Distribution of chirality in the quantum walk: Markov process and entanglement

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The asymptotic behavior of the quantum walk on the line is investigated, focusing on the probability distribution of chirality independently of position. It is shown analytically that this distribution has a longtime limit that is stationary and depends on the initial conditions. This result is unexpected in the context of the unitary evolution of the quantum walk as it is usually linked to a Markovian process. The asymptotic value of the entanglement between the coin and the position is determined by the chirality distribution. For given asymptotic values of both the entanglement and the chirality distribution, it is possible to find the corresponding initial conditions within a particular class of spatially extended Gaussian distributions.

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I. INTRODUCTION

The quantum walk (QW) on the line [1] is a natural generalization of the classical random walk in the frame of quantum computation and quantum-information processing and is receiving much attention [2–4]. It has the property of spreading over the line linearly in time, as characterized by the standard deviation $\sigma(t) \sim t$, while its classical analog spreads as $\sigma(t) \sim t^{1/2}$. This property, as well as quantum parallelism and quantum entanglement, could be used to increase the efficiency of quantum algorithms. As an example, the QW has been used as the basis for optimal quantum search algorithms [5,6] on several topologies. On the other hand, some experimental implementations of the QW have been reported [7], and others have been proposed by a number of authors [8].

The concept of entanglement is an important element in the development of quantum communication, quantum cryptography, and quantum computation. In this context, several authors have studied the QW subjected to different types of coin operators and/or sources of decoherence to analyze the longtime entanglement between the coin and the position and its relation with the initial conditions [9,10]. Carneiro *et al.* [11] investigated entanglement between the coin and the position, calculating the entropy of the reduced density matrix of the coin. The relation between asymptotic entanglement and nonlocal initial conditions (in the one- and two-dimensional QW) is treated in Refs. [12–17]. References [18–20] analyze the effect of entanglement on the initial coin state, which is measured by the mean value of the walk, and the relation between the entanglement and the symmetry of the probability distribution. In Ref. [21], the relation between entanglement and decoherence is studied numerically. Refereneces [22,23] propose to use the QW as a tool for quantum algorithm development and as an entanglement generator, potentially useful for testing quantum hardware.

In previous works [11–23], QW evolution was studied using the amplitude of probability to evaluate the dynamics. In this work, I introduce a new probability distribution, the global chirality distribution (GCD), that is the distribution of chirality independently of the walker's position. I show that the GCD has an asymptotic limit, and I connect this limit with the entropy of entanglement between the coin and the position. The asymptotic behavior of GCD is an unexpected result because, owing to the unitary evolution, the QW does not converge to any stationary state, as would be the case, for example, with a Markov chain. In order to show these results, I rewrite the QW evolution equation as the sum of two different terms, one responsible for the classical diffusion and the other for the quantum coherence [24]. As we shall see, the first term obeys a master equation, as is typical of Markovian processes, while the second term includes the interference needed to preserve the unitary character of the quantum evolution. This approach provides a more intuitive framework which proves useful for analyzing the behavior of quantum systems with decoherence. It allows us to study the quantum evolution together with the associated classical Markovian process at all times and, in particular, the asymptotic behavior of the GCD.

The article is organized as follows. In the next section, I develop the standard QW model; in the third section, I build the master equation for the GCD; in the fourth section, I present the asymptotic solution for the QW; in the fifth section, the entropy of entanglement is connected with the GCD; and in the last section, I draw conclusions.

II. THE STANDARD QW

The QW on the line corresponds to a one-dimensional evolution of a quantum system in a direction which depends on an additional degree of freedom, the chirality, with two possible states: "left" $|L\rangle$ or "right" $|R\rangle$. The global Hilbert space of the system is the tensor product $H_s \otimes H_c$, where H_s is the Hilbert space associated with the motion on the line and H_c is the chirality Hilbert space. Let us call T_- (T_+) the operators in H_s that move the walker one site to the left (right) and $|L\rangle\langle L|$ and $|R\rangle\langle R|$ the chirality projector operators in H_c. We consider the unitary transformations

$$U(\theta) = \{T_- \otimes |L\rangle\langle L| + T_+ \otimes |R\rangle\langle R|\} \circ \{I \otimes K(\theta)\}, \quad (1)$$

where $K(\theta) = \sigma_z \cos\theta + i\sigma_x \sin\theta$, I is the identity operator in H_s, and σ_z and σ_x are Pauli matrices acting in H_c. The unitary operator $U(\theta)$ evolves the state in one time step as

$$|\Psi(t+1)\rangle = U(\theta)|\Psi(t)\rangle. \quad (2)$$

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The wave vector can be expressed as the spinor

$$|\Psi(t)\rangle = \sum_{k=-\infty}^{\infty} \begin{bmatrix} a_k(t) \\ b_k(t) \end{bmatrix} |k\rangle, \tag{3}$$

where the upper (lower) component is associated with the left (right) chirality. Substituting Eqs. (3) and (1) into Eq. (2) and projecting over the position vector $|k\rangle$, the unitary evolution is written as the map

$$\begin{aligned} a_k(t+1) &= a_{k+1}(t)\cos\theta + b_{k+1}(t)\sin\theta, \\ b_k(t+1) &= a_{k-1}(t)\sin\theta - b_{k-1}(t)\cos\theta. \end{aligned} \tag{4}$$

III. UNITARY EVOLUTION AND MASTER EQUATION FOR THE CHIRALITY

In Refs. [24,25], it is shown how a unitary quantum mechanical evolution can be separated into Markovian and interference terms. Here we use this method to recognize a master equation in chirality starting from the original map Eqs. (4). First I define the left and right distributions of position as $P_{kL}(t) = |a_k(t)|^2$ and $P_{kR}(t) \equiv |b_k(t)|^2$, respectively. Combining the two components of Eqs. (4), and after some simple algebra, we obtain

$$\begin{aligned} P_{k,L}(t+1) &= P_{k+1,L}(t)\cos^2\theta + P_{k+1,R}(t)\sin^2\theta \\ &\quad + \beta_{k+1}(t)\sin 2\theta, \\ P_{k,R}(t+1) &= P_{k-1,L}(t)\sin^2\theta + P_{k-1,R}(t)\cos^2\theta \\ &\quad - \beta_{k-1}(t)\sin 2\theta, \end{aligned} \tag{5}$$

where $\beta_k \equiv \mathrm{Re}[a_k(t)b_k^*(t)]$ is an interference term, with $\mathrm{Re}(z)$ indicating the real part of z. Of course, the probability distribution for the position is $P_k(t) = P_{kL}(t) + P_{kR}(t)$. I define the global left and right chirality probabilities as

$$\begin{aligned} P_L(t) &\equiv \sum_{k=-\infty}^{\infty} P_{kL}(t) = \sum_{k=-\infty}^{\infty} |a_k(t)|^2 , \\ P_R(t) &\equiv \sum_{k=-\infty}^{\infty} P_{kR}(t) = \sum_{k=-\infty}^{\infty} |b_k(t)|^2 , \end{aligned} \tag{6}$$

with $P_R(t) + P_L(t) = 1$, and the GCD is defined as the distribution formed by the couple

$$\begin{bmatrix} P_L(t) \\ P_R(t) \end{bmatrix}.$$

Using the definition Eq. (6) in Eq. (5), we have

$$\begin{aligned} \begin{bmatrix} P_L(t+1) \\ P_R(t+1) \end{bmatrix} &= \begin{pmatrix} \cos^2\theta & \sin^2\theta \\ \sin^2\theta & \cos^2\theta \end{pmatrix} \begin{bmatrix} P_L(t) \\ P_R(t) \end{bmatrix} \\ &\quad + \mathrm{Re}[Q(t)]\sin 2\theta \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \end{aligned} \tag{7}$$

where

$$Q(t) \equiv \sum_{k=-\infty}^{\infty} a_k(t) b_k^*(t). \tag{8}$$

In Eq. (7), the two-dimensional matrix can be interpreted as a transition probability matrix for a classical two-dimensional random walk as it satisfies the necessary requirements, namely, all its elements are positive, and the sum over the elements of any column or row is equal to 1. On the other hand, it is clear that $Q(t)$ accounts for the interferences. When $Q(t)$ vanishes, the behavior of the GCD can be described as a classical Markovian process. However, $Q(t) = 0$ does not necessarily imply the loss of unitary evolution; such a loss requires the vanishing of all the $\beta_k(t)$ [see Eq. (5)]. As shown in Ref. [26], the primary effect of decoherence is to make the interference terms $\beta_k(t)$ negligible; in this case, Eq. (5) becomes a true master equation. On the other hand, when $Q(t)$ is time independent, that is, $Q(t) = Q =$ constant, then Eq. (7) is solved using the methods developed in [27]; its solution as a function of the initial GCD is

$$\begin{aligned} \begin{bmatrix} P_L(t) \\ P_R(t) \end{bmatrix} &= \frac{1}{2} \begin{pmatrix} 1+\cos^t 2\theta & 1-\cos^t 2\theta \\ 1-\cos^t 2\theta & 1+\cos^t 2\theta \end{pmatrix} \begin{bmatrix} P_L(0) \\ P_R(0) \end{bmatrix} \\ &\quad + \mathrm{Re}[Q]\, \frac{1-\cos^t 2\theta}{\tan\theta} \begin{bmatrix} 1 \\ -1 \end{bmatrix}. \end{aligned} \tag{9}$$

Taking the limit $t \to \infty$ in Eq. (9), it is possible to obtain the asymptotic value of the GCD as a function of its initial value and Q.

In the generic case, $Q(t)$ is a time-dependent function, but in this system (as will be seen in the next section), $Q(t)$, $P_L(t)$, and $P_R(t)$ have longtime limiting values which are determined by the initial conditions of Eqs. (4). Therefore we can solve Eq. (7) in this limit, defining

$$\begin{aligned} \Pi_L &\equiv P_L(t \to \infty), \\ \Pi_R &\equiv P_R(t \to \infty), \\ Q_0 &\equiv Q(t \to \infty), \end{aligned} \tag{10}$$

and substituting these asymptotic values in Eq. (7) to obtain the stationary solution for the GCD:

$$\begin{bmatrix} \Pi_L \\ \Pi_R \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + 2\mathrm{Re}(Q_0)/\tan\theta \\ 1 - 2\mathrm{Re}(Q_0)/\tan\theta \end{bmatrix}. \tag{11}$$

This interesting result for the QW shows that the longtime probability to find the system with left or right chirality has a limit.

In the next section, I show that it is possible to have $Q_0 = 0$, choosing adequately the initial conditions. In this case, Eq. (7) approaches a Markov chain [27] with two states, and the dynamics of the GDC turns into an example of dependent Bernoulli trials in which the probabilities of success or failure at each trial depend on the outcome of the previous trial. Now the only asymptotic solution is $\Pi_L = \Pi_R = 1/2$ [see Eq. (11)].

If we look back at Eq. (2) in connection with Eq. (11), a paradoxical situation arises. The dynamical evolution of the QW is unitary, but the evolution of its GCD has an asymptotic value characteristic of a diffusive behavior. This situation is further surprising if we compare our case with the case of the QW on finite graphs [28], where it is shown that there is no convergence to any stationary distribution.

IV. ASYMPTOTIC SOLUTION FOR THE QW

In previous works [3,25], an alternative analytical approach was presented to obtain the asymptotic behavior of the QW on the line. The discrete map was substituted by two continuous differential equations for $a_k(t)$ and $b_k(t)$, starting from a characteristic time $t_0 \gg 1$. The initial conditions for these equations are not necessarily the same as those used in the discrete map of Eqs. (4) because the approximation of a finite difference by a derivative does not hold for small times. However, these initial conditions must ensure the same asymptotic behavior as that of the discrete map.

The asymptotic solutions of Eqs. (4) given by the differential equations are

$$\begin{aligned} a_k(t) &\simeq \sum_{l=-\infty}^{\infty} (-1)^{k-l}\, a_l^0\, J_{k-l}(t\cos\theta), \\ b_k(t) &\simeq \sum_{l=-\infty}^{\infty} (-1)^{k-l}\, b_l^0\, J_{k-l}(t\cos\theta), \end{aligned} \tag{12}$$

where J_l is the lth-order cylindrical Bessel function and a_k^0 and b_k^0 are initial amplitudes for the differential equations. To ensure that the behavior of the discrete map and the differential equations are the same in the asymptotic regime, we should choose a_k^0 and b_k^0 to be smoothly extended in space.

Replacing Eq. (12) in Eqs. (6) and (8) and noting that the Bessel functions satisfy $\sum_{j=-\infty}^{\infty} J_j(t)J_{j-k}(t) = \delta_{k0}$, we have

$$Q(t) = \sum_{k=-\infty}^{\infty} a_k^0 b_k^{0*} = Q_0, \tag{13}$$

$$P_L(t) = \sum_{j=-\infty}^{\infty} \left|a_k^0\right|^2 = \Pi_L, \tag{14}$$

$$P_R(t) = \sum_{k=-\infty}^{\infty} \left|b_k^0\right|^2 = \Pi_R. \tag{15}$$

The time independence of $Q(t)$, $P_L(t)$, and $P_R(t)$ is a consequence of the asymptotic approach given by Eq. (12), and evidently their values are Q_0, Π_L, and Π_R, respectively. When $Q(t)$, $P_L(t)$, and $P_R(t)$ are calculated with the map Eqs. (4), they have a transient time dependence (for $t < t_0$), after which they attain their asymptotic values Q_0, Π_L, and Π_R, as shown in [25].

I propose for the initial conditions a_k^0 and b_k^0 the following extended Gaussian distributions [29]:

$$a_k^0 \equiv \left\{\frac{1}{\sigma_0\sqrt{2\pi}} \exp\left[-\frac{(k-k_0)^2}{2\sigma_0^2}\right]\right\}^{\frac{1}{2}} \cos\alpha, \tag{16}$$

$$b_k^0 \equiv a_k^0 \tan\alpha \exp(i\delta), \tag{17}$$

where σ_0 is the initial standard deviation, k_0 is the central position of the Gaussian distribution, α is a parameter that determines the initial proportion of the left and right chiralities, and δ is a phase to be determined later, as a function of α and θ.

Now I evaluate Q_0, Π_L, and Π_R using the initial conditions Eqs. (16) and (17) in Eqs. (13), (14), and (15) and noting that $\sum_{k=-\infty}^{\infty} \exp[-k^2/2\sigma_0^2] \cong \sqrt{2\pi}\sigma_0$, for $\sigma_0 \gg 1$:

$$Q_0 = \tfrac{1}{2}\sin 2\alpha \cos\delta, \tag{18}$$

$$\Pi_L = \cos^2\alpha, \tag{19}$$

$$\Pi_R = \sin^2\alpha. \tag{20}$$

On the other hand, from Eq. (11), we see that Q_0 and Π_L are not independent; then, substituting Eqs. (18), (19), and (20) into Eq. (11), we have

$$\cos\delta = \frac{\tan\theta}{\tan 2\alpha}. \tag{21}$$

Then I rewrite Eq. (18) as a function of the two independent parameters of the model θ and α:

$$Q_0 = \tfrac{1}{2}\cos 2\alpha \tan\theta; \tag{22}$$

note that Q_0 vanishes for $\alpha = \pi/4$. In order to verify the approximations made in our analytical treatment, I shall compare the result of Eq. (19) with the numerical evaluation of the asymptotic behavior of $P_L(t)$ using the map Eqs. (4) and the initial conditions given by Eqs. (16) and (17). This calculation is presented in Fig. 1. Our selection of the initial amplitudes ensures that the asymptotic value for $P_L(t)$ is equal to the initial one, which in turn is the same as that given by Eq. (19). Thus the asymptotic behaviors of Eqs. (4) are in excellent agreement with our theoretical approach. Our treatment works very well for values of $\sigma_0 > 10$. The asymptotic regime of $P_L(t)$ sets in at the time t_0 after some strong oscillations. The value of t_0 depends on the parameters of the problem.

To sum up, the dynamical evolution of the QW is defined by Eqs. (4), but it is possible to obtain a predetermined asymptotic value of the GCD

$$\begin{bmatrix} \Pi_L \\ \Pi_R \end{bmatrix},$$

using as initial conditions Eqs. (16) and (17), where the parameters α and δ are determined by Eqs. (19) and (21) and the parameters k_0 and σ_0 are free to be adjusted.

V. ENTROPY OF ENTANGLEMENT

The unitary evolution of the QW generates entanglement between the coin and position degrees of freedom. This entanglement will be characterized [11,12] by the von Neumann entropy of the reduced density operator, called entropy of entanglement. The quantum analog of the Shannon entropy is the von Neumann entropy

$$S_N(\rho) = -\mathrm{tr}(\rho\log\rho), \tag{23}$$

where $\rho = |\Psi(t)\rangle\langle\Psi(t)|$ is the density matrix of the quantum system. Owing to the unitary dynamics of the QW, the system remains in a pure state, and this entropy vanishes. However, for these pure states, the entanglement between the chirality and

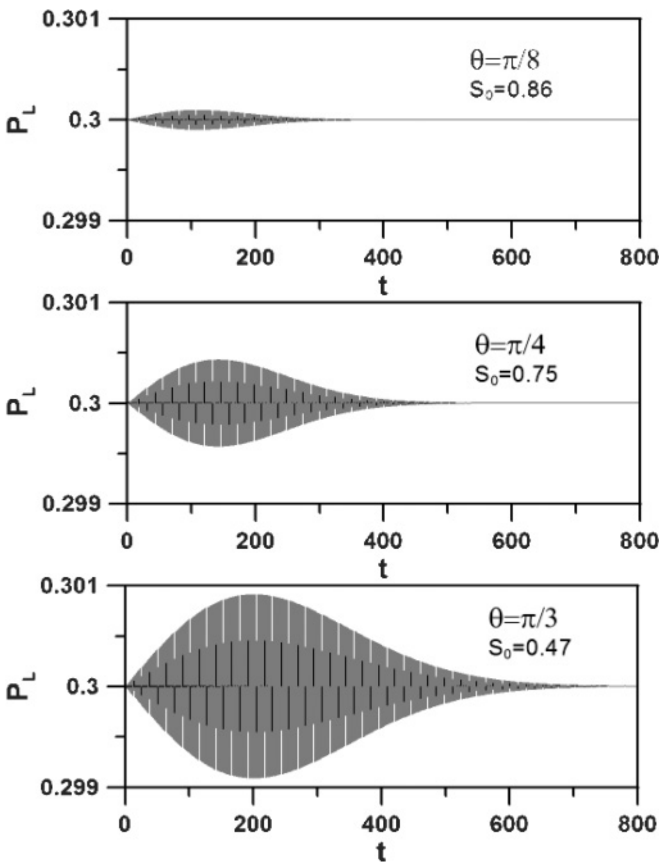

FIG. 1. The global left probability $P_L(t)$ as a function of the dimensionless time t calculated with the map Eqs. (4). The initial conditions are given by Eqs. (16) and (17). It is shown for three values of θ that $\sigma_0 = 100$, $k_0 = 0$, and $\cos^2\alpha = 0.3$. The approximate values of t_0 are, from top to bottom, 300, 500, and 700. The asymptotic values for the dimensionless entropy S_0 are also presented.

the position can be quantified by the associated von Neumann entropy for the reduced density operator:

$$S(\rho) = -\mathrm{tr}(\rho_c \log \rho_c), \tag{24}$$

where $\rho_c = \mathrm{tr}(\rho)$ and the partial trace is taken over the positions. Using the wave function Eq. (3) and its normalization properties, the reduced density operator is explicitly expressed as

$$\rho_c = \begin{bmatrix} P_L(t) & Q(t) \\ Q(t)^* & P_R(t) \end{bmatrix}. \tag{25}$$

The reduced entropy can be expressed through the two eigenvalues $\{\lambda_+, \lambda_-\}$ of the reduced density matrix as

$$S(t) = -\lambda_+ \log_2 \lambda_+ - \lambda_- \log_2 \lambda_-. \tag{26}$$

The expressions for the eigenvalues are

$$\lambda_\pm = \frac{1}{2}\{1 \pm \sqrt{1 + 4[|Q(t)|^2 - P_L(t)P_R(t)]}\}. \tag{27}$$

In the asymptotic regime $\lambda_\pm \to \Lambda_\pm$,

$$\Lambda_\pm = \frac{1}{2}[1 \pm \sqrt{1 + 4(|Q_0|^2 - \Pi_L \Pi_R)}], \tag{28}$$

and the corresponding entropy $[S(t) \to S_0]$ is

$$S_0 = -\Lambda_+ \log_2 \Lambda_+ - \Lambda_- \log_2 \Lambda_-. \tag{29}$$

Using the initial conditions Eqs. (16) and (17) in Eq. (28), we have

$$\Lambda_\pm = \frac{1}{2}\left[1 \pm \frac{\cos 2\alpha}{\cos\theta}\right]. \tag{30}$$

For $\alpha = \pi/4$, both eigenvalues are $\Lambda_\pm = 1/2$, and from Eqs. (19), (20), and (22), $\Pi_L = \Pi_R = 1/2$ and $Q_0 = 0$. For this value, the entropy of entanglement Eq. (29) has its maximum value $S_0 = 1$. Therefore the maximum value of the entropy of entanglement is achieved for the classical Markovian process ($Q_0 = 0$). Note that this result is true for all initial conditions that satisfy $Q(t) \to 0$ as it follows from Eqs. (7), (11), (28), and (29).

For $\alpha = \theta/2$, the entropy attains its minimum value $S_0 = 0$ [see Eqs. (29) and (30)]. Then, in this case, there is no entanglement between coin and position.

Using the results of the previous section, it is clear that starting from given initial conditions, the asymptotic values Π_L and Q_0 are obtained, and then the entropy of entanglement is calculated using Eqs. (28) and (29). The inverse path is also possible; that is, starting from a predetermined value of the entropy of entanglement [Eq. (29)], it is possible to obtain the initial conditions [Eqs. (16) and (17)] of the system that produce this entanglement asymptotically.

The previous ideas are numerically implemented using Eqs. (11), (28), and (29) and taking Q_0 as a real constant, and the results are presented in Figs. 2 and 3. Figure 2 shows that for each value of S_0, there are two values of Π_L, and

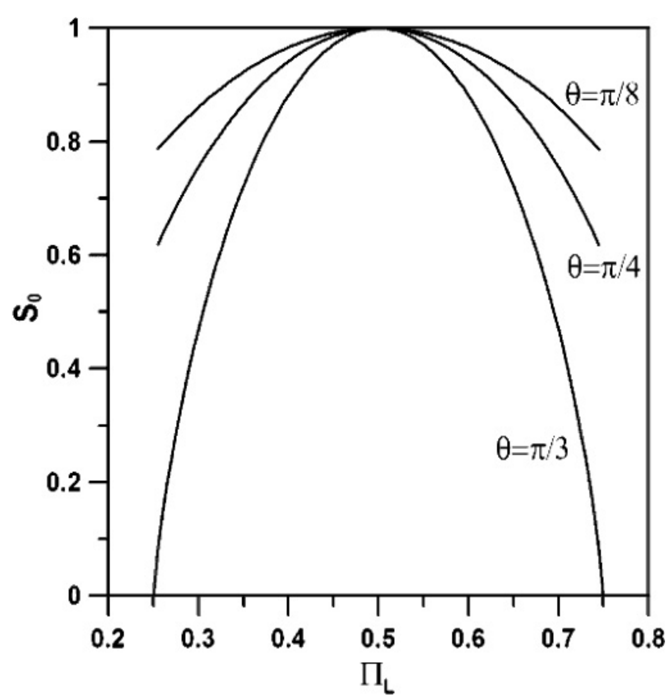

FIG. 2. The dimensionless entropy of entanglement S_0 as a function of the asymptotic global left probability Π_L for three different values of θ.

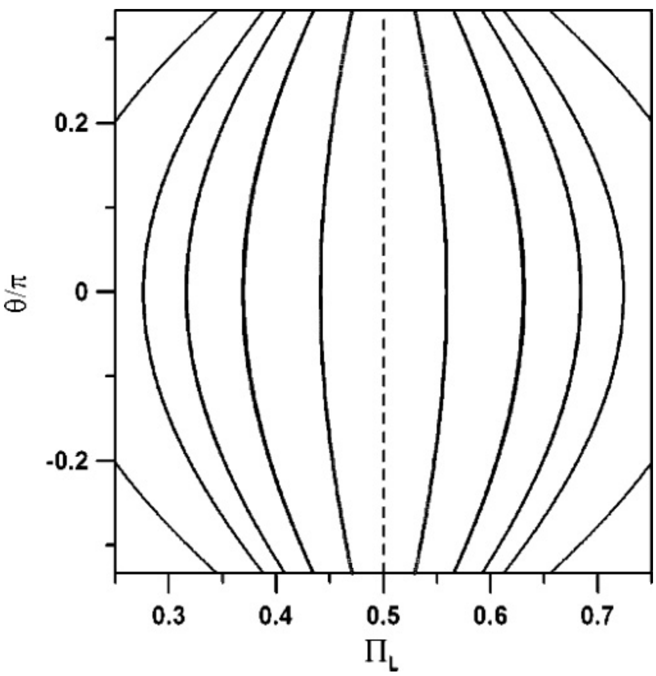

FIG. 3. Level curves for the dimensionless entropy of entanglement S_0 as a function of the dimensionless angle θ/π and the asymptotic global left probability Π_L. Five curves, in full line, are presented; each curve has two branches placed symmetrically on both sides of the central straight dashed line $\Pi_L = 0.5$. Starting from this line, where $S_0 = 1$, the values of S_0 are 0.99, 0.95, 0.90, 0.85, and 0.70.

that the width of the entropy curve grows inversely with θ. In Fig. 3, the level curves of the entropy as a function of θ and Π_L are presented as projections of the three-dimensional surface. From these figures, it is clear that the maximum of the entropy of the entanglement is achieved for the classical Markovian process ($\Pi_L = 1/2$)

To conclude this section, it is interesting to compare the entropy of entanglement with the usual Shannon entropy used in the theory of communication. In particular, one could wonder if the entropy of the entanglement may be used as a measurement of the degree of disorder of chirality. The Shannon entropy, in the asymptotic GCD model, is

$$S_S \equiv -\Pi_L \log_2 \Pi_L - \Pi_R \log_2 \Pi_R, \tag{31}$$

where Π_L and Π_R are given by Eq. (11).

It is clear from Eqs. (29) and (31) that when $Q_0 = 0$ ($\Pi_L = \Pi_R = 1/2$), both entropies attain the maximum value $S_0 = S_S = 1$. However, for other values of Q_0, they are different, in particular, when there is perfect statistical order; that is, when $\Pi_L = 1$ and $\Pi_R = 0$ (or $\Pi_L = 0$ and $\Pi_R = 1$), the Shannon entropy vanishes as it should, but the entropy of entanglement does not vanish. Therefore, although the behavior of the entropy of entanglement is correlated with the behavior of the GCD, it does not describe correctly the degree of disorder of the GCD.

VI. CONCLUSION

This article provides a different view of QW dynamics. It studies the QW, focusing on the probability distribution of the chirality independently of the position (GCD), and connects this distribution with the entropy of entanglement. Using an alternative analytical approach for the QW on the line, developed in previous works [3,25], I show analytically that the GCD converges to a stationary solution. The asymptotic behavior of the GCD looks like the behavior of the two-dimensional classical random walk, but unlike the latter, the asymptotic GCD depends on the initial conditions. The coexistence of the unitary evolution of the amplitude together with the asymptotic value of the GCD is a striking result about the behavior of the system.

I study the entanglement between the coin and the position in the QW on the line and show that the behavior of the entropy of entanglement depends on the GCD. I also show that the asymptotic entanglement is maximized when the evolution of the GCD follows a Markovian process. However, the entropy of entanglement does not describe correctly the degree of disorder of the GCD; this is well described by the Shannon entropy. In previous works [11–13,21], the dependence of the asymptotic entropy of entanglement on the initial conditions was studied; here I provide an analytical recipe to obtain a predetermined entanglement using extended Gaussian initial conditions. In other words, starting from a given value of the entropy of entanglement, it is possible to choose the corresponding initial conditions. These exact expressions can also be used to obtain a predetermined asymptotic GCD; that is, starting from a given asymptotic limit of the GCD, one can obtain the corresponding initial conditions for the QW.

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