Thermodynamic behavior of the quantum walk

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A thermodynamic theory is developed to describe the behavior of the entanglement between the coin and position degrees of freedom of the quantum walk on the line. It is shown that, in spite of the unitary evolution, a steady state is established after a Markovian transient stage. This study suggests that if a quantum dynamics develops in a composite Hilbert space (i.e., the tensor product of several subspaces), then the behavior of an operator that belongs only to one of the subspaces may camouflage the unitary character of the global evolution.

I. INTRODUCTION

The concept of isolated system plays a fundamental role in the formulation of quantum mechanics. It is an idealization that was constructed as an aid to understand some phenomena displayed by real systems that may be regarded as approximately isolated. However, since about 50 years ago, the study of quantum decoherence has acquired a central position in the formulation of quantum mechanics. In fact, concepts such as thermodynamic equilibrium seem impossible to coordinate with the idea of an isolated system because such a system follows a unitary evolution and it cannot reach a final equilibrium state at $t \to \infty$.

In this context we ask ourselves if it is possible to introduce the concept of temperature for an isolated quantum system that evolves in a composite Hilbert space. In this paper the quantum walk on the line [1] has been chosen as a model to answer this question. The quantum walk (QW) is a natural generalization of the classical random walk in the frame of quantum computation and quantum information processing, and it is receiving permanent attention [2–4]. It has the property to spread over the line linearly in time as characterized by the standard deviation $\sigma(t) \sim t$, while its classical analog spreads out 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 [5,6]. Recently, we have been investigating [7–9] the asymptotic behavior of the QW on the line, focusing on the probability distribution of chirality independently of position. We showed that this distribution has a stationary long-time limit that depends on the initial conditions. This result is unexpected in the context of the unitary evolution of the QW because such a behavior is usually associated with a Markovian process. In this paper we further explore the behavior of the chirality distribution and define a thermodynamic equilibrium between the degrees of freedom of position and chirality. This equilibrium allows us to introduce a temperature concept for this unitary closed system. We obtain a master equation with a time-dependent population rate that describes the transient behavior of the reduced density operator of the QW toward thermodynamic equilibrium. This reduced density operator shows a surprising feature: its behavior looks diffusive in spite of the unitarity of the global evolution of the system.

This paper is organized as follows. In the next section the standard QW model is presented. In Sec. III the entanglement temperature is defined. Then in Secs. IV and V the entanglement temperature is obtained for localized initial conditions and for distributed initial conditions, respectively. In Sec. VI the transient behavior toward thermal equilibrium is studied, and finally, in the last section some conclusions are drawn.

II. QW ON THE LINE

The composite Hilbert space of the QW is the tensor product $\mathcal{H}_s \otimes \mathcal{H}_c$, where $\mathcal{H}_s$ is the Hilbert space associated to the motion on the line and $\mathcal{H}_c$ is the chirality (or coin) Hilbert space. In this composite space the walker moves, at discrete time steps $t \in \mathbb{N}$, along a one-dimensional lattice of sites $k \in \mathbb{Z}$. The direction of motion depends on the state of the chirality, with the eigenstates R and L. The wave vector can be expressed as the spinor

$$|\Psi(t)\rangle = \sum_{k=-\infty}^{\infty} \begin{bmatrix} a_k(t) \\ b_k(t) \end{bmatrix} |k\rangle, \qquad (1)$$

where the upper (lower) component is associated with the left (right) chirality.

Then $P_{kL}(t) = |a_k(t)|^2$ and $P_{kR}(t) = |b_k(t)|^2$ denote the probability of finding the walker at (k,t) and the coin in states R and L, respectively. The probability of finding the walker at (k,t) is

$$P(k,t) = \langle \Psi_{k,t} | \Psi_{k,t} \rangle = |a_k(t)|^2 + |b_k(t)|^2, \qquad (2)$$

and $\sum_k P(k,t) = 1$.

The QW is ruled by a unitary map whose standard form is [10–13]

$$a_k(t+1) = a_{k+1}(t) \cos\theta + b_{k+1}(t) \sin\theta,$$
$$b_k(t+1) = a_{k-1}(t) \sin\theta - b_{k-1}(t) \cos\theta, \qquad (3)$$

where $\theta \in [0, \pi/2]$ is a parameter defining the bias of the coin toss ($\theta = \frac{\pi}{4}$ for an unbiased or Hadamard coin). The global left- and right-chirality probabilities are defined as

$$P_L(t) \equiv \sum_{k=-\infty}^{\infty} P_{kL}(t) = \sum_{k=-\infty}^{\infty} |a_k(t)|^2,$$
$$P_R(t) \equiv \sum_{k=-\infty}^{\infty} P_{kR}(t) = \sum_{k=-\infty}^{\infty} |b_k(t)|^2, \qquad (4)$$

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with $P_R(t) + P_L(t) = 1$. The global chirality distribution (GCD) is defined as the distribution formed by the couple $\begin{bmatrix} P_L(t) \\ P_R(t) \end{bmatrix}$. It is shown in Ref. [7] that the GCD satisfies the following map:

$$\begin{bmatrix} P_L(t+1) \\ P_R(t+1) \end{bmatrix} = \begin{pmatrix} \cos^2\theta & \sin^2\theta \\ \sin^2\theta & \cos^2\theta \end{pmatrix} \begin{bmatrix} P_L(t) \\ P_R(t) \end{bmatrix}$$
$$+ \mathrm{Re}[Q(t)]\sin 2\theta \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \qquad (5)$$

where

$$Q(t) \equiv \sum_{k=-\infty}^{\infty} a_k(t) b_k^*(t). \qquad (6)$$

The two-dimensional matrix in Eq. (5) 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, in the generic case $Q(t)$ together with $P_L(t)$ and $P_R(t)$ are time-dependent functions that have long-time limiting values [7] that are determined by the initial conditions of Eq. (3). Equation (5) can be solved in this limit. We define

$$\Pi_L \equiv \lim_{t \to \infty} P_L(t),$$
$$\Pi_R \equiv \lim_{t \to \infty} P_R(t), \qquad (7)$$
$$Q_0 \equiv \lim_{t \to \infty} Q(t),$$

and then we obtain the asymptotic stationary solution for the GCD as

$$\begin{bmatrix} \Pi_L \\ \Pi_R \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 + 2\mathrm{Re}(Q_0)/\tan\theta \\ 1 - 2\mathrm{Re}(Q_0)/\tan\theta \end{bmatrix}. \qquad (8)$$

This interesting result for the QW shows that the long-time probability to find the system with left or right chirality has a limit. Therefore, although the dynamical evolution of the QW is unitary, the evolution of its GCD has an asymptotic-limit characteristic of a diffusive behavior. This situation is further surprising if we compare our case with the case of the QW on finite graphs [14], where it is shown that there is no convergence to any stationary distribution.

III. ENTANGLEMENT AND TEMPERATURE

The concept of entanglement is an important element in the development of quantum communication, quantum cryptography, and quantum computation. In this context some authors [15,16] have proposed to use the QW as a tool for quantum algorithm development and as an entanglement generator, potentially useful for testing quantum hardware. On the other hand, the relation between the asymptotic coin-position entanglement and the initial conditions of the

QW has been investigated by several authors [17–27]. In this work we also study this last kind of entanglement, which, as we shall show, can be seen as a system-environment entanglement and as such is not useful, in general, for quantum computing.

The unitary evolution of the QW generates entanglement between the coin and position degrees of freedom. To characterize this entanglement we start with the von Neumann entropy. which is the quantum analog of the Gibbs entropy,

$$S_N(\rho) = -\mathrm{tr}(\rho \log_{10} \rho), \qquad (9)$$

where $\rho = |\Psi(t)\rangle\langle\Psi(t)|$ is the density matrix of the quantum system. Due 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 the position can be quantified by the associated von Neumann entropy for the reduced density operator [17,18] that defines the entropy of entanglement,

$$S(\rho) = -\mathrm{tr}(\rho_c \log_{10} \rho_c), \qquad (10)$$

where

$$\rho_c = \mathrm{tr}(\rho), \qquad (11)$$

and the partial trace is taken over the positions. Using the wave-function equation (1) and its normalization properties, we obtain the reduced density operator [17]

$$\rho_c = \begin{pmatrix} P_L(t) & Q(t) \\ Q(t)^* & P_R(t) \end{pmatrix}. \qquad (12)$$

The density operator ρ_c has the eigenvalues

$$\lambda_\pm = \tfrac{1}{2}[1 \pm \sqrt{1 - 4[P_L(t)\,P_R(t) - |Q(t)|^2]}]. \qquad (13)$$

Then the entanglement entropy equation (10) is expressed through these two eigenvalues as

$$S(\rho) = -\lambda_+ \log_{10} \lambda_+ - \lambda_- \log_{10} \lambda_-. \qquad (14)$$

In the asymptotic regime $t \to \infty$ the eigenvalues go to a stationary limit, $\lambda_\pm \to \Lambda_\pm$, and

$$\Lambda_\pm = \tfrac{1}{2}[1 \pm \sqrt{1 - 4(\Pi_L\,\Pi_R - |Q_0|^2)}]. \qquad (15)$$

Further from Eq. (8) it follows that

$$\Pi_L\,\Pi_R = \frac{1}{4} - \left(\frac{\mathrm{Re}(Q_0)}{\tan\theta}\right)^2, \qquad (16)$$

which is substituted in Eq. (15), and then the asymptotic eigenvalues are expressed as

$$\Lambda_\pm = \tfrac{1}{2} \pm \sqrt{\chi}, \qquad (17)$$

with

$$\chi \equiv |Q_0|^2 + [\mathrm{Re}(Q_0)/\tan\theta]^2. \qquad (18)$$

Note that the values of the interference term Q_0 are constrained to satisfy the condition

$$0 < \Lambda_+\Lambda_- < 1, \qquad (19)$$

and then

$$0 < \chi < \tfrac{1}{4}. \qquad (20)$$

The entanglement entropy has an asymptotic limit as well,

$$S_0 = -\Lambda_+ \log_{10} \Lambda_+ - \Lambda_- \log_{10} \Lambda_-, \tag{21}$$

which only depends on the initial conditions through the interference term Q_0. Therefore we are led to consider that after some transient time the QW achieves a thermodynamic equilibrium between the position and chirality degrees of freedom.

In order to make a fuller description of this equilibrium it is necessary to connect the eigenvalues of ρ_c with its associated Hamiltonian operator H_c. To obtain this connection we shall use the quantum Brownian motion model of Ref. [28]. We considered the system associated with the chirality degrees of freedom and characterized by the density matrix ρ_c in thermal contact (entanglement) with the bath system associated with the position degrees of freedom, the lattice. In this context ρ_c satisfies the equation

$$\frac{\partial \rho_c}{\partial t} = \frac{1}{i\hbar}[H_c, \rho_c] + \Gamma \rho_c, \tag{22}$$

where $[H_c, \rho_c]$ is the commutator and $\Gamma \rho_c$ represents the Brownian motion of ρ_c induced by the noise (fluctuating forces) exerted on ρ_c by the lattice (position degrees of freedom). In the equilibrium (stationary) situation we must have $\partial \rho_c / \partial t = 0$ and $\Gamma \rho_c = 0$ [28], that is,

$$[H_c, \rho_c] = 0. \tag{23}$$

Therefore, in the asymptotic regime, the density operator ρ_c is an explicit function of the Hamiltonian operator, which must be time independent. Let us call $\{\Phi_+, \Phi_-\}$ the eigenfunctions of the density matrix, so the operators H_c and ρ_c are both diagonal in this basis. Then the eigenvalues Λ_+ and Λ_- depend on the corresponding eigenvalues of H_c. We take these eigenvalues to be $\{-\epsilon, \epsilon\}$ without any loss of generality; they represent the possible values of the entanglement energy. This interpretation agrees with the fact that $\Lambda_\pm$ are the probabilities that the system is in the eigenstates $\Phi_\pm$, respectively.

It is interesting to point out that, in the context of classical random walks, it is natural to view the entanglement entropy of heads vs tails as the entropy of mixing. Here the values Π_L and Π_R [Eq. (8)] depend on the basis used for the reduced density matrix; however, the asymptotic reduced density matrix is characterized by the eigenvalues $\Lambda_\pm$, and these are independent of the basis. Therefore, as in the classical case, these eigenvalues can be interpreted as an excess density of heads vs tails chirality in the basis where the density matrix is diagonal.

The precise dependence between $\Lambda_\pm$ and $\pm\epsilon$ is determined by the type of ensemble we construct. The main proposal of this paper is that this equilibrium corresponds to a quantum canonical ensemble. Therefore we propose that

$$\Lambda_\pm \equiv \frac{e^{\pm\beta\epsilon}}{e^{\beta\epsilon} + e^{-\beta\epsilon}}, \tag{24}$$

which defines the entanglement temperature $T \equiv 1/\beta$. Of course, in Eq. (24) only the ratio ϵ/T is well defined; however, we chose to introduce the temperature as this concept strengthens the idea of asymptotic equilibrium between the position and chirality degrees of freedom. Note that while temperature makes sense only in the mentioned equilibrium

state, the entropy concept can be introduced without such a restriction.

The probability that a state chosen at random from the ensemble $\{\Phi_+, \Phi_-\}$ possesses an energy ϵ is determined by the Boltzmann factor $e^{-\beta\epsilon}$. Let us call $\widetilde{\rho_c}$ the diagonal expression of the density operator ρ_c; then

$$\widetilde{\rho_c} = \begin{pmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{pmatrix} = \frac{1}{e^{\beta\epsilon} + e^{-\beta\epsilon}} \begin{pmatrix} e^{\beta\epsilon} & 0 \\ 0 & e^{-\beta\epsilon} \end{pmatrix}. \tag{25}$$

This operator is formally the same density operator that corresponds to an electron that possesses an intrinsic spin and a magnetic moment in an external magnetic field [29]. Therefore, we may consider the QW chirality in thermal contact (entanglement) with its position space, the lattice. The lattice itself is a large system, which can be regarded as being always very close to internal equilibrium at the absolute temperature T.

In general the Hilbert space of a quantum-mechanical model factors as a tensor product $\mathcal{H}_{\text{sys}} \otimes \mathcal{H}_{\text{env}}$ of the spaces describing the degrees of freedom of the system and environment. The evolution of the system is determined by the reduced density operator that results from taking the trace over $\mathcal{H}_{\text{env}}$ to obtain $\varrho_{\text{sys}} = \text{tr}_{\text{env}}(\rho)$. The simple toy models similar to our model studied in Refs. [30–32] show how the correlations of a quantum system with other systems may cause one of its observables to behave in a classical manner. In this sense the fact that the partial trace over the QW positions leads to a system effectively in thermal equilibrium agrees with those previous results.

Starting from Eq. (25), it is possible to build the thermodynamics for the QW entanglement. The partition function of the system is then given by

$$\mathcal{Z} = e^{\beta\epsilon} + e^{-\beta\epsilon} = 2\cosh(\beta\epsilon). \tag{26}$$

Accordingly, and also using Eqs. (15) and (24), the temperature is given by

$$T = 2\epsilon / \ln\left(\frac{1 + 2\sqrt{\chi}}{1 - 2\sqrt{\chi}}\right), \tag{27}$$

the Helmholtz free energy is given by

$$A = -\frac{1}{\beta}\ln[2\cosh(\beta\epsilon)] = \frac{T}{2}\ln\left(\frac{1}{4} - \chi\right), \tag{28}$$

the internal energy is given by

$$U = -\epsilon\tanh(\beta\epsilon) = -2\epsilon\sqrt{\chi}, \tag{29}$$

and, finally, the entropy is given by

$$S_0 = \beta U - \beta A, \tag{30}$$

where this last thermodynamic definition for the entropy of course agrees with the previous Shannon expression in Eq. (21). To finish this section, in Fig. 1 we present the dependence of these thermodynamic magnitudes on the interference parameter χ.
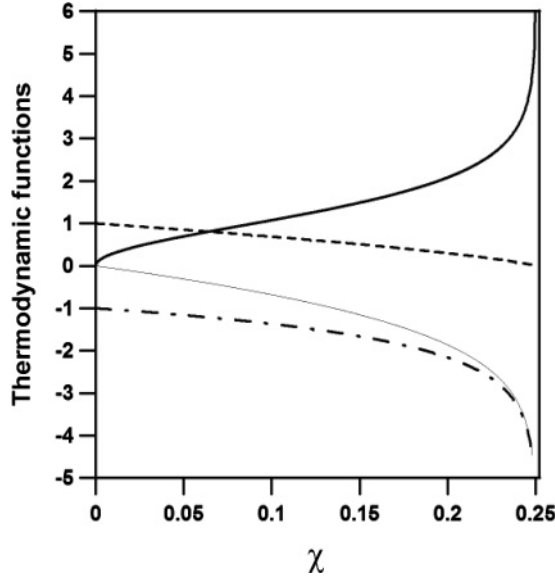
FIG. 1. Dimensionless thermodynamic function normalized by $\log(2)$ as a function of the dimensionless parameter χ. From the top to the bottom they are as follows: thick solid line, $\beta\epsilon$; dashed line, the entropy S_0; thin solid line, the energy βU; dash-dotted line, the Helmholtz free energy βA.

IV. LOCALIZED INITIAL CONDITIONS

As seen in the previous section, the thermodynamics of entanglement only depends on the interference term Q_0, which in turn only depends on the initial conditions, as shown in [7].

In order to investigate this dependence on the initial conditions of the system we consider first the localized case. The initial state of the walker is assumed to be sharply localized at the origin with arbitrary chirality; thus

$$|\Psi(0)\rangle = \begin{pmatrix} \cos(\gamma/2) \\ \exp i\varphi \ \sin(\gamma/2) \end{pmatrix} |0\rangle, \qquad (31)$$

where $\gamma \in [0,\pi]$ and $\varphi \in [0,2\pi]$ define a point on the unit three-dimensional Bloch sphere. The expression for Q_0 was obtained in Ref. [18], fixing the bias of the coin toss $\theta = \pi/4$, following the method developed by Nayak and Vishwanath [33]:

$$Q_0 = \frac{1}{2}\left(1 - \frac{1}{\sqrt{2}}\right)[\cos\gamma \ + \sin\gamma \ (\cos\varphi + i\sqrt{2}\sin\varphi)]. \tag{32}$$

Using this result in Eq. (18), the dependence of χ with the initial conditions is given by

$$\chi = \chi_0(1 + \cos\varphi \sin 2\gamma), \qquad (33)$$

where $\chi_0 = 3/4 - 1/\sqrt{2}$.

It is useful to define a characteristic temperature (in units of ϵ)

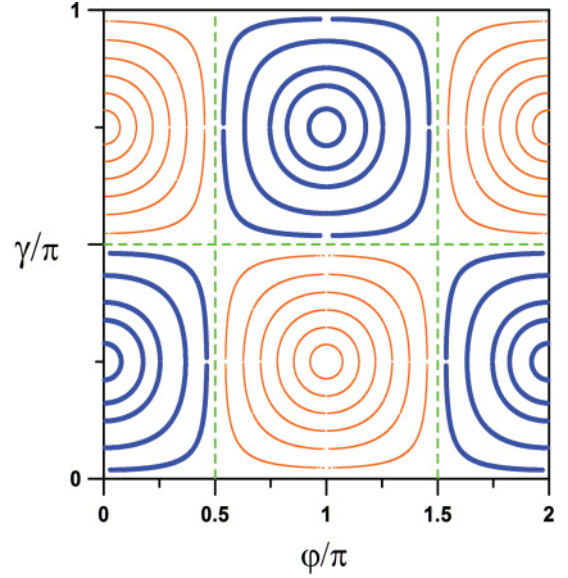$$T_0 = 2 / \left[\ln\left(\frac{1 + 2\sqrt{\chi_0}}{1 - 2\sqrt{\chi_0}}\right) \right] \qquad (34)$$

FIG. 2. (Color online) Isothermal curves as functions of the dimensionless angles γ and φ. Due to the rotation symmetry in the angle φ only four zones are distinguished: two "cold" and two "hot." The hot zones (thin orange lines) have six isotherms, and their temperatures are, from inside to outside, $T/T_0 = 6.5, 3.2, 2.2, 1.6, 1.3$, and 1.1. The cold zones (thick blue lines) have five isotherms, and their temperatures are, from outside to inside, $T/T_0 = 0.9, 0.8, 0.7, 0.68$, and 0.66. The straight dashed green lines correspond to $T/T_0 = 1$ [see Eq. (35)].

in order to express any other temperature in terms of $T_0 = 1/\beta_0$. Then from Eq. (27) we obtain an expression for β as a function of the angles γ and φ:

$$\cos\varphi \sin 2\gamma = \left(\frac{\tanh\beta}{\tanh\beta_0}\right)^2 - 1. \qquad (35)$$

Figures 2 and 3 show the level curves (isotherms) for the entanglement temperature as a function of the QW initial position, Eqs. (27) and (33). In Fig. 2 the initial position is defined through the angles γ and φ, and in Fig. 3 it is defined through the position on the Bloch sphere [see Eq. (31)]. Both Figs. 2 and 3 show four regions, two of them corresponding to temperatures $T > T_0$ (thin orange lines) and the other two to temperatures $T < T_0$ (thick blue lines). The longest isotherms (dashed green lines) correspond to the temperature $T = T_0$, and their initial conditions are $\gamma = 0, \pi/2, \pi$ and $\varphi = \pi/2, 3\pi/2$. It is interesting to point out that the marked asymmetry of Fig. 3 is related to the fact that the Hadamard gate is a combination of σ_z and σ_x Pauli matrices acting in the Hilbert space of the QW. As a result, in the asymptotic limit, Fig. 3 has a symmetry in the XZ plane for $\theta = \pi/4$, but it has anisotropy in the Y direction.

Figures 2 and 3 also show the dependence on the initial conditions γ and φ for any function of χ, in particular for $\Lambda_{\pm}$ [see Eqs. (17) and (33)].

V. DISTRIBUTED INITIAL CONDITIONS

In previous works [7,34] we have studied the QW with extended initial conditions. Now the entanglement temperature
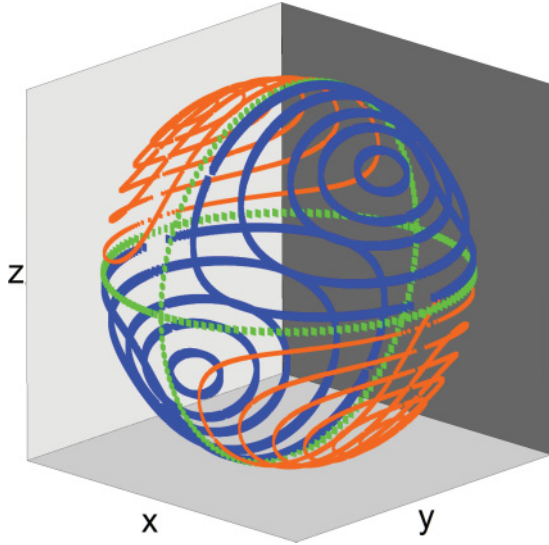
FIG. 3. (Color online) The isothermal curves of Fig. 2 are shown on the Bloch sphere. The initial chirality of the QW determines the entanglement temperature [see Eqs. (27), (31), and (33)].

is studied in such a case. The following extended Gaussian distributions is proposed:

$$a_k^0 \equiv \left[\frac{1}{\sigma_0 \sqrt{2\pi}} \exp\left(-\frac{k^2}{2\sigma_0^2} \right) \right]^{\frac{1}{2}} \cos(\gamma/2), \qquad (36)$$

$$b_k^0 \equiv e^{i\varphi} \left[\frac{1}{\sigma_0 \sqrt{2\pi}} \exp\left(-\frac{k^2}{2\sigma_0^2} \right) \right]^{\frac{1}{2}} \sin(\gamma/2), \qquad (37)$$

where σ_0 is the initial standard deviation, $\gamma \in [0,\pi]$ determines the initial proportion of the left and right chirality, and $\varphi \in [0,2\pi]$ is a global phase. Using these initial conditions, Eqs. (36) and (37), the asymptotic value of $Q(t)$, see Eqs. (6) and (7), was obtained [7] as

$$Q_0 = \tfrac{1}{2} \cos\gamma \, \tan\theta \,, \qquad (38)$$

with the restrictions

$$\sigma_0 \gg 1 \qquad (39)$$

and

$$\cos\varphi = \frac{\tan\theta}{\tan\gamma}. \qquad (40)$$

Replacing Eq. (38) in Eq. (18), we obtain

$$\chi = \left(\frac{\cos\gamma}{2\cos\theta} \right)^2, \qquad (41)$$

and then using Eq. (27), we have

$$\beta\epsilon = \frac{1}{2} \ln\left(\frac{|\cos\theta| + |\cos\gamma|}{|\cos\theta| - |\cos\gamma|} \right), \qquad (42)$$

where, taking into account Eqs. (20) and (41), the initial condition satisfies the constraint

$$|\cos\gamma| < |\cos\theta|. \qquad (43)$$

The functions Q_0, χ, and β vanish for $\gamma = \pi/2$ [see Eqs. (38), (41), and (42)], and simultaneously, the entanglement entropy, Eq. (14), has its maximum value $S_0 = 1$.
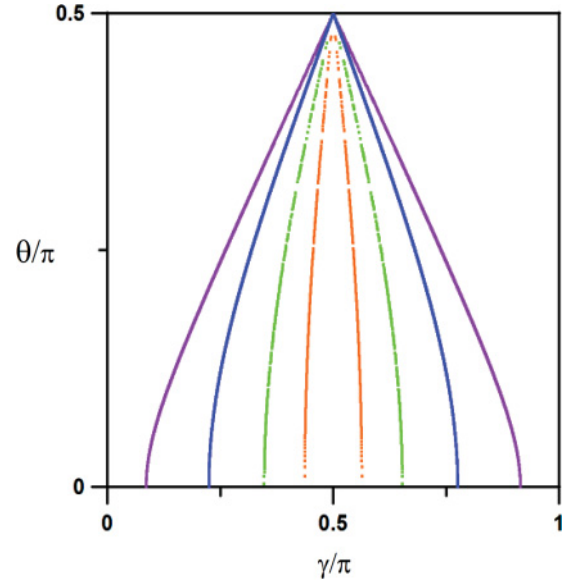

FIG. 4. (Color online) Isothermal curves as functions of the dimensionless angles γ (initial conditions) and θ (bias of the coin). Four curves are presented; each curve has two branches placed symmetrically on both sides of $\gamma = \pi/2$, where $T = \infty$. The values of T are given by Eq. (42). From left to right the values of T are, in units of ϵ, 0.5 (purple), 1 (blue), 2 (green), and 5 (orange). The diagram has two discontinuities in $\theta = \pi/2$ and in $\gamma = \pi/2$ [see Eqs. (42) and (43)].

This maximum value is achieved when the entanglement temperature is $T = \infty$. Under these conditions the system behaves as a classical Markov process [7]. On the other hand, the initial conditions γ and φ are not independent [see Eq. (40)], and for each value of γ there is only one value of T; then for fixed θ it is not possible to have isotherms as functions of γ and φ. Instead, the entanglement temperature depends on θ and γ from Eq. (42); i.e., the choice of the bias of the coin toss θ or of the initial proportion of the chirality γ could lead to the same entanglement temperature. Figure 4 shows the isotherms as functions of γ and θ.

VI. TRANSIENT BEHAVIOR

In the QW a stationary entanglement is established between the chirality and position degrees of freedom after a transient time. This fact allowed us to introduce the concept of entanglement temperature. The transient behavior of the system is studied using the original map equation (3) in a numerical code with initial conditions given by Eq. (31). These numerical calculations are summarized in Figs. 5 and 6. Figure 5 presents the difference between the transient (λ_+) and the stationary (Λ_+) eigenvalues of the density matrix as a function of time [see Eqs. (13) and (15)]. Figure 5 only presents the envelope of the curves because the real eigenvalue dynamics is very intricate; it presents quick oscillations with a high density of paths, and it is only possible distinguish its global contour. However, the average evolution of the system is determined by the envelope dynamics. Each envelope has two branches placed symmetrically on both sides of $\lambda_+ - \Lambda_+ = 0$. Two pairs of curves are presented with solid and dashed lines. In
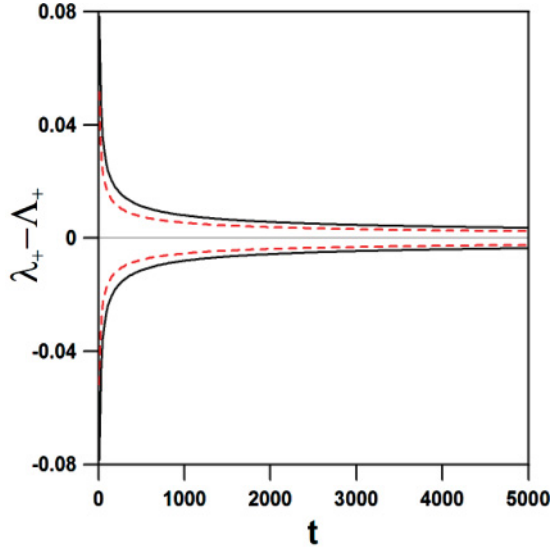
FIG. 5. (Color online) Envelope of the probability $\lambda_+ - \Lambda_+$ as a function of the dimensionless time t for two different initial conditions. Each initial condition is established by the couple (φ, γ) in Eq. (31). Their values are $(\pi/8, \pi/4)$ for the solid black line and $(\pi/4, \pi/3)$ for the dashed red line. In both cases, the temperature is $T = 0.79T_0$.

both cases, the envelopes decay for $t \to \infty$ as a power law $1/t^c$, with $c = 0.490$ for the dashed red line and $c = 0.486$ for the solid black line. The envelopes of $\lambda_\pm$ will be called $\widetilde{\lambda}_\pm$, respectively.

It was numerically verified for several initial conditions given by Eq. (31) that the transient behavior of $\widetilde{\lambda}_\pm - \Lambda_\pm$ can be adjusted by a time power law. Figure 6 shows the power-law exponent c as a function of the initial condition γ for the same temperature. Remember that, for T and γ given, φ is determined by Eq. (35). Therefore, the exponent c has a
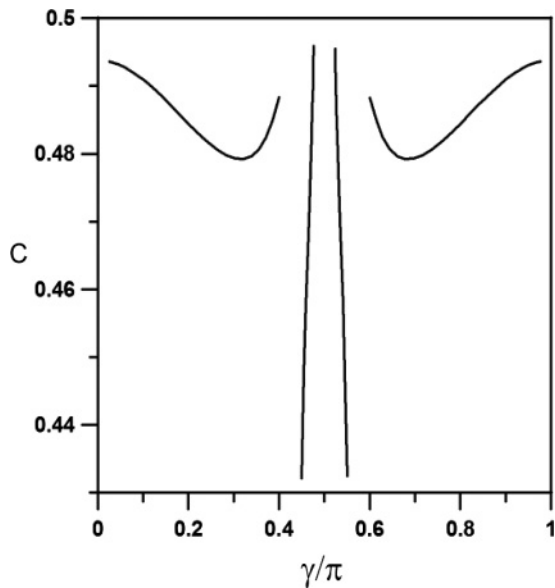

FIG. 6. The power-law exponent as a function of the dimensionless angle γ. The initial conditions (φ, γ) correspond to the isotherms $T = 1.1T_0$.

dependence on the initial conditions; however, this dependence is not determined by the asymptotic temperature value.

Additionally, the transient behavior of $\widetilde{\lambda}_\pm - \Lambda_\pm$ was numerically studied using initial conditions given by Eqs. (36) and (37), with $\sigma \gg 1$. In these cases, the system showed a negligible transient dynamics, in agreement with the calculation developed in Ref. [7]. Therefore, for these initial conditions, the reduced density matrix is essentially always in thermodynamic equilibrium.

With the aim to understand the transient behavior of the system we develop an analytic theory implementing a parallelism between the reduced density operator Eq. (25) and the density operator of an electron in an external magnetic field. With this picture in mind we propose the following master equation for the probabilities λ_+ and λ_-:

$$\frac{d\lambda_-}{dt} = \lambda_+ \, w_{+-} - \lambda_- \, w_{-+},$$
$$\frac{d\lambda_+}{dt} = \lambda_- \, w_{-+} - \lambda_+ \, w_{+-}, \tag{44}$$

where w_{+-} and w_{-+} are transition probabilities per unit of time, which can be understood as population rates. w_{+-} corresponds to the transition $\lambda_+ \to \lambda_-$ and w_{-+} corresponds to the transition $\lambda_- \to \lambda_+$. These rates are time-dependent functions, and their behaviors are known in the limit $t \to \infty$ when $d\lambda_\pm/dt \to 0$. In this limit, the stationary solution of Eq. (44) must be the couple Λ_- and Λ_+, given by Eq. (15). Then the asymptotic values of the population rates satisfy

$$\frac{w_b}{w_a} = \frac{\Lambda_-}{\Lambda_+}, \tag{45}$$

where w_a and w_b are defined by

$$w_a \equiv \frac{\lim}{t \to \infty} w_{-+}, \tag{46}$$

$$w_b \equiv \frac{\lim}{t \to \infty} w_{+-}. \tag{47}$$

Equation (45) expresses a condition of detailed balance that says that the rate of occurrence for any transition equals the rate for the inverse transition. Using our knowledge about the transient and asymptotic behaviors, the following population rates are proposed:

$$w_{+-} = w_b + \xi(t), \tag{48}$$
$$w_{-+} = w_a - \xi(t), \tag{49}$$

where

$$\xi(t) = \frac{K}{t^c} \left[\omega \sin(\omega t + \delta) + \left(\frac{c}{t} - w_a - w_b \right) \cos(\omega t + \delta) \right], \tag{50}$$

with $c > 0$, K, ω, and δ being constants. The general solution of Eq. (44) with these population rates is

$$\lambda_+ = \Lambda_+ + \frac{K}{t^c} \cos(\omega t + \delta) + d \, e^{-(w_a + w_b)t}, \tag{51}$$

$$\lambda_- = \Lambda_- - \frac{K}{t^c} \cos(\omega t + \delta) - d \, e^{-(w_a + w_b)t}, \tag{52}$$

where d is an additional constant. Note that $e^{-(w_a + w_b)t} \to 0$ faster than $1/t^c$ for $t \to \infty$; then Eqs. (51) and (52) verify the

asymptotic behavior obtained numerically. All the constants K, c, ω, δ, and d depend on the initial conditions; however, their values should be compatible with the positive character of the functions λ_+, λ_-, w_{+-}, and w_{-+}. In particular, to describe correctly the numerical results, K takes a finite value for localized initial conditions, and it takes a negligible value for distributed initial conditions. In summary, the Brownian motion equation for our reduced density matrix, Eq. (22), takes the form of a master equation, Eq. (44).

Finally, it is important to point out that the asymptotic behavior found here is similar to the behavior of the simple cellular automaton known as *sandpile* [35]. Such behaviors are characteristic of extended dynamical systems with spatial degrees of freedom. They naturally evolve to self-organized states with correlations that decay with a power law.

VII. CONCLUSION

The unitary evolution of the QW in a composite Hilbert space is studied. In particular, the entanglement between chirality and position degrees of freedom is investigated. After a transient time the system establishes a stationary entanglement between the coin and the position that allows us to develop a thermodynamic theory. The asymptotic reduced density operator is used to introduce the entanglement thermodynamic functions in the canonical equilibrium. These thermodynamic functions characterize the asymptotic entanglement, and the system can be seen as a spin-1/2 particle coupled to an infinite bath, the $|k\rangle$ position states.

It is shown that the QW initial condition determines the system's temperature as well as other thermodynamic functions. A map for the isotherms is analytically built for arbitrary localized initial conditions. Additionally, it is shown that, choosing appropriately the bias of the coin toss, it is possible to obtain a predetermined entanglement temperature.

The transient dynamics of the reduced density operator outside the thermodynamic equilibrium is also studied. We show numerically that this transient behavior can be adjusted with a power law whose exponent depends on the initial conditions. We built a master equation to describe this behavior where the population rates have a time dependence. The accuracy of the master equation solution is numerically verified, and it is shown that the reduced density has a cellular automaton behavior.

The behavior of the reduced density operator looks diffusive, but it has a dependence on the initial conditions, the global evolution of the system being unitary. Then, if an observer only had information related to the chirality degrees of freedom, it would be very difficult for him to recognize the unitary character of the quantum evolution. In general, from this simple model we can conclude that if the quantum system dynamics occurs in a composite Hilbert space, then the behavior of the operators that only belong to one subspace could camouflage the unitary character of the global evolution.

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