Average position in quantum walks with a U(2) coin

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We investigated discrete-time quantum walks with an arbitrary unitary coin. Here we discover that the average position \( \langle x \rangle = \max\langle x \rangle \sin(\alpha + \gamma) \), while the initial state is \( 1/\sqrt{2} | 0L \rangle + i | 0R \rangle \). We prove the result and get some symmetry properties of quantum walks with a U(2) coin with \( | 0L \rangle \) and \( | 0R \rangle \) as the initial state.

I. INTRODUCTION

Quantum walks (QWs) were first introduced in 1993 \(^1\) as a generalization of classical random walks. According to the time evolution, QWs can be divided into discrete-time and continuous-time \(^2\) QWs. Recently, both continuous-time \(^3\) and discrete-time \(^4\) QWs are found to be universal for quantum computation. A number of quantum algorithms based on QWs have already been proposed in \(^3\)–\(^10\). In addition, QWs in graph \(^11\), on a line with a moving boundary \(^12\), with multiple coins \(^13\) or decoherent coins \(^14\) have been discussed also.

QWs using a SU(2) coin was introduced by Chan-drakshar, et al. \(^15\), where the standard deviation and measurement entropy properties were discussed. Here we discuss the symmetry and average position properties for the QWs with a U(2) coin.

II. HADAMARD QUANTUM WALKS

In this paper, we always discuss within the discrete-time QWs. The total Hilbert space for QWs is given by \( \mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C \), where \( \mathcal{H}_P \) is spanned by the orthonormal states \( \{|x\} \) and \( \mathcal{H}_C \) is the two-dimensional coin space spanned by two orthonormal states \( |L\rangle \) and \( |R\rangle \).

Each step of the QWs can be split into two operations: the evolution of coin state and the particle movement according to the coin state.

Here the Hadamard walk, the coin is evolved by applying the Hadamard operation:

\[
H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},
\]

the particle movement operator is given by

\[
S = e^{ip\sigma_z} = \sum_x S_x,
\]

where \( p \) is the momentum operator, \( \sigma_z \) is the Pauli-\( z \) operator.

III. GENERALIZED DISCRETE TIME QUANTUM WALKS

An arbitrary one-qubit unitary operation can be written as a U(2) matrix:

\[
U_{\alpha,\beta,\gamma,\theta} = e^{i\theta} \begin{pmatrix} e^{i\alpha} \cos \beta, & -e^{-i\gamma} \sin \beta \\ e^{i\gamma} \sin \beta, & e^{-i\alpha} \cos \beta \end{pmatrix}
\]

For example, the Hadamard operator can be described in the form \( H = U_{\pi/4,\pi/2,0,\pi/4} \). By replacing the Hadamard coin with an operator \( U_{\alpha,\beta,\gamma,\theta} \), we can obtain the generalized QWs \(^15\), which can be written as

\[
|\Psi_t\rangle = [S(I_P \otimes H_C)]^t |\Psi_0\rangle
\]

Lemma 1. The quantum walks have the same probability distribution with a U(2) coin or a SU(2) coin which has the same parameters \( \alpha, \beta \) and \( \gamma \) in the U(2) matrix.

Proof. The SU(2) coin operator can be written as

\[
U_{\alpha,\beta,\gamma}^S = \begin{pmatrix} e^{i\alpha} \cos \beta, & -e^{-i\gamma} \sin \beta \\ e^{i\gamma} \sin \beta, & e^{-i\alpha} \cos \beta \end{pmatrix}
\]

Then the U(2) coin \( U_{\alpha,\beta,\gamma,\theta} = e^{i\theta} U_{\alpha,\beta,\gamma}^S \). The probability distribution for QWs with a U(2) coin after \( t \) steps:

\[
P(x,t) = |\langle x|\Psi_t\rangle|^2 = |e^{i\theta} \langle x| \Psi_t^S \rangle|^2
\]

\[
\equiv P^S(x,t),
\]

where \( |\Psi_t^S\rangle \) and \( P^S(x,t) \) are the state and the probability distribution for QWs with a SU(2) coin after \( t \) steps respectively.

\[\square\]
Corollary 2. The average position is the same in quantum walks with a $U(2)$ coin and a $SU(2)$ coin if the two coins have the same parameters $\alpha$, $\beta$ and $\gamma$ with the $U(2)$ coin.

Proof. From Lemma 1 we can know that the average position for a $U(2)$ coin $(x) = \sum_x xP(x,t) = \sum_x xP^S(x,t) \equiv \langle x \rangle^S$, where $\langle x \rangle^S$ is the average position for QWs with a $SU(2)$ coin.

With corollary 2 if we want to know the average position property in QWs with an arbitrary unitary operator, we only need to study the quantum walk with a $SU(2)$ coin instead, for the rest part of this paper, we always use the $SU(2)$ coin as denoted in Eq. 4.

Following the analysis in Ref. [16], the state after $t$ steps QWs with a $SU(2)$ coin

$$\Psi_t = [S(I_P \otimes U^S_{\alpha,\beta,\gamma})]_t \Psi_0,$$

the spatial Fourier transformation for of the wave function $\Psi(x,t)$ over $Z$ is given by

$$\tilde{\Psi}(k,t) = \sum_{x=-\infty}^{\infty} \Psi(x,t)e^{ikx},$$

where $k \in [-\pi, \pi]$. We can know

$$\tilde{\Psi}(k,t) = (M_k)^t \tilde{\Psi}(k,0),$$

where

$$M_k = e^{ik}M_+ + e^{-ik}M_- = (e^{-i(k-\alpha)} \cos \beta, -e^{-i(k+\gamma)} \sin \beta, e^{i(k-\alpha)} \cos \beta).$$

The eigenvalues of $M_k$ is

$$\lambda_a = e^{-i\omega},$$

$$\lambda_b = e^{i\omega},$$

where $\cos \omega = \cos(k-\alpha) \cos \beta$. And the eigenstates

$$\begin{align*}
\tilde{\Psi}_k^a &= \frac{1}{c_k} \begin{pmatrix} P_k \\ Q_k^a \end{pmatrix}, \\
\tilde{\Psi}_k^b &= \frac{1}{c_k} \begin{pmatrix} P_k \\ Q_k^b \end{pmatrix},
\end{align*}$$

where

$$\begin{align*}
P_k &= -e^{-i(k+\gamma)} \sin \beta, \\
Q_k^a &= -i \sin \omega_k + i \sin(k-\alpha) \cos \beta, \\
Q_k^b &= i \sin \omega_k + i \sin(k-\alpha) \cos \beta.
\end{align*}$$

IV. THE AVERAGE POSITION IN QUANTUM WALKS

Fig. 1 and Fig. 2 show the average position after $t = 100$ steps QWs with a $SU(2)$ coin in the case of $\beta = \pi/6$, while the initial state is $\ket{1/L} + i \ket{0R}$). From Fig. 1 we can know that $\langle x \rangle$ only depends on the sum of $\alpha$ and $\gamma$. Fig. 2 shows that the actual $\langle x \rangle$ exactly match the function of $f(\phi) = \max(\langle x \rangle) \sin(\phi)$, then we conject that $\langle x \rangle = G(\beta, t) \sin(\alpha + \gamma)$. 

$$C_k^b = \sqrt{P_k^* P_k + (Q_k^*)^* Q_k^b}$$

$$= \sqrt{2(\sin^2 \omega_k - \cos \beta \sin(k-\alpha) \sin \omega_k)}.$$
V. PROOF IN MATHEMATICS

Theorem 3. The probability distribution for quantum walks with a SU(2) coin is independent of the parameter \( \alpha \) and \( \gamma \), when the initial state is \( |0L \rangle \) or \( |0R \rangle \). i.e.

\[
\begin{align*}
P_{|0L\rangle}(\alpha, \beta, \gamma, x, t) &= P_{|0L\rangle}(\beta, x, t) \\
P_{|0R\rangle}(\alpha, \beta, \gamma, x, t) &= P_{|0R\rangle}(\beta, x, t) ,
\end{align*}
\]  

(17)

for any \( \alpha \) and \( \gamma \).

Proof. If the initial state \( |\Psi_0\rangle = |0L\rangle \), then \( \tilde{\Psi}(k, 0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \). The probability of \( |x\rangle \) :

\[
P_{|0L\rangle}(\alpha, \beta, \gamma, x, t) = P_L(\alpha, \beta, \gamma, x, t) + P_R(\alpha, \beta, \gamma, x, t) \\
= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} g_L(k_1, k_2, \alpha, \beta, \gamma, x, t) dk_1 dk_2 + \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} g_R(k_1, k_2, \alpha, \beta, \gamma, x, t) dk_1 dk_2 ,
\]

(18)

where \( g_j(k_1, k_2, \alpha, \beta, \gamma, x, t) = \tilde{\psi}_j^*(k_1, t) \tilde{\psi}_j(k_2, t) e^{i(k_1-k_2)x} \), \( j \in \{L, R\} \). If we set \( h = k + \alpha \), then we can know \( g_j(h_1, h_2, \alpha, \beta, \gamma, x, t) = g_j(h_1 + 2\pi, h_2, \beta, \gamma, x, t) \), and \( g_j(h_1, h_2, \beta, \gamma, x, t) = g_j(h_1 + 2\pi, h_2, \beta, \gamma, x, t) \).

\[
P_j(\alpha, \beta, \gamma, x, t) = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} g_j(h_1, h_2, \beta, x, t) dh_1 dh_2 \\
= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} g_j(h_1, h_2, \beta, x, t) dh_1 dh_2 \\
= P_j(\beta, x, t) .
\]

(19)

Further more we can know \( P_{|0L\rangle}(\alpha, \beta, \gamma, x, t) = P_{|0L\rangle}(\beta, x, t) \). In the same way, we can also get \( P_{|0R\rangle}(\alpha, \beta, \gamma, x, t) = P_{|0R\rangle}(\beta, x, t) \).

\[
\begin{align*}
\left\{ \begin{array}{l}
P^L(x) = |m|^2 P^L_{|0L\rangle} + |n|^2 P^L_{|0R\rangle} - (e^{-i(\alpha+\gamma)}m^*n + e^{i(\alpha+\gamma)}mn^*)G^L(\beta, x, t) \\
P^R(x) = |m|^2 P^R_{|0L\rangle} + |n|^2 P^R_{|0R\rangle} - (e^{-i(\alpha+\gamma)}m^*n + e^{i(\alpha+\gamma)}mn^*)G^R(\beta, x, t)
\end{array} \right. ,
\end{align*}
\]

(23)

where \( G^L \) and \( G^R \) are indepent of \( \alpha \) and \( \gamma \).

\[
P^L_{|0L\rangle+n|0R\rangle}(x) = \frac{1}{4\pi^2} \int \int \tilde{\psi}_L^*(k_1, t) \tilde{\psi}_L(k_2, t) e^{i(k_1-k_2)x} dk_1 dk_2 \\
= |m|^2 P^L_{|0L\rangle}(\beta, x, t) + |n|^2 P^L_{|0R\rangle}(\beta, x, t) \\
(\sum_{i=1}^{4} G_i + e^{i(\alpha+\gamma)}mn^* \sum_{i=1}^{4} G_i) ,
\]

(24)

Proof. The probability at state \( |xL\rangle \) after \( t \) steps:

\[
\begin{align*}
\left\{ \begin{array}{l}
\Psi^L_{|0L\rangle}(x, t) + \Psi^L_{|0R\rangle}(-x, t) = \Psi^L_{|0L\rangle}(x, t) \\
\Psi^R_{|0L\rangle}(x, t) - \Psi^R_{|0R\rangle}(-x, t) = \Psi^R_{|0L\rangle}(x, t) ,
\end{array} \right.
\end{align*}
\]

(20)

where \( \Psi^m(x, t) \) denotes the coefficient of the \( |x \rangle \) state after \( t \) steps quantum walk with the initial state \( |n \rangle \).

Proof.

\[
\begin{align*}
\Psi^L_{|0L\rangle}(x, t) &\pm \Psi^L_{|0R\rangle}(-x, t) \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} \tilde{\psi}^L_{|0L\rangle}(k, t)e^{-ikx} dk + \frac{1}{2\pi} \int_{-\pi}^{\pi} \tilde{\psi}^L_{|0R\rangle}(k, t)e^{ikx} dk \\
&= \frac{1}{2\pi} \int_{-\pi}^{\pi} Q_k^\alpha [P_k e^{-ikx} \mp P_k e^{ikx}] [e^{-i\omega_k t} - e^{i\omega_k t}] dk ,
\end{align*}
\]

(22)

As \( Q_k^\alpha \in \mathbb{R} \), we can know \( \Psi^L_{|0L\rangle}(x, t) + \Psi^L_{|0R\rangle}(-x, t) \in \mathbb{R} \), and \( \Psi^L_{|0L\rangle}(x, t) - \Psi^L_{|0R\rangle}(-x, t) \in \mathbb{R} \). Similarly, we can get Eq. (21).

Corollary 5. The symmetry property of distribution between quantum walks with a U(2) coin in initial state \( |0L \rangle \) and \( |0R \rangle \): For an arbitrary \( t \), \( P^R_{|0L\rangle}(\beta, x, t) = P^L_{|0R\rangle}(\beta, x, t), P^L_{|0L\rangle}(\beta, x, t) = P^R_{|0R\rangle}(\beta, x, t) \).

Proof. We set \( \Psi^R_{|0L\rangle}(x) = C + Di \), where \( C, D \in \mathbb{R} \). From Theorem 4 we can know \( \Psi^L_{|0R\rangle}(-x) = C - Di \), then we can know \( P^R_{|0L\rangle}(\beta, x, t) = P^L_{|0R\rangle}(\beta, x, t) \). Similarly, we can also get \( P^R_{|0L\rangle}(\beta, x, t) = P^L_{|0R\rangle}(\beta, x, t) \).

Theorem 6. If the initial state \( |\Psi_0\rangle = m |0L \rangle + n |0R \rangle \), where \( |m|^2 + |n|^2 = 1 \), the probability at state \( |xL \rangle \) or \( |xR \rangle \) after \( t \) steps quantum walk is

\[
\begin{align*}
P^L(x) = |m|^2 P^L_{|0L\rangle} + |n|^2 P^L_{|0R\rangle} - (e^{-i(\alpha+\gamma)}m^*n + e^{i(\alpha+\gamma)}mn^*)G^L(\beta, x, t) \\
P^R(x) = |m|^2 P^R_{|0L\rangle} + |n|^2 P^R_{|0R\rangle} - (e^{-i(\alpha+\gamma)}m^*n + e^{i(\alpha+\gamma)}mn^*)G^R(\beta, x, t)
\end{align*}
\]
where
\[
G_1(\beta, x, t) = \frac{1}{4\pi^2} \int \int e^{i(\omega_{h_1} - \omega_{h_2})t} \frac{1}{(\omega_{h_1} - \omega_{h_2})^2} e^{i(h_1 - h_2)x} e^{-ih_1}(Q^b_{h_2})^* dh_1 dh_2
\]
\[
= \frac{1}{4\pi^2} \int \int \frac{Q^b_{h_2} \sin^3 \beta}{(\omega_{h_1} - \omega_{h_2})^2} \sin((\omega_{h_1} - \omega_{h_2}) + (h_1 - h_2) + (h_1 - h_2)x - h_1)|dh_1 dh_2| \in R.
\] (25)

As the same of \(G_1(\beta, x, t)\), we can know \(G_i(\beta, x, t) \in R\), where \(i \in \{1, 2, 3, 4\}\). So Eq. (24) can be written as
\[
P^L(x) = |m|^2 P^L_{|0L\rangle} + |n|^2 P^L_{|0R\rangle} - (e^{-i(\alpha+\gamma)}m^* n + e^{i(\alpha+\gamma)}mn^*)G^L(\beta, x, t),
\] (26)

where \(G^L(\beta, x, t) = \sum_{i=1}^4 G_i\). In the same way as \(P^L(x)\), we can get \(P^R(x)\) in Eq. (23).

**Theorem 7.** If the initial state \(|\Psi_0\rangle = 1/\sqrt{2}(|0L\rangle + i |0R\rangle)\). The average position after \(t\) steps quantum walk:
\[
\langle x \rangle = G(\beta, t)\sin(\alpha + \gamma), \text{ where } G(\beta, t) \text{ only depends on } \beta \text{ and } t.
\]

**Proof.** From Corollary 5, we can know
\[
\sum_{x=-t}^t x[P^R_{|0L\rangle}(\beta, x, t) + P^L_{|0L\rangle}(\beta, x, t)] = 0
\]
and
\[
\sum_{x=-t}^t x[P^L_{|0L\rangle}(\beta, x, t) + P^R_{|0L\rangle}(\beta, x, t)] = 0.
\] (27)

Using Eq. (27) and Theorem 6, we can know
\[
\langle x \rangle = \sum_{x=-t}^t x(P^L(\alpha, \beta, \gamma, x, t) + P^R(\alpha, \beta, \gamma, x, t))
\]
\[
= G(\beta, t)\sin(\alpha + \gamma),
\] (28)
where \(G(\beta, t) = -\sum_{x=-t}^t x[G^L(\beta, x, t) + G^R(\beta, x, t)]\) only depends on \(\beta \) and \(t\), regardless of \(\alpha \) or \(\gamma\). 

**VI. CONCLUSIONS**

In this paper, we discussed the properties of the average position in QWs with an arbitrary unitary coin. With a SU(2) coin, if the initial state is \(|0L\rangle \) or \(|0R\rangle\), the probability distribution is independent on \(\alpha \) and \(\gamma\). Some symmetry properties between different initial states \(|0L\rangle \) and \(|0R\rangle\) were proved, we get that \(P^R_{|0L\rangle}(\beta, x, t) = P^L_{|0R\rangle}(\beta, -x, t)\) and \(P^L_{|0L\rangle}(\beta, x, t) = P^R_{|0R\rangle}(\beta, -x, t)\). If the initial state \(|\Psi_0\rangle = 1/\sqrt{2}(|0L\rangle + i |0R\rangle)\), we can know the average \(\langle x \rangle = G(\beta, t)\sin(\alpha + \gamma)\), so if we replace the Hadamard operator with an arbitrary unitary operator, the average position is always not equal to 0, unless \(\alpha + \beta = n\pi, n \in \mathbb{Z}\).

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