Mapping quantum random walks onto a Markov chain by mapping a unitary transformation to a higher dimension of an irreducible matrix

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Here, a new two-dimensional process, discrete in time and space, that yields the results of both a random walk and a quantum random walk, is introduced. This model describes the distribution of four coin states $|1>, -|1>, |0>, -|0>$ in space without interference, instead of two coin states $|1>, |0>$. For the case of no boundary conditions, the model is similar to a Markov process, namely, it conserves the probability distribution of the four coin states, and by using a proper transformation, yields probability distributions of the two quantum states $|1>, |0>$ in space, similar to a unitary operator. Numerical results for a quantum random walk on infinite and finite lines are introduced.
Various problems of quantum random walks have been investigated by many groups. For example, Aharonov et al. [1] explored the notion of quantum random walks; Ambainis et al. [2–4] examined quantum walks on graphs; Bach et al. [5] investigated one-dimensional quantum walks with absorbing boundary conditions; Dür et al. [6] discussed quantum random walks in optical lattices; Konno et al. [7] examined absorption problems and the eigenvalues of two-state quantum walks [8]; Mackay et al. [9] explored quantum walks in higher dimensions; and Bartlet et al. [10] examined quantum topology identification and various other problems [11,12]. Several studies have discussed the differences between random walks and quantum random walks, such as those conducted by Childs et al. [13] and Motes et al. [14]. The differences are manifested in various distribution functions that influence all the moments of the dynamics. For example, the probability distribution function of a symmetric random walk starting at the origin behaves like a Gaussian distribution around the origin, namely, there is a high probability of the walker being found at the origin, while in the case of a quantum random walk, there is a low probability of being found at the origin, mainly because of interference [1,7].

Here, a new two-dimensional model, discrete in time and in space, that yields the results of both a random walk and a quantum random walk, is introduced. This model describes the distribution of four coin states \(|1\rangle, -|1\rangle, |0\rangle, -|0\rangle\) in space without interference, instead of two coin states \(|1\rangle, |0\rangle\). Using a proper transformation (introduced below) on the four coin state distributions yields the amplitude distributions of the two quantum states, \(|1\rangle, |0\rangle\), similar to a unitary operator. The model shows that the asymptotic behaviour of the distribution of each of the four coin states behaves like a Gaussian distribution. The model also enables us to extend it with different boundary conditions, such as a reflecting point or a trap, and obtain the distribution of each of the four coin states separately, thereby gaining a better understanding of the entire system.
Equivale
once between a Hadamard operator and a Markov chain

The discrete-time quantum random walk is defined by two operators: The coin flip operator and the shift operator, where the Hilbert space that governs the walk is a tensor product of 

\[ \mathcal{H}_T = \mathcal{H}_C \otimes \mathcal{H}_S, \]

so that \( \mathcal{H}_C \) is a Hilbert space that can be defined by the two canonical bases 

\[ |0 \rangle \quad \text{and} \quad |1 \rangle \]

as follows:

\[ |0 \rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1 \rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \]

(1)

and \( \mathcal{H}_S \) is a Hilbert space defined by an infinite canonical base

\[ |k \rangle = (0,0,0,\ldots,1,0,0)^T, \]

where 1 stands for the kth position in space.

The amplitude of a particle at location kth at any time step n, defined by a 2D vector, is as follows:

\[ |\psi_k(n)\rangle = \alpha |0 \rangle_c + \beta |1 \rangle_c \]

(2)

where the subscript c denotes that these states belong to the \( \mathcal{H}_C \) space.

The probability that the particle is at location k at time step n is given by the square of the modulus of \( |\psi_k(n)\rangle \), namely, \( ||\psi_k(n)||^2 \)

The Hadamard operator is defined by the following unitary operator:

\[ H = \frac{1}{\sqrt{2}} H_d, \]

(3)

where \( H_d \) is the Hadamard matrix:

\[ H_d = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \]

(4)

In order to build our model, the \( H \) operator was applied to the following coin states:

\[ |0 \rangle_c, |1 \rangle_c, -|1 \rangle_c, -|0 \rangle_c, \]

which yields

\[ H|0 \rangle_c = \frac{\sqrt{2}}{2} (|0 \rangle_c + |1 \rangle_c), \]

(5)

\[ H|1 \rangle_c = \frac{\sqrt{2}}{2} (|0 \rangle_c - |1 \rangle_c), \]

(6)

\[ H(-|1 \rangle_c) = \frac{\sqrt{2}}{2} (-|0 \rangle_c + |1 \rangle_c), \]

(7)

\[ H(-|0 \rangle_c) = \frac{\sqrt{2}}{2} (-|0 \rangle_c - |1 \rangle_c), \]

(8)
Using these results, the Hadamard operator can be described by the following Markov chain with two reflecting points and transition probabilities of \( p = q = 0.5 \), as shown in Figure 1.

Figure 1. A four-site Markov chain that represents the transitions between the coin states \(|0\rangle_c, |1\rangle_c, -|1\rangle_c, -|0\rangle_c\).

The analogy between a Hadamard operator and the model depicted in Figure 1 is explained as follows:

When starting at coin state \(|0\rangle_c\), the walker can stay at \(|0\rangle_c\) or jump to state \(|1\rangle_c\) (Eq. (5)).

When starting at coin state \(|1\rangle_c\), the walker can jump backward to state \(|0\rangle_c\) or jump to state \(-|1\rangle_c\) (Eq. (6)).

When starting at coin state \(-|1\rangle_c\), the walker can jump backward to state \(|1\rangle_c\) or jump to state \(-|0\rangle_c\) (Eq. (7)).

When starting at coin state \(-|0\rangle_c\), the walker can stay at that state or jump to state \(-|1\rangle_c\) (Eq. (8)).

Stated formally: The transition probabilities matrix that represents the Markov chain depicted in Figure 1 is as follows:

\[
A = \begin{bmatrix}
0.5 & 0.5 & 0 & 0 \\
0.5 & 0 & 0.5 & 0 \\
0 & 0.5 & 0 & 0.5 \\
0 & 0 & 0.5 & 0.5 \\
\end{bmatrix},
\]

\[ (9) \]

In order to present the mathematical relation between the transition matrix \( A \) and the Hadamard operator, the interference matrix \( B \) is defined as follows:

\[
B = \begin{bmatrix}
1 & 0 & 0 & -1 \\
0 & 1 & -1 & 0 \\
\end{bmatrix},
\]

\[ (10) \]

Several properties of the interference matrix will be utilized, including the following:
\[ BB^T = 2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = 2I_2, \]  
(11)

and

\[ B^T B = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} = I_4 - J_4, \]  
(12)

where \( I_4 \) is the identity matrix, \( J_4 \) is a reversal matrix, and the subscript denotes its dimension.

Using the interference matrix \( B \), the Hadamard matrix can be presented as

\[ H = \frac{1}{\sqrt{2}} BAB^T, \]  
(13)

which can be shown explicitly by multiplication as follows:

\[ \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & -1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 0.5 & 0.5 & 0 & 0 \\ 0.5 & 0 & 0.5 & 0 \\ 0 & 0.5 & 0 & 0.5 \\ 0 & 0 & 0.5 & 0.5 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & -1 \\ -1 & 0 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \]  
(14)

In other words, the unitary Hadamard operator is mapped onto a higher dimension of a symmetric Markov process (Note that \( \text{Det}(H) \neq 0 \), while \( \text{Det}(A) = 0 \)).

**The power of \( A^n \)**

The mathematical relation between \( A^n \) and \( H^n \), where \( n \) is the step number, is explained in the following equations:

Based on Eq. (13), \( H^2B \) can be written as

\[ H^2B = \left( \frac{1}{\sqrt{2}} \right)^2 (BAB^T)(BAB^T)B, \]  
(15)

Since \( B^T B \) commutes with the transition matrix \( A \) [15], Eq. (15) can be rearranged to

\[ H^2B = \left( \frac{1}{\sqrt{2}} \right)^2 B(B^T B)^2A^2, \]  
(16)

and similar to Eq. (16), the following relation can be written in general for any positive integer \( n \):

\[ H^nB = \left( \frac{1}{\sqrt{2}} \right)^n B(B^T B)^nA^n, \]  
(17)

Note that \( B^T B/2 = \frac{1}{2} (I_4 - J_4) \) from Eq. (12), and \( (B^T B/2)^2 \) satisfies
\[
(B^T B/2)^2 = \frac{1}{4} (I_4 I_4 - I_4 J_4 - J_4 I_4 + J_4 J_4) = \frac{1}{4} (I_4 - 2J_4 + I_4) = \frac{1}{2} (I_4 - J_4),
\]
which means that \( B^T B / 2 \) is an idempotent matrix (M is idempotent if \( M^2 = M \)), and in general, \((B^T B/2)^n = B^T B / 2\), which yields
\[
(B^T B)^n = 2^{n-1} B^T B
\] (19)

Substituting Eq. (19) into Eq. (17) yields:
\[
H^n B = \left( \frac{1}{\sqrt{2}} \right)^n 2^{n-1} B B^T B A^n,
\] (20)
and using the property of Eq. 11, \( BB^T = 2I \), yields the desired relation:
\[
H^n B = B \sqrt{2^n A^n}.
\] (21)

Consider the following arbitrary initial condition of the Markov chain:
\[
P(0) = \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix},
\] (22)
where \( P(0) \) describes the four coin states: \(|0 >_c, 1 >_c, -1 >_c, -|0 >_c \) at step \( n = 0 \).

This initial condition corresponds to
\[
|\psi(0) >= \alpha |0 >_c + \beta |1 >_c - \gamma |1 >_c - \delta |0 >_c ,
\] (23)
Applying Eq. (21) to the initial condition yields
\[
H^n B P(0) = B \sqrt{2^n A^n} P(0),
\] (24)
Rearranging the left side yields
\[
H^n |\psi(0) >= B \sqrt{2^n A^n} P(0),
\] (25)
and in general yields
\[
|\psi(n + 1) >= H |\psi(n) >= B \sqrt{2^{n+1} A^n} P(n).
\] (26)
Note that:
(a) The interference matrix operates only at the end of the process.
(b) The solution of the Markov chain conserves the distribution of the four coin states:
\[
[1,1,1,1] P(n) = [1,1,1,1] P(0).
\] (27)
(c) By using the interference matrix, the square modulus of the quantum state \( |\psi(n) > \) is preserved as a unitary operator:
\[ ||\psi(n) >||^2 = \left| B \sqrt{2^n} P(n) \right|^2 = ||\psi(0) >||^2. \]  

\textbf{A random walk and quantum random walk model}

The process of a quantum random walk includes a shift operator [1], which is a unitary operator that acts on a different Hilbert space, \( H_S \). The two processes, Hadamard and the shift operators, can be described by the following model depicted in Figure 2, where the horizontal direction (X axis) describes the movements due to the shift operator, and the vertical direction (Y axis) describes the movements due to the Hadamard operator, which are described by the transition matrix \( A \).

![Figure 2. A two-step Markovian model. The horizontal direction (X axis) describes the movements due to the shift operator, and the vertical direction (Y axis) describes the movements due to the transition matrix A.](image)

The main points of the model are as follows:

1. The shift operator is responsible for the movement in the horizontal direction described by a birth and death process.
2. The Hadamard operator presented by transition matrix \( A \) is responsible for movements in the vertical direction.
3. The movements in the horizontal direction and vertical direction occur one after the other, rather than simultaneously.
4. The same state can be populated without interference. Thus, it is possible to propagate $|0\rangle_c, -|0\rangle_c$ at the same kth site.

5. Interference occurs at the end of the dynamics.

6. In order to obtain the amplitude of the quantum state after $n$ steps, the distribution of states is multiplied by a factor of $\sqrt{2^n}$ (Eq. 26).

Returning now to the quantum random walk, the following equation describes its dynamics [7]:

$$|\psi_k(n + 1)\rangle = |0\rangle \langle 0| H |\psi_{k-1}(n)\rangle + |1\rangle \langle 1| H |\psi_{k+1}(n)\rangle,$$

(29)

In this equation, the shift operator “moves” the coin state $|0\rangle$ to the right and $|1\rangle$ to the left, whereas the sign of the quantum state does not change its direction.

Similarly, the shift operator described in Figure 2 moves the coin state $|0\rangle$ and $-|0\rangle$ to the right and $|1\rangle$ and $-|1\rangle$ to the left, so that the dynamics of this system can be formulated as follows:

$$P_k(n + 1) = |U1 \rangle \langle U1| A P_{k-1}(n) + |U4 \rangle \langle U4| A P_{k-1}(n) +$$

$$|U2 \rangle \langle U2| A P_{k+1}(n) + |U3 \rangle \langle U3| A P_{k+1}(n),$$

(30)

whereby $P_k(n)$ is a 4-dimensional column vector describing the four coin states at the kth site. $U1, U2, U3, U4$ are the canonical bases of the Markovian system, specifically:

$< U1 | = [1, 0, 0, 0], < U2 | = [0, 1, 0, 0], < U3 | = [0, 0, 1, 0], < U4 | = [0, 0, 0, 1]$

Each of these bases represents the coin states $|0\rangle, |1\rangle, -|1\rangle, -|0\rangle$ correspondingly.

Multiplying both sides of Eq. (30) by the interference matrix $B$ yields

$$B P_k(n + 1) = B |U1 \rangle \langle U1| A P_{k-1}(n) + B |U4 \rangle \langle U4| A P_{k-1}(n) +$$

$$B |U2 \rangle \langle U2| A P_{k+1}(n) + B |U3 \rangle \langle U3| A P_{k+1}(n),$$

(31)

using the following equalities, which can be proved explicitly by multiplication [16]

$$B (|U1 \rangle \langle U1| + |U4 \rangle \langle U4|) = |0\rangle \langle 0| B,$$

(32)

$$B (|U2 \rangle \langle U2| + |U3 \rangle \langle U3|) = |1\rangle \langle 1| B,$$

(33)

into Eq. (32,33), and multiplying both sides by $\sqrt{2}^{n+1}$ yields

$$\sqrt{2}^{n+1} B P_k(n + 1) = \sqrt{2}^n (|0\rangle \langle 0| B \sqrt{2}A P_{k-1}(n)) + |1\rangle \langle 1| B \sqrt{2}A P_{k+1}(n))$$

(34)

Substituting $HB = B\sqrt{2}A$ obtained from Eq. (21) for $n = 1$ yields

$$\sqrt{2}^{n+1} B P_k(n + 1) = \sqrt{2}^n (|0\rangle \langle 0| H B P_{k-1}(n)) + |1\rangle \langle 1| H B P_{k+1}(n)),$$

(35)
Finally, using the relation of Eq. (26) $|\psi(n + 1)\rangle = \sqrt{2}^{n+1} B P(n + 1)$ returns the same dynamics as in Eq. (29):

$$|\psi_k(n + 1)\rangle = |0\rangle + |1\rangle + |0\rangle - |1\rangle \propto |\psi_{k-1}(n)\rangle + |\psi_{k+1}(n + 1)\rangle.$$  

The following figures describe the distributions of the four coin states. Figures 3 and 4 present a numerical result after 100 steps, starting at the origin in state $|0\rangle_c$

$$|\psi_k=0(0)\rangle = |0\rangle + |1\rangle + |0\rangle - |1\rangle = |0\rangle_c$$

whereas the amplitude distribution of the quantum random walk at the kth sites of states

$$|0\rangle_c, |1\rangle_c, -|0\rangle_c, -|1\rangle_c \text{ is calculated as follows:}$$

$$\sqrt{2^n} < U1|P_k(n)> \sqrt{2^n} < U1|P_k(n)> \sqrt{2^n} < U1|P_k(n)> \sqrt{2^n} < U1|P_k(n)> , \text{ respectively.}$$

The three graphs in the first row describe:

(a) The Markov distribution of state $|0\rangle$ in space: $< U1|P_k(n)>$.

(b) The Markov distribution of state $-|0\rangle$ in space: $< U4|P_k(n)>$.

(c) The probability distribution of the quantum state $|0\rangle$ being at the kth site:

$$2^n (< U1|P_k(n)> - < U4|P_k(n)>)^2.$$  

The second row of the graphs describes:

(d) The distribution of state $|1\rangle$ in space: $< U2|P_k(n)>$.

(e) The distribution of state $-|1\rangle$ in space: $< U3|P_k(n)>$.

(f) The probability distribution of the quantum state $|1\rangle$ being at the kth site:

$$2^n (< U2|P_k(n)> - < U3|P_k(n)>)^2.$$
Figure 3. Graphs (a), (b), (d), (e) present the Markov chain distribution of the four coin states \(|0_c\), \(|-0_c\), \(|1_c\), \(|-1_c\), respectively. Graphs (c) and (f) present the probability distribution of the quantum states \(|0_c\), \(|1_c\).

Figure 3 shows that, prior to the interference, all the states behave like Gaussian distributions. Adding the distributions of Figure 3a,b,c,d yields the probability of the random walk being at the kth site (depicted as a black line in Figure 4), and adding the distributions of Figure 3c,f describes the probability of the quantum random walk being at the kth site (depicted as the blue line in Figure 4).
FIGURE 4. A random walk vs. a quantum random walk after 100 steps starting at the origin.

Note that this system conserves the properties of the Markovian and unitary system; therefore,

\[
\sum_k <[1 1 1 1]|P_k(n)> = \sum_k <[1 1 1 1]|P_k(0)>
\]

(37)

\[
2^n \sum_k |B|P_k(n)>|^2 = \sum_k |B|P_k(0)>|^2
\]

(38)

**Finite cases**

It is possible to embed boundary conditions in the model described in Figure 2, such as a trap:

\[
\text{Trap} = \begin{bmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix}
\]

(39)

or to apply a reflecting point. In the latter case, there are two kinds of reflecting barriers described by switching between the states \(|0>_c, |1>_c\) and \(\neg|0>_c, \neg|1>_c\), presented by

\[
RP1 = \frac{1}{\sqrt{2}} \begin{bmatrix}
0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0
\end{bmatrix}
\]

(40)
or switching between the states $|0\rangle_c, -|1\rangle_c$ and between $-|0\rangle_c, |1\rangle_c$, presented by

$$RP2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$  \hspace{1cm} \text{(41)}$$

The factor $1/\sqrt{2}$ is added, since the amplitude of each of the four coin states are multiplied by $\sqrt{2}$ in each step. Note that the reflecting point matrix is not a stochastic matrix; therefore, in this case, the system is not considered Markovian (the sum of the population will not be conserved); nevertheless, the model preserves its unitary properties.

The y axis operator of a system with $n$ sites bounded by two reflecting points at both ends can be written as

$$Y = (I_n - Z) \otimes A + Z \otimes RP1$$  \hspace{1cm} \text{(42)}$$

where the product is a Kronecker product and the $Z$ matrix is an $n \times n$ matrix, except the two elements at the beginning and the end of the diagonal elements, namely $Z(1,1) = 1; Z(n, n) = 1$.

The x axis operator, meaning the Shift Operator, can be formulated as

$$X = \text{right} \otimes \text{Zerostate} + \text{left} \otimes \text{Onestate}$$  \hspace{1cm} \text{(43)}$$

where

$$\text{Zerostate} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \hspace{1cm} \text{Onestate} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$  \hspace{1cm} \text{(44)}$$

and the right and the left matrix are an $n \times n$ zero matrix, except those that appear above the main diagonal and those that appear beneath the main diagonal, respectively:

$$\text{right} (j, j + 1) = 1, \text{left}(j + 1, j) = 1$$  \hspace{1cm} \text{(45)}$$

for integer $j$ between 1 to $n - 1$ (inclusive)

The dynamics of the system are the scalar product of the two operators $U = XY$ [17].

In this case, the initial condition and the results unfold in such a way that the first four elements describe the four coin states of the first site and the next four elements describe the four coin states of the second site, and so on; therefore, the results must be reshaped to a $4 \times n$ matrix.

In any case, the model is illustrated in Figure 2 above.
Figure 5 presents the results of the probability distribution of a quantum random walk on a finite line of 25 sites after 35 and 65 steps, where each site initializes at \((|0\rangle - |1\rangle)/\sqrt{46}\), except for the boundaries.

![Figure 5](image)

Figure 5. Probability distribution of a quantum random walk on a finite line of 25 sites after 35 and 65 steps, starting at site 2–24 with the state \((|0\rangle - |1\rangle)/\sqrt{46}\).

Note that the system began equally distributed with states \(|0\rangle\) and \(-|1\rangle\), then switched after 35 steps mostly to state \(|0\rangle\), and after 65 steps mostly went back to state \(|1\rangle\).

**Summary**

We presented a two-dimensional model that mapped both a random and a quantum random walk onto the same system. The system conserves the distribution of states for the case of an infinite line, similar to a Markovian process, and by using a proper transformation, yields the amplitude distribution of the two quantum states \(|1\rangle, |0\rangle\), similar to a unitary operator. The model shows that for a large \(n \gg 1\), the amplitudes of each of the four quantum states behave like a Gaussian distribution. The model also enables us to embed different boundary conditions, such as a reflecting point or a trap \(n\), and has the advantage of revealing each of the four coin states without interference, thereby acquiring a deeper understanding of the process.
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[15] In an explicit way by matrix multiplication: $B^TBA - ABA^T = 0$ or note that $B^T = I_4 - J_4$ and both the identity matrix, $I_4$, and the reversal matrix, $J_4$, commute with $A$.
[16] For example: $B(|U1><U1| + |U4><U4|) = |0><0|B$

$B(|U1><U1| + |U4><U4|) = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$

And $|0><0|B = \begin{bmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \end{bmatrix}$ as expected.
The X operator behaves as a unitary operator for the sites located between the reflecting points. However, for the left boundary it conserves only states $|0\rangle_c$ and $-|0\rangle_c$, which are the only ones that “live” there and for the right boundary it conserves only states $|1\rangle_c$ and $-|1\rangle_c$, which are also the only states that “live” there; thus, all of the quantum states are conserved.