A Simulator for Discrete Quantum Walks on Lattices

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Abstract

We present a simulator for two-particle quantum walks on the line and one particle on a two-dimensional squared lattice. It can be used to investigate the equivalence between the two cases (one- and two-particle walks) for various boundary conditions (open, circular, reflecting, absorbing and their combinations). For the case of a single walker on a two-dimensional lattice, the simulator can also implement the Möbius strip. Furthermore, other topologies for the walker are also simulated by the proposed tool, like certain types of planar graphs with degree up to 4, by considering missing links over the lattice. The main purpose of the simulator is to study the genuinely quantum effects on the global properties of the two-particle joint probability distribution on the entanglement between the walkers/axis. For that purpose, the simulator is designed to compute various quantities such as: the entanglement and classical correlations, (classical and quantum) mutual information, the average distance between the two walkers, different hitting times and quantum discord. These quantities are of vital importance in designing possible algorithmic applications of quantum walks, namely in search, 3-SAT problems, etc. The simulator can also implement the static partial measurements of particle(s) positions and dynamic breaking of the links between certain nodes, both of which can be used to investigate the effects of decoherence on the walker(s). Finally, the simulator can be used to investigate the dynamic Anderson-like particle localization by varying the coin operators of certain nodes on the line/lattice. We also present some illustrative and relevant examples of one- and two-particle quantum walks in various scenarios. The tool was implemented in C and is available on-line at http://qwsim.weebly.com/.

1 Introduction

Quantum walks[1] are the quantum analog of classical random walks. They have been used both to develop quantum-based algorithms and to model vari-
ous physical systems and processes. It was shown that under certain assumptions and scenarios, continuous-time quantum walks can be exponentially faster than classical ones, see Ref. [2, 3]. They have been used in designing search algorithms,[4] and showed to be quadratically faster than any known classical counterparts [6]. Discrete-time quantum walks have also been shown to be useful in searching spatial regions under realistic assumptions, and moreover, to clearly surpass, at least quadratically, common search algorithms, see Ref. [7], [8], [9], [10], [11], [12]. Similar results were obtained when quantizing classical algorithms based on random walks, namely when the underlying Markov chain is ergodic and symmetric,[11] or even to a larger class of Markov chains.[12]

Multi-particle quantum walks were first introduced in Ref. [13] where it was shown that certain joint two-particle properties, such as the mean distance between the walkers and the hitting time for at least one walker, can be for walkers initially entangled between each other larger or smaller than in the case of unentangled walkers. Further work studied the meeting problem[14] and the generation of the entanglement between the walkers,[15] confirming the genuine quantum mechanical influence of entanglement on the joint features of quantum walks, which in turn might affect the performance of the above mentioned computational applications.

Analytical results concerning quantum walks, like hitting, mixing and dispersion time (among others), were extensively studied for single-particle quantum walks (see for example Ref. [16], [17]). Also, the tools for the numerical study of one particle quantum walks in one and two dimensions have been presented before (see Ref. [18], [19]). Yet, although the entanglement between the coin and the position degrees of freedom have been studied in detail both numerically and analytically (see for example Ref. [20] and [21], respectively), a very little work has been done concerning the effects of the entanglement between the walkers. In order to address these issues, we designed a tool for numerical simulation of two-particle quantum walks.

Herein, we present the main result of the paper – a simulator for two-particle quantum walks in one dimension and one-particle quantum walks in two dimensions. The simulator computes quantities that measure the global features that are influenced by the entanglement between the two walkers, such as correlations, classical (Shannon) and quantum (von Neumann) mutual information between the two walkers, average distance between the walkers, various hitting times for at least one walker, etc. It can include various boundary conditions – open, reflecting and absorbing – and combine them for each particle independently, resulting in different two-particle geometries, such as torus, cylinder, finite squared lattice with reflecting boundaries, etc. For one particle on a two-dimensional lattice, a new boundary conditions resulting in a Möbius strip and Klein bottle topologies are possible to consider, which would in the case of two particles in one dimension require non-local shift operation for at least one particle. By implementing the static partial position measurements (constant during the walk) and/or dynamic breaking links between certain nodes (random choice of links broken at each step of the walk), our simulator can be used to study the effects of decoherence. The dynamic change of coin operators can also be
implemented and used to study various types of particle localizations[22], such as those of Anderson type and others.[23] The simulator can perform up to $10^7$ steps of a discrete-time quantum walk on the open line. The memory needed to encode an arbitrary state of such walk after $10^8$ steps would be around 12000 Gbits of RAM, which exceeds the memory of standard computers available in the market. Thus our simulator saturates the current technological limits of an average consumer. When restricting the memory needed to encode the walk by considering reflecting boundaries in the nodes, say -4000 and +4000, the simulator performs $10^8$ steps in about two weeks on a standard 3 Ghz computer, which is reasonable for a well defined scientific research.

Other results, presented as examples in Section 4, confirm the expected dependence of the above mentioned joint quantities on entanglement, in accordance with the Theorems 1–3 from Section 3. Also, we explicitly showed the examples of Anderson-like localizations in the presence of various static and dynamic decoherence mechanisms (i.e., partial position measurements, broken links and varying coin operations).

The paper is organized as follows. After this Introduction, in Section 2 we present a mathematical description of a discrete-time quantum walk on a line with one and two particles, and show the equivalence of the latter with a one-particle quantum walk on a square lattice. We discuss different boundary conditions (circular, reflecting, absorbing, etc.) and for the case of a one-particle walk on a lattice, different topologies (Möbius strip, Klein bottle, etc.). Finally, we describe two models for a noise in a quantum walk: dynamic breaking of links between certain nodes, and varying coins for random nodes. In Section 3 we describe the quantities that our simulator is calculating and analyze their relevance, with the emphasis to a two-particle quantum walk picture where joint properties depending on correlation and entanglement can exhibit specific non-classical quantum features. In Section 4 we present some illustrative examples. Finally, in Section 5 we present conclusions and possible future improvements to the code.

## 2 Discrete-time quantum walk

In a discrete-time quantum walk on a line, we consider the movement of a walker along discrete positions, labeled on a line $x \in \mathbb{Z}$. At each step this particle can move to the left or to the right of the line. The direction is controlled by an internal degree of freedom, commonly called the coin degree of freedom. Both position and coin states of a given particle can be modelled using Hilbert spaces $\mathcal{H}_P = \text{span}\{|x\rangle : x \in \mathbb{Z}\}$ and $\mathcal{H}_C = \text{span}\{|R\rangle, |L\rangle\}$, for the position space and the coin space respectively. The total Hilbert space of a particle doing a discrete-time quantum walk on a line is given by $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C$. The one-step time evolution of the system is described by the unitary operator

$$\hat{U} = \hat{S} \left( \hat{I}_P \otimes \hat{U}_C \right),$$

(1)
where $\hat{S}$ is the shift operator given by

$$\hat{S} = \left( \sum_x |x + 1\rangle \langle x| \right) \otimes |R\rangle \langle R| + \left( \sum_x |x - 1\rangle \langle x| \right) \otimes |L\rangle \langle L| , \quad (2)$$

$\hat{I}_p$ is the identity operator on $H_p$, and $\hat{U}_C \in U(2)$ acts on $H_C$.

Now, consider two non-interacting particles on a line. The joint Hilbert space of the composite system, consisting of two distinguishable particles 1 and 2 doing a quantum walk over the same line, is

$$H_{12} = H_1 \otimes H_2$$

where $H_1 = H_{p,1} \otimes H_{c,1}$ and $H_2 = H_{p,2} \otimes H_{c,2}$ represent the Hilbert spaces of particles 1 and 2, respectively. The joint one-step time evolution of this system is simply the tensor product between the unitary operators for time evolutions of each particle

$$\hat{U}_{12} = \hat{U}_1 \otimes \hat{U}_2 = \left[ \hat{S}_1 \left( \hat{I}_{p,1} \otimes \hat{U}_{c,1} \right) \right] \otimes \left[ \hat{S}_2 \left( \hat{I}_{p,2} \otimes \hat{U}_{c,2} \right) \right]$$

$$= \hat{S}_{12} \left( \left( \hat{I}_{p,1} \otimes \hat{I}_{p,2} \right) \otimes \hat{U}_{c,12} \right) ,$$

where $\hat{S}_{12} = \hat{S}_1 \otimes \hat{S}_2$ has the form

$$\hat{S}_{12} = \sum_{x_1, x_2} |x_1 + 1, x_2 + 1\rangle \langle x_1, x_2| \otimes |RR\rangle_{12} \langle RR|$$

$$+ |x_1 + 1, x_2 - 1\rangle \langle x_1, x_2| \otimes |RL\rangle_{12} \langle RL|$$

$$+ |x_1 - 1, x_2 + 1\rangle \langle x_1, x_2| \otimes |LR\rangle_{12} \langle LR|$$

$$+ |x_1 - 1, x_2 - 1\rangle \langle x_1, x_2| \otimes |LL\rangle_{12} \langle LL| \quad (3)$$

and the joint coin operator is

$$\hat{U}_{c,12} = \hat{U}_{c,1} \otimes \hat{U}_{c,2}.$$ 

Note that the labels of ket states denote the joint and single-particle Hilbert spaces $H_{12}, H_1$ and $H_2$, such that $|x_1, x_2\rangle_{12} \equiv |x_1\rangle_1 |x_2\rangle_2$, etc.

It is easy to see that a quantum walk of two particles on a line, in which initial positions of both walkers are equal, say 0, is equivalent to a quantum walk of one particle along a two-dimensional square lattice $xOy$, whose nodes

\footnote{From mathematical point of view, it is irrelevant whether two particles are performing the walk over the same or different lines: both descriptions are identical. Yet, it is crucial for the applications. For example, in the study of the effects of entanglement between the two walkers on the features of quantum walk-based search algorithms, in which the two walkers are performing a search over the same data-base. For the same reason, we assume that the walks are performed simultaneously, which is the reason for requiring particle distinguishability: otherwise, the states of two identical particles would be subject to bosonic and fermionic symmetrization and anti-symmetrization rules. On the other hand, such states are possible to study in the case of distinguishable particles as well.}
are labeled by their coordinates \(#\{(x, y) : x, y \in \mathbb{Z}\}\) along two perpendicular axes \(#x\) and \(#y\). Indeed, if the positions of the two particles on a line represent the two orthogonal coordinates, along the axes 1 and 2, of a node in the square lattice, then the two-particle configuration \((1, 1)\) corresponds to a position \((1, 0)\) of a particle on the \(xOy\) lattice whose axes \(#x\) and \(#y\) are rotated by \(\pi/4\) with respect to the axes 1 and 2, see Figure 1.

In general, the correspondence between a two-particle configuration \((x_1, x_2)\) and a position \((x, y)\) of a node in a rotated \(xOy\) lattice is given by:

\[
\begin{align*}
x &= \frac{1}{2} (x_2 + x_1), \\
y &= \frac{1}{2} (x_2 - x_1),
\end{align*}
\]

which establishes the correspondence between the states from a two-particle position Hilbert space \(\mathcal{H}_{P,12} \equiv \mathcal{H}_{P,1} \otimes \mathcal{H}_{P,2}\) and a position Hilbert space \(\mathcal{H}_{P,xy} = \text{span}\{\langle x, y \rangle : x, y \in \mathbb{Z}\}\) of a single particle on a square lattice \(xOy\).

According to this, moving both particles to the right along a line is equivalent to a particle on a lattice moving East (to the right with respect to the \(x\)-axis). This induces the following correspondence between the states from a two-particle coin Hilbert space \(\mathcal{H}_{C,12} \equiv \mathcal{H}_{C,1} \otimes \mathcal{H}_{C,2}\) and the one-particle coin space \(\mathcal{H}_{C,xy} = \text{span}\{\langle E \rangle, \langle S \rangle, \langle N \rangle, \langle W \rangle\}\):

\[
\begin{align*}
|E\rangle &= |RR\rangle_{12}, |S\rangle = |RL\rangle_{12} \\
|N\rangle &= |LR\rangle_{12}, |W\rangle = |LL\rangle_{12}.
\end{align*}
\]

Therefore, the overall Hilbert space of a single particle doing a quantum walk along the \(xOy\) squared lattice is \(\mathcal{H}_{xy} \equiv \mathcal{H}_{P,xy} \otimes \mathcal{H}_{C,xy}\) (note that, for reasons of simplicity, we drop the labels of the ket states form \(\mathcal{H}_{xy}\)). The above correspondences (4) and (5) give the shift operator equivalent to \(\hat{S}_{12}\):

\[
\hat{S}_{xy} = \sum_{xy} |x + 1, y\rangle \langle x, y| \otimes |E\rangle \langle E|
+ |x, y - 1\rangle \langle x, y| \otimes |S\rangle \langle S|
+ |x, y + 1\rangle \langle x, y| \otimes |N\rangle \langle N|
+ |x - 1, y\rangle \langle x, y| \otimes |W\rangle \langle W|,
\]

while the coin operator for a quantum walk of a particle on the lattice, equivalent to a given two-particle walk on a line, is unchanged: \(\hat{U}_{C,xy} = \hat{U}_{C,12}\). Note that in general \(\hat{U}_{C,xy} \in U(4) \supset U(2) \otimes U(2)\), which in the case of two particles on a line would correspond to a global coin operation that could increase the entanglement between the coins of two particles. The unitary time evolution of each step of the quantum walk is given by:

\[
\hat{U}_{xy} = \hat{S}_{xy} \otimes (\hat{I}_{P,xy} \otimes \hat{U}_{C,xy}),
\]
Figure 1: Relation between the representations of quantum walks of one particle on a lattice and two particles on a line.

where $I_{P,xy}$ is the identity operator on $H_{P,xy}$.

Note that the above correspondence between a two-particle walk on a line and a single-particle walk on a square lattice is valid as long as initial positions of two particles on a line are of the same parity. Otherwise, using (4) we see that the two-particle walk is equivalent to a walk on a different square lattice whose node positions are half-integers. This way, we can use our simulator for two particles on a line to simulate quantum walks of two distinguishable particles on the same lattice, as long as their joint state is a product between one-particle states.

2.1 Quantum walks with specific boundary conditions and topologies

Quantum walks with certain boundary conditions are quite interesting. Firstly, from the theoretical point, it is essential to understand how these boundaries affect the features of quantum walks, in particular the entanglement between the particles as well as the other mentioned quantities that we study. Moreover, from a practical point of view, these boundaries might reduce significantly the state space, which leads to a numerically feasible analysis. Finally, quantum walks with particular boundaries can be used to simulate various (finite-size) physical systems.
First, we will consider boundary conditions for particles on a line. Then, we turn to the case of the square lattice. The correspondence between the two cases is given by (4) and (5).

For a particle on a line, two simplest cases are circular and the reflecting boundary conditions. In the case of circular boundary conditions, we connect two points $M$ and $-M$. Our system is finite (a circle with $2M+1$ points), which affects the shift operator: the sum in (2) goes from $-(M-1)$ to $(M-1)$, while the connected points $-M$ and $M$ are represented by adding the term
\[
\hat{C} = |M\rangle \langle M| \otimes |R\rangle \langle R| + |M\rangle \langle -M| \otimes |L\rangle \langle L| + |M-1\rangle \langle M| \otimes |R\rangle \langle R| + |M\rangle \langle -M-1\rangle \langle -M| \otimes |L\rangle \langle L|.
\] (7)

For reflecting boundary conditions at positions $M$ and $-M$, a coin operator that describes the reflection of particle's direction of movement (i.e. coin state) is changed at the points of reflection:
\[
(\hat{I}_P \otimes \hat{U}_C) \rightarrow \left( \sum_{x_1=-(M-1)}^{x_1=M-1} |x_1\rangle \langle x_1| \otimes \hat{U}_C \right) + (|M\rangle \langle -M| + |M\rangle \langle M|) \otimes (|L\rangle \langle R| + |R\rangle \langle L|). \] (8)

Note that a general case of different two positions is equivalent to moving the initial position. One can also consider reflection in a single position $M$ as well.

Combining the above two circular and reflecting (finite) together with open (infinite) boundary conditions, one can in the case of two particles on a line obtain different topologies: torus (two circles), finite and infinite cylinder (circular and reflection/open), square (both particles reflect on both sides of 0), etc. The corresponding corrected shift operators are obtained as a tensor product between the two single-particle corrected operators.

Analogously, one can study the circular and reflecting boundary conditions for the case of one particle on a two-dimensional lattice as well. For example, the correction of the shift operator for the case of circular conditions connecting points with different positions on the $x$-axis ($M$ and $-M$), resulting in the (infinite) cylinder geometry, is given by
\[
\hat{C}_x = \sum_y |M, y\rangle \langle M, y| \otimes |E\rangle \langle E| + |M, y\rangle \langle -M, y| \otimes |W\rangle \langle W|
- (M-1), y\rangle \langle -M, y| \otimes |E\rangle \langle E| + |M-1, y\rangle \langle M, y| \otimes |W\rangle \langle W|,
\] (9)
while the reflection over the lines $x = \pm M$ results in the correction of the coin operator given by:
\[
\hat{R}_x = \sum_y |M, y\rangle \langle M, y| \otimes |W\rangle \langle E| + |M, y\rangle \langle -M, y| \otimes |E\rangle \langle W| +
+ \sum_{x=-(M-1)}^{x=M-1} \sum_{y=-M}^{y=M} |x, y\rangle \langle x, y| \otimes \hat{U}_C.
\] (10)
In addition to the above two cases, for a two-dimensional lattice one more option of a boundary along one axis occur, presenting us with the Möbius strip. Connecting the points \((M, y)\) of the line \(x = M\), and \((-M, -y)\) of the line \(x = -M\), results in the shift operator for which the sum for the \(x\) component is again going as above (from \(-M + 1\) to \(M - 1\)), while the correction term is

\[
\hat{M}_x = \sum_y \langle -M, -y | M, y \rangle \otimes |E\rangle \langle E | + \langle -M, -y | M, y \rangle \otimes |W\rangle \langle W |
\]

\[
|M - 1, y \rangle \langle M, y| \otimes |W\rangle \langle W | + \langle -(M - 1), y | -M, y \rangle \langle E \rangle \langle E |
\]

and analogously for connecting the \(y = M\) and \(y = -M\) axes according to Möbius topology. Combining the two results in the topology of Klein bottle.

Note that the Möbius boundary conditions for the case of two particles on a line would require a non-local shift operation, connecting distant sites \(x_2\) and \(-x_2\) of a second particle, whenever the first one is in the position \(x_1 = M\) or \(x_1 = -M\). Clearly, the shift operation is not a simple product of two one-particle operations. It is rather a controlled operation: conditioned to a position of the first particle, the second one is moving either locally (\(x_2 \rightarrow j \pm 1\)), if \(x_1 \neq \pm M\), or non-locally, otherwise. This can bring interesting consequences for the properties of a quantum walk, as it may introduce entanglement between the walkers.

Another type of boundary conditions are absorbing ones. They are modeled by measurements at certain points (of a line or a lattice) at each step of the walk. For example, an absorption at point \(x_1\) on a line of a particle, coming from the left or right, is modeled by performing a measurement given by the projector \(\hat{P}(x_1) = |x_1\rangle \langle x_1| \otimes \hat{I}_C\). If a particle is found at position \(i\), it is absorbed and a walk stopped. Otherwise, a particle is for sure not in a position \(x_1\), its state \(|\psi(n)\rangle\) after \(n\) steps of the walk, is collapsed onto \(\hat{I}_PC - \hat{P}(x_1) = (\hat{I}_P - |x_1\rangle \langle x_1|) \otimes \hat{I}_C |\psi(n)\rangle\), renormalized to unity, and evolved by the one step evolution operator described above. Such walks, known as measured walks, were studied before in Ref. [3], [25] in relation to various hitting times (see our discussion in the next section).

Partial measurements modeling absorption of a particle can be also used to model noise and decoherence effects. The other two ways to model noise and decoherence effects are breaking the links between certain nodes, or using different coins for different nodes and/or steps.

### 2.2 Noise and decoherence: broken links and different coins

Studying decoherence effects by breaking the links between two nodes was first introduced in Ref. [26] for the case of a walk on a line, and later generalized to a two-dimensional case.[27] In a one-dimensional case, breaking the link between two neighboring nodes \(x_0\) and \(x_0 + 1\), at a step \(n\) of a walk, is equivalent to imposing the reflecting boundary conditions in between the two nodes, for
particle coming from both directions. In other words, a particle coming from
the node $x_0$ to the right will, instead of arriving to node $x_0 + 1$, change its
direction (coin state, from $|R\rangle$ to $|L\rangle$) and return back to $x_0$, and analogously
for the particle coming from the node $x_0 + 1$ to the left. Therefore, breaking
the link between the nodes $x_0$ and $x_0 + 1$, at a step $n$ of the walk, changes the
shift operator $\hat{S}$ at that step from (2) to:
\[
\hat{S} = \left( \sum_{x_1 \neq x_0} |x_1 + 1\rangle \langle x_1| \right) \otimes |R\rangle \langle R| + |x_0\rangle \langle x_0| \otimes |L\rangle \langle L| \\
+ \left( \sum_{x_1 \neq x_0 + 1} |x_1 - 1\rangle \langle x_1| \right) \otimes |L\rangle \langle L| + |x_0 + 1\rangle \langle x_0 + 1| \otimes |R\rangle \langle R|.
\]

Analogously, the shift operator (6) for the case of a single walker in two-
dimensions is changed as well. For example, breaking the link between the nodes
$(x_0, y_0)$ and $(x_0 + 1, y_0)$ changes $|x_0 + 1, y_0\rangle \langle x_0, y_0| \otimes |E\rangle \langle E|$ to $|x_0, y_0\rangle \langle x_0, y_0| \otimes |W\rangle \langle W|$, and $|x_0, y_0\rangle \langle x_0 + 1, y_0| \otimes |W\rangle \langle W|$ to $|x_0 + 1, y_0\rangle \langle x_0 + 1, y_0| \otimes |E\rangle \langle E|W\rangle$.

Note that in the case of two walkers on a line, breaking of the links has
to be identical for both walkers, if we want them to walk over the same line.
Also, note that breaking of one link of only one of the two lines correspond to
breaking of infinitely many links in the corresponding two-dimensional walk on
the $xOy$ plane.

If in every step different (possibly randomly chosen) links are broken, the
shift operation changes from step to step and the breaking is dynamic. Breaking
of the links can be either static or dynamic. If links (given by the pairs of nodes
that are supposed to be connected by them) that are broken are fixed throughout
the whole walk, the shift operator is changed according to the above description
and fixed as well: in every step of the walk the same shift operation is applied
(breaking is static). Otherwise, if in every step different (possibly randomly
chosen) links are broken, the shift operation changes from step to step and the
breaking is dynamic. Note that static breaking of the links allow to study walks
over planar graphs with nodes having at most degree 4.

The other possibility of studying noise and decoherence effects is by intro-
ducing different coin operation for different nodes. In the one-dimensional case
(analogously for two dimensions and higher), changing the unique coin operation $\hat{U}_C$ to $\hat{U}_{C_i}$, for each node $i$, changes the one-step evolution (1), from
$\hat{U} = \hat{S} \left( I_P \otimes \hat{U}_C \right)$ to
\[
\hat{U} = \hat{S} \left( \sum_{x_i} |x_i\rangle \langle x_i| \otimes \hat{U}_{C_{x_i}} \right)
\]
\[
= \left( \sum_{x_i} |x_i + 1\rangle \langle x_i| \otimes |R\rangle \langle R| \hat{U}_{C_{x_i}} + |x_i - 1\rangle \langle x_i| \otimes |L\rangle \langle L| \hat{U}_{C_{x_i}} \right),
\]
and analogously for one particle on the lattice.
Again, altering coin operations can be either static or dynamic. Quantum-to-classical transition driven by many coins was studied in Ref. [28]. The particle localization due to varying coin in time was also studied in Ref. [22], [23, 24]. The physical explanation of the particle localization can be explained as follows: a quantum walk, say on a lattice, can be seen as a model for a scattering process of a particle (say, electron) over the ions of a crystal lattice, such that a coin operators model the transition amplitudes between the neighboring ions. Introducing for some nodes coins different from the common one corresponds to introducing impurities (ions different from the one of a crystal lattice), which in the static case (impurities fixed in time) leads to Anderson-type particle localization.[29]

3 Quantities computed by the simulator

In this section, we describe the quantities that characterize quantum walk that our simulator is computing. Since the emphasis of the program is to study the joint properties of a multi-particle quantum walk, we will use notation compatible with the case of two walkers on a line. Using (4) and (5), one can easily obtain the corresponding quantities for the case of a single walker in two dimensions.

A pure state of two walkers is a unit vector in a two-particle Hilbert space $H_{12} \equiv H_1 \otimes H_2$, where one-particle mutually isomorphic spaces $H_i = H_{P,i} \otimes H_{C,i}$, with $i \in \{1, 2\}$, have each a position and a coin factor space. Writing $H_{12} = (H_{P,1} \otimes H_{P,2}) \otimes (H_{C,2} \otimes H_{C,2}) = H_{P,12} \otimes H_{C,12}$, one can talk of a two-particle position and coin (generally mixed) states.

If the initial state is $|\psi(0)\rangle_{12} \in H_{12}$, then after $n$ steps the state is $|\psi(n)\rangle_{12} = \hat{U}_{12}^n |\psi(0)\rangle_{12}$.

Partial one-particle mixed states, after $n$ steps of a walk, are given by density operators obtained by performing partial trace, $\hat{\rho}_i(n) = \text{Tr}_2 |\psi(n)\rangle \langle \psi(n)|_{12}$, and analogously for the second particle. The joint position state is evaluated by performing partial trace over the joint coin space $H_{C,12}$, $\hat{\rho}_{P,12}(n) = \text{Tr}_{C,12} |\psi(n)\rangle \langle \psi(n)|_{12}$, while to obtain the coin state, we do a partial trace over the joint position space $H_{P,12}$. $\hat{\rho}_{C,12}(n) = \text{Tr}_{P,12} |\psi(n)\rangle \langle \psi(n)|_{12}$. The one-particle position and coin states are obtained analogously, from one-particle states $\hat{\rho}_i(n)$, with $i \in \{1, 2\}$.

The main quantity from which we compute relevant joint properties is a joint two-particle probability distribution $p_{12}(i, j; n)$, a probability that the position $x_1$ of the first particle is $i$, and the position $x_2$ of the second is $j$. It is easily computed from the overall position state $\hat{\rho}_{P,12}(n)$ as

$$p_{12}(i, j; n) =_{12} \langle i, j | \hat{\rho}_{P,12}(n) | i, j \rangle_{12}.$$  \hspace{1cm} (12)

Often, for reasons of simplicity, we assume the time dependence (i.e. step $n$) as implicit, and write $p_{12}(i, j)$, $\hat{\rho}_{P,12}$, etc. Also, sometimes we will drop the
labels 12, 1 and 2 that denote whether a given quantity is a two-particle or a single-particle quantity: for example $p(i, j)$ instead of $p_{12}(i, j; n)$, or $\hat{\rho}_P$ instead of $\hat{\rho}_{P,12}(n)$.

Marginal probability, $p_1(i; n) = \sum_j p_{12}(i, j; n)$ can also be obtained from partial one-particle state, $p_1(i; n) = \langle i | \hat{\rho}_1(n) | i \rangle$, and analogously for particle 2.

In Ref. [13] it was shown that joint probability distributions obtained from initial states entangled in the coin degree of freedom cannot be achieved by initial separable states, while the marginal probabilities are nothing but a weighted sum of single-particle probability distributions. As this is the key result showing the difference between classical and quantum states at the level of joint, rather than single-walker level, we present it as a theorem (as well as the results regarding the average squared distance and the one-shot probability to hit, presented below):

**Theorem 1:** Let $p_{12}^{\pm}(i, j; n)$ be the joint probability distributions obtained after $n$ steps from the initial states $|\psi(0)\rangle_{12} = |00\rangle (|RL\rangle \pm |LR\rangle)/\sqrt{2}$ maximally entangled in the coin degree of freedom, starting from the initial position (0, 0). Then, no initial state separable in the coin degree of freedom can produce either of the two joint probabilities $p_{12}^{\pm}(i, j; n)$.

As the evolution of quantum walks in unitary, there exist no stationary state of the system, a fixed point of the evolution, as in the case of classical random walks. Therefore, there exist no stationary probability distribution (for detailed discussion, see for example Ref. [16] or [17]). Yet, the time (or rather, step) average of the probability distribution, $\bar{p}_{12}(i, j; n) = \frac{1}{n} \sum_{k=1}^{n} p_{12}(i, j; k)$, does converge to a limiting distribution (analogously for one-particle distribution):

$$\pi_{12}(i, j) = \lim_{n \to \infty} \bar{p}_{12}(i, j; n).$$

One can thus study how fast (in steps $n$) an average distribution $\bar{p}_{12}(i, j; n)$ approaches the limiting one $\pi_{12}(i, j)$, globally (mixing time), point-wise (sampling time), etc. (for definitions of the mixing, sampling, filling and dispersion time, see for example Ref. [17]).

The first global quantity of the two walker to consider is the average distance between the two:

$$\langle \hat{d} \rangle = \langle |\hat{x}_1 - \hat{x}_2| \rangle = \sum_{i,j} p_{12}(i, j; n) |i - j|.$$

Note that the $n$-dependence is implicit as the average is an expectation value of an operator $\hat{d} = |\hat{x}_1 - \hat{x}_2|$ taken for the state $|\psi(n)\rangle_{12}$. This is clearly a global quantity that is not dependent only on marginal probability distributions $p_1(i; n)$ and $p_2(i; n)$, but on the correlations between the two random variables $x_1$ and $x_2$, which can in this case have particular entanglement-induced quantum features different from any classical-like correlations, analogously as in the case of the average squared distance $\langle \hat{d}^2 \rangle = \langle (\hat{x}_1 - \hat{x}_2)^2 \rangle$, as first shown in Ref. [13]. We present this result as a theorem:
Theorem 2: Let $\langle \hat{d}^2 \rangle^\pm$ be the average squared distance obtained from the initial states $|\psi(0)\rangle^\pm = |00\rangle (|RL\rangle \pm |LR\rangle)/\sqrt{2}$. Then, no initial state separable in the coin degree of freedom can produce either of the two expected values. Moreover, if by $\langle \hat{d}^2 \rangle^S$ we denote the average squared distance of a generic initial state separable in the coin degree of freedom, then we have the following strict inequalities:

$$\langle \hat{d}^2 \rangle^+ < \langle \hat{d}^2 \rangle^S < \langle \hat{d}^2 \rangle^-.$$ 

Next, we discuss various types of the so-called mixing times. First, we describe the one-particle case, then we move to the case of two walkers.

In algorithmic applications of quantum walks, like in search problems, a solution to the problem is given by a particular node $i_0$ (or more than one node, but the generalization is straightforward) and one is interested in the probability of finding this solution. In other words, we are interested in the probability of finding the walker in the position $i_0$.

Let us define two (one-particle) orthogonal projectors, $\hat{P}_0 = |i_0\rangle \langle i_0| \otimes \hat{I}_c$ and $\hat{P}_1 = \hat{I} - \hat{P}_0$, where $\hat{I}_c$ is the identity in the coin space. Then, the one-shot hitting time for a given probability $p$ is the number of steps $N^{(1)}(i_0, p)$ for which the probability of the walker to be found in position $i_0$ is bigger or equal than $p$ (see Ref. [3]). It is determined by the (one-particle) one-shot probability to hit:

$$P^{(1)}_{f}(i_0; n) = \|\hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n-1} |\psi(0)\rangle\|^2.$$ 

(13)

The above definition of hitting time is useful in cases one can estimate step $n$ around which the one-shot probability to hit $P^{(1)}_{f}(i_0; n)$ is relatively high, like it was the case of Shor’s algorithm.[30]

If we check after each step whether the particle is in position $i_0$, we effectively perform the above measurement $M(i_0) = 0 \cdot \hat{P}_0 + 1 \cdot \hat{P}_1$ after each step. Such a walk, in which after each step the measurement given by $M(i_0)$ is performed, is called the $|i_0\rangle$-measured walk:[3] if the particle is collapsed (absorbed) onto the ray $|i_0\rangle (result 0 obtained)$, the solution to the problem (data-base search, etc.) is found and the walk terminated; otherwise, if the result is 1, the walk is evolved one more step by $\hat{U}$.

For $|i_0\rangle$-measured walk, let $P^{(1)}_{f}(i_0; n)$ be the probability to detect (for the first time) the particle at position $i_0$, at step $n$ (first-time probability to hit):

$$P^{(1)}_{f}(i_0; n) = \|\hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n-1} |\psi(n)\rangle\|^2.$$ 

(14)

Then, the average hitting time of the $|i_0\rangle$-measured walk is:[25]

$$N^{(1)}_{a}(i_0) = \sum_{n=1}^{\infty} n P^{(1)}_{f}(i_0; n).$$ 

(15)

The above hitting time corresponds to a typical (average, expected) running time for the quantum-walk based algorithm.[25]

Finally, one might be interested in a number of steps $N^{(1)}_{c}(i_0, p)$ after which a $|i_0\rangle$-measured walk has probability to stop greater or equal than certain given
p. Such $\mathcal{N}_c^{(1)}(i_0, p)$ is called the concurrent hitting time[3], and is given by the concurrent probability to hit $P_c^{(1)}(i_0; n)$ for the walk to stop at any of the steps $n' \leq n$:

$$P_c^{(1)}(i_0; n) = \sum_{n'=1}^{n} \| \hat{P}_0 \hat{U}^{n'} |\psi(0)\rangle \|^2.$$  \hspace{1cm} (16)

As noted in Ref. [25], the concurrent hitting time corresponds to the number of steps after which the probability to find the solution is greater or equal than $p$.

The above hitting times were defined for one-particle quantum walks and are given by the probabilities (13) – (16). For two particles, the corresponding hitting times are given by the analogous two-particle probabilities $P_o^{(2)}(i_0; n)$, $P_f^{(2)}(i_0; n)$ and $P_c^{(2)}(i_0; n)$ that at least one of the two particles is detected in position $i_0$. Indeed, if the solution to the problem is given by the marked position $i_0$, it is enough if only one of the two walkers finds it. The two-particle probabilities and hitting times are obtained as in the case of one-particle walks, by substituting one-particle $\hat{P}_0$ (and its complement $\hat{P}_1$) by its two-particle equivalent

$$\hat{P}_0 = \left( |i_0\rangle \langle i_0| \right)_{P_1} \otimes \hat{I}_{P_2} + \hat{I}_{P_1} \otimes |i_0\rangle \langle i_0| - |i_0\rangle \langle i_0| \otimes |i_0\rangle \langle i_0|$$

in equations (13) – (16). Note the subtraction of the term $|i_0\rangle \langle i_0| \otimes |i_0\rangle \langle i_0|$ which is twice counted in the sum of the first two terms of the expression. Formally, without the subtraction this would not be an idempotent projector for which $\hat{P}_0^2 = \hat{P}_0$.

In finding solutions by searching certain data base, for example, we would prefer if the two particles search different regions at each given moment: if the two walkers are following each other, than there is little help of such "parallel processing". In other words, the probability that both walkers are found in the same position should be as small as possible; their average distance as big as possible. In Ref. [13] it was shown that the maximal/minimal one-shot probability $P_o^{2}(i_0; n)$ to find at least one particle in position $i_0$ corresponds to the case of maximal/minimal average distance, when the initial coin state is the maximally entangled. This is a content of the following theorem:

**Theorem 3:** Let $P_o^{2}(i_0; n)^\pm$ be the average squared distance obtained from the initial states $|\psi(0)\rangle_{12} = |00\rangle (|RL\rangle \pm |LR\rangle)/\sqrt{2}$. Then we have the following strict inequalities:

$$P_o^{2}(i_0; n)^+ < P_o^{2}(i_0; n)^S < P_o^{2}(i_0; n)^-,$$

where $P_o^{2}(i_0; n)^S$ is the one-shot probability of a generic initial state separable in the coin degree of freedom.

Global quantities do not depend on marginal probability distributions, but on the correlations between the random variables, in our case the positions of the two walkers. They are given by the covariance. For the case of the positions $x_1$ and $x_2$ of the two walkers, the covariance is given by:

$$\text{Cov}(x_1, x_2) = \langle (x_1 - \langle x_1 \rangle)(x_2 - \langle x_2 \rangle) \rangle = \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle,$$  \hspace{1cm} (17)
The other way to quantify correlations between two walkers is by classical (Shannon) and quantum (von Neumann) mutual information. Classical (Shannon) mutual information between the two random variables, say positions $x_1$ and $x_2$, is (note the implicit dependence on the step $n$):

$$I(x_1 : x_2) = H(x_1) + H(x_2) - H(x_1, x_2),$$  \hspace{1cm} (18)

where $H(x_p) = -\sum_i p_1(i) \log p_1(i)$, with $p = 1, 2$, is the Shannon entropy of the random variable $x_p$ taking the values $i \in \mathbb{Z}$, and

$$H(x_1, x_2) = -\sum_{i,j} p_{12}(i, j) \log p_{12}(i, j)$$  \hspace{1cm} (19)

is the joint (Shannon) entropy of $x_1$ and $x_2$.

The corresponding quantum (von Neumann) mutual information between the position degrees of freedom of two walkers is given in terms of their global and partial position states $\hat{\rho}_{P,12}, \hat{\rho}_{P,1}$ and $\hat{\rho}_{P,2}$:

$$I(\hat{\rho}_{P,12}) = S(\hat{\rho}_{P,1}) + S(\hat{\rho}_{P,2}) - S(\hat{\rho}_{P,12}),$$  \hspace{1cm} (20)

where $S(\hat{\rho}_{P,1}) = -\text{Tr}(\hat{\rho}_{P,1} \log \hat{\rho}_{P,1})$, and analogously for other two mixed states.

As it was shown in Ref. [13], the initial entanglement in the joint two-particle coin state can, starting from the initially product position state $|0,0\rangle_{12}$, bring about correlations between the positions of the two, the correlations beyond those achievable by any classical (i.e. mixed, but separable) initial state. In other words, a two-particle quantum walk can, in the course of steps, transfer the entanglement, and thus correlations, from the coin to the position degree of freedom. Therefore, one might be interested in analyzing the dynamics of mutual information (Shannon and von Neumann) between the (joint) coin and position degrees of freedom, or between the coins of the two walkers, or finally between the two walkers. They are given by expressions analogous to (18) and (20).

Finally, one can directly study entanglement between the two degrees of freedom. This is, being purely quantum feature, the most interesting quantity to study since it brings, in some settings, features of quantum walks classically impossible to achieve.[13] Nevertheless, unlike the correlations or (classical and quantum) mutual information, entanglement is more complex to characterize and quantify. In the case of pure bipartite states, entanglement between the two degrees of freedom is well defined and easy to evaluate: it is nothing but the von Neumann entropy of either of the two partial mixed states. Thus, if the initial state is pure, entanglement between the coin and position degree of freedom is given by:

$$E_{C,P} = S(\hat{\rho}_{C,12}) = S(\hat{\rho}_{P,12}).$$  \hspace{1cm} (21)

Obviously, from the numerical point of view, it is much easier, and more accurate, to use the first equality and deal with much smaller $4 \times 4$ matrix representation of $\hat{\rho}_{C,12}$. Writing the joint two-particle state $|\psi\rangle$ in the Schmidt
bi-orthogonal expansion between the joint position and coin degrees of freedom

\[ |\psi\rangle = \sum_{k=1}^{4} \sqrt{r_k} |\varphi_k\rangle_p |k\rangle_C, \]

the partial coin and position mixed states are given as

\[ \hat{\rho}_C = \sum_{k=1}^{4} r_k |k\rangle_C \langle k| \]

and \[ \hat{\rho}_P = \sum_{k=1}^{4} r_k |\varphi_k\rangle_p \langle \varphi_k|_P \] (note that, for reasons of simplicity, we dropped the step \( n \) dependence, and subscripts 12).

Calculating the coin state is computationally easy, its complexity is only quadratic in the number of steps \( n \), as one has to evaluate \(|\psi(n)\rangle\) and then a simple trace \( \hat{\rho}_C(n) = Tr_P |\psi(n)\rangle \langle \psi(n)| \). Solving the characteristic equation and finding eigenvalues \( r_k \) and eigenvectors \(|k\rangle_c\) of a four-dimensional system given by \( \hat{\rho}_C \) is easy task as well. Finally, the eigenvectors \(|\varphi_k\rangle_p\) are easily calculated by obtaining the partial scalar product, \(|\varphi_k\rangle_p = \frac{1}{\sqrt{r_k}} \langle k| \langle \psi| \).

Finally, the partial position state is \( \hat{\rho}_P = \sum_{k=1}^{4} r_k |\varphi_k\rangle_p \langle \varphi_k|_P \) and the entanglement between the position and the coin degree of freedom is:

\[ E_{C,P} = S(\hat{\rho}_{C,12}) = S(\hat{\rho}_{P,12}) = -\sum_{k=1}^{4} r_k \log(r_k). \]

But, finding the entanglement between the positions of two walkers, or the two coins, is much more difficult problem. The partial position and coin states, \( \hat{\rho}_{P,12} \) and \( \hat{\rho}_{C,12} \), are mixed, and mixed-state entanglement is neither unique, nor easy to evaluate. One possible mixed-state entanglement measure is the entanglement of formation.[31] For the case of two-particle position state, one possible upper bound to the entanglement of formation could be given as:

\[ E_F(\hat{\rho}_{P,12}) = \sum_{k=1}^{4} r_k E(|\varphi_k\rangle_p,_{12}), \]

with \( E(|\varphi_k\rangle_p,_{12}) = S(Tr_{P,2} |\varphi_k\rangle_p \langle \varphi_k|_{P,12}). \)

A relevant measure for the quantumness of correlations is the quantum discord.[33] In classical information theory, we have that the mutual information between random variables \( X \) and \( Y \) is given by \( I(X : Y) = H(X) + H(Y) - H(X,Y) \) or, equivalently, \( J(X : Y) = H(Y) - H(Y|X) \).

For the general joint state \( \hat{\rho}_{XY} \) a subsystem’s partial state after a measurement performed on the other sub-system is determined by the choice of the measurement and its outcome. Let \( M_x = \sum_i i\Pi_i^X \) be a sub-system’s \( X \) observable, where \( \Pi_i^X = |i\rangle \langle i| \) represent one-dimensional orthogonal projectors corresponding to the measurement outcome \( i \). Upon measuring \( \hat{M}_X \otimes \hat{I}_Y \) onto the joint state \( \hat{\rho}_{XY} \), and obtaining the result \( i \), the partial state of the subsystem \( Y \) is

\[ \hat{\rho}_{Y|i\Pi_i^X} = Tr_X \frac{(\Pi_i^X \otimes \hat{I}_Y)\hat{\rho}_{XY}(\Pi_i^X \otimes \hat{I}_Y)}{p_i}, \]
where \( p_i = \text{Tr}_{XY}(\hat{\rho}_{XY}(\hat{\Pi}_X^i \otimes \hat{I}_Y)) \). The expected entropy of the sub-system \( Y \), conditioned by the measurement \( \hat{M}_X \) performed on the sub-system \( X \) is:

\[
S(Y|\hat{M}_X^i) = \sum_i p_i S(\hat{\rho}_{Y|iX^i}).
\]

The difference between the uncertainty of the state of the sub-system \( Y \) (measured by the von-Neumann entropy) before the sub-system measurement \( \hat{M}_X \) was performed, and the expected uncertainty after it has been performed is

\[
\mathcal{J}(X : Y)_{\hat{M}_X} = S(\hat{\rho}_Y) - S(Y|\hat{M}_X),
\]

where \( \hat{\rho}_Y = \hat{\rho}_{XY} \). The quantum discord, with respect to the measurement \( \hat{M}_X \), is given by

\[
\delta(X : Y)_{\hat{M}_X} = I(X : Y) - \mathcal{J}(X : Y)_{\hat{M}_X}
\]

\[
= S(\hat{\rho}_Y) - S(\hat{\rho}_{XY}) + S(Y|\hat{M}_X). \tag{22}
\]

In the case of two particles on the line, \( X \) denotes the position of particle 1 and \( Y \) the position of particle 2. For one particle on the lattice, \( X \) and \( Y \) denote the positions of the particle along the \( x \) and \( y \) axes, respectively.

## 4 The simulator at work

Here, we illustrate the simulator at work. The simulator is constituted by three main programs: one for simulating one particle on a square lattice; another for simulating two particles on a line; and, finally, one to simulate a single particle on a line. All the quantities described in Section 3 can be outputted by the simulator, and are chosen in a configuration file. The configuration file is parsed by the simulator and contains the following information: dimension of the grid, number of steps to simulate, initial state for the particles, broken links in the grid, boundary conditions of the grid, measurement points, distribution of random quantum coins over the grid, quantities to simulate.

Next, we present several examples of usage of the simulator, one for each program.

### 4.1 A particle on a square lattice

For this case we illustrate the simulator by computing several relevant quantities for a quantum walk over a square lattices with several broken links. The idea is to get a picture of the effect of broken links (or impurities) in the simulated quantities. In particular we verify Anderson-like localization by noticing that the average probability distribution is concentrated around the initial position.

For this particular simulation we consider:

- a grid of size 61 × 61;
- a number of steps 30;
- broken link probability of 0.48;
- initial state $|\psi(0)\rangle = |0,0\rangle |E\rangle$.

The plots output by the program concerning the quantities are depicted in Figure 2, 3, 4 and 5.

![Figure 2](image1.png)

Figure 2: (Color online) Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Probability on plane after 30 steps. (Right) Average probability distribution.

![Figure 3](image2.png)

Figure 3: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Shannon entropy for variables $X$ and $Y$. (Right) Shannon mutual information for position variables $X$ and $Y$. 
Figure 4: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) von Neumann mutual information of $\hat{\rho}_{P,XY}$. (Right) Quantum discord of $Y$ given measurements $\Pi_i^X$ on $X$.

Figure 5: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Mean distance of variables $X$ and $Y$. (Right) Covariance of variables $X$ and $Y$.

4.2 Two particles on a line

The effect of entanglement on quantum walks is a relevant problem which is hard to tackle analytically. For this reason the simulator is designed to determine various information theoretical quantities, such as entropy, mutual information, (upper-bound) entanglement of formation, which quantify the effect of entanglement between the coins on the joint position probability distribution of two walkers. Indeed, one can check that entangled particles evolve differently than non entangled ones.[13].

For this particular simulation we consider:

- a grid of size 61 × 61;
• a number of steps 30;
• initial state $|\psi(0)\rangle_{12} = |0, 0\rangle_{12} (|RR\rangle - |LL\rangle)$.

The results of the quantities are depicted in Figures 6, 7, 8 and 9.

Figure 6: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Probability on plane after 30 steps. (Right) Average probability distribution.
Figure 7: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Shannon entropy for variables $x_1$ and $x_2$. (Right) Shannon mutual information for position variables $x_1$ and $x_2$.

Figure 8: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) von Neumann mutual information of $\hat{\rho}_{P,12}$. (Right) Quantum Discord.

Figure 9: Evolution of one particle on a square lattice with broken link probability of 0.48 for 30 steps. (Left) Mean distance of variables $x_1$ and $x_2$. (Right) Covariance of variables $x_1$ and $x_2$. 20
4.3 A particle on a line

Although the case of a particle on a line is quite well studied, we also included it in the simulator. To take profit of the features of the simulator we considered an absorbing boundary condition. For this particular simulation we consider:

- a line of length 100;
- a number of steps 10000;
- absorbing boundary condition;
- initial state \(|\phi_0\rangle = |0\rangle |R\rangle\).

The results of the quantities are depicted in Figure 10.

![Probability Distribution](image1)
![Average Probability Distribution](image2)

Figure 10: Evolution of one particle on a line of length 201, for 10000 steps with absorbing boundary. (Left) Probability distribution for position. (Right) Average probability distribution for position.

Compared to the DTQW in Ref. [34], our program can perform simulation of a walk for up to \(10^7\) steps, which might seem as a disadvantage. Nevertheless, the two types of quantum walks differ significantly in their long-time behavior, as the cited paper thoroughly analyses: while the standard DTQW has a ballistic behavior, i.e. its diffusion scales as \(\sigma \sim t\), the feed-forward DTQW diffusion scales as \(\sigma \sim t^{0.4}\). Consequently, the memory needed to encode the relevant part of the state is just a fraction of the memory needed to encode a state of a standard 1D DTQW after \(10^8\) steps (see figure 2A of Ref. [34], where the x-axis goes from -4500 to +4500). Indeed, the memory needed to encode a quantum state of a standard DTQW after \(10^8\) steps would be 12800 Gbits, which exceeds the limits of any conceivable computer memory that can be found on the market.

Nevertheless, when posing similar constraints to a standard 1D DTQW, for example reflecting boundary conditions, thus effectively limiting the area of a walk, our simulator can perform many more steps. In particular, for a line that goes from node -4000 to node +4000, our program was able to finish the
simulation for $10^6$ steps in roughly 3 hours, while to simulate $10^7$ steps took roughly 30 hours. Consequently, running time for $10^8$ steps would take roughly about two weeks, which is reasonable for a well defined scientific research. In Figure 11, we present the probability distribution and the average probability distribution of particle position for the mentioned simulation of $10^7$ steps.

Figure 11: Probability distribution (left) and average probability distribution (right) of the particle position for one-particle quantum walk on the open line after $10^7$ steps. The initial state is $|\psi(0)\rangle = |0\rangle |L\rangle$, and the random coin parameters are set within the interval $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$.

4.4 Example: Anderson localization

Here we simulate the effect of two types of decoherence due to random broken links and random coins, in order to see if Anderson localization will occur, as well as to find some difference between the two models. In the case of random broken link, the broken link factor gives the probability of each link to be broken. For random coins, the random coin factor is the probability of the coin operator, at each position, to be randomly chosen.

For this particular simulation we consider:

- a 2D lattice of size $61 \times 61$;
- a number of steps 100;
- Klein Bottle boundary condition;
- initial state $|\phi_0\rangle = |0\rangle (|E\rangle + |S\rangle)$.

Simulations ran for 9 cases: random coin factors of 0.2, 0.48 and 0.9, random broken link factors of 0.2, 0.48 and 0.9 and random coin and broken link factors of 0.2, 0.48 and 0.9.

The results of the quantities are depicted in Figures 12 and 13.
Figure 12: Position probability distribution of one particle on the lattice of dimension $61 \times 61$, for 100 steps with different random coin factors and random broken link factors. (First row left) Probability distribution for position with random coin factor 0.2. (First row right) Probability distribution for position with random broken link factor 0.2. (Second row left) Probability distribution for position with random coin factor 0.48. (Second row right) Probability distribution for position with random broken link factor 0.48. (Third row left) Probability distribution for position with random coin factor 0.9. (Third row right) Probability distribution for position with random broken link factor 0.9.
Figure 13: Position probability distribution of particle on the lattice of dimension $61 \times 61$, for 100 steps with same both broken link and random coin factors. (First) Position probability distribution with broken link and random coin factors 0.2. (Second) Position probability distribution with broken link and random coin factors 0.48. (Third) Position probability distribution with broken link and random coin factors 0.9.

Figures 12 and 13 suggest that both random broken link and random coin can lead to Anderson localization. Moreover, based on figure 12 one can conclude that for the same factors, the localization is sharper for random broken links compared to random coins. Figure 13 shows the Anderson localization due to both random broken links and coins. Further analysis/simulation is needed to characterize Anderson localization.

Anderson localization for quantum walk on the line can be achieved by defining static random coins of parameters $\theta, \zeta, \xi \in \left[\frac{\pi}{8} - \frac{\pi}{8}, \frac{\pi}{8} + \frac{\pi}{8}\right]$, illustrated in Figure 14 with the following conditions:

- a line of size 8001;
- a number of steps 4000;
- reflecting boundary condition;
• initial state $|0\rangle |R\rangle$;
• static random coin with parameters $\theta, \zeta, \xi \in \left[\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}\right]$;
• the probability that at each step a link will be broken (index broken link) is 0.3.

Figure 14: Probability distribution (left) and average probability distribution (right) of the particle position for one-particle quantum walk on the open line after 4000 steps. The initial state is $|\psi(0)\rangle = |0\rangle |R\rangle$, the probability that at each step a link will be broken (index broken link) is 0.3 and the random coin parameters are set within the interval $\theta, \zeta, \xi \in \left[\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}\right]$. The respective parse file can be found in Appendix A.

In the case of two particles on separate lines we can simulate two different types of decoherences leading to localization. In Figure 15 one particle is under the influence of static random coins, the other is under the influence of random coins at random positions.

• two lines of size 201;
• a number of steps 100;
• reflecting boundary conditions;
• initial state $\sqrt{2} |0, 0\rangle |RR\rangle$;
• static random coin with parameters $\theta, \zeta, \xi \in \left[\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}\right]$ for the first walker;
• broken link index of 0.3 for the second walker, with Hadamard coin.
Figure 15: Probability distribution (left) and average probability distribution (right) of the particles positions for two-particle quantum walk on open lines after 100 steps. The initial state is $|\psi(0)\rangle = |0,0\rangle |RR\rangle$, for the first walker the random coin parameters are set within the interval $\theta, \zeta, \xi \in \left[\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}\right]$, while for the second walker the fixed coin is given by the Hadamard operator and the index broken link is 0.3. The respective parse file can be found in Appendix B.

4.5 Example: Static Broken Links

To illustrate the usage of static broken links, we consider a 2D lattice with nine boxes of equal dimensions and slits between them, as indicated below:

- 2D lattice of size $91 \times 91$;
- a number of steps 1000;
- reflecting boundary conditions;
- initial state $\frac{1}{2}(|-30,-30\rangle (|E\rangle + i |N\rangle) + |30,30\rangle (|W\rangle + i |S\rangle))$;
- Hadamard coin;
- The static broken links are set between positions $(-15,y) & (-14,y)$ and $(14,y) & (15,y)$, for $y \in \{-45,\ldots,45\}\setminus\{-30,0,30\}$, and positions $(x,-15) & (x,-14)$ and $(x,14) & (x,15)$, for $x \in \{-45,\ldots,45\}\setminus\{-30,0,30\}$;
Figure 16: Probability distribution (left) and average probability distribution (right) of particle position for one-particle quantum walk on a lattice with reflecting boundary conditions at $x, y = \pm 45$ after 1000 steps. The initial state is $|\psi(0)\rangle = \frac{1}{2} (|−30, −30\rangle (|E\rangle + i|N\rangle) + |30, 30\rangle (|W\rangle + i|S\rangle))$, with the fixed coin given by the Hadamard operator. The static broken links are set between positions $(-15, y) \& (-14, y)$ and $(14, y) \& (15, y)$, for $y \in \{-45, \ldots, 45\}\{-30, 0, 30\}$, and positions $(x, -15) \& (x, -14)$ and $(x, 14) \& (x, 15)$, for $x \in \{-45, \ldots, 45\}\{-30, 0, 30\}$. Note that the entire grid is divided into 9 equally-sized loosely connected squares, and the initial state of the walker is a linear superposition of two distant positions (and the corresponding coin states) located in different squares.

5 Conclusions

We developed a simulator for a two-particle quantum walk on a line and one particle on a two-dimensional squared lattice. The simulator can be used to investigate the equivalence between the two cases (one- and two- particle walks) for various boundary conditions (open, circular, reflecting, absorbing and their combinations). For the case of a single walker on a two-dimensional lattice, the simulator can implement the Möbius strip and other similar boundary conditions. Furthermore, other topologies for the walker are also simulated by the proposed tool, like planar graphs with degree up to 4, by considering missing links over the lattice. The simulator is able to compute a vast number of relevant quantities, namely: average position probability distribution, standard deviation/covariances, Shannon and von Neumann entropy and mutual information, upper bound for the entanglement formation, as well as quantum discord. The simulator is available at \url{http://qwsim.weebly.com/} and allows for computational experiments for quantum walks covering new aspects and quantities that were not available before.
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