1 Files

The simulator is composed of 3 separate programs located in separate folders:

- *qwsim_1D*: contains all files needed to simulate the one particle quantum walk on the line;
- *qwsim_1D_2_walkers*: contains all files needed to simulate two particles on the line;
- *qwsim_2D_1_walker*: contains all files needed to simulate one particle on a square lattice;

Each of the programs is in a separate folder. In each folder there are 6 files:

- Makefile;
- main.c;
- qwsim.c;
- qwsim.h;
- *parse_file.txt*: file of the simulation parameters;
- plots.m: matlab file for graph plotting;

2 Running the program

To run the program, one should follow the steps below:

- Compile the program;
- open parse file and change the parameters as described in the next sections;
- save the parse file;
- type *./main* and enter;

Once the simulator finishes, it will output data files as described in the next sections.
There is a matlab program in each folder named *plots.m* to plot the graphs. It's only necessary to open matlab, access the folder of the program and type plots on the terminal.

3 One Particle Quantum Walk on the Line

This section describes the fields of the parse file and the output files. The parse file looks like this:

M

Steps

points

i

c

real_value

complex_value

index_brokenlink_imp

fixed_broken_links

I_0

coin

varying_coin_each_step

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp

fixed_coins

K

theta_0

theta_1

zeta_0

```
zeta_1

xi_0

xi_1

ref 1

dim_absorb 0

i_0

c

gnu_plot
```

3.1 parser_file.txt fields

- M: size of the line, from $-M$ to M;
- steps: number of steps of the quantum walk;
- points: number of initial points where the wave amplitudes are nonzero. Note that a pair $(position, point)$ counts as a single point;
- i: positions on the line where the amplitudes are nonzero;
- c: coin states where the amplitudes are nonzero-0 means *right* and 1 means $left$;
- *real_value*: real part of the amplitude of the wave;
- *complex_value*: complex part of the amplitude of the wave;

  For example

  ```
  points 2

  i 0 3

  c 0 1

  real_value 1 2

  complex_value  3 4
  ```

  ---

  means that at point $(0, 0)$ the wave amplitude is $\frac{1}{\sqrt{1^2+2^2+3^2+4^2}} 1 + \imath 3$ and at point $(3, 1)$ it is $\frac{1}{\sqrt{1^2+2^2+3^2+4^2}} 2 + \imath 4$.

- *index_brokenlink_imp*: fraction of the links that are broken. The links are chosen at random in each step;
- *fixed_broken_links*: number of fixed broken links.
- *I_0*: set of nodes such that $i_0 \in I_0$ means there is a broken link between i_0 and $i_0 + 1$. Note that $-M \leq i_0 \leq M - 1$.

  If the number of fixed broken links is 0 then this field must be empty.
- *coin*: sets the coin operator for the particle in every position;
  - -2 sets the identity matrix;
  - -1 sets the reflection coin;
  - 0 sets the Hadamard coin;
  - 3 sets the random matrix that varies at each step;
- *varying_coin_each_step*: if set to 1, in each step the coin operator will be set according to the following parameters:
  - *theta_0* and *theta_1* sets an interval for θ;
  - *zeta_0* and *zeta_1* sets an interval for ζ;
  - *xi_0* and *xi_1* sets an interval for ξ;
    Note that if *varying_coin_each_step* = 0 then these fields must be empty.
- *index_coin_imp*: fraction of the positions on the line where the coin state is randomly chosen. The position and the matrices are chosen at random at each step;
- *fixed_coins*: number of static random coins.
  - K: positions of static random coins
  - *theta_0* and *theta_1*
  - *zeta_0* and *zeta_1*
  - *xi_0* and *xi_1*.
    Note that if *fixed_coins* = 0 then these fields must be empty.

  For example

```
fixed_coins 2

i 9 -5

theta_0 0 0.75

theta_1 0.75 1.23

zeta_0 0 0.75
```

```
zeta_1 0.75 1.23

xi_0 0.25 0.75

xi_1 0.25 0.95
```

---

means that at position 9 the random matrix is defined with parameters $\theta \in [0, 0.75]$, $\zeta \in [0, 0.75]$ and $\xi = 0.25$ and at position -5 with $\theta \in [0.75, 1.23]$, $\zeta \in [0.75, 1.23]$ and $\xi \in [0.75, 0.95]$.

- ref: if set to 1 reflection boundary is activated. If set to 0 circular boundary condition is activated.
- *dim_absorb*: number of absorbing points;
  - i: position of the absorbing point on the line;
  - c: coin state of the absorbing point;

    Note that if *dim_absorb* is 0 then these fields must be empty.
- *gnu* : *plot*:if set to 1 the output files will be plotted using GNUplot.

3.2 Default files generated

- *mean_x*: mean value of variable x;
- *probability_distribution*: probability distribution of the particle position;
- *average_probability_distribution*: average probability distribution of the particle position;
- *Von_Newman_entropy*: von Neumann entropy of the coin state density matrix;
- *standard_deviation*: standard deviation of x;
- *Shannon_entropy*: Shannon entropy of the coin state density matrix diagonal.

4 Two-particle Quantum Walk on a line

Folder *qwsim_1D_2_walkers*

The parse file has the following form:

```
M

steps

points

i

j

c

real_value

complex_value

different_lines

index_brokenlink_imp_1

fixed_broken_link_1

I_0

coin1

varying_coin_each_step_1

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp_1

fixed_coin_1
```

```
K_1

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

rf1

index_brokenlink_imp_2

fixed_broken_link_2

J_0

coin2

varying_coin_each_step_2

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp_2

fixed_coin_2

K_2

theta_0

theta_1

zeta_0
```

```
zeta_1

xi_0

xi_1


rf2

dim

i_0

j_0

m_options

vn_x

vn_y

vn_m_info

q_discord

ent_form

gnu_plot
```

4.1 parser_file.txt fields

- M: Size of the grid, from $-M$ to M;
- *steps*: number of steps of the quantum walk;
- *points*: number of points where the wave amplitudes are nonzero. Note thatNote that a pair $(position, coin)$ fonts as a single point;
- i: initial position of the first particle;
- j: initial position of the second particle;
- c: coin state where the amplitudes are nonzero-0 means RR, 1 means RL, 2 means LR and 3 is LL, where L stands for left and R stands for right.
- *real_value*: real part of the amplitude of the wave;
- *complex_value*: complex part of the amplitude of the wave;

  As an example, the first 8 items of the parse file as follows

---

```
M 20

steps 100

points 2

i 0 0

j -2 -1

c 0 1

real_value 1 0

complex_value 0 1
```

---

mean that at $(0, -2, RR)$ the amplitude is $\frac{1}{\sqrt{2}}$ and at $(0, -1, RL)$ the amplitude is $\frac{\imath}{\sqrt{2}}$.

- $different\_lines$: 0 means the walkers are in the same line and 1 means they are in different lines;
- $index\_brokenlink\_imp\_1$: index of broken link impurities of the first particle if $different\_lines$ is set to 1. If $different\_lines$ is set to 0, this index will be used for both walkers.
- $fixed\_broken\_link\_1$: number of fixed broken links for the first walker.
- I_0: set of nodes such that $i_0 \in I_0$ means there is a broken link between i_0 and $i_0 + 1$. Note that $-M \leq i_0 \leq M - 1$.
- $coin1$: Sets the coin for the first particle. If $different\_lines$ is set to 0, it sets the coin for both walkers.
  - -2 sets the identity matrix;
  - -1 sets the reflection coin;
  - 0 sets the Hadamard coin;
  - 3 sets the random matrix that varies at each step;
- $fixed\_coin\_1$: number of static random coins to be defined with the following parameters.
  - K_1: positions of static random coins.
    * $theta\_0$ and $theta\_1$ set an interval for θ;
    * $zeta\_0$ and $zeta\_1$ set an interval for ζ;
    * xi_0 and xi_1 set an interval for ξ;
      If $fixed\_coin\_1$ is 0 then these fields must be empty.

```
fixed_coins1 2

K_1 9 -5

theta_0 0 0.75

theta_1 0.75 1.23

zeta_0 0 0.75

zeta_1 0.75 1.23

xi_0 0.25 0.75

xi_1 0.25 0.75
```

---

means that at position 9 the random matrix is defined with parameters $\theta \in [0, 0.75]$, $\zeta \in [0, 0.75]$ and $\xi = 0.25$ and at position -5 with $\theta \in [0.75, 1.23]$, $\zeta \in [0.75, 1.23]$ and $\xi = 0.75$ as in the $1D$ case.

- *varying_coin_each_step_1*: if set to 1, in each step the coin operator will be set according to the following parameters:
  - *theta_0* and *theta_1* sets an interval for θ;
  - *zeta_0* and *zeta_1* sets an interval for ζ;
  - *xi_0* and *xi_1* sets an interval for ξ;

    If *varying_coin_each_step_1* is 0 then these fields must be empty.
- *index_coin_imp_1*: if $different\_lines$ is set to 1 this is the index of coin operator impurities of first particle . If $different\_lines$ is set to 0, this index will be used for both walkers.
- $rf1$: if set to 1 reflection boundary is activated for the first walker. If set to 0 circular boundary condition is activated.
- *index_coin_imp_2*: if $different\_coin$ is set to 1 this is the index of coin operator impurities of the second particle.
- *index_brokenlink_imp_2*: index of broken link impurities of the second particle if $different\_lines$ is set to 1.
- *fixed_broken_link_2*: number of fixed broken links for second walker.
- J_0: set of nodes such that $j_0 \in J_0$ means there is a broken link between j_0 and $j_0 + 1$. Note that $-M \leq j_0 \leq M - 1$.
- *coin*2 Sets the coin for the second particle.
  - -2 sets the identity matrix;
  - -1 sets the reflection coin;

- 0 sets the Hadamard coin;
- 3 sets the random matrix that varies at each step;

- *fixed_coin_2*: number of static random coins to be defined with the following parameters.
  - *K_2*: positions of static random coins.
  - *theta_0*, *theta_1*: sets an interval for θ;
  - *zeta_0*, *zeta_1*: sets an interval for ζ;
  - *xi_0*, *xi_1*: sets an interval for ξ;
    If *fixed_coin_2* $= 0$ then these fields must be empty.

- *varying_coin_each_step_2*: If set to 1, in each step the coin operator will be set according to the following parameters:
  - *theta_0*, *theta_1*: sets an interval for θ;
  - *zeta_0*, *zeta_1*: sets an interval for ζ;
  - *xi_0*, *xi_1*: sets an interval for ξ; If *varying_coin_each_step_2* $= 0$ then these fields must be empty.

- *rf2*: if set to 1 reflection boundary is activated for the second walker. If set to 0 circular boundary condition is activated.

- *dim*: number of measuring positions.
  - *i_0*: Positions of measurement for the first walker.
  - *j_0*: Positions of measurement for the second walker.
    If *dim* is 0 then these fields must be empty.

- *m_options*: Measure options.
  - *m_options* $= 0$: no measures calculated;
  - *m_options* $= 1$: determines one shot probability to hit;
  - *m_options* $= 2$: determines first time probability to hit;
  - *m_options* $= 3$: determines first time probability to hit, average hitting time and concurrent probability to hit;

- *vn_x*: if set to 1 the simulator calculates $S(\hat{\rho}_{P,1})$ in each step.

- *vn_y*: if set to 1 the simulator calculates $S(\hat{\rho}_{P,2})$ in each step.

- *vn_m_info*: if set to 1 (works properly only when *vn_x* and *vn_y* are set to 1), calculates $\mathcal{I}(\hat{\rho}_{P,12}) = S(\hat{\rho}_{P,1}) + S(\hat{\rho}_{P,2}) - S(\hat{\rho}_{P,12})$ in each step.

- *q_discord*: If set to 1 it determines $\delta(P1 : P2)_{\{\hat{\Pi}_i^{P1}\}} = S(\hat{\rho}_{P2}) - S(\hat{\rho}_{P,12}) + S(P2|\hat{M}^{P1})$ where $\{\hat{\Pi}_i^{P1}\}$ is the set of one-dimensional orthogonal projectors corresponding to the measurement outcome i of the first particle.

- *ent_form*: if set to 1 it determines $E_F(\hat{\rho}_{P,12}) = \sum_{k=1}^{4} r_k E(|\varphi_k\rangle_{P,12})$ with $E(|\varphi_k\rangle_{P,12}) = S(\mathrm{Tr}_{P,2} |\varphi_k\rangle \langle\varphi_k|_{P,12})$.

- *gnu_plot*:if set to 1 the output files will be plotted using GNUplot.

4.2 Default files generated

- *Average_hitting_time*: average hitting time
- *Average$_P$robability_Distribution*: average position probability on plane;
- *Concurrence_hitting_time*: concurrent probability to hit;
- *E_f*: upper bound of E_f;
- *First time to hit*: first-time probability to hit;
- *H_x*: Shannon entropy of the marginal probability distribution of positions x_1;
- *H_xy*: Shannon entropy of the marginal probability distribution of positions x_1 and x_2;
- *H_y*: Shannon entropy of the marginal probability distribution of positions x_2;
- *I_xy*: Shannon mutual information of the marginal probability distribution of position variables x_1 and x_2;
- *Iv_xy*: von Neumann mutual information $\hat{\rho}_{P,12}$;
- *mean_dist*: mean distance of variables x_1 and x_2;
- *mean_x*: mean value of variable x_1;
- *mean_y*: mean value of variable x_2;
- *one shot probability hit*: one-shot probability to hit $\mathcal{P}_o^1(i_0; n)$;
- *Probability_distribution*: position probability on plane;
- *Quantum Discord*: Quantum discord of x_2 with respect to measurements $\hat{\Pi}_i^{x_1}$ on x_1;
- *S_x*: von Neumann entropy of $\hat{\rho}_{P,1}$;
- *S_y*: von Neumann entropy of $\hat{\rho}_{P,2}$;
- *Shannon_entropy of coin state*: Shannon entropy of the coin state density matrix diagonal;
- *Von_Neuman_entropy of coin state*: von Neumann entropy of $\hat{\rho}_{C,12}$;
- *xy_cov*: covariance of variables x_1 and x_2;

5 One Particle Quantum Walk on a 2D Lattice

Folder *qwsim_2D_1_walker*

The parse file has the following form:

```
M

steps

points

i

j

c

real_value

complex_value

moi

moj

index_brokenlink_imp

fixed_broken_link

i

j

c

coin 0

varying_coin_each_step

theta_10

theta_11

theta_20

theta_21

zeta_10
```

zeta_11

zeta 20

zeta_21

xi_10

xi_11

xi_20

xi_21

index_coin_imp

fixed_coins

K_i

K_j

theta_10

theta_11

zeta_10

zeta_11

xi_10

xi_11

theta_20

theta_21

zeta_20

zeta_21

xi_20

xi_21

refi 0

refj 0

```
dim 0

i_0

j_0

m_options

vn_x

vn_y

vn_m_info

q_discord

ent_form

gnu
```

5.1 parser_file.txt fields

- M: Size of the grid, from $-M$ to M;
- *steps*: number of steps of the quantum walk;
- *points*: number of points where the wave amplitudes are nonzero. Note that a pair $(position, point)$ counts as a single point;
- i: initial position in coordinate x;
- j: initial position in coordinate y;
- c: coin state where the amplitudes are nonzero - 0 means $East$, 1 means $South$, 2 means $North$ and 3 is $West$;
- *real_value*: real part of the amplitude of the wave;
- *complex_value*: complex part of the amplitude of the wave;

  For example

  ```
  M 20

  steps 100

  points 2

  i 0 0

  j -2 -1
  ```

```
c 2 3

real_value 1 2 0 0

complex_value 0 0 3 4
```

---

means that at $(0, -2, N)$ the amplitude is $\frac{1}{\sqrt{2}}$ and at $(0, -1, W)$ the amplitude is $\frac{\imath}{\sqrt{2}}$.

$$
\begin{aligned}
|\psi\rangle = & \frac{1}{\sqrt{1^2+2^2+3^2+4^2}}(|0,-2\rangle\,|E\rangle + 2\,|0,-1\rangle\,|S\rangle \\
& + 3\imath\,|1,0\rangle\,|N\rangle + 4\imath\,|2,0\rangle\,|W\rangle)
\end{aligned}
$$

- *moi*: if set to 1 the moebios topology is set for coordinate x;
- *moj*: if set to 1 the moebios topology is set for coordinate y;
- *index_brokenlink_imp*: fraction of the links that are broken. The links are chosen at random in each step;
- *fixed_broken_links*: number of fixed broken links given by the triplets (i, j, c)
  - i: any position from $-M$ until $M-1$
  - j: any position from $-M$ until $M-1$
  - c: coin states can be either 0 ($East$) or 2 ($North$).
    If *fixed_broken_links* is set to 0 then these fields must be empty.
- *coin*: Sets the coin operator for the particle in every position;
  - -2 sets the identity matrix;
  - -1 sets the reflection coin;
  - 0 sets the Hadamard coin;
  - 1 sets the Fourier coin;
  - 2 sets the Grover coin;
  - 3 sets the random matrix that varies at each step;
- *index_coin_imp*: fraction of the positions on the grid where the coin state is randomly chosen. The position and the matrices are chosen at random at each step;
- *fixed_coins*: number of static coins to be defined with the following parameters
  - *K_i*: any position from $-M$ until M;
  - *K_j*: any position from $-M$ until M;

- *theta_10*, *theta_11*: sets an interval for θ_1;
- *zeta_10*, *zeta_11*: sets an interval for ζ_1;
- *xi_10*, *xi_11*: sets an interval for ξ_1;
- *theta_20*, *theta_21*: sets an interval for θ_2;
- *zeta_20*, *zeta_21*: sets an interval for ζ_2;
- *xi_20*, *xi_21*: sets an interval for ξ_2;
  If *fixed_coins* is set to 0 then these fields must be empty.

For example

```
fixed_coins 2

K_i 0 1

K_j 1 0

theta_10 0 0.25

theta_11 0.5 0.30

zeta_10  0.5 0.30

zeta_11  1 0.35

xi_10  1 0.35

xi_11  1.5 0.40

theta_20 0 0.45

theta_21 0.25 0.50

zeta_20 0.25 0.55

zeta_21 0.5 0.60

xi_20 0.5 0.65

xi_21 0.75 0.70
```

---

means that at position $(0,1)$ we fix the parameters $\theta_1 \in [0,0.5], \zeta_1 \in [0.5,1], \xi_1 \in [1,1.5], \theta_2 \in [0,0.25], \zeta_2 \in [0.25,0.5], \xi_2 \in [0.5,0.75]$.

and at position $(1,0)$, $\theta_1 \in [0.25,0.30], \zeta_1 \in [0.30,0.35], \xi_1 \in [0.35,0.40], \theta_2 \in [0.45,0.50], \zeta_2 \in [0.55,0.60], \xi_2 \in [0.65,0.70]$.

- *varying_coin_each_step*;

- *theta_10*, *theta_11*: sets an interval for θ_1;
- *zeta_10*, *zeta_11*: sets an interval for ζ_1;
- *xi_10*, *xi_11*: sets an interval for ξ_1;
- *theta_20*, *theta_21*: sets an interval for θ_2;
- *zeta_20*, *zeta_21*: sets an interval for ζ_2;
- *xi_20*, *xi_21*: sets an interval for ξ_2;
  If *varying_coin_each_step* is set to 0 then these fields must be empty.

- $refi$: if set to 1 reflecting boundary is set;
- $refj$: if set to 1 reflecting boundary is set;
- *dim* Number of measuring positions;
  - *i_0*: positions of measurement for the coordinate x;
  - *j_0*: positions of measurement for the coordinate y;
    If $dim = 0$ then these fields must be empty.
- *m_options*: Measure options.
  - *m_options* $= 0$: no measures calculated;
  - *m_options* $= 1$: determines one shot probability to hit;
  - *m_options* $= 2$: determines first time probability to hit;
  - *m_options* $= 0$: determines first time probability to hit, average hitting time and concurrent probability to hit;
- *moi*: if set to 1 the moebius topology is set for coordinate x;
- *moj*: if set to 1 the moebius topology is set for coordinate y;
- *vn_x*: if set to 1 the simulator calculates $S(\hat{\rho}_X)$ on each step;
- *vn_y*: if set to 1 the simulator calculates $S(\hat{\rho}_Y)$ on each step;
- *vn_m_info*: If set to 1 (works properly only when *vn_x* and *vn_y* are set to 1), calculates $\mathcal{I}(\hat{\rho}_{XY})) = S(\hat{\rho}_X) + S(\hat{\rho}_Y) - S(\hat{\rho}_{XY})$;
- *q_discord*: If set to 1 it determines $\delta(X:Y)_{\{\hat{\Pi}_i^X\}} = S(\hat{\rho}_Y) - S(\hat{\rho}_{XY}) + S(Y|\hat{M}^X)$;
- *ent_form*: If set to 1 it determines $E_F(\hat{\rho}_{XY}) = \sum_{k=1}^{4} r_k E(|\varphi_k\rangle_{XY})$ with $E(|\varphi_k\rangle_{XY}) = S(\mathrm{Tr}_Y\,|\varphi_k\rangle\,\langle\varphi_k|_{XY})$;
- *gnu_plot*:if set to 1 the output files will be plotted using GNUplot.

5.2 Default files generated

- $Average\_hitting\_time$: average hitting time.
- $Average_Probability\_Distribution$: average position probability on plane;
- $Concurrence\_hitting\_time$: concurrent probability to hit
- E_f: upper bound of E_f;
- $First\ time\ to\ hit$: first-time probability to hit;
- H_x: Shannon entropy of the marginal probability distribution of positions X;
- H_xy: Shannon entropy of the marginal probability distribution of positions X and Y;
- H_y: Shannon entropy of the marginal probability distribution of positions Y;
- I_xy: Shannon mutual information of the marginal probability distribution of position variables X and Y;
- Iv_xy: von Neumann mutual information of $\hat{\rho}_{P,XY}$;
- $mean\_dist$: mean distance of variables X and Y;
- $mean\_x$: mean value of variable X;
- $mean\_y$: mean value of variable Y;
- *one shot probability hit*: one-shot probability to hit $\mathcal{P}^1_o(i_0; n)$;
- $Probability\_distribution$: position probability on plane;
- *Quantum Discord*: Quantum discord of Y with respect to measurements $\hat{\Pi}^X_i$ on X;
- S_x: von Neumann entropy of $\hat{\rho}_{P,X}$;
- S_y: von Neumann entropy of $\hat{\rho}_{P,Y}$;
- $Shannon\_entropy\ of\ coin\ state$: Shannon entropy of coin state;
- $Von\_Newman\_entropy\ of\ coin\ state$: von Neuwmann entropy of $\hat{\rho}_{C,XY}$;
- xy_cov: covariance of variables X and Y;

6 examples

6.1 Example for One Particle Quantum Walk on the Line

6.1.1 Random broken links and Reflecting Boundary

- a line of length 201;
- a number of steps 1000;
- reflecting boundary condition on both ends;
- index of random broken link of $0,3$;
- initial state $|\psi_0\rangle = \frac{1}{\sqrt{2,25}} \left(|0\rangle \left(|R\rangle - |L\rangle\right) + 0,5\,|5\rangle\,|R\rangle\right)$.

parse file looks like this:

```
M 100

Steps 1000

points 3

i 0 0 5

c 0 1 1

real_value 1.0 -1.0 0.5

complex_value 0.0 0.0 0.0

index_brokenlink_imp 0

fixed_broken_links 0

I_0

coin 0

varying_coin_each_step 0

theta_0

theta_1

zeta_0

zeta_1

xi_0
```

```
xi_1

index_coin_imp 0

fixed_coins 0

i

theta_0

theta_1

zeta_0

zeta_0

xi_0

xi_1

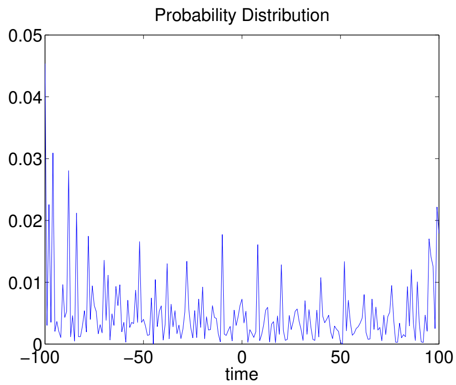
ref 1

dim_absorb 0

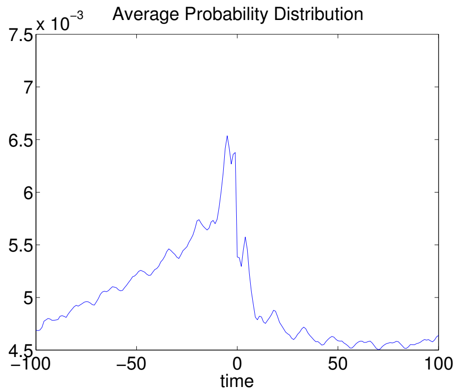
i

c

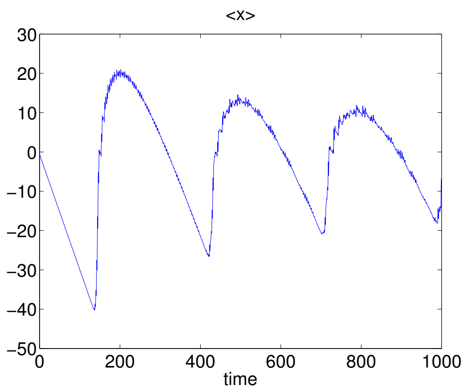
gnu_plot 0
```



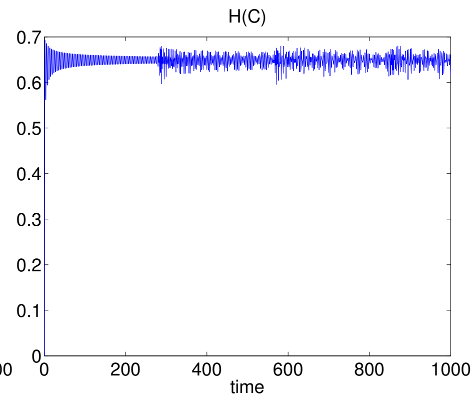
(a) Probability distribution for position.



(b) Average probability distribution for position.

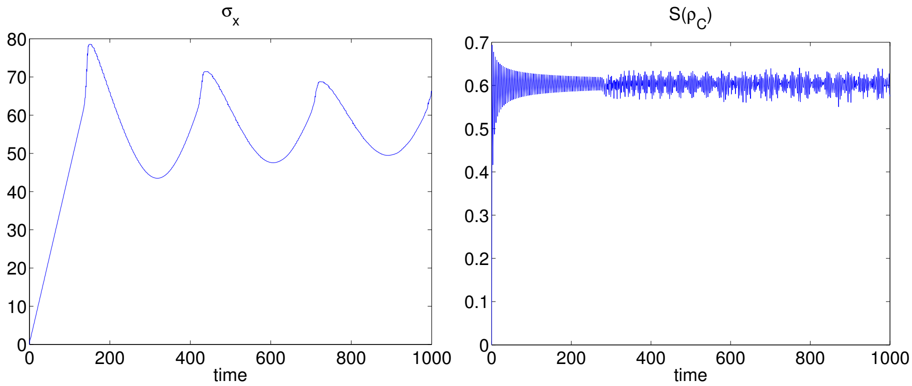


(c) Mean value of variable x.



(d) Shannon entropy of coin state density matrix.

Figure 1: Evolution of one particle for the example of *qwsim_1D*



(a) Standard deviation of x.

(b) von Neumann entropy of coin state density matrix

Figure 2: Evolution of one particle for the example of *qwsim_1D*

6.1.2 Static random coin and Reflecting Boundary

- a line of size 8001;
- a number of steps 4000;
- reflecting boundary condition;
- initial state $|0\rangle|R\rangle$;
- static random coin with parameters $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$.

```
M 4000

Steps 4000

points 1

i 0

c 0

real_value 1

complex_value 0

index_brokenlink_imp 0.3

fixed_broken_links 0

I_0

coin 0

varying_coin_each_step 1

theta_0 0.3927

theta_1 1.1781

zeta_0 0.3927
```

```
zeta_1 1.1781

xi_0 0.3927

xi_1 1.1781

index_coin_imp 0

fixed_coins 0

i

theta_0

theta_1

zeta_0

zeta_0

xi_0

xi_1

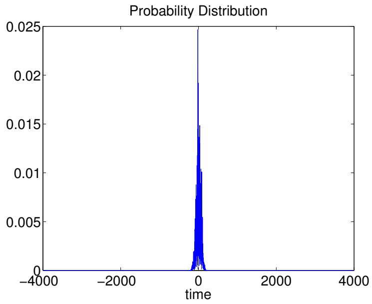
ref 1

dim_absorb 0

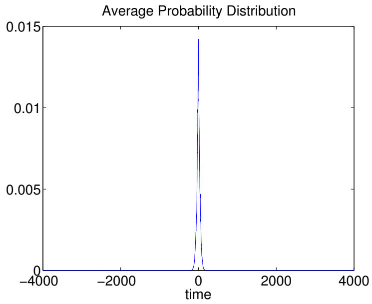
i

c

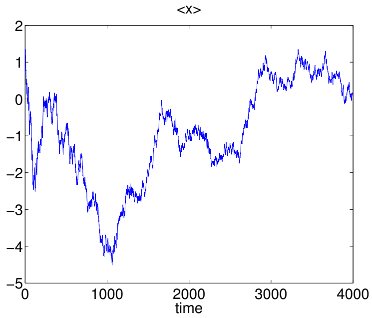
gnu_plot 0
```



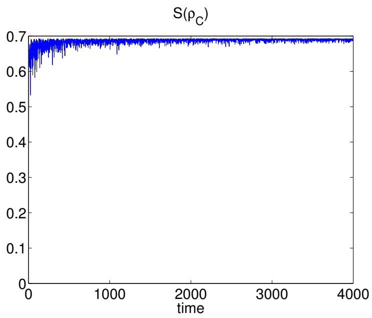
(a) Probability distribution for position.



(b) Average probability distribution for position.



(c) Mean value of variable x.



(d) von Neumann entropy of coin state density matrix.

Figure 3: Evolution of quantum walk for the example of one particle quantum walk on the line for 4000 steps, initial state given by $i\,|0\rangle\,|R\rangle$, index broken link 0.3 and varying coin of parameters $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$. The respective parse file can be found in appendix A

6.2 Example for One Particle Quantum Walk on a Square Lattice

6.2.1 Random Coins at Random Positions and Random Broken Links

- a grid of size 61×61;
- a number of steps 30;
- initial state $|\psi(0)\rangle = \frac{1}{2}\,|-5,-5\rangle_{12}\,(|E\rangle - |S\rangle) + \frac{1}{2}\,|5,5\rangle_{12}\,(|N\rangle - |W\rangle)$.
- random matrix index of 0.2;
- random broken link index of 0.2;
- klein bottle;

Parse file looks like this:

```
N 30

steps 60
```

```
points 4

i -5 -5 5 5

j -5 -5 5 5

c 0 1 2 3

real_value 1 -1 1 -1

complex_value 0 0 0 0

moi 1

moj 1

index_brokenlink_imp 0.2

fixed_broken_links 0

i

j

c

coin 0

varying_coin_each_step 0

theta_10

theta_11

theta_20

theta_21

zeta_10

zeta_11

zeta_20

zeta_21

xi_10

xi_11
```

```
xi_20

xi_21

index_coin_imp 0

fixed_coins 0

i

j

theta_10

theta_11

theta_20

theta_21

zeta_10

zeta_11

zeta_20

zeta_21

xi_10

xi_11

xi_20

xi_21

refI 1

refJ 1

dim 0

i_0

j_0

m_options 0

vn_x 0
```

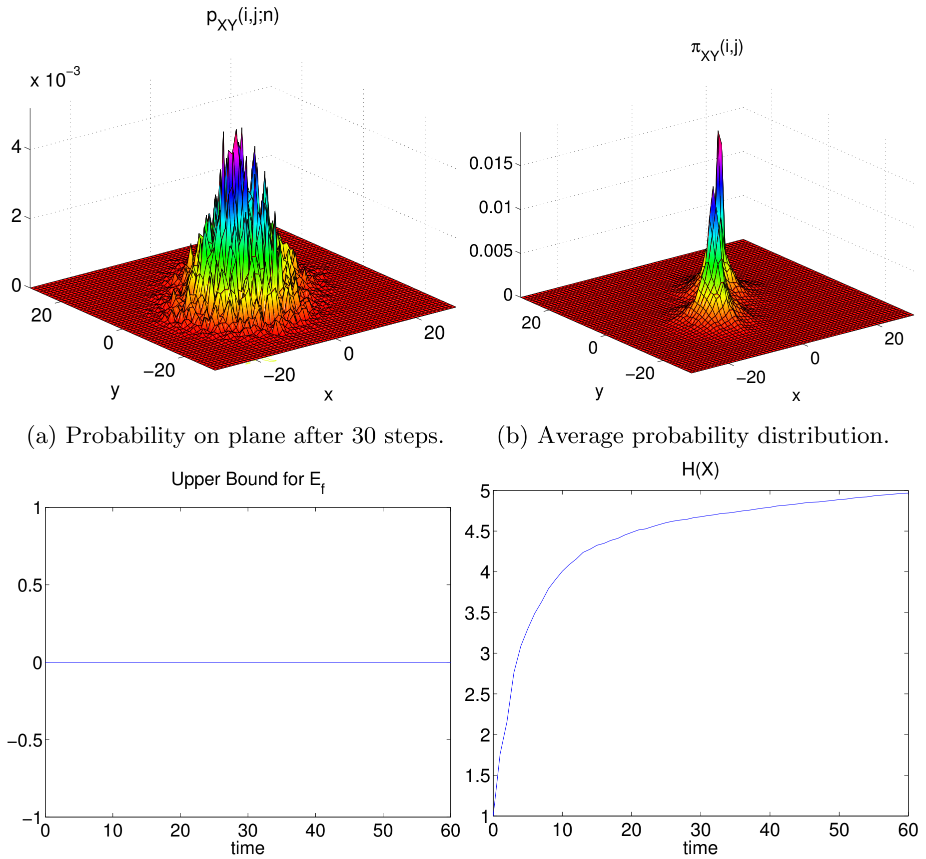
```
vn_y 0

vn_m_info 0

q_discord 0

ent_form 0

gnu_plot 0
```



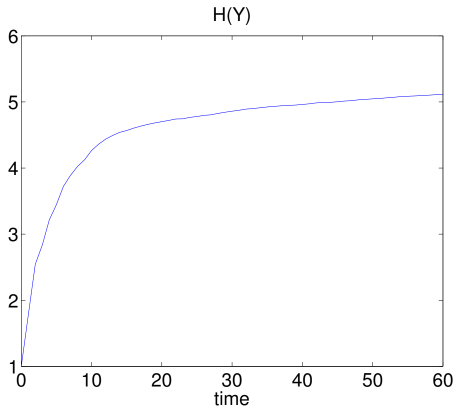
(a) Probability on plane after 30 steps.

(b) Average probability distribution.

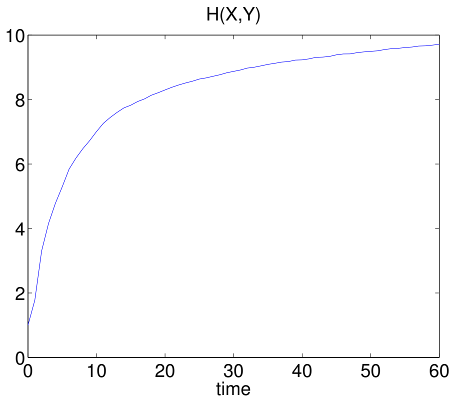
(c) Upper bound of E_f.

(d) Shannon entropy for positions X.

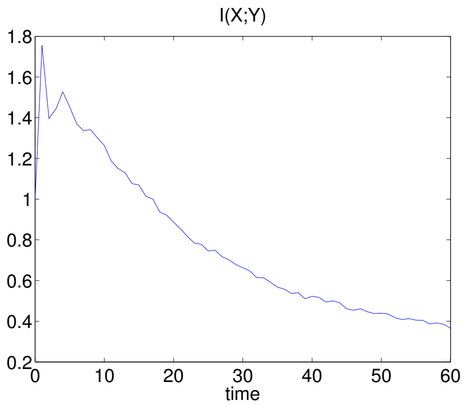
Figure 4: Evolution of quantum walk for the example of one particle quantum walk on a lattice.



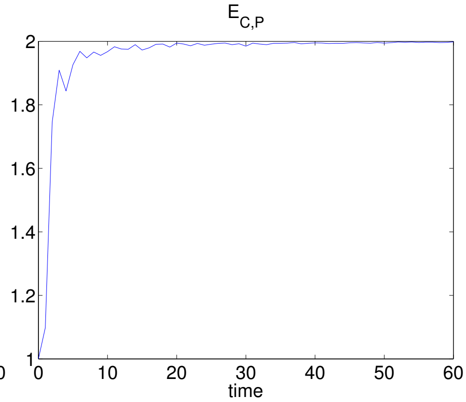
(a) Shannon entropy for positions Y.



(b) Shannon entropy for variables X and Y.

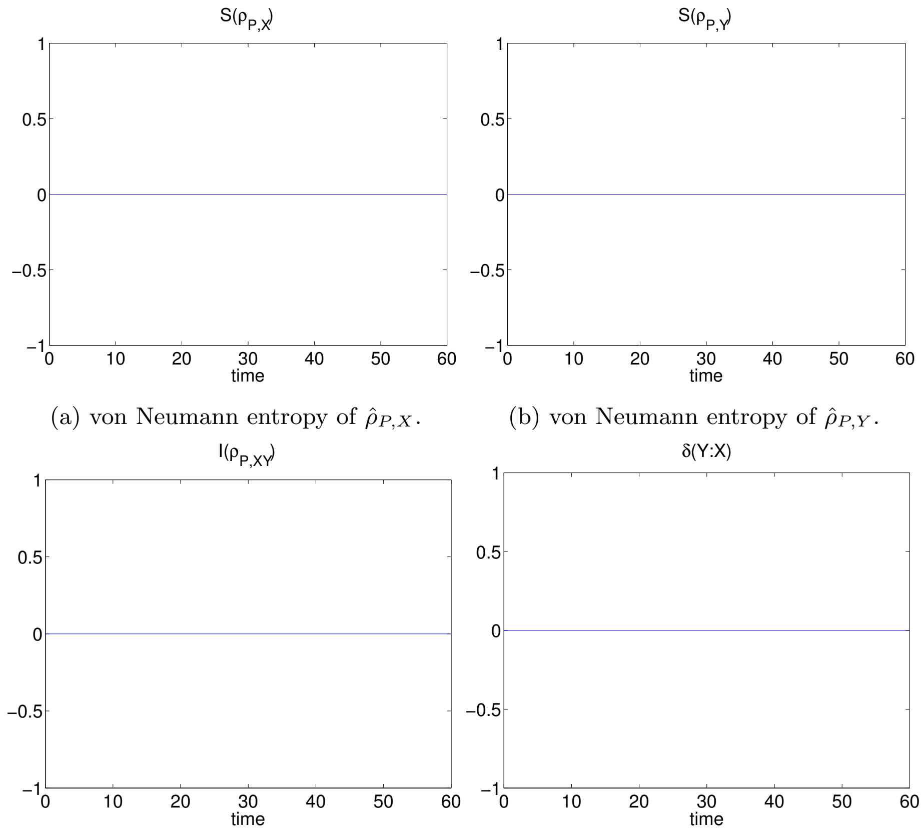


(c) Shannon mutual information for position variables X and Y.



(d) von Neumann entropy of $\hat{\rho}_{C,XY}$.

Figure 5: Evolution of quantum walk for the example of one particle quantum walk on a lattice.



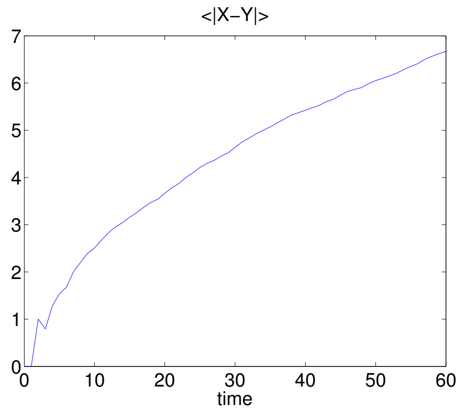
(a) von Neumann entropy of $\hat{\rho}_{P,X}$.

(b) von Neumann entropy of $\hat{\rho}_{P,Y}$.

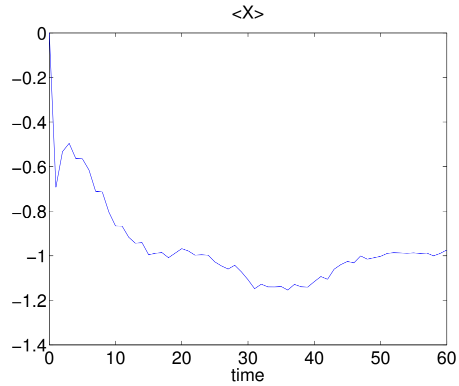
(c) von Neumann mutual information of $\hat{\rho}_{P,XY}$.

(d) Quantum discord of Y given measurements $\hat{\Pi}_i^X$ on X.

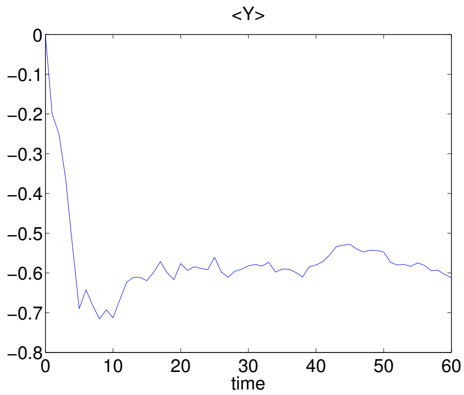
Figure 6: Evolution of quantum walk for the example of one particle quantum walk on a lattice.



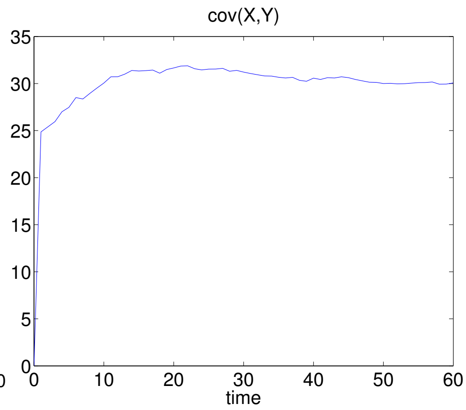
(a) Mean distance of variables X and Y.



(b) Mean value of variable X.

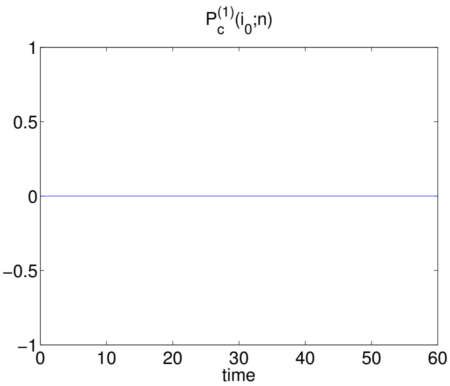


(c) Mean value of variable Y.

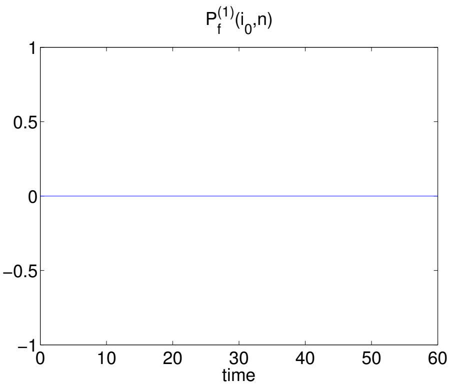


(d) Covariance of variables X and Y.

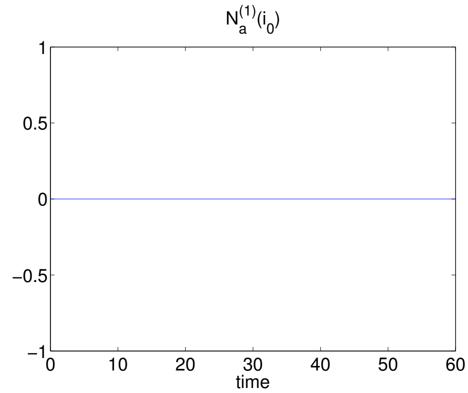
Figure 7: Evolution of quantum walk for the example of one particle quantum walk on a lattice.



(a) concurrent probability to hit.



(b) First time probability to hit.



(c) Average hitting time.

Figure 8: Evolution of quantum walk for the example of one particle quantum walk on a lattice.

6.2.2 Static Broken Links

- 2D lattice of size 91×91;
- 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 $y \in \{-45, \ldots, 45\}\backslash\{-30, 0, 30\}$, and positions $(x, -15)\&(x, -14)$ and $(x, 14)\&(x, 15)$, for $x \in \{-45, \ldots, 45\}\backslash\{-30, 0, 30\}$;

```
N 45

steps 1000
```

points 4

i −30 −30 30 30

j −30 −30 30 30

c 0 2 3 1

real_value 1 0 1 0

complex_value 0 1 0 1

moi 0

moj 0

index_brokenlink_imp 0

fixed_broken_links 352

i −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14 14 14 14 14 14 −45 −44 −43 −42 −41 −40 −39
−38 −37 −36 −35 −34 −33 −32 −31 −29 −28 −27 −26 −25 −24 −23 −22 −21
−20 −19 −18 −17 −16 −15 −14 −13 −12 −11 −10 −9 −8 −7 −6 −5 −4 −3
−2 −1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23
24 25 26 27 28 29 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 −45
−44 −43 −42 −41 −40 −39 −38 −37 −36 −35 −34 −33 −32 −31 −29 −28 −27
−26 −25 −24 −23 −22 −21 −20 −19 −18 −17 −16 −15 −14 −13 −12 −11
−10 −9 −8 −7 −6 −5 −4 −3 −2 −1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
16 17 18 19 20 21 22 23 24 25 26 27 28 29 31 32 33 34 35 36 37 38
39 40 41 42 43 44 45

j −45 −44 −43 −42 −41 −40 −39 −38 −37 −36 −35 −34 −33 −32 −31 −29 −28
−27 −26 −25 −24 −23 −22 −21 −20 −19 −18 −17 −16 −15 −14 −13 −12 −11
−10 −9 −8 −7 −6 −5 −4 −3 −2 −1 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15
16 17 18 19 20 21 22 23 24 25 26 27 28 29 31 32 33 34 35 36 37 38
39 40 41 42 43 44 45 −45 −44 −43 −42 −41 −40 −39 −38 −37 −36 −35
−34 −33 −32 −31 −29 −28 −27 −26 −25 −24 −23 −22 −21 −20 −19 −18 −17
−16 −15 −14 −13 −12 −11 −10 −9 −8 −7 −6 −5 −4 −3 −2 −1 1 2 3 4 5 6
7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29
31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15 −15
−15 −15 −15 −15 −15 −15 14 14 14 14 14 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14 14
14 14 14 14 14 14 14 14

c 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
0 0 0 0 0 0 0 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
2 2 2 2 2 2 2 2 2 2 2 2 2 2 2

coin 0

```
varying_coin_each_step 0

theta_10

theta_11

theta_20

theta_21

zeta_10

zeta_11

zeta_20

zeta_21

xi_10

xi_11

xi_20

xi_21

index_coin_imp 0

fixed_coins 0

i

j

theta_10

theta_11

theta_20

theta_21

zeta_10

zeta_11

zeta_20

zeta_21

xi_10

xi_11

xi_20

xi_21

refI 1

refJ 1

dim 0

i_0

j_0

m_options 0

vn_x 0

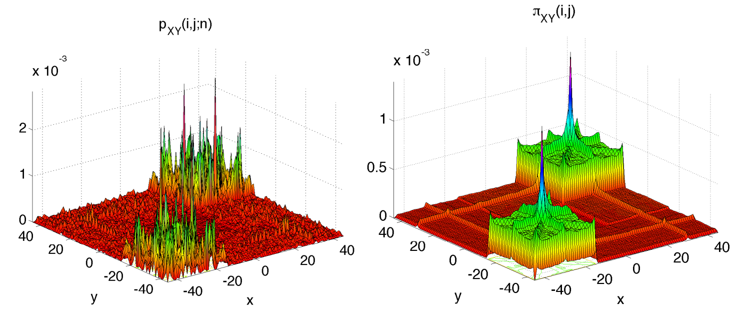
vn_y 0
```

```
vn_m_info 0

q_discord 0

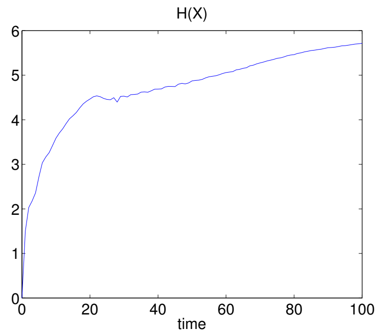
ent_form 0

gnu_plot 0
```



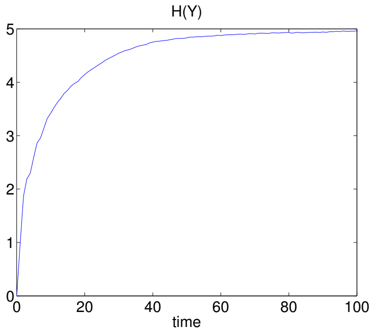
(a) Probability on plane after 30 steps.

(b) Average probability distribution.

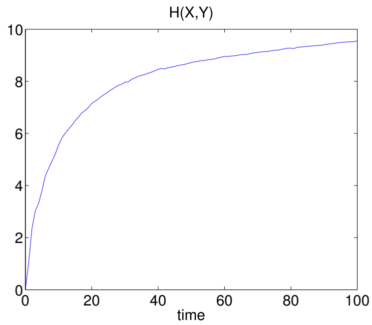


(c) Shannon entropy for positions x_1.

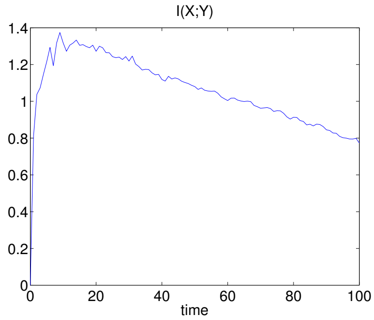
Figure 9: Evolution of quantum walk for the example of one particle quantum walk on a lattice with Hadamard coin operator and broken links at positions $x = -15, 15$ and $y = -15, 15$ and with slits located at $x = -30, 0, 30$ when $y = -15, 15$ and for $y = -30, 0, 30$ when $x = -15, 15$. The initial state is $\frac{1}{2}(|-30,-30\rangle\,(|E\rangle + i\,|N\rangle) + |30,30\rangle\,(|W\rangle + i\,|S\rangle))$. The parse can be found in appendix C



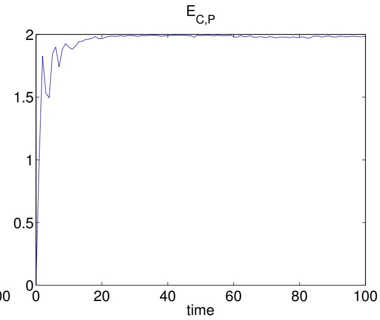
(a) Shannon entropy for positions x_2.



(b) Shannon entropy for variables x_1 and x_2.

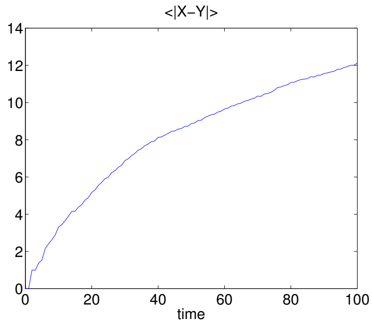


(c) Shannon mutual information for position variables x_1 and x_2.

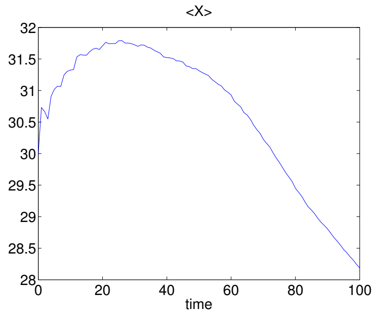


(d) von Neumann entropy of $\hat{\rho}_{C,12}$.

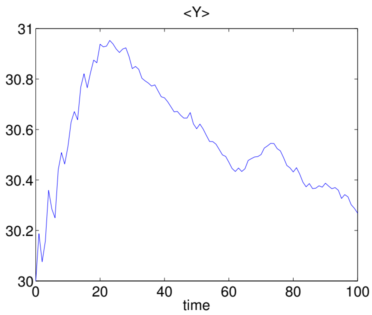
Figure 10: Evolution of quantum walk for the example of one particle quantum walk on a lattice with Hadamard coin operator and broken links at positions $x = -15, 15$ and $y = -15, 15$ and with slits located at $x = -30, 0, 30$ when $y = -15, 15$ and for $y = -30, 0, 30$ when $x = -15, 15$. The initial state is $\frac{1}{2}(|-30,-30\rangle\,(|E\rangle + i\,|N\rangle) + |30,30\rangle\,(|W\rangle + i\,|S\rangle))$. The parse can be found in appendix C



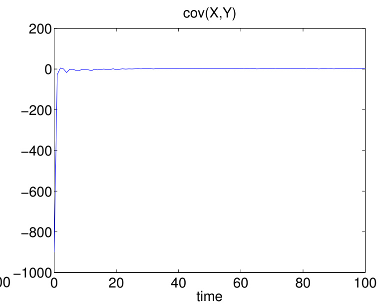
(a) Mean distance of variables x_1 and x_2.



(b) Mean value of variable x_1.



(c) Mean value of variable x_2.



(d) Covariance of variables x_1 and x_2.

Figure 11: Evolution of quantum walk for the example of one particle quantum walk on a lattice with Hadamard coin operator and broken links at positions $x = -15, 15$ and $y = -15, 15$ and with slits located at $x = -30, 0, 30$ when $y = -15, 15$ and for $y = -30, 0, 30$ when $x = -15, 15$. The initial state is $\frac{1}{2}(|{-30}, -30\rangle (|E\rangle + i\,|N\rangle) + |30, 30\rangle (|W\rangle + i\,|S\rangle))$. The parse can be found in appendix C

6.3 Example for 2 Particles Quantum Walk on the Line

6.3.1 different Random Broken Link indexes for the particles and Measurement

- a grid of size 61×61;
- a number of steps 30;
- initial state $|\psi(0)\rangle_{12} = \frac{1}{2}\,|{-5}, -5\rangle_{12}\,(|RR\rangle - |LL\rangle) + \frac{1}{2}\,|5, 5\rangle_{12}\,(|RR\rangle - |LL\rangle)$..
- reflecting boundary conditions;
- random matrix index of 0.6 on line 1 and 0.3 on line 2;
- measures in point 10 of first line with option 3;
- first walker with circular topology and second particle with reflecting boundaries.

```
M 30

steps 60

points 4

i -5 -5 5 5

j -5 -5 5 5

c 0 3 0 3

real_value 1 -1 1 -1

complex_value 0 0 0 0

different_lines 1

index_brokenlink_imp_1 0.6

fixed_broken_link_1 0

I_0

coin1 0

varying_coin_each_step_1 0

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp_1 0

fixed_coin_1 0

K

theta_0
```

```
theta_1

zeta_0

zeta_1

xi_0

xi_1

rf1 1

index_brokenlink_imp_2 0.3

fixed_broken_link_2 0

J_0

coin2 0

varying_coin_each_step_2 0

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp_2 0

fixed_coin_2 0

K

theta_0

theta_1

zeta_0

zeta_1

xi_0
```

```
xi_1

rf2 1

dim 61

i_0 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10
10 10 10 10 10 10 10 10 10 10 10 10 10 10 10 10

j_0 -30 -29 -28 -27 -26 -25 -24 -23 -22 -21 -20 -19
-18 -17 -16 -15 -14 -13 -12 -11 -10 -9 -8 -7 -6 -5 -4
-3 -2 -1 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17
18 19 20 21 22 23 24 25 26 27 28 29 30

m_options 3

vn_x 1

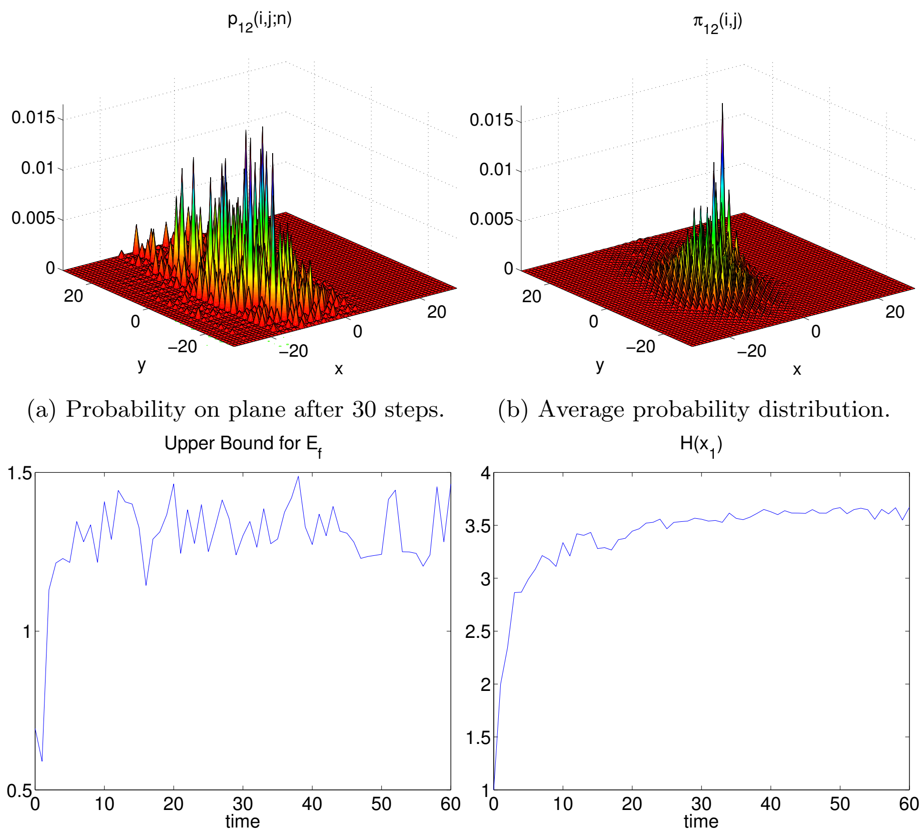
vn_y 1

vn_m_info 1

q_discord 1

ent_form 1

gnu_plot 0
```



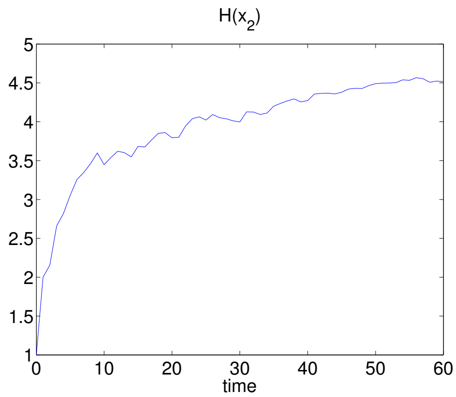
(a) Probability on plane after 30 steps.

(b) Average probability distribution.

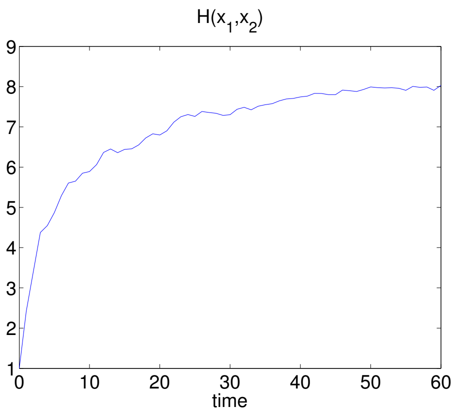
(c) Upper bound of E_f.

(d) Shannon entropy for positions x_1.

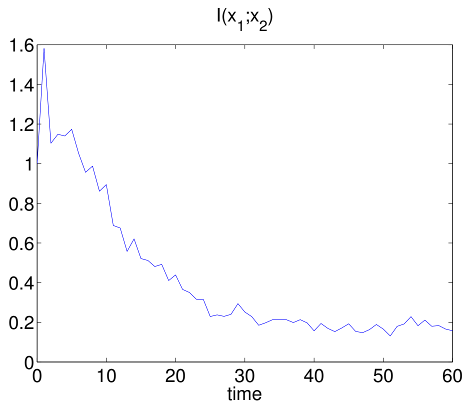
Figure 12: Evolution of quantum walk for the example of two particles quantum walk on a line.



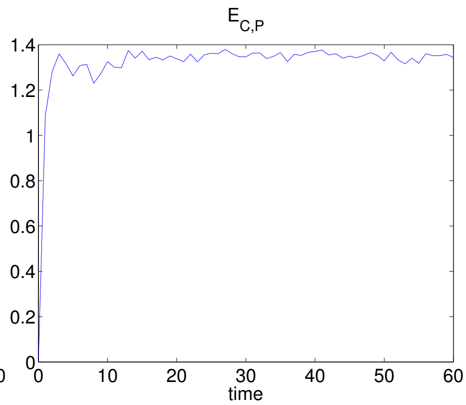
(a) Shannon entropy for positions x_2.



(b) Shannon entropy for variables x_1 and x_2.

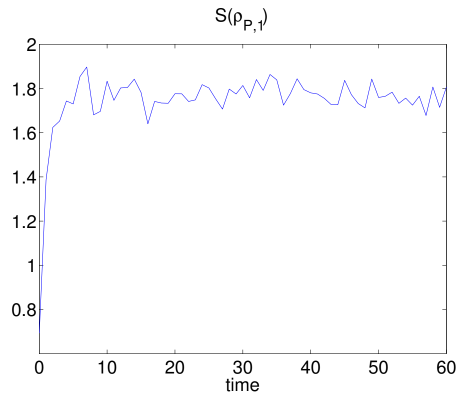


(c) Shannon mutual information for position variables x_1 and x_2.

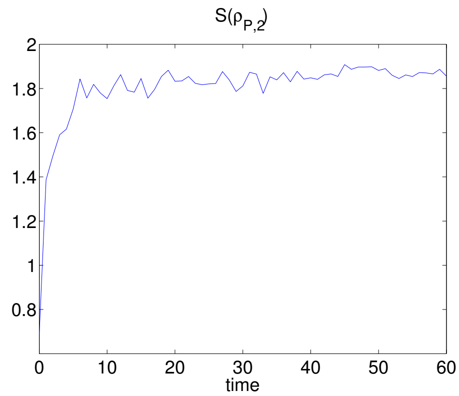


(d) von Neumann entropy of $\hat{\rho}_{C,12}$.

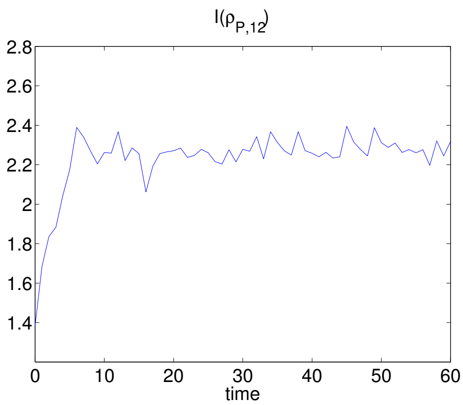
Figure 13: Evolution of quantum walk for the example of two particles quantum walk on a line.



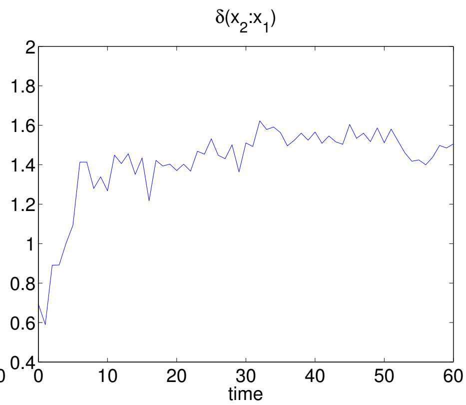
(a) von Neumann entropy of $\hat{\rho}_{P,1}$.



(b) von Neumann entropy of $\hat{\rho}_{P,2}$.

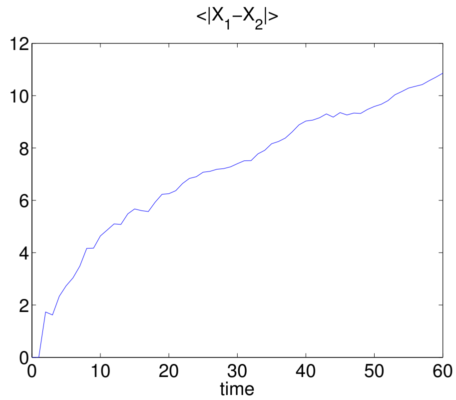


(c) von Neumann mutual information of $\hat{\rho}_{P,12}$.

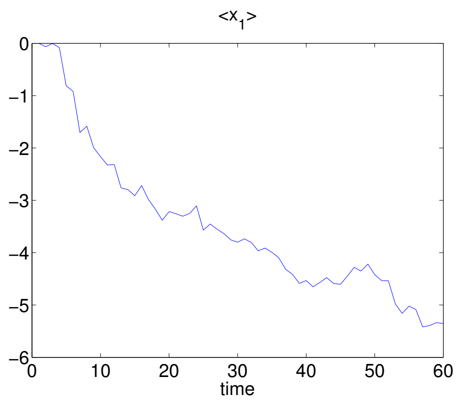


(d) Quantum Discord...

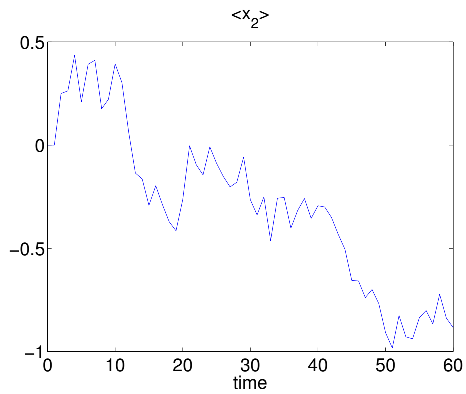
Figure 14: Evolution of quantum walk for the example of two particles quantum walk on a line.



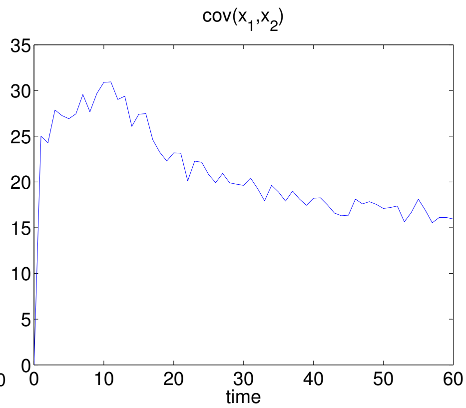
(a) Mean distance of variables x_1 and x_2.



(b) Mean value of variable x_1.

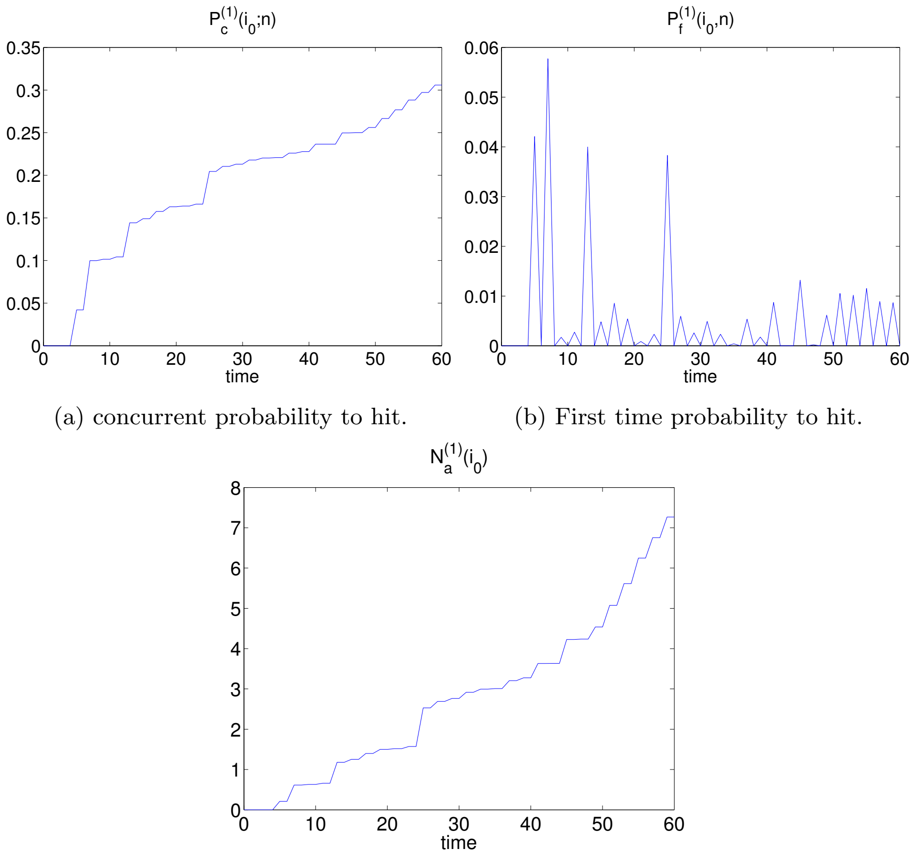


(c) Mean value of variable x_2.



(d) Covariance of variables x_1 and x_2.

Figure 15: Evolution of quantum walk for the example of two particles quantum walk on a line.



(a) concurrent probability to hit.

(b) First time probability to hit.

(c) Average hitting time.

Figure 16: Evolution of quantum walk for the example of two particles quantum walk on a line.

6.3.2 Static Random Coin for First Walker and Random Broken links for Second Walker

- two lines of size 201;
- a number of steps 100;
- reflecting boundary conditions;
- initial state $|0,0\rangle\,|RR\rangle$;
- static random coin with parameters $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$ for the first walker;
- broken link index of 0.3 for the second walker, with Hadamard coin.

M 100

```
steps 100

points 1

i 0

j 0

c 0

real_value 1

complex_value 0

different_lines 1

index_brokenlink_imp_1 0

fixed_broken_link_1 0

I_0

coin1 0

varying_coin_each_step_1 0

theta_0

theta_1

zeta_0

zeta_1

xi_0

xi_1

index_coin_imp_1 0

fixed_coin_1 201

K -100 -99 -98 -97 -96 -95 -94 -93 -92 -91 -90 -89 -88 -87 -86 -85 -84
    -83 -82 -81 -80 -79 -78 -77 -76 -75 -74 -73 -72 -71 -70 -69 -68 -67
    -66 -65 -64 -63 -62 -61 -60 -59 -58 -57 -56 -55 -54 -53 -52 -51
    -50 -49 -48 -47 -46 -45 -44 -43 -42 -41 -40 -39 -38 -37 -36 -35 -34
    -33 -32 -31 -30 -29 -28 -27 -26 -25 -24 -23 -22 -21 -20 -19 -18
    -17 -16 -15 -14 -13 -12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3
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    28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49
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    72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93
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fixed_broken_link_2 0

J_0

coin2 0
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zeta_1
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xi_1
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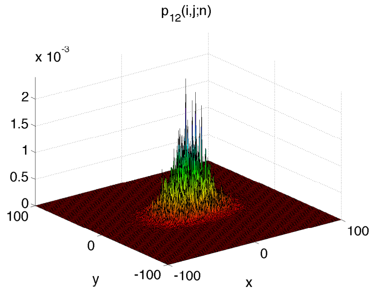
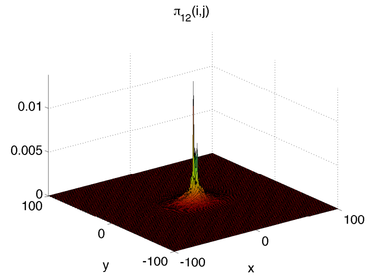
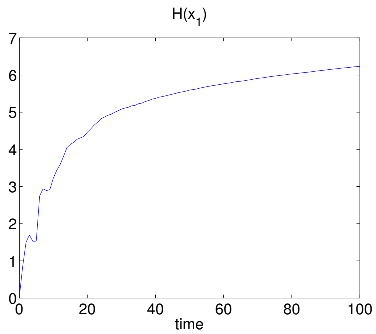




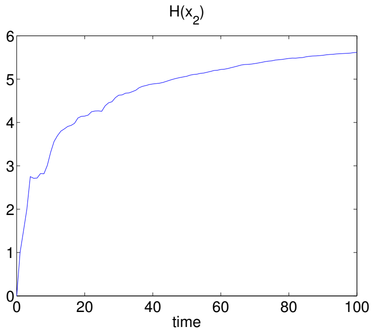
(a) Probability on plane after 30 steps.

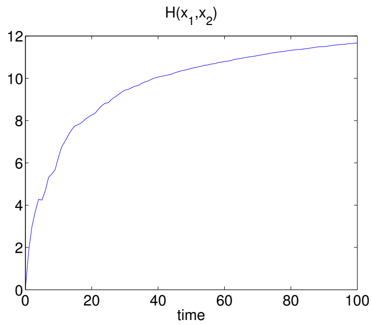
(b) Average probability distribution.



(c) Shannon entropy for positions x_1.

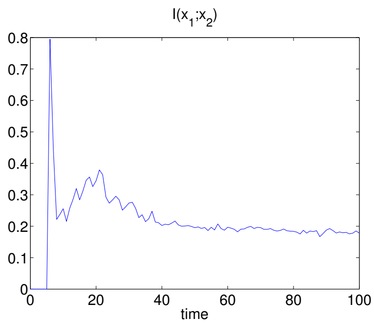
Figure 17: Evolution of quantum walk for two particles quantum walk on different lines, for 100 steps, initial state given by $\frac{1+i}{\sqrt{2}} |0,0\rangle |RR\rangle$, the first walker being influenced by a random coin with $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$ and the second coin with Hadamard coin operator and a broken link index of 0.3.The parse file is in appendix B.

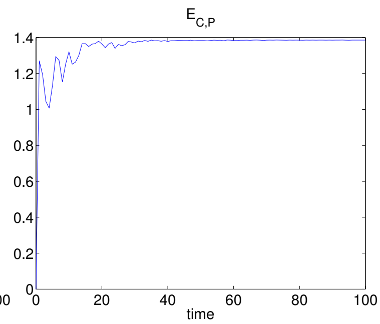




(a) Shannon entropy for positions x_2.

(b) Shannon entropy for variables x_1 and x_2.

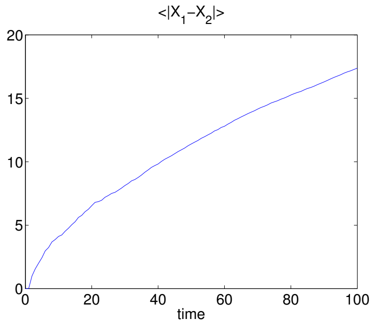




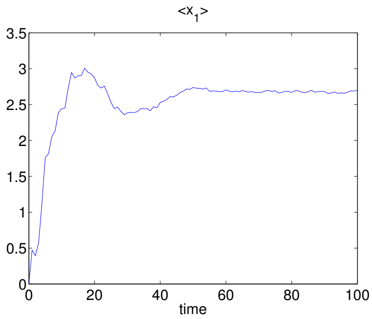
(c) Shannon mutual information for position variables x_1 and x_2.

(d) von Neumann entropy of $\hat{\rho}_{C,12}$.

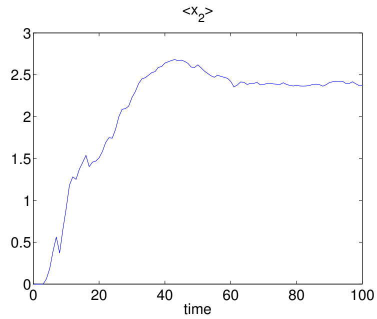
Figure 18: Evolution of quantum walk for two particles quantum walk on different lines, for 100 steps, initial state given by $\frac{1+i}{\sqrt{2}} |0,0\rangle |RR\rangle$, the first walker being influenced by a random coin with $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$ and the second coin with Hadamard coin operator and a broken link index of 0.3.The parse file is in appendix B.



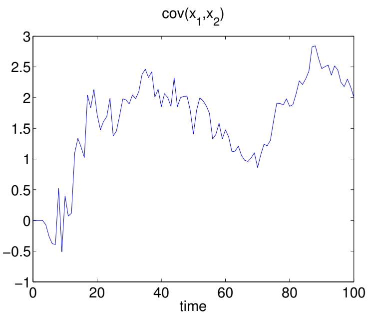
(a) Mean distance of variables x_1 and x_2.



(b) Mean value of variable x_1.



(c) Mean value of variable x_2.



(d) Covariance of variables x_1 and x_2.

Figure 19: Evolution of quantum walk for two particles quantum walk on different lines, for 100 steps, initial state given by $\frac{1+i}{\sqrt{2}} |0,0\rangle |RR\rangle$, the first walker being influenced by a random coin with $\theta, \zeta, \xi \in [\frac{\pi}{4} - \frac{\pi}{8}, \frac{\pi}{4} + \frac{\pi}{8}]$ and the second coin with Hadamard coin operator and a broken link index of 0.3.The parse file is in appendix B.

References

[1] J. Rodrigues, N. Paunkovic, P. Mateus, A simulator for Discrete Quantum Walk on Lattices