Randomizing Quantum Walk

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Abstract

The conditional shift operator in Discrete-time Quantum Walk (DTQW) shifts the position of the walker by unit shift-size depending on the coin state. This scenario can be generalized by choosing the shift-size different from the unit size. The first generalization made in this work is that shift-size is greater than unit size. The second variant is made out of allowing shift-size in positive and negative directions to be not equal to each other. The third type is developed by choosing the shift-size randomly at each step. We have calculated several parameters for these walks. The probability in each case evolves depending on the choice of the shift-sizes. All three walks spread faster than the standard DTQW. In the case of random shift-size, the probability becomes random but still follows some specific pattern. The increase in shift-size, on one hand, preserves the overall behavior but on other hand increases standard deviations $\sigma$ for random choice of shift-size. For all these variants the Shannon entropy remains the same for the initial steps and then becomes small (after a few steps) than the Shannon entropy of standard DTQW. The Shannon entropy for random shift-size is of random behavior. The entanglement entropy remains the same as that of DTQW with small variations at higher steps. For the special case of the walk with a left-side shift-size greater than the right-side shift-size, the entropy reduces drastically after a few initial steps.

Keywords Quantum walk · Position-coin entanglement entropy · Standard deviation · Shannon entropy

1 Introduction

Classical Random Walks (CRWs) are used to model a wide variety of physical phenomena e.g. the Brownian motion \cite{1} and to find out the solution of the Laplace, equation \cite{2}. The quantum mechanical version, known as Quantum Walks (QWs), has been implemented experimentally in nuclear magnetic resonance (NMR) \cite{3}, superconducting circuits \cite{4} and in so many other fields.
There are two main types of QWs, “Continuous-time Quantum Walk (CTQW)” and “Discrete-time Quantum Walk (DTQW)”. The CTQW was introduced in 1998 [5], in such a walk, evolution is ruled by the Schrödinger equation. The DTQW was introduced later in 2001 [6–9] governed by two unitary operators, “coin operator” and “shift operator” that control the evolution of the walker’s state. DTQWs have gained considerable attention due to their ability to model physical systems of diverse nature. The straightforward construction of quantum walks makes them suitable tools for simulating other quantum systems as well [10, 11].

The DTQWs have got vast applications, e.g. they are used to develop fast algorithms for quantum computation tasks [12–18]. They are also used for the simulation of the topological phenomenon in condensed matter systems [19–22]. Many such applications motivated researchers to study the behavior of quantum walks and related aspects [23–29].

In the traditional DTQW, shift-size is usually taken as a unit and fixed for each step. QWs with shift-sizes different than a unit is considered, e.g. in ref. [30], the stability of the recurrence of quantum walk on a line is tested against bias. While the quantum walks with sequential periodic jumps are recently analyzed [31].

Here, we generalize DTQW in three different ways. The first generalization is made by allowing shift-sizes to be greater than the unit. This quantum walk is named as “Discrete-time Un-biased Quantum Walk (DTUBQW)” as shown in Fig. 1 (a). The second generalization is made by choosing the biased shift-size (unequal for left and right shifts) is used for the different outcomes of the coin. We call this walk “Discrete-time Biased Quantum Walk (DTBQW)” as shown in Fig. 1 (b). In the third generalization, we allow the shift-size to be greater than the unit and to be randomly chosen at each step. We call this type of walk “Discrete-time Random Shift-size Quantum Walk (DTRSSQW)” as illustrated in Fig. 1 (c).

We analyze these variants, discussed above, by calculating the Shannon entropy (SE), in our case SE is the amount of uncertainty in the position of the particle, and by calculating Standard Deviation (SD) to check their spread. Another quantity we analyzed is Von Neuman entropy which is coin-position entanglement entropy. Some of the variants show random behavior, to analyze it we have shown average probability distribution of 1000 walks.

This article is organized in the following way. In Section 2, the probability distribution of three variants of DTQW are presented. We introduce the DTUBQW and the corresponding probability distribution in Section 2.1. The second type of walk, DTBQW with an unequal shift-size on right and left is introduced in Section 2.2. In Section 2.3, the third variant of a quantum walk, DTRSSQW with unequal shift-size for different outcomes of the coin is discussed. In Section 3, the standard deviation and in Section 4 the Shannon Entropy of all walks are analyzed. In Section 5 Neuman entropy of the vairants are showed. In Section 6, conclusions of this work are presented.

![Fig. 1](image-url) Diagrams of walker that moves to either left or right depending upon the outcome of a coin a (DTUBQW): equal shift-size that can be different than unit shift-size. b (DTBQW): shift-size can be different for left and right movement. c (DTRSSQW): the shift-size is randomly chosen at each step
### 2 Probability Distribution

In the DTQW, the evolution of a walker is determined by (Coin and Shift) unitary operators. The coin operator acts on internal states and the conditional shift operator acts on the external states of the walker. The shift-size is usually taken to be a unit size. Three generalizations are proposed to this shift-size.

#### 2.1 Discrete-time Un-biased Quantum Walk (DTUBQW)

Here, we generalize the DTQW by selecting shift-size $k$, where $k \in \mathbb{Z}$ that can be different from unity. As in DTQW for a single-qubit walker, the coin (Hilbert) space, $\mathcal{H}_c$, is spanned by $|0\rangle, |1\rangle$. The position (Hilbert) space, $\mathcal{H}_p$, is spanned by $|x\rangle : x \in \mathbb{Z}$. Thus the total Hilbert space of the walker is $\mathcal{H}_p \otimes \mathcal{H}_c$. In DTUBQW, the coin operator is

$$\hat{C} = \cos \theta |0\rangle_c \langle 0| + \sin \theta |1\rangle_c \langle 1|$$

$$+ \sin \theta |0\rangle_c \langle 1| - \cos \theta |1\rangle_c \langle 0| \otimes |x\rangle_p \langle x|$$ (1)

and shift operator is defined as in the following

$$\hat{S} = |0\rangle_c \langle 0| \otimes \sum_x |x - k\rangle_p \langle x|$$

$$+ |1\rangle_c \langle 1| \otimes \sum_x |x + k\rangle_p \langle x|$$ (2)

The walk operator, $\hat{U} = \hat{S} \hat{C}$, acts on the initial state ($\phi_{int}$) of the walker and leads it to the final state, i.e.

$$|\phi_T\rangle = \hat{U}^T |\phi_{int}\rangle$$ (3)

here, $T$ is the number of steps. In Fig. 2(a) we have shown the probability distribution of DTUBQW for rotation angle $\theta = \pi/4$. The probability depends upon the rotation angle as well as on shift-size. The initial state $\phi_{int}$ is defined as

$$|\phi_{int}\rangle = (a(0,0)|0\rangle_C + b(0,0)|1\rangle_C) \otimes |0\rangle_p$$ (4)

where

$$a(x = 0, T = 0) = \frac{1}{\sqrt{2}}, b(x = 0, T = 0) = -\frac{i}{\sqrt{2}}$$

This fact can be useful for constructing algorithms that search for particular data at already determined sites. Figure 2(a) shows the probability for two shift-sizes i.e. 1 and 3, we see that for larger step size walker can reach farthermost positions in the same number of steps. We get the peaked probability, the relation between shift-size($k$), peak number ($N_{peak}$), and peak position ($X_{peak}$) has been found to obey a specific formula.

$$X_{peak} = 2kN_{peak}$$ (5)

This fact can be useful for constructing algorithms that search for particular data at already determined sites.
2.2 Discrete-time Biased Quantum Walk (DTBQW)

In this sub-section, we analyze the biased quantum walk by selecting the un-equal shift-size to right and left

$$\hat{S} = |0\rangle_c |0\rangle \otimes \sum_x |x - k_L\rangle_p \langle x|$$

$$+ |1\rangle_c |1\rangle \otimes \sum_x |x + k_R\rangle_p \langle x|$$

(6)

where $k_R$ is shift-size to the right and $k_L$ is to the left, so $k_L \neq k_R$. Figure 2(b) depicts the probability distribution of a DTBQW for rotation angles ($\theta = \pi/4$). The probability distribution is asymmetric when we exchange left and right step-sizes. The probability depends upon the size of the shift as well the difference between the Left Shift-size (LSS) and Right Shift-size (RSS).

This walk offers a large number of possibilities as shift-size can be selected differently for left and right shifts.

2.3 Discrete-time Random Shift-size Quantum Walk (DTRSSQW)

The quantum walk is generated by selecting shift-size randomly at each step. The conditional shift operator is modified to the following form
\[ \hat{S}_{\text{rand}} = |0\rangle_C \langle 0| \otimes \sum_x |x - k_j\rangle_P \langle x| + |1\rangle_C \langle 1| \otimes \sum_x |x + k_j\rangle_P \langle x| \] (7)

The integer “\(k_j\)” is randomly chosen from interval [1, n] at each step where n is another integer. In Fig. 2(c) we have shown the probability distribution for angle \(\theta = \pi/4\), the shift-size is chosen randomly from the interval [1, 3] and the walker has shifted accordingly. At each position, the shift-size of the next step is again chosen randomly from the same interval. We have shown two runs to illustrate that in each run the probability distribution changes randomly and the quantum walk is partially randomized. Higher probabilities peaks are found in every run, around the center, and at the ends of the probability distribution. Now to find out the behavior of such a walk the average probability distribution for 1000 walks is obtained. The evolution after 60 steps is plotted in Fig. 2(d). It shows a hybrid kind of behavior with the central peak around zero position is like Gaussian distribution of classical random walk and two smaller peaks at the ends giving quantum behavior.

3 Standard Deviation

In this section, \(\sigma_T\) for all the three types of walks for rotation angle \(\theta = \pi/4\) are presented. The mean \(\mu\) can be calculated from \(P(x)\) i.e.

\[ \mu_T = \sum [x \cdot P_T(x)] \] (8)

while the variance in terms of \(\mu\),

\[ \sigma^2_T = [\sum x^2 \cdot P_T(x)] - \mu^2_T \] (9)

which implies that

\[ \sigma_T = \sqrt{[\sum x^2 \cdot P_T(x)] - \mu^2_T} \] (10)

It is observed that generally, they all spread faster than the standard DTQW except the biased walk when the right shift-size is large. In Fig. 3(a) the \(\sigma_T\) of DTQW with unit shift-size, DTUBQW with \(k = 3\), DTBQW with \(K_R = 1\) and \(K_L = 3\) and DTBQW with \(K_R = 3\) and \(K_L = 1\) are shown. In Fig. 3(b) the \(\sigma_T\) of DTQW with unit shift-size and two runs of DTRSSQW with \(j\) from the interval [1,3] is depicted. It can be seen that the \(\sigma_T\) of DTRSSQW is random but the general trend remains the same for each run.

The deviation behaviors for DTUBQW and DTBQW resemble sawtooth having tooth size getting bigger with shift-size. The number of jumps as well as \(\sigma_T\) increases with shift-size. The \(\sigma_T\) of DTUBQW with \(K_R = 1\) and \(K_L = 3\) and DTBQW behave similarly and higher than the \(\sigma_T\) of DTQW. The \(\sigma_T\) of DTUBQW with \(K_R = 3\) and \(K_L = 1\) is lesser then the \(\sigma\) of DTQW.

4 Shannon Entropy

In 1948, the idea of Shannon Entropy (SE) was presented by Claude Shannon [32]. The SE was introduced in QWs for various kinds of coins. For each step of QW, the Shannon
entropy is determined from the probability of positions and internal degrees of freedom occupied by a state. SE can be calculated by tracking probability \( P_T(x) \), where \( T \) is the number of steps while \( x \) is the position, i.e.

\[
S_T = - \sum_{-T}^{T} P_T(x) \log_2 P_T(x).
\]  

(11)

The evolution in SE in all the variants of QWs are calculated. In Fig. 4(a), we have shown the SE for DTQW with unit shift-size, DTUBQW with \( K_L = 3, K_R = 1 \) and \( K_L = 1, K_R = 3 \), and with \( K_L = 3, K_R = 1 \). While in Fig. 4(b) SE for DTQW with unit shift-size and DTRSSQW with \( j \) interval \([1, 3]\) are depicted for two runs.

![Fig. 3](image1)

**Fig. 3**  
(a) Standard Deviation of DTQW with unit shift-size (Black solid line), DTUBQW with shift-size=3 (Black Dotted line), DTBQW with \( K_L = 1, K_R = 3 \) (Blue Dashed line) and \( K_L = 3, K_R = 1 \) (Red Dot-Dashed),  
(b) Standard Deviation of DTQW with unit shift-size (Black solid line), DTRSSQW with \( j \) interval \([1, 3]\) for two runs (Red, Blue line)

![Fig. 4](image2)

**Fig. 4**  
(a) Shannon Entropy (SE) of DTQW with unit shift-size (Blue line), DTUBQW with shift-size=3 (Black Dotted), DTBQW with \( K_L = 3 \) and \( K_R = 1 \) (Red Dashed line) and DTBQW with \( K_L = 1 \) and \( K_R = 3 \) (Green Dashed line),  
(b) SEs of DTQW with unit shift-size(Blue line), DTRSSQW with \( j \) interval \([1, 3]\) (for two runs (Blue Dashed, Red Dashed))
5 Entanglement Entropy between Position and Coin

The Entanglement Entropy between the position of the particle and the coin state (PCEE) follows the standard definition of von Neumann Entropy for a bipartite pure state \[33\] and it is calculated as

\[ S_N = -tr(\rho_c \ln(\rho_c)). \] (12)

Here, \( \rho_c \) is reduced operator and \( \rho_c = tr(\rho) \), \( \rho \) is a density operator i.e. \( \rho = |\Psi\rangle\langle\Psi| \). Note that, in general \( tr(\rho^2) < 1 \). Step-dependent density operator for our walker state can be expressed as

\[
\rho(T) = |\phi(T)\rangle\langle\phi(T)|
\] (13)

\[
= \sum_x (a(x, T)|0\rangle + b(x, T)|1\rangle)(a(x, T)^*|0\rangle
+b(x, T)^*|1\rangle \otimes |x\rangle\langle x|
\] (14)

The reduced density matrix is

\[
\rho_c(T) = \sum_x \langle x|\rho(T)|x\rangle.
\]

\[
= \sum_x \begin{bmatrix}
|a(x, T)|^2 & a(x, T)b(x, T)^* \\
a(x, T)^*b(x, T) & |b(x, T)|^2
\end{bmatrix}
\] (15)

By defining

\[
\beta(T) = \sum_x |b(x, T)|^2,
\]

\[
\alpha(T) = \sum_x |a(x, T)|^2,
\]

\[
\gamma(T) = \sum_x a(x, T) \cdot b(x, T)^*
\] (16)

reduced density matrix becomes

\[
= \begin{bmatrix}
\alpha(T) & \gamma(T) \\
\gamma(T)^* & \beta(T)
\end{bmatrix}
\] (17)

with eigenvalues

\[
\Lambda_{\pm}(T) = \frac{1}{2} \pm \frac{1}{2} \sqrt{1 - 4(\alpha(T)\beta(T) + |\gamma(T)|^2)}
\] (18)

Consequently, the PCEE is explicitly given by

\[
S_N(T) = -(\Lambda_+(T) \log_2(\Lambda_+(T)) + \Lambda_-(T) \log_2(\Lambda_-(T))).
\] (19)

In Fig. 5(a), \( S_N(T) \) of DTQW with unit shift-size, DTUBQW with \( k = 3 \), DTBQW with \( K_R = 1 \) and \( K_L = 3 \), and with \( K_R = 3 \) and \( K_L = 1 \) are shown. While in Fig. 5(b)
Fig. 5  a Position Coin Entanglement Entropy (PCEE) of DTQW with unit shift-size (Black Solid line), DTUBQW with shift-size=3 (Red Dotted Line), DTBQW with $K_L = 3$ and $K_R = 1$ (Blue Dashed Dotted line), DTBQW with $K_R = 1$ and $K_L = 3$ (Pink Dashed line), b Position Coin Entanglement Entropy (PCEE) of DTQW with unit shift-size (Black Solid line), DTRSSQW with $j$ chosen from the interval $[1, 3]$ for two runs (Blue Dotted, Red Dashed)

$S_N(T)$ of DTQW with unit shift-size and for two runs of DTRSSQW with $j \in \{1, 2, 3\}$ are presented. PCEE of DTQW and DTUBQW are same for initial 20 steps then value of PCEE becomes larger than DTQW’s. While PCEE of DTBQW with $K_R = 1$ and $K_L = 3$ are similar as DTQW’s. While PCEE of DTBQW with $K_R = 3$ and $K_L = 1$ is similar with DTQW for initial steps, similarity reduces with increase in $K_R$, then there PCEE value becomes smaller i.e. $\sim 0.2$. The PCEE for random shift-size is larger and random.

6 Conclusion

Three different types of quantum walks are introduced in this work. The first walk is called DTUBQW, it is built using a shift-size larger than DTQW. The probability spreads away faster as compared to DTQW. Its standard deviation is larger than the standard DTQW and, shows the sawtooth behavior. Initially, the SE of this walk increases faster but becomes slower after a few steps. Their PCEE is similar to DTQW for some initial steps, but the PCEE becomes large as the number of steps increase. The second type of walk is called DTBQW, having asymmetric shift-sizes for the left and right sides. It gives different probability distributions for the exchange of shift-sizes from left to right. The walker probability in direction of a bigger shift reaches farther away from the center. The SD of DTBQW depends upon the choice of the shift-size in the right or left directions and is sawtooth-like. SE is smaller than SE of DTQW in both cases independent of which side has a bigger shift-size. On the other hand, when shift-size in the left direction is bigger, PCEE is similar to DTQW but when the shift-size in the right direction is larger, PCEE suddenly starts to reduce after a few initial steps. The third walk is called DTRSSQW, having shift-size randomly chosen from an interval at each step. It gives random probability distribution with the probability peaks at the center and on both ends. The SD of this variant is random and greater than that of DTQW. The SE is larger than DTQW and has high uncertainty than the other two variants. The PCEE for DTRSSQW is random and larger than DTQW.

This study of one-dimensional quantum walks can be generalized to quantum walks with entangled coins and for higher dimensions with single and multi-particles. It can also
be generalized to more than two entangled qubits. It will be interesting to use different coins for these walks. We will leave these matters for future work.

 Declarations

 Conflict of Interests  The authors have no conflicts to disclose.

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