoint)
measurement_nonsymmetric = nm_measurement(rho_nonsymmetric, vset)
println(sum(positions .* measurement_nonsymmetric))
```


should print 0. However, the output is approximately -0.5698 . Further analysis would show that the situation happens even after removing `Hlocal` or `H` operators.

The key is to add another Lindbladian operator, which make the evolution symmetric again. This can be done by proper adjustment of `nm_lind`.

```
linddescription1 = Dict{1 => ones(1,1), 2 => [1 1; 1 -1]}
linddescription2 = Dict{1 => ones(1,1), 2 => [1 1; -1 1]}
lind1, vset = nm_lind(adjacency, linddescription1)
lind2, vset = nm_lind(adjacency, linddescription2)
hglocal = nm_glob_ham(adjacency)
hlocal = nm_loc_ham(vset)
opsymmetric = evolve_generator(hglocal, [lind1, lind2], hlocal, w)
rhoinit = nm_init(vset[[midpoint]], vset)
```

If we leave the rest of the code unchanged, then we will receive approximately $-6.759E-9$ as an output, which can be treated as numerical zero. Note that for `nm_lind` we can either make a dictionary for all degrees, or for all vertices. Similarly, `nm_glob_ham` can be generalized for all pairs of degrees or all pairs of vertices.

4.5. Performance analysis

At the moment of writing, the only package developed for simulating the evolution of quantum stochastic walks is `QSWALK.M` package for *Wolfram Mathematica*. Hence we compared the performance of computing non-moralizing evolution on path graph for various orders.

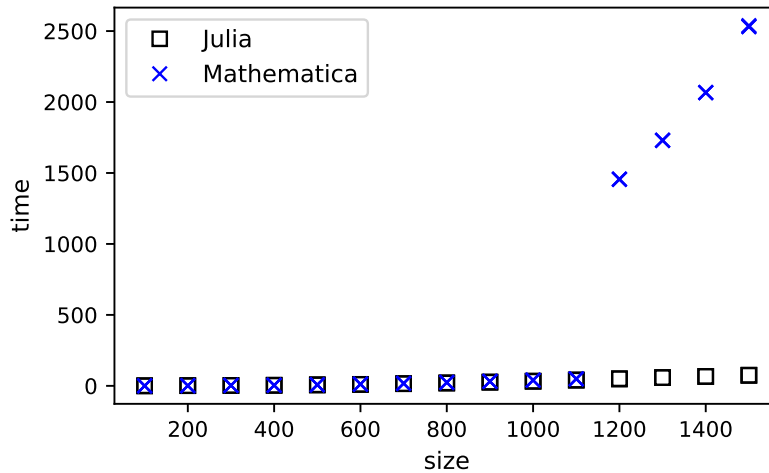


Figure 4: Comparison of time required to simulated quantum stochastic walk on the line in Julia with `QSWALK.JL` and in *Mathematica*, using the package described in [10]. Parameter `size` denotes the size of the graph.

Results presented in Fig. 4 demonstrate that for small enough graphs `JULIA` and *Mathematica* compute the result in similar time. However, after some order threshold we can

observe sudden drop of efficiency of *Mathematica*. Our in-depth analysis showed that the main reason is the change of `MatrixExp` function behavior. Unfortunately, *Mathematica* is not an open source programming language, hence we cannot find any explanation of the phenomena. Most probably then inefficiency calculation of the results from internal aspects of *Mathematica* implementation. The calculations were executed on three different architectures and all of them yield efficiency drop for QSWALK.M package for *Wolfram Mathematica* for the same order of the input matrix.

5. Concluding remarks and future work

In this paper we have provided the description of QSWALK.JL module developed for the purpose of studying quantum stochastic walks. The package is focused on the graph-based evolution and provides many functions typically used for quantum walks on graphs. We have utilized JULIA programming language and the package demonstrates an advantage over the existing software in terms of the performance. The nonmoralizing evolution first implemented in the package enables the study of quantum procedures developed using quantum stochastic walks on arbitrary directed graphs. As such, the package can be used to gain more insight into the properties of quantum evolution on this type of graphs. While the name of the presented package refers to Quantum Stochastic Walk, it is not limited to this type of evolution only. Many of the presented functions can be used for arbitrary quantum evolution with constant H and \mathcal{L} .

Acknowledgements. This work has been supported by the Polish Ministry of Science and Higher Education under project number IP 2014 031073. Authors would like to thank Piotr Gawron for valuable remarks concerning the usage of type system in JULIA.

References

- [1] K. Domino, A. Glos, M. Ostaszewski, Superdiffusive quantum stochastic walk definable of arbitrary directed graph, *Quantum Inform. Comput* 17 (11-12) (2017) 973–986.
- [2] J. Bezanson, S. Karpinski, V. Shah, A. Edelman, Julia: A fast dynamic language for technical computing, *arXiv:1209.5145* (2012).
- [3] Julia documentation, <https://docs.julialang.org/en/latest/> (Accessed on 18/12/2017) (2018).
- [4] J. Bezanson, A. Edelman, S. Karpinski, V. B. Shah, Julia: A fresh approach to numerical computing, *SIAM Review* 59 (1) (2017) 65–98.
- [5] K. Domino, A. Glos, M. Ostaszewski, Ł. Paweła, P. Sadowski, Properties of quantum stochastic walks from the asymptotic scaling exponent, *arXiv:1611.01349* (2016).
- [6] A. Glos, J. Mischczak, M. Ostaszewski, Limiting properties of stochastic quantum walks on directed graphs, *J. Phys. A: Math. Theor.* 51 (2018) 035304, *arXiv:1703.01792*. doi: 10.1088/1751-8121/aa9a4a.

- [7] C. Liu, R. Balu, Steady states of continuous-time open quantum walks, *Quantum Inf. Process.* 16 (7) (2017) 173. doi:10.1007/s11128-017-1625-8.
- [8] H. Bringuier, Central limit theorem and large deviation principle for continuous time open quantum walks, *Annales Henri Poincaré* 18 (10) (2017) 3167–3192. doi:10.1007/s00023-017-0597-7.
- [9] E. Sánchez-Burillo, J. Duch, J. Gómez-Gardenes, D. Zueco, Quantum navigation and ranking in complex networks, *Sci. Rep.* 2. doi:10.1038/srep00605.
- [10] P. Falloon, J. Rodriguez, J. Wang, QSWalk: a Mathematica package for quantum stochastic walks on arbitrary graphs, *Comput. Phys. Commun.* doi:10.1016/j.cpc.2017.03.014.
- [11] T. Loke, J. Tang, J. Rodriguez, M. Small, J. Wang, Comparing classical and quantum PageRanks, *Quantum Inf. Process.* 16 (1) (2017) 25. doi:10.1007/s11128-016-1456-z.
- [12] F. Caruso, A. Chin, A. Datta, S. Huelga, M. Plenio, Highly efficient energy excitation transfer in light-harvesting complexes: The fundamental role of noise-assisted transport, *J. Chem. Phys.* 131 (10) (2009) 09B612. doi:10.1063/1.3223548.
- [13] M. Mohseni, P. Rebentrost, S. Lloyd, A. Aspuru-Guzik, Environment-assisted quantum walks in photosynthetic energy transfer, *J. Chem. Phys.* 129 (17) (2008) 11B603. doi:10.1063/1.3002335.
- [14] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd, A. Aspuru-Guzik, Environment-assisted quantum transport, *New J. Phys.* 11 (3) (2009) 033003. doi:10.1088/1367-2630/11/3/033003.
- [15] J. Whitfield, C. Rodríguez-Rosario, A. Aspuru-Guzik, Quantum stochastic walks: A generalization of classical random walks and quantum walks, *Phys. Rev. A* 81 (2) (2010) 022323. doi:10.1103/PhysRevA.81.022323.
- [16] List of QC simulators, <https://quantiki.org/wiki/list-qc-simulators> (Accessed on 18/12/2017) (2012-).
- [17] F. Marquezino, R. Portugal, The QWalk simulator of quantum walks, *Comput. Phys. Commun.* 179 (5) (2008) 359–369. doi:10.1016/j.cpc.2008.02.019.
- [18] S. Berry, P. Bourke, J. Wang, qwViz: Visualisation of quantum walks on graphs, *Comput. Phys. Commun.* 182 (10) (2011) 2295–2302. doi:10.1016/j.cpc.2011.06.002.
- [19] J. Izaac, J. Wang, pyCTQW: A continuous-time quantum walk simulator on distributed memory computers, *Comput. Phys. Commun.* 186 (2015) 81–92. doi:10.1016/j.cpc.2014.09.011.

- [20] V. Gorini, A. Kossakowski, E. Sudarshan, Completely positive dynamical semigroups of N-level systems, *J. Math. Phys.* 17 (5) (1976) 821–825. doi:10.1063/1.522979.
- [21] A. Kossakowski, On quantum statistical mechanics of non-hamiltonian systems, *Rep. Math. Phys.* 3 (4) (1972) 247–274. doi:10.1016/0034-4877(72)90010-9.
- [22] G. Lindblad, On the generators of quantum dynamical semigroups, *Commun. Math. Phys.* 48 (2) (1976) 119–130. doi:10.1007/BF01608499.
- [23] J. Miszczak, Singular value decomposition and matrix reorderings in quantum information theory, *Int. J. Mod. Phys. C* 22 (09) (2011) 897–918. doi:10.1142/S0129183111016683.
- [24] Julia implementations of some routines contained in EXPOKIT, <https://github.com/acroy/Expokit.jl> (Accessed on 18/12/2017) (2018).
- [25] R. Sidje, Expokit: a software package for computing matrix exponentials, *ACM Trans. Math. Software* 24 (1) (1998) 130–156. doi:10.1145/285861.285868.
- [26] S. Bromberger, J. Fairbanks, et al., JuliaGraphs/LightGraphs.jl: LightGraphs (2017). doi:10.5281/zenodo.889971.
- [27] PyPlot.jl – plotting for Julia based on matplotlib.pyplot, <https://github.com/JuliaPy/PyPlot.jl> (Accessed on 18/12/2017) (2017).
- [28] S. Albeverio, R. Høegh-Krohn, Frobenius theory for positive maps of von Neumann algebras, *Commun. Math. Phys.* 64 (1) (1978) 83–94. doi:10.1007/BF01940763.