1 1D Quantum Walk

1.1 Basic Dynamics

The state of the single particle quantum walk, here named quantum walk in 1D, is written as

$$|\psi\rangle = \sum_{i,c} \alpha_{i,c} |i\rangle |c\rangle . \tag{1}$$

where $|i\rangle \in \mathcal{H}_P$, $|c\rangle \in \mathcal{H}_C$ and $\mathcal{H}_P = \text{span}\{|x\rangle : x \in \mathbb{Z}\}$ and $\mathcal{H}_C = \text{span}\{|R\rangle, |L\rangle\}$ are Hilbert spaces. The overall Hilbert space is denoted $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C$.

The dynamics of the walk is described by the shift operator

$$\hat{S} = \left(\sum_i |i+1\rangle \langle i|\right) \otimes |R\rangle \langle R| + \left(\sum_i |i-1\rangle \langle i|\right) \otimes |L\rangle \langle L| \tag{2}$$

and the coin operator, which is a 2 by 2 unitary matrix, denoted here as $\hat{C}$.

The usual description of the unitary dynamics of quantum walk is given by

$$\hat{U}_1 = \hat{S} \otimes \hat{C} = \hat{S} \left(\sum_i |i\rangle \langle i| \otimes \hat{C}\right) .$$

1.1.1 Shift Operator and Topologies

The shift operator can also be altered if one defines the boundary condition to be at positions $-N$ and N (which is the case for every simulation):

$$\hat{S}_1 = \left(\sum_{i=-N}^{N-1} |i+1\rangle \langle i|\right) \otimes |R\rangle \langle R| + \left(\sum_{i=-N+1}^{N} |i-1\rangle \langle i|\right) \otimes |L\rangle \langle L| . \tag{3}$$

On the other hand, it is possible do define circular topology simply by connecting both ends of the line, only by adding to $\hat{S}_1$ the following terms

$$\hat{B}_1 = |-N\rangle \langle N| \otimes |R\rangle \langle R| + |N\rangle \langle -N| \otimes |L\rangle \langle L| \tag{4}$$

Another constrain that can be imposed on the shift operator are broken links. When there is a broken link from positions i_0 to $i_0 + 1$, we get

$$\begin{aligned} \hat{G}_{i_0} = &- (|i_0+1\rangle \langle i_0| \otimes |R\rangle \langle R| + |i_0\rangle \langle i_0+1| \otimes |L\rangle \langle L|) \\ &+ |i_0\rangle \langle i_0| \, |L\rangle \langle R| + |i_0+1\rangle \langle i_0+1| \, |R\rangle \langle L| . \end{aligned}$$

If we have broken links between nodes (i_0^1, i_0^1+1), ..., (i_0^k, i_0^k+1), and define $I_0 = \{i_0^1, i_0^2, \ldots, i_0^k\}$, the resulting Operator will be

$$\hat{G}_{I_0} = \sum_{i_0 \in I_0} \hat{G}_{i_0}.$$

When broken links are fixed from the beginning and are unchanged during the walk, we are dealing with static broken links. Here, I_0 is fixed right at the beginning and remains unchanged throughout the quantum walk.

Given a specific shift operator, If broken links appear at random positions, then one is dealing with dynamic broken links. At each step, on top of the shift operator, random broken links are chosen according to a fixed parameter p which gives the probability of breaking any link. At each step, for each $i \in \{-N, \ldots, N-1\}$ a number r is picked at random from $[0,1]$. For each i, if $r \leq p$, then $i \in I_0$, otherwise $i \notin I_0^{t,p}$. Then, $\hat{G}_{I_0^{t,p}}$ will will change the shift operator in step t.

Since the shift operator can vary at each step t, we denote it by $\hat{S}_t$ to ease the notation.

1.1.2 Coin Operators

A generalization of this unitary evolution can be done by assigning to each position i a coin operator $\hat{C}_i$:

$$\hat{U}_2 = \hat{S}\left(\sum_i |i\rangle\langle i| \otimes \hat{C}_i\right)$$

where the coin operators can be written more generally as

$$\begin{bmatrix} e^{\imath\xi}\cos(\theta) & e^{\imath\zeta}\sin(\theta) \\ e^{\imath\zeta}\sin(\theta) & -e^{\imath\xi}\cos(\theta) \end{bmatrix}$$

with $\xi, \theta, \zeta \in [0, \pi/2]$.

static random coins occur when at fixed positions, at each step the coins are randomly chosen. A random coin can be defined by choosing ranges $[\xi_0, \xi_1]$, $[\theta_0, \theta_1]$ and $[\zeta_0, \zeta_1]$ and

$$\begin{aligned} \hat{C}_t &= \begin{bmatrix} e^{\imath\xi}\cos(\theta) & e^{\imath\zeta}\sin(\theta) \\ e^{\imath\zeta}\sin(\theta) & -e^{\imath\xi}\cos(\theta) \end{bmatrix} \\ \xi &= \xi_0 + (\xi_1 - \xi_0) \times r_1 \\ \theta &= \theta_0 + (\theta_1 - \theta_0) \times r_2 \\ \zeta &= \zeta_0 + (\zeta_1 - \zeta_0) \times r_3 \\ r_1, r_2, r_3 &\in U(0,1). \end{aligned}$$

where the subscript t means the coin is altered at each step.

Additionally, one can define for specific position k a random coin as $\hat{C}_t$ which we denote here as $\hat{C}_{k,t}$ and the set of such positions, K.

The general dynamic will be given by

$$\hat{U}_2 = \hat{S}_t \left(\sum_{i \notin K} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K} |i\rangle \langle i| \otimes \hat{C}_{i,t} \right)$$

In the dynamic case random coins appears at random positions at each step. First, every coin operator for every position must be specified at the beginning. Then, positions are chosen randomly, as for the case of dynamic broken links, in order to select at each step the positions for the random coins. For each $s \in \{-N, \ldots, N\}$, pick a random number $r \in [0,1]$. If $r < p$ then $s \in S^{t,p}$, otherwise do nothing. Then for each selected position, the following matrix

$$\begin{aligned}
\hat{C}^p_{k,t} &= \begin{bmatrix} e^{\imath\xi}\cos(\theta) & e^{\imath\zeta}\sin(\theta) \\ e^{\imath\zeta}\sin(\theta) & -e^{\imath\xi}\cos(\theta) \end{bmatrix} \\
\xi &= \frac{\pi}{2} r_1 \\
\theta &= \frac{\pi}{2} r_2 \\
\zeta &= \frac{\pi}{2} r_3 \\
r_1&, r_2, r_3 \in U(0,1).
\end{aligned}$$

is computed and used at that position for that step and at each step we get

$$\hat{U}_2 = \hat{S}_t \left(\sum_{i \notin K, K^{t,p}} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K, i \notin K^{t,p}} |i\rangle \langle i| \otimes \hat{C}_{i,t} + \sum_{i \notin K, i \in K^{t,p}} |i\rangle \langle i| \otimes \hat{C}^p_{i,t} \right)$$

1.1.3 Measurements

Measure operator, in this context, is a projective measurement of the form $|i,c\rangle \langle i,c|$ for position i, coin state c.

For specific pairs of numbers $\mathcal{M} = \{(i_1, c_1), \ldots, (i_l, c_l)\}$, the measure projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,c) \in \mathcal{M}} |i,c\rangle \langle i,c| \,.$$

The general dynamic of the quantum walk can be summarized in the following formula

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,c} \alpha_{i,c}(n) |i\rangle |c\rangle .$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle \langle\psi(n)| .$$

1.2 *qwsim_1D*

Here we describe how to choose the dynamics for the quantum walk by introducing parameters in the parse file.

1.2.1 Inputs

N refers to the dimension of the line that goes from $-N$ until N. It fixes the dimension of the Hilbert space (overall state). The initial state is introduced in the simulator by specify how much non-zero amplitudes $\alpha_{i,c}$ there is, the respective positions i and coin state c. Then for each pair i, c the numbers $\mathrm{Re}(\alpha_{i,c})$ and $\mathrm{Im}(\alpha_{i,c})$ need to be defined.

By fixing N the simulator fixes the shift operator to (3). Moreover, due to memory management, circular boundary condition is selected by default, hence we ad the circular boundary condition term (4), yielding

$$\hat{S}_t = \hat{S}_1 + \hat{B}_1.$$

By choosing p_1 we change the shift operator to

$$\hat{S}_t = \hat{S}_1 + \hat{B}_1 + \hat{G}^{t,p_1}_{I_0}$$

If one fixes broken links, one defines specific positions as described above and we get

$$\hat{S}_t = \hat{S}_1 + \hat{B}_1 + \hat{G}^{t,p_1}_{I_0} + \hat{G}_{I_0}.$$

After selection of initial state and boundary conditions for the shift operator, one can choose from a set of standard operators a coin operator $\hat{C}$ for all the positions of the walker. The options for $\hat{C}$ are Hadamard, identity and the overall unitary evolution is set to

$$\hat{U}_1 = \hat{S}_t \otimes \hat{C} = \hat{S}_t \left(\sum_i |i\rangle \langle i| \otimes \hat{C} \right).$$

p_2 changes the coin operators accordingly, yielding

$$\hat{U}_2 = \hat{S}_t \left(\sum_{i \notin K^{t,p_2}} |i\rangle \langle i| \otimes \hat{C} + \sum_{i \in K^{t,p_2}} |i\rangle \langle i| \otimes \hat{C}^p_{i,t} \right).$$

By fixing a static random coin one is defining the matrix $\hat{C}_t$ and we get

$$\hat{U}_2 = \hat{S}_t \left(\sum_{i \notin K^{t,p_2}} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K^{t,p_2}} |i\rangle \langle i| \otimes \hat{C}^p_{i,t} \right).$$

If, in addition, we define specific coins at specific positions we get

$$\hat{U}_2 = \hat{S}_t \left(\sum_{i \notin K, K^{t,p}} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K, i \notin K^{t,p}} |i\rangle \langle i| \otimes \hat{C}_{i,t} + \sum_{i \notin K, i \in K^{t,p}} |i\rangle \langle i| \otimes \hat{C}^p_{i,t} \right).$$

Measure points can also be set in any position for any coin state. Parameter *dim_absorb* refers to the number of points one wishes to measure (absorb the probability amplitude). By choosing $dim\_absorb = l$, l pairs of numbers $\mathcal{M} = \{(i_1, c_1), \ldots, (i_l, c_l)\}$ will be specified and mathematically the projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,c) \in \mathcal{M}} |i, c\rangle \langle i, c|.$$

The general dynamic of the quantum walk can be summarized as

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,c} \alpha_{i,c}(n) |i\rangle |c\rangle$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle \langle \psi(n)|.$$

1.2.2 Output Data

The output data is obtained from the following two density matrices:

$$\begin{aligned} Tr(\rho(n))_P &= \sum_c (I_P \otimes \langle c|) \rho(n) (I_P \otimes |c\rangle) \\ &= \sum_c \left(\sum_{i_1} \alpha_{i_1,c}(n) |i, j\rangle \right) \left(\sum_{i_2} \alpha^*_{i_1,c}(n) \langle i, j| \right) = \rho_P(n) \end{aligned}$$

and
$Tr(\rho(n))_P =$

$$
\begin{aligned}
&= \sum_i (\langle i| \otimes I_C)\rho(|i\rangle \otimes I_C) \\
&= \sum_i \left(\sum_{c_1} \alpha_{i,c_1} \langle i|i\rangle |c_1\rangle \right) \left(\sum_{c_2} \alpha^*_{i_2,c_2} \langle i|i\rangle \langle c_2| \right) \\
&= \sum_i \left(\sum_{c_1} \alpha_{i,c_1} |c_1\rangle \right) \left(\sum_{c_2} \alpha^*_{i,c_2} \langle c_2| \right) = \rho_C .
\end{aligned}
$$

The output files are:

- The file *probability_distribution* at line $b = i + N$ gives the value for

$$P_i(steps) = \sum_c \left(\alpha_{i,c} \alpha^*_{i,c} \right)$$

- The *average_probability_distribution* where at line $b = i + N$ gives the value

$$P_{av,i}(n) = \frac{1}{steps} \sum_c \left(\alpha_{i,c} \alpha^*_{i,c} \right)$$

- *mean_x* refers to the mean distance where at line n gives

$$\langle i\rangle (n) = \sum_i i \times P_i(n)$$

- *standard_deviation* where at line n gives

$$\sigma_x(n) = \sqrt{\sum_i (\langle i\rangle - i \times P_i(n))^2}$$

- *Shannon_entropy* where at line n gives

$$
\begin{aligned}
p_c(n) &= \langle c| \rho_c(n) |c\rangle \\
H(C) &= -\sum_c p_c(n) \log(p_c(n))
\end{aligned}
$$

- *von_Neumann_entropy* where at line n gives

$$S(\rho_c(n)) = \sum_s \lambda_s \ln(\lambda_s)$$

where λ_s are the eigenvalues of $\rho_c(n)$.

2 Two particles Quantum Walk on the Line

2.1 Basic Dynamics

The state of two particles quantum walk, is written as

$$|\psi\rangle = \sum_{i,j,c_1,c_2} \alpha_{i,,c_1,j,c_2} |i, c_1\rangle |j, c_2\rangle . \tag{5}$$

where$|i, c_1\rangle \in \mathcal{H}_1$ and $|j, c_2\rangle \in \mathcal{H}_2$, with $\mathcal{H}_k = \mathcal{H}_{P,k} \otimes \mathcal{H}_{C_k}$. The overall Hilbert space is described as $\mathcal{H}_1 \otimes \mathcal{H}_2$. The dynamics of the walk for each particle is described as the case of 1D quantum walk.

The same options for 1D quantum walk here can be described by $\hat{U} = \hat{U}_1 \otimes \hat{U}_2$ where

$$\hat{U}_1 = \hat{S}^1_t \left(\sum_{i \notin K_1, K^{t,p_{2,1}}} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K_1, i \notin K^{t,p}} |i\rangle \langle i| \otimes \hat{C}_{i,t} + \sum_{i \notin K_1, i \in K^{t,p_{2,1}}} |i\rangle \langle i| \otimes \hat{C}^{p_{2,1}}_{i,t} \right)$$

with

$$\hat{S}^1_t = \hat{S} + \hat{B}_1 + \hat{G}^{t,p_{1,1}}_{I^1_0} + \hat{G}_{I^1_0}$$

and

$$\hat{U}_2 = \hat{S}^2_t \left(\sum_{i \notin K_2, K^{t,p_{2,2}}} |i\rangle \langle i| \otimes \hat{C}_t + \sum_{i \in K_2, i \notin K^{t,p_{2,2}}} |i\rangle \langle i| \otimes \hat{C}_{i,t} + \sum_{i \notin K_2, i \in K^{t,p_{2,2}}} |i\rangle \langle i| \otimes \hat{C}^{p_{2,2}}_{i,t} \right)$$

with

$$\hat{S}^2_t = \hat{S} + \hat{B}_1 + \hat{G}^{t,p_{1,2}}_{I^2_0} + \hat{G}_{I^2_0}.$$

This is the general case when the two particles are on different lines. When they are in the same line, $\hat{U}_2 = \hat{U}_1$.

2.1.1 Measurement

Measure points can also be set in any position for any coin state. Measure operator, in this context, is a projective measurement of the form $(|i\rangle\langle i| \otimes I) \otimes (|j\rangle\langle j| \otimes I)$ for position (i, j).

For l measuring points, $\mathcal{M} = \{(i_1, j_1), \ldots, (i_l, j_l)\}$, the projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,j)\in\mathcal{M}} (|i\rangle\langle i| \otimes I) \otimes (|j\rangle\langle j| \otimes I).$$

The general dynamic of the quantum walk can be summarized as

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,j,c} \alpha_{i,j,c}(n) |i, j\rangle |c\rangle$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle\langle\psi(n)|.$$

2.2 *qwsim_1D_2_walkers*

Here we describe how to choose the dynamics for the quantum walk by introducing parameters in the parse file. For brevity, and since the "composition" of operators is similar to the case of *qwsim_1D*, we omit the explicit operators formula.

2.2.1 Inputs

N refers to the dimension of the line that goes from $-N$ until N. Then one selects if the particles are in the same line or not.

The choices for $\hat{U}_1$ and $\hat{U}_2$ is done in the same fashion as in *qwsim_1D*.

Measure points can also be set in any position for any coin state. Parameter *dim_absorb* refers to the number of points one wishes to measure (absorb the probability amplitude). Measure operator, in this context, is a projective measurement of the form $|i, c\rangle\langle i, c|$ for position i, coin state c.

More than one measure point can be defined and are fixed throughout the walk. By choosing $dim\_absorb = l$, l pairs of numbers $\mathcal{M} = \{(i_1, j_1), \ldots, (i_l, j_l)\}$ will be specified and mathematically the projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,j)\in\mathcal{M}} |i, j\rangle\langle i, j| \otimes I.$$

The general dynamic of the quantum walk can be summarized as

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,c} \alpha_{i,c}(n) |i\rangle |c\rangle$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle \langle\psi(n)| .$$

2.2.2 Output Data

The output data is obtained from the following two density matrices:

$$\begin{aligned} Tr(\rho(n))_P &= \sum_c (I_P \otimes \langle c|)\rho(n)(I_P \otimes |c\rangle) \\ &= \sum_c \left(\sum_{i_1,j_1} \alpha_{i_1,j_1,c}(n) |i_1, j_1\rangle \right) \left(\sum_{i_2,j_2} \alpha^*_{i_1,j_2,c}(n) \langle i_2, j_2| \right) = \rho_P(n) \end{aligned}$$

and

$$\begin{aligned} Tr(\rho(n))_P &= \\ &= \sum_{i,j} (\langle i,j| \otimes I_C)\rho(|i,j\rangle \otimes I_C) \\ &= \sum_{i,j} \left(\sum_{c_1} \alpha_{i,j,c_1} \langle i,j|i,j\rangle |c_1\rangle \right) \left(\sum_{c_2} \alpha^*_{i_2,c_2} \langle i,j|i,j\rangle \langle c_2| \right) \\ &= \sum_{i,j} \left(\sum_{c_1} \alpha_{i,j,c_1} |c_1\rangle \right) \left(\sum_{c_2} \alpha^*_{i,j,c_2} \langle c_2| \right) = \rho_C . \end{aligned}$$

The output files are:

- The file *probability_distribution* at line l, according to $l = (j+N)+(2N+1)(i+N)$, is

$$P_{i,j}(steps) = \sum_c \left(\alpha_{i,j,c}\alpha^*_{i,j,c} \right)$$

- The *average_probability_distribution* where at line l gives the value

$$P_{av,i,j}(n) = \frac{1}{steps} \sum_c \left(\alpha_{i,j,c}\alpha^*_{i,j,c} \right)$$

- *mean_x* refers to the mean distance where at line n gives

$$\langle i \rangle (n) = \sum_i i \times \left(\sum_j P_{i,j}(n) \right)$$

- *mean_y* refers to the mean distance where at line n gives

$$\langle j \rangle (n) = \sum_j j \times \left(\sum_i P_{i,j}(n) \right)$$

- *Covariance* where at line n gives

$$\mathrm{Cov}(x(n), y(n)) = \left(\sum_{i,j} P_{i,j}(n) \times (i \times j) \right) - \langle i \rangle (n) \times \langle j \rangle (n)$$

- *mean_distance*

$$\langle i - j \rangle = \sum_{i,j} (i-j) P_{i,j}$$

- *one shot probability to hot*

$$\mathcal{P}_o^{(1)}(i_0; n) = \| \hat{P}_0 \left| \psi(n) \right\rangle \|^2 = \| \langle i_0 | \psi(n) \rangle \|^2$$

- *Average hitting time*

$$\mathcal{P}_f^{(1)}(i_0; n) = \| \hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n-1} \left| \psi(0) \right\rangle \|^2$$
$$\mathcal{N}_a^{(1)}(i_0) = \sum_{n=1}^{\infty} n \mathcal{P}_f^{(1)}(i_0; n)$$

- *Concurrent hitting time*

$$\mathcal{P}_c^{(1)}(i_0; n) = \sum_{n'=1}^{n} \| \hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n'-1} \left| \psi(0) \right\rangle \|^2$$

- $H(X)$

$$p_i = \sum_j P_{i,j}$$
$$H(X) = -\sum_i p_i \log(p_i)$$

- $H(Y)$

$$p_j = \sum_i P_{i,j}$$
$$H(Y) = -\sum_j p_j \log(p_j)$$

- $H(C)$

$$p_c = \langle c| \rho_c |c\rangle$$
$$H(C) = -\sum_c p_c \log(p_c)$$

- $H(X,Y)$

$$H(X,Y) = -\sum_{i,j} P_{i,j} \log(P_{i,j})$$

- $I(X:Y)$

$$I(X:Y) = H(X) + H(Y) - H(X,Y)$$

- $Von\_Newman\_entropy\ of\ coin\ state$

$$S(\rho_P) = S(\rho_c) = -\sum r_k \log(r_k)$$

- S_x

$$S(\rho_x) = Tr[\rho_x \ln \rho_x] = -Tr[R_x \ln R_x] = \sum_s \lambda_s \ln(\lambda_s)$$

- S_y

$$S(\rho_y) = Tr[\rho_y \ln \rho_y] = -Tr[R_y \ln R_y] = \sum_s \lambda_s \ln(\lambda_s)$$

- Iv_xy

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

- $Quantum\ Discord$

$$\delta_{\hat{\Pi}_i^X} = I(\hat{\rho}_{P,12}) - J(X:Y)$$

- E_f is the upper bound for the entanglement of formation

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

3 1 Particle on a 2D Lattice

3.1 Basic Dynamics

The state of the single particle quantum walk, on a 2D lattice, is written as

$$|\psi\rangle = \sum_{x,y,c} \alpha_{x,y,c} |x, y\rangle |c\rangle . \tag{6}$$

The dynamics of the walk is described by the shift operator

$$\begin{aligned}
\hat{S}_{xy} = \sum_{xy} & |x+1, y\rangle \langle x, y| \otimes |E\rangle \langle E| \\
& + |x, y-1\rangle \langle x, y| \otimes |S\rangle \langle S| \\
& + |x, y+1\rangle \langle x, y| \otimes |N\rangle \langle N| \\
& + |x-1, y\rangle \langle x, y| \otimes |W\rangle \langle W|
\end{aligned}$$

and the coin operator, which is a 4 by 4 unitary matrix, denoted here as $\hat{C}$.

The usual description of the unitary dynamics of quantum walk is given by

$$\hat{U}_1 = \hat{S}_{xy} \otimes \hat{C} = \hat{S}_{xy} \left(\sum_{i,j} |i, j\rangle \langle i, j| \otimes \hat{C} \right) .$$

3.2 Shift Operator and Topologies

The shift operator can also be altered if one defines the boundary condition to be at positions $-N$ and N (which is the case for every simulation):

$$\begin{aligned}
\hat{S}_{xy} = & \sum_{x=-N}^{N-1} \sum_{y=-N}^{N} |x+1, y\rangle \langle x, y| \otimes |E\rangle \langle E| \\
& + \sum_{x=-N}^{N} \sum_{y=-N+1}^{N} |x, y-1\rangle \langle x, y| \otimes |S\rangle \langle S| \\
& + \sum_{x=-N}^{N-1} \sum_{y=-N}^{N-1} |x, y+1\rangle \langle x, y| \otimes |N\rangle \langle N| \\
& + \sum_{x=-N+1}^{N-1} \sum_{y=-N}^{N} |x-1, y\rangle \langle x, y| \otimes |W\rangle \langle W|
\end{aligned} \tag{7}$$

On the other hand, it is possible do define cylinder topology simply by connecting the ends $x = -N$ to $x = N$, yielding

$$\hat{B}_{x,1} = \sum_{y=-N}^{N} \left|-N,y\right\rangle \left\langle N,y\right| \otimes \left|E\right\rangle \left\langle E\right| + \sum_{y=-N}^{N} \left|N,y\right\rangle \left\langle -N,y\right| \otimes \left|W\right\rangle \left\langle W\right| \qquad (8)$$

or by connecting the ends $y = -N$ to $y = N$, giving

$$\hat{B}_{y,1} = \sum_{x=-N}^{N} \left|x,N\right\rangle \left\langle x,-N\right| \otimes \left|S\right\rangle \left\langle S\right| + \sum_{x=-N}^{N} \left|x,-N\right\rangle \left\langle x,N\right| \otimes \left|N\right\rangle \left\langle N\right|. \qquad (9)$$

Another possible boundary condition is the Möbius strip when we connect boundaries $x = -N$ and $x = N$

$$\hat{B}_{x,2} = \sum_{y} \left|-N,-y\right\rangle \left\langle N,y\right| \otimes \left|E\right\rangle \left\langle E\right| + \sum_{y} \left|N,-y\right\rangle \left\langle -N,y\right| \otimes \left|W\right\rangle \left\langle W\right| \qquad (10)$$

or boundaries $y = -N$ and $y = N$

$$\hat{B}_{y,2} = \sum_{x} \left|-x,-N\right\rangle \left\langle x,N\right| \otimes \left|N\right\rangle \left\langle N\right| + \sum_{x} \left|x,-N\right\rangle \left\langle -x,N\right| \otimes \left|S\right\rangle \left\langle S\right| \qquad (11)$$

When both Möbis strip are in use, we get the Klein bottle.

Another constrain that can be imposed on the shift operator are broken links. When there is a broken link from positions (x_0, y_0) to (x_0+1, y_0) we get

$$\begin{aligned}\hat{G}_{x,x_0} = &-(\left|x_0+1,y_0\right\rangle \left\langle x_0,y_0\right| \otimes \left|E\right\rangle \left\langle E\right| + \left|x_0,y_0\right\rangle \left\langle x_0+1,y_0\right| \otimes \left|W\right\rangle \left\langle W\right|) \\ &+ \left|x_0,y_0\right\rangle \left\langle x_0,y_0\right| \otimes \left|W\right\rangle \left\langle E\right| + \left|x_0+1,y_0\right\rangle \left\langle x_0+1,y_0\right| \otimes \left|E\right\rangle \left\langle W\right|\end{aligned}$$

whereas if the broken link is in positions (x_0, y_0) and (x_0, y_0+1), then

$$\begin{aligned}\hat{G}_{y,y_0} = &-(\left|x_0,y_0+1\right\rangle \left\langle x_0,y_0\right| \otimes \left|N\right\rangle \left\langle N\right| + \left|x_0,y_0\right\rangle \left\langle x_0,y_0+1\right| \otimes \left|S\right\rangle \left\langle S\right|) \\ &+ \left|x_0,y_0\right\rangle \left\langle x_0,y_0\right| \otimes \left|S\right\rangle \left\langle N\right| + \left|x_0,y_0+1\right\rangle \left\langle x_0,y_0+1\right| \otimes \left|N\right\rangle \left\langle S\right|.\end{aligned}$$

If we have broken links between nodes $(i_0^1, j_0^1), (i_0^1+1, j_0^1), \ldots, (i_0^k, j_0^k), (i_0^k+1, j_0^k)$, and define $I_0 = \{(i_0^1, j_0^1), \ldots, (i_0^k, j_0^k)\}$ the resulting shift operator will be

$$\hat{G}_{x,I_0} = \sum_{x_0 \in I_0} \hat{G}_{x_0}$$

whereas if we have broken links between nodes $(i_0^1, j_0^1), (i_0^1, j_0^1+1), \ldots, (i_0^k, j_0^k), (i_0^k, j_0^k+1)$, and define $J_0 = \{(i_0^1, j_0^1), \ldots, (i_0^k, j_0^k+1)\}$ we get

$$\hat{G}_{y,J_0} = \sum_{y_0 \in I_0} \hat{G}_{x_0}$$

When broken links are fixed from the beginning and are unchanged during the walk, we are dealing with static broken links. Here, I_0 and J_0 are fixed right at the beginning and remains unchanged throughout the quantum walk.

Given a specific shift operator, If broken links appear at random positions, then one is dealing with dynamic broken links. At each step, on top of the shift operator, random broken links are chosen according to a fixed parameter p which gives the probability of breaking any link. At each step, for each $(x, y, c) \in \{-N, \ldots, N-1\}^2 \times \{E, N\}$ a number r is picked at random from $[0, 1]$. For each (x, y, E), if $r \leq p$, then $(x, y, E) \in I_0^{t,p}$, otherwise $(x, y, E) \notin I_0^{t,p}$. For each (x, y, N), if $r \leq p$, then $(x, y) \in J_0^{t,p}$, otherwise $(x, y) \notin J_0^{t,p}$.

$$\hat{G}_{I_0^{t,p}, J_0^{t,p}} = \hat{G}_{x, I_0^{t,p}} + \hat{G}_{y, J_0^{t,p}}.$$

3.2.1 Coin Operators

A generalization of this unitary evolution can be done by assigning to each position (i, j) a coin operator $\hat{C}_{i,j}$:

$$\hat{U}_2 = \hat{S}\left(\sum_{i,j} |i, j\rangle \langle i, j| \otimes \hat{C}_{i,j}\right)$$

where the coin operators can be written more generally as

$$\begin{bmatrix} e^{\imath\xi_1}\cos(\theta_1) & e^{\imath\zeta_1}\sin(\theta_1) \\ e^{\imath\zeta_1}\sin(\theta_1) & -e^{\imath\xi_1}\cos(\theta_1) \end{bmatrix} \otimes \begin{bmatrix} e^{\imath\xi_2}\cos(\theta_2) & e^{\imath\zeta_2}\sin(\theta_2) \\ e^{\imath\zeta_2}\sin(\theta_2) & -e^{\imath\xi_2}\cos(\theta_2) \end{bmatrix}$$

and $\xi_1, \zeta_1, \theta_1, \xi_2, \zeta_2, \theta_2 \in [0, \pi/2]$.

static random coins occur when at fixed positions, at each step the coins are randomly chosen. A random coin can be defined by ranges $[\xi_{10}, \xi_{11}]$, $[\theta_{10}, \theta_{11}]$, $[\zeta_{10}, \zeta_{11}]$, $[\xi_{20}, \xi_{21}]$, $[\theta_{20}, \theta_{21}]$ and $[\zeta_{20}, \zeta_{21}]$ as

$$\begin{aligned}
\hat{C}_t &= \begin{bmatrix} e^{\imath\xi_1}\cos(\theta_1) & e^{\imath\zeta_1}\sin(\theta_1) \\ e^{\imath\zeta_1}\sin(\theta_1) & -e^{\imath\xi_1}\cos(\theta_1) \end{bmatrix} \otimes \begin{bmatrix} e^{\imath\xi_2}\cos(\theta_2) & e^{\imath\zeta_2}\sin(\theta_2) \\ e^{\imath\zeta_2}\sin(\theta_2) & -e^{\imath\xi_2}\cos(\theta_2) \end{bmatrix} \\
\xi_1 &= \xi_{10} + (\xi_{11} - \xi_{10}) \times r_1 \\
\theta_1 &= \theta_{10} + (\theta_{11} - \theta_{10}) \times r_2 \\
\zeta_1 &= \zeta_{10} + (\zeta_{11} - \zeta_{10}) \times r_3 \\
\xi_2 &= \xi_{20} + (\xi_{21} - \xi_{20}) \times r_4 \\
\theta_2 &= \theta_{20} + (\theta_{21} - \theta_{20}) \times r_5 \\
\zeta_2 &= \zeta_{20} + (\zeta_{21} - \zeta_{20}) \times r_6 \\
r_i &\in U(0, 1).
\end{aligned}$$

Additionally, one can define for specific position k a random coin as $\hat{C}_t$ which we denote here as $\hat{C}_{(x,y),t}$ and the set of such positions, K.

The general dynamic will be given by

$$\hat{U}_2 = \hat{S}^t_{x,y} \left(\sum_{(x,y)\notin K} |x,y\rangle \langle x,y| \otimes \hat{C}_t + \sum_{(x,y)\in K} |x,y\rangle \langle x,y| \otimes \hat{C}_{(x,y),t} \right)$$

In the dynamic case random coins appears at random positions at each step. Positions are chosen randomly, as for the case of dynamic broken links, in order to select at each step the positions for the random coins. Then for each selected position, the following matrix

$$\begin{aligned}
&\hat{C}^{(x,y)}_{t,p} \begin{bmatrix} e^{\imath\xi_1}\cos(\theta_1) & e^{\imath\zeta_1}\sin(\theta_1) \\ e^{\imath\zeta_1}\sin(\theta_1) & -e^{\imath\xi_1}\cos(\theta_1) \end{bmatrix} \otimes \begin{bmatrix} e^{\imath\xi_2}\cos(\theta_2) & e^{\imath\zeta_2}\sin(\theta_2) \\ e^{\imath\zeta_2}\sin(\theta_2) & -e^{\imath\xi_2}\cos(\theta_2) \end{bmatrix}\\
&\xi_1 = \frac{\pi}{2} \times r_1\\
&\theta_1 = \frac{\pi}{2} \times r_2\\
&\zeta_1 = \frac{\pi}{2} \times r_3\\
&\xi_2 = \frac{\pi}{2} \times r_4\\
&\theta_2 = \frac{\pi}{2} \times r_5\\
&\zeta_2 = \frac{\pi}{2} \times r_6\\
&r_i \in U(0,1).
\end{aligned}$$

is computed and used at position (x,y) for step t.

3.2.2 Measurement

Measure points can also be set in any position for any coin state. Measure operator, in this context, is a projective measurement of the form $|x,y\rangle \langle x,y| \otimes I$ for position (x,y).

For l measuring points, $\mathcal{M} = \{(i_1,j_1),\ldots,(i_l,j_l)\}$, the projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,j)\in\mathcal{M}} |i,j\rangle \langle i,j| \otimes I.$$

The general dynamic of the quantum walk can be summarized as

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,j,c} \alpha_{i,j,c}(n) |i,j\rangle |c\rangle$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle \langle\psi(n)| \, .$$

3.3 *qwsim_2D_1_walker*

Here we describe how to choose the dynamics for the quantum walk by introducing parameters in the parse file. For brevity, and since the "composition" of operators is similar to the case of *qwsim_1D*, we omit the explicit operators formula.

3.3.1 Inputs

N refers to the dimension of the line that goes from $-N$ until N. In order to define the initial state, one has to specify how much non-zero amplitudes $\alpha_{i,j,c}$ there is, the positions the respective positions (i, j) and coin state c. Then for each $tuple(i, j, c)$ the numbers $\mathrm{Re}(\alpha_{i,j,c})$ and $\mathrm{Im}(\alpha_{i,j,c})$ need to be defined.

By fixing N the simulator fixes the shift operator to (7). Moreover, due to memory management, cylinder boundary condition is selected by default (for $x = \pm N$ and $y = \pm N$) , hence we get for shift operator

$$\hat{S}_{xy,t} = \hat{S}_{xy,1} + \hat{B}_{x,1} + \hat{B}_{y,1}.$$

By choosing p_1 we define the sets I_0^{t,p_1}, I_1^{t,p_1}, J_0^{t,p_1} and J_0^{t,p_1} and change the shift operator accordingly.

$$\hat{S}_{xy,t} = \hat{S}_{xy,1} + \hat{B}_{x,1} + \hat{B}_{y,1} + \hat{G}_{I_0^{t,p_1},J_0^{t,p_1}}.$$

If one fixes broken links, one defines specific positions as described above, I_0 and J_0

$$\hat{S}_{xy,t} = \hat{S}_{xy,1} + \hat{B}_{x,1} + \hat{B}_{y,1} + \hat{G}_{I_0^{t,p_1},J_0^{t,p_1}} + \hat{G}_{I_0,J_0}.$$

One can choose a set of standard coin operator $\hat{C}$ for all the positions of the walker. The options for $\hat{C}$ are Hadamard, identity, Fourier and Grover Matrices and the overall unitary evolution is set to

$$\hat{U}_1 = \hat{S}_{xy,t} \otimes \hat{C} = \hat{S}_3 \left(\sum_{i,j} |i,j\rangle \langle i,j| \otimes \hat{C} \right).$$

p_2 changes the coin operators accordingly, by defining the set K^{t,p_2}.

$$\hat{U}_2 = \hat{S}_{xy,t}\left(\sum_{i\notin K^{t,p_2}} |i\rangle\langle i| \otimes \hat{C} + \sum_{i\in K^{t,p_2}} |i\rangle\langle i| \otimes \hat{C}^{p}_{i,t}\right).$$

By fixing a static random coin one is defining the matrix $\hat{C}_t$.

$$\hat{U}_2 = \hat{S}_{xy,t}\left(\sum_{i\notin K^{t,p_2}} |i\rangle\langle i| \otimes \hat{C}_t + \sum_{i\in K^{t,p_2}} |i\rangle\langle i| \otimes \hat{C}^{p}_{i,t}\right).$$

If, in addition, we define specific coins at specific positions we fix the set K.

$$\hat{U}_2 = \hat{S}_{xy,t}\left(\sum_{(x,y)\notin K^{t,p_2},K} |x,y\rangle\langle x,y| \otimes \hat{C}_t + \sum_{(x,y)\in K^{t,p_2}} |x,y\rangle\langle x,y| \otimes \hat{C}^{p_2}_{ij,t} + \sum_{(i,j)\in K} |i\rangle\langle i| \otimes \hat{C}_{ij,t}\right).$$

Measure points can also be set in any position for any coin state. Parameter *dim_absorb* refers to the number of points one wishes to measure (absorb the probability amplitude). Measure operator, in this context, is a projective measurement of the form $|i,c\rangle\langle i,c|$ for position i, coin state c.

More than one measure point can be defined and are fixed throughout the walk. By choosing $dim\_absorb = l$, l pairs of numbers $\mathcal{M} = \{(i_1, j_1), \ldots, (i_l, j_l)\}$ will be specified and mathematically the projector operator will take the form

$$M_{\mathcal{M}} = \sum_{(i,j)\in\mathcal{M}} |i,j\rangle\langle i,j| \otimes I.$$

The general dynamic of the quantum walk can be summarized as

$$|\psi(n)\rangle = ([I - M_{\mathcal{M}}]\hat{U}_2)^n |\psi\rangle = \sum_{i,c} \alpha_{i,c}(n) |i\rangle |c\rangle$$

Note that $|\psi(n)\rangle$ must be renormalized after each step if $\mathcal{M} \neq \emptyset$. The respective density matrix is given by

$$\rho(n) = |\psi(n)\rangle\langle\psi(n)|.$$

3.3.2 Output Data

The output data is obtained from the following two density matrices:

$$
\begin{aligned}
Tr(\rho(n))_P &= \sum_c (I_P \otimes \langle c|)\rho(n)(I_P \otimes |c\rangle) \\
&= \sum_c \left(\sum_{i_1,j_1} \alpha_{i_1,j_1,c}(n) \left| i_1, j_1 \right\rangle \right) \left(\sum_{i_2,j_2} \alpha^*_{i_1,j_2,c}(n) \left\langle i_2, j_2 \right| \right) = \rho_P(n)
\end{aligned}
$$

and

$$
\begin{aligned}
&Tr(\rho(n))_P = \\
&= \sum_{i,j} (\langle i,j| \otimes I_C)\rho(|i,j\rangle \otimes I_C) \\
&= \sum_{i,j} \left(\sum_{c_1} \alpha_{i,j,c_1} \langle i,j|i,j\rangle \left| c_1 \right\rangle \right) \left(\sum_{c_2} \alpha^*_{i_2,c_2} \langle i,j|i,j\rangle \left\langle c_2 \right| \right) \\
&= \sum_{i,j} \left(\sum_{c_1} \alpha_{i,j,c_1} \left| c_1 \right\rangle \right) \left(\sum_{c_2} \alpha^*_{i,j,c_2} \left\langle c_2 \right| \right) = \rho_C.
\end{aligned}
$$

The output files are:

- The file *probability_distribution* at line l, according to $l = (j+N)+(2N+1)(i+N)$, is

$$P_{i,j}(steps) = \sum_c \left(\alpha_{i,j,c}\alpha^*_{i,j,c} \right)$$

- The *average_probability_distribution* where at line l gives the value

$$P_{av,i,j}(n) = \frac{1}{steps} \sum_c \left(\alpha_{i,j,c}\alpha^*_{i,j,c} \right)$$

- *mean_x* refers to the mean distance where at line n gives

$$\langle i \rangle (n) = \sum_i i \times \left(\sum_j P_{i,j}(n) \right)$$

- *mean_y* refers to the mean distance where at line n gives

$$\langle j \rangle (n) = \sum_j j \times \left(\sum_i P_{i,j}(n) \right)$$

- *Covariance* where at line n gives

$$\mathrm{Cov}(x(n), y(n)) = \left(\sum_{i,j} P_{i,j}(n) \times (i \times j)\right) - \langle i \rangle (n) \times \langle j \rangle (n)$$

- *mean_distance*

$$\langle i - j \rangle = \sum_{i,j} (i - j) P_{i,j}$$

- *one shot probability to hot*

$$\mathcal{P}_o^{(1)}(i_0; n) = \|\hat{P}_0 \left|\psi(n)\right\rangle \|^2 = \|\langle i_0 | \psi(n) \rangle\|^2$$

- *Average hitting time*

$$\mathcal{P}_f^{(1)}(i_0; n) = \|\hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n-1} \left|\psi(0)\right\rangle \|^2$$
$$\mathcal{N}_a^{(1)}(i_0) = \sum_{n=1}^{\infty} n \mathcal{P}_f^{(1)}(i_0; n)$$

- *Concurrent hitting time*

$$\mathcal{P}_c^{(1)}(i_0; n) = \sum_{n'=1}^{n} \|\hat{P}_0 \hat{U} [\hat{P}_1 \hat{U}]^{n'-1} \left|\psi(0)\right\rangle \|^2$$

- $H(X)$

$$p_i = \sum_j P_{i,j}$$
$$H(X) = -\sum_i p_i \log(p_i)$$

- $H(Y)$

$$p_j = \sum_i P_{i,j}$$
$$H(Y) = -\sum_j p_j \log(p_j)$$

- $H(C)$

$$p_c = \left\langle c\right| \rho_c \left|c\right\rangle$$
$$H(C) = -\sum_c p_c \log(p_c)$$

- $H(X,Y)$

$$H(X,Y) = -\sum_{i,j} P_{i,j} \log(P_{i,j})$$

- $I(X:Y)$

$$I(X:Y) = H(X) + H(Y) - H(X,Y)$$

- $Von\_Newman\_entropy\ of\ coin\ state$

$$S(\rho_P) = S(\rho_c) = -\sum r_k \log(r_k)$$

- S_x

$$S(\rho_x) = Tr[\rho_x \ln \rho_x] = -Tr[R_x \ln R_x] = \sum_s \lambda_s \ln(\lambda_s)$$

- S_y

$$S(\rho_y) = Tr[\rho_y \ln \rho_y] = -Tr[R_y \ln R_y] = \sum_s \lambda_s \ln(\lambda_s)$$

- Iv_xy

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

- $Quantum\ Discord$

$$\delta_{\hat{\Pi}_i^X} = I(\hat{\rho}_{P,12}) - J(X:Y)$$

- E_f is the upper bound for the entanglement of formation

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