Thermodynamics of N-dimensional quantum walks

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The entanglement between the position and the coin state of an N-dimensional quantum walker is shown to lead to a thermodynamic theory. The entropy, in this thermodynamics, is associated with the reduced density operator for the evolution of chirality, taking a partial trace over positions. From the asymptotic reduced density matrix it is possible to define thermodynamic quantities, such as the asymptotic entanglement entropy, temperature, and Helmholz free energy. We study in detail the case of a two-dimensional quantum walk, in the case of two initial conditions: a nonseparable coin-position initial state and a separable one. The resulting entanglement temperature is presented as a function of the parameters of the system and those of the initial conditions.

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I. INTRODUCTION

The coined quantum walk (QW) model on the line was introduced by Aharonov *et al.* [1] and its properties in graphs were studied in Ref. [2]. In this model, the particle jumps from site to site in a direction which depends on the value of an internal degree of freedom called chirality. QWs on multidimensional lattices have been studied by many authors [3–6] and display the key feature of spreading quadratically faster, in terms of the probability distribution, compared to the classical random walk model on the same underlying structure [7]. These models were successfully applied to develop quantum algorithms, especially for searching a marked node in graphs [8–10]. There are other models of QWs and some of them do not use an auxiliary Hilbert space and have no coin. The continuous-time QW model introduced by Farhi and Gutman [11] and the coinless QW model introduced by Patel *et al.* [12] are examples of such models. The latter model can be used to search a marked node on two-dimensional finite lattices with the same number of steps (asymptotically in terms of the system size) compared to the coined model, with the advantage of using a smaller Hilbert space [13].

The thermodynamics of QWs on the line was introduced in Refs. [14,15] using the coined QW model, which has two subspaces, namely, the coin and spatial parts. Taking the model's whole Hilbert space, the dynamics is unitary, with no change in the entropy. On the other hand, the coin subspace evolves entangled with its environment. In the asymptotic limit ($t \to \infty$), after tracing out the spatial part, the coin reaches a final equilibrium state which, if we consider the quantum canonical ensemble, can be seen to have an associated temperature. This procedure allows the introduction of thermodynamical quantities and helps to clarify the physics behind the dynamics. In most cases, the thermodynamical quantities depend on the initial condition, in stark contrast with the classical Markovian behavior.

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 $\varrho_{\text{sys}} = \text{tr}_{\text{env}}(\rho)$. A simple toy model, similar to our model studied in Refs. [16] and [17], shows 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 these previous results.

In this work, we focus our attention on the thermodynamics of coined QWs on multidimensional lattices. The analysis of the dynamics is greatly simplified by using the Fourier basis (momentum space). In the computational basis, the evolution operator is in a Hilbert space of infinite dimensions, while in the Fourier basis we use a new operator in the finite coin subspace. The temperature of the QW is obtained by taking the asymptotic limit ($t \to \infty$) of the reduced density matrix of the coin subspace and by making a correspondence with a quantum canonical ensemble. Using the saddle-point expansion theorem [18], we obtain the expression of the entanglement temperature in terms of the coin entries and the initial state. This analysis generalizes the results in Ref. [14] and allows us to obtain many new examples due to the increased number of degrees of freedom.

The paper is organized as follows. In Sec. II we review the dynamics of multidimensional coined QWs in terms of the Fourier basis. In Sec. III we describe the thermodynamics of QWs on lattices and show how to obtain the temperature and other thermodynamical quantities. In Sec. IV we obtain an explicit expression for the temperature in terms of the initial condition. In Sec. V we give some examples in two dimensions. In the last section we draw conclusions.

II. N-DIMENSIONAL DISCRETE QUANTUM WALKS

In this section, following Ref. [19], we present a brief theoretical development to obtain the wave function of the system. The system moves at discrete time steps $t \in \mathbb{N}$ across an N-dimensional lattice of sites $\mathbf{x} \equiv (x_1, \ldots, x_N) \in \mathbb{Z}^N$. Its evolution is governed by a unitary time operator. This operator can be written as the application of two simpler operators, one representing the unitary operator due to the $2N$-dimensional

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coin which determines the direction of displacement and the other being specifically the unitary operator of the displacement. The Hilbert space of the whole system then has the form

$$\mathcal{H} = \mathcal{H}_{\mathrm{P}} \otimes \mathcal{H}_{\mathrm{C}}, \tag{1}$$

where the position space, $\mathcal{H}_{\mathrm{P}}$, is spanned by the unitary vectors $\{|\mathbf{u}_\alpha\rangle \equiv |\delta_{1\alpha},\ldots,\delta_{N\alpha}\rangle; \alpha = 1,\ldots,N\}$, and the coin space, $\mathcal{H}_{\mathrm{C}}$, is spanned by $2N$ orthonormal quantum states $\{|\alpha_\eta\rangle : \alpha = 1,\ldots,N; \eta = \pm\}$. Therefore α is associated with the axis, and η with the direction. In the usual QW on the line ($N = 1$), $|1_-\rangle$ and $|1_+\rangle$ are the right and left states, $|\mathrm{R}\rangle$ and $|\mathrm{L}\rangle$. The state of the system at any time t is represented by the ket $|\psi_t\rangle$, which can be expressed as

$$|\psi_t\rangle = \sum_{\mathbf{x}\in\mathbb{Z}^{\mathbf{N}}} \sum_{\alpha=1}^{N} \sum_{\eta=\pm} \psi_{\mathbf{x},t}^{\alpha,\eta}\, |\mathbf{x}\rangle \otimes |\alpha_\eta\rangle, \tag{2}$$

where

$$\psi_{\mathbf{x},t}^{\alpha,\eta} = (\langle\alpha_\eta| \otimes \langle\mathbf{x}|)|\psi_t\rangle. \tag{3}$$

We define, at each point $\mathbf{x}$, the ket

$$|\psi_{\mathbf{x},t}\rangle = \langle\mathbf{x}|\psi_t\rangle = \sum_{\alpha=1}^{N} \sum_{\eta=\pm} \psi_{\mathbf{x},t}^{\alpha,\eta} |\alpha_\eta\rangle, \tag{4}$$

which is a coin state, so that

$$\psi_{\mathbf{x},t}^{\alpha,\eta} = \langle\alpha_\eta|\psi_{\mathbf{x},t}\rangle. \tag{5}$$

As $|\psi_{\mathbf{x},t}^{\alpha,\eta}|^2 = |(\langle\alpha_\eta| \otimes \langle\mathbf{x}|)|\psi_t\rangle|^2$ is the probability of finding the walker at $(\mathbf{x},t)$ and the coin in state $|\alpha_\eta\rangle$, the probability of finding the walker at $(\mathbf{x},t)$ irrespective of the coin state is then

$$P_{\mathbf{x},t} = \sum_{\alpha=1}^{N} \sum_{\eta=\pm} \left|\psi_{\mathbf{x},t}^{\alpha,\eta}\right|^2 = \langle\psi_{\mathbf{x},t}|\psi_{\mathbf{x},t}\rangle, \tag{6}$$

where we have used the fact that $\sum_{\alpha=1}^{N}\sum_{\eta=\pm} |\alpha_\eta\rangle\langle\alpha_\eta|$ is the identity in $\mathcal{H}_{\mathrm{C}}$. Clearly $\sum_{\mathbf{x}} P_{\mathbf{x},t} = 1$ because $\sum_{\mathbf{x}} |\mathbf{x}\rangle\langle\mathbf{x}|$ is the identity in $\mathcal{H}_{\mathrm{P}}$.

The dynamical evolution of the system is ruled by

$$|\psi_{t+1}\rangle = \hat{U}|\psi_t\rangle, \tag{7}$$

where the unitary operator

$$\hat{U} = \hat{D} \circ (\hat{I} \otimes \hat{C}) \tag{8}$$

is given in terms of the identity operator in $\mathcal{H}_{\mathrm{P}}$, $\hat{I}$, and two more unitary operators. First, the so-called coin operator $\hat{C}$, which acts in $\mathcal{H}_{\mathrm{C}}$, can be written in its more general form as

$$\hat{C} = \sum_{\alpha=1}^{N}\sum_{\eta=\pm}\sum_{\alpha'=1}^{N}\sum_{\eta'=\pm} C_{\alpha',\eta'}^{\alpha,\eta} |\alpha_\eta\rangle\langle\alpha'_{\eta'}|, \tag{9}$$

where the matrix elements $C_{\alpha',\eta'}^{\alpha,\eta} \equiv \langle\alpha_\eta|\hat{C}|\alpha'_{\eta'}\rangle$ can be arranged as a $2N\times 2N$ unitary square matrix C. Then $\hat{D}$ is the conditional displacement operator in $\mathcal{H}$:

$$\hat{D} = \sum_{\mathbf{x}} \sum_{\alpha=1}^{N} \sum_{\eta=\pm} |\mathbf{x} + \eta\mathbf{u}_\alpha\rangle\langle\mathbf{x}| \otimes |\alpha_\eta\rangle\langle\alpha_\eta|. \tag{10}$$

Note that, depending on the coin state $|\alpha_\eta\rangle$, the walker moves one site to the positive or negative direction of x_α if $\eta = +$ or $\eta = -$, respectively.

Projecting Eq. (7) onto $\langle\mathbf{x}|$ and using Eqs. (3) and (8)–(10) we obtain

$$|\psi_{\mathbf{x},t+1}\rangle = \sum_{\alpha=1}^{N}\sum_{\eta=\pm} |\alpha_\eta\rangle\langle\alpha_\eta|\hat{C}|\psi_{\mathbf{x}-\eta\mathbf{u}_\alpha,t}\rangle, \tag{11}$$

which, further projected onto $\langle\alpha_\eta|$, leads to

$$\psi_{\mathbf{x},t+1}^{\alpha,\eta} = \sum_{\alpha'=1}^{N}\sum_{\eta'=\pm} C_{\alpha',\eta'}^{\alpha,\eta}\, \psi_{\mathbf{x}-\eta\mathbf{u}_\alpha,t}^{\alpha',\eta'}. \tag{12}$$

Equation (12) is the N-dimensional QW map in the position representation. It shows that for any given time step the wave function at each point is the coherent linear superposition of the wave functions at the neighboring points calculated in the previous time step, the weights of the superposition being given by the coin operator matrix elements $C_{\alpha',\eta'}^{\alpha,\eta}$.

Given the linearity of the map and the fact that it is space invariant, i.e., the matrix elements $C_{\alpha',\eta'}^{\alpha,\eta}$ do not depend on the space coordinates, the spatial discrete Fourier transform (DFT), which has been used many times in QW studies [20,21], is a very useful technique.

The DFT is defined as

$$|\tilde{\psi}_{\mathbf{k},t}\rangle \equiv \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}} |\psi_{\mathbf{x},t}\rangle, \tag{13}$$

where $\mathbf{k} = (k_1,\ldots,k_N)$; $k_\alpha \in [-\pi,\pi]$, is the quasimomentum vector. The DFT satisfies

$$|\psi_{\mathbf{x},t}\rangle \equiv \int \frac{d^N\mathbf{k}}{(2\pi)^N} e^{i\mathbf{k}\cdot\mathbf{x}} |\tilde{\psi}_{\mathbf{k},t}\rangle. \tag{14}$$

Following Eq. (4) we define the components of the wave function in momentum space as

$$|\tilde{\psi}_{\mathbf{k},t}\rangle = \sum_{\alpha=1}^{N}\sum_{\eta=\pm} \tilde{\psi}_{\mathbf{k},t}^{\alpha,\eta} |\alpha_\eta\rangle, \tag{15}$$

$$\tilde{\psi}_{\mathbf{k},t}^{\alpha,\eta} = \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}} \psi_{\mathbf{x},t}^{\alpha,\eta}. \tag{16}$$

Applying the previous definitions to the map, (12), and using

$$\sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}} |\psi_{\mathbf{x}-\eta\mathbf{u}_\alpha,t}\rangle = \exp(-i\eta\mathbf{k}\cdot\mathbf{u}_\alpha)|\tilde{\psi}_{\mathbf{k},t}\rangle, \tag{17}$$

we obtain

$$|\tilde{\psi}_{\mathbf{k},t+1}\rangle = \hat{C}_{\mathbf{k}}|\tilde{\psi}_{\mathbf{k},t}\rangle, \tag{18}$$

where we have defined a coin operator in momentum space,

$$\hat{C}_{\mathbf{k}} \equiv \sum_{\alpha=1}^{N}\sum_{\eta=\pm} |\alpha_\eta\rangle\langle\alpha_\eta|\hat{C}\exp(-i\eta k_\alpha). \tag{19}$$

Above, $k_\alpha = \mathbf{k}\cdot\mathbf{u}_\alpha$.

The matrix elements of the coin operator in this space are

$$\langle\alpha_\eta|\hat{C}_{\mathbf{k}}|\alpha'_{\eta'}\rangle \equiv (C_{\mathbf{k}})_{\alpha',\eta'}^{\alpha,\eta} = \exp(-i\eta k_\alpha) C_{\alpha',\eta'}^{\alpha,\eta}. \tag{20}$$

Projecting Eq. (18) onto $\langle\alpha_\eta|$ and using (19) and (20) leads to

$$\tilde{\psi}^{\alpha,\eta}_{\mathbf{k},t+1} = \sum_{\alpha'=1}^{N}\sum_{\eta'=\pm} \exp(-i\eta k_\alpha) C^{\alpha,\eta}_{\alpha',\eta'} \tilde{\psi}^{\alpha',\eta'}_{\mathbf{k},t}. \tag{21}$$

As we see, the nonlocal maps (11) and (12) become local in the momentum representation given by Eqs. (18) and (21). This allows us to easily obtain a formal solution to the QW dynamics, since the map (18), implies

$$|\tilde{\psi}_{\mathbf{k},t}\rangle = (\hat{C}_{\mathbf{k}})^t |\tilde{\psi}_{\mathbf{k},0}\rangle. \tag{22}$$

Therefore the set of eigenvalues and eigenvectors of $\hat{C}_{\mathbf{k}}$ is most useful to solve the QW evolution dynamics.

Since, according to Eq. (22) the operator $\hat{C}_{\mathbf{k}}$ must be unitary, all its eigenvalues $\{\lambda^{(s)}_{\mathbf{k}} : s = 1,2,3,\ldots,2N\}$ can be written in the form $\lambda^{(s)}_{\mathbf{k}} = \exp(-i\omega^{(s)}_{\mathbf{k}})$, with $\omega^{(s)}_{\mathbf{k}}$ real. In addition to these eigenvalues, we also need to know the corresponding eigenvectors $\{|\phi^{(s)}_{\mathbf{k}}\rangle\}$. These eigenvectors satisfy the orthogonality condition

$$\langle\phi^{(s)}_{\mathbf{k}}|\phi^{(s')}_{\mathbf{k}}\rangle = \delta_{ss'}, \tag{23}$$

where $\delta_{ss'}$ is the Kronecker δ. Once the eigenvalues and eigenvectors of $\hat{C}_{\mathbf{k}}$ are known, implementing Eq. (22) is straightforward. Given the initial distribution of the walker in the position representation, $|\psi_{\mathbf{x},0}\rangle$, we compute its DFT $|\tilde{\psi}_{\mathbf{k},0}\rangle$ via Eq. (13), as well as the projections

$$\tilde{f}^{(s)}_{\mathbf{k}} = \langle\phi^{(s)}_{\mathbf{k}}|\tilde{\psi}_{\mathbf{k},0}\rangle, \tag{24}$$

so that $|\tilde{\psi}_{\mathbf{k},0}\rangle = \sum_s \tilde{f}^{(s)}_{\mathbf{k}}|\phi^{(s)}_{\mathbf{k}}\rangle$. Using Eq. (22), we obtain

$$|\tilde{\psi}_{\mathbf{k},t}\rangle = \sum_{s=1}^{2N} \exp\left(-i\omega^{(s)}_{\mathbf{k}}t\right)\tilde{f}^{(s)}_{\mathbf{k}}|\phi^{(s)}_{\mathbf{k}}\rangle. \tag{25}$$

In the position representation we get, using Eq. (14),

$$|\psi_{\mathbf{x},t}\rangle = \sum_{s=1}^{2N} |\psi^{(s)}_{\mathbf{x},t}\rangle, \tag{26}$$

$$|\psi^{(s)}_{\mathbf{x},t}\rangle = \int \frac{d^N\mathbf{k}}{(2\pi)^N} \exp\left[i\left(\mathbf{k}\cdot\mathbf{x} - \omega^{(s)}_{\mathbf{k}}t\right)\right]\tilde{f}^{(s)}_{\mathbf{k}}|\phi^{(s)}_{\mathbf{k}}\rangle. \tag{27}$$

In this way the time evolution of the QW is formally solved: all we must do is to compute the set of eigenvalues and eigenstates of $\hat{C}_{\mathbf{k}}$ and the initial state in reciprocal space $|\tilde{\psi}_{\mathbf{k},0}\rangle$, which determines the weight functions $\tilde{f}^{(s)}_{\mathbf{k}}$ through Eq. (24).

III. ENTANGLEMENT AND THERMODYNAMICS

Entanglement in quantum mechanics is associated with the nonseparability of the degrees of freedom of two or more particles. The degrees of freedom involved in entangled states are usually discrete, such as the spins of electrons or nuclei. However, there is also interest in continuous degrees of freedom, such as the position or the moment of a particle, due to their potential to increase storage capacity and information processing in quantum computation [22]. The unitary evolution of the QW generates entanglement between the coin and the position degrees of freedom. The asymptotic coin-position entanglement and its dependence on the initial conditions of the QW have been investigated by several authors [14,15,23–34]. In particular, in Ref. [15] it has been shown that the coin-position entanglement can be seen as a system-environment entanglement and it allows us to define the entanglement temperature. In the present work we also study this subject using the N-dimensional QW as a system.

Let us briefly review the usual definition of entropy with the aim of clarifying the emergence of the concept of entanglement entropy. The density matrix of the quantum system is

$$\widehat{\rho}(t) = |\psi_t\rangle\langle\psi_t|. \tag{28}$$

The quantum analog of the Gibbs entropy is the von Neumann entropy,

$$S_N(t) = -\mathrm{tr}[\widehat{\rho}(t)\log\widehat{\rho}(t)]. \tag{29}$$

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

$$S(t) = -\mathrm{tr}(\widehat{\rho}_c(t)\log\widehat{\rho}_c(t)), \tag{30}$$

where

$$\widehat{\rho}_c(t) = \mathrm{tr}_p(\widehat{\rho}) = \sum_{\mathbf{x}}\langle\mathbf{x}|\psi_t\rangle\langle\psi_t|\mathbf{x}\rangle \tag{31}$$

is the reduced density operator for the chirality evolution and the partial trace, tr_p, is taken over the positions. Note that, in general, $\mathrm{tr}(\widehat{\rho}_c^2) < 1$, i.e., the reduced operator $\widehat{\rho}_c(t)$ corresponds to a statistical mixture. The expression for the entropy given by Eq. (30) will be used as a measure of entanglement between the position and the chirality of the system. Using the properties of the wave function $|\psi_{\mathbf{x},t}\rangle = \langle\mathbf{x}|\psi_t\rangle$ and the identity

$$\sum_{\mathbf{x}} e^{i(\mathbf{k}-\mathbf{k}_0)\cdot\mathbf{x}} = (2\pi)^N\delta^N(\mathbf{k}-\mathbf{k}_0), \tag{32}$$

for the N-dimensional δ, it is straightforward to obtain the following expression for Eq. (31), the reduced density operator:

$$\widehat{\rho}_c(t) = \sum_{s=1}^{2N}\sum_{s'=1}^{2N}\int \exp\left[i\left(\omega^{(s')}_{\mathbf{k}} - \omega^{(s)}_{\mathbf{k}}\right)t\right] \times \tilde{f}^{(s)}_{\mathbf{k}}\left(\tilde{f}^{(s')}_{\mathbf{k}}\right)^*|\phi^{(s)}_{\mathbf{k}}\rangle\langle\phi^{(s')}_{\mathbf{k}}|\frac{d^N\mathbf{k}}{(2\pi)^N}. \tag{33}$$

This expression can be evaluated in the asymptotic limit $t\to\infty$ using the stationary phase theorem (see Ref. [21]), where only terms with $\omega^{(s')}_{\mathbf{k}} = \omega^{(s)}_{\mathbf{k}}$ contribute in Eq. (33). Therefore, in the asymptotic limit the reduced density operator is

$$\widehat{\varrho} \equiv \widehat{\rho}_c(t\to\infty) = \sum_{s=1}^{2N}\int \frac{d^N\mathbf{k}}{(2\pi)^N}\left|\tilde{f}^{(s)}_{\mathbf{k}}\right|^2|\phi^{(s)}_{\mathbf{k}}\rangle\langle\phi^{(s)}_{\mathbf{k}}|. \tag{34}$$

As the density operator is positive definite, its associated matrix, Eq. (34), has real and positive eigenvalues. We let $\{|\Phi_s\rangle\}$ be the basis that makes this matrix diagonal. Therefore, in this basis, the corresponding asymptotic density matrix has the simple shape

$$\varrho_{ss'} = \Lambda_s\delta_{ss'}, \tag{35}$$

where $\Lambda_s \geqslant 0$ are the eigenvalues of the asymptotic density matrix, which satisfy

$$\sum_{s=1}^{2N} \Lambda_s = 1. \tag{36}$$

In order to make a more complete description of this equilibrium in the asymptotic limit, it is necessary to connect the eigenvalues of ρ_c with an unknown associated Hamiltonian operator H_c. To obtain this connection we use the quantum Brownian motion model from Ref. [35]. In this theory one considers that the entanglement between the system associated with the chirality degrees of freedom, characterized by the density matrix ρ_c, and the system associated with the position degrees of freedom, the lattice, is equivalent to the thermal contact between the system and a thermal bath. In equilibrium,

$$[H_c, \rho_c] = 0 \tag{37}$$

should be satisfied. As a consequence, in the asymptotic regime the density operator ρ_c is an explicit function of a time-independent Hamiltonian operator. If we note by $\{|\Phi_s\rangle\}$ the set of eigenfunctions of the density matrix, the operators H_c and ρ_c are both diagonal in this basis. Therefore the eigenvalues Λ_s depend on the corresponding eigenvalues of H_c. We denote this set of eigenvalues $\{\epsilon_s\}$; they can be interpreted as the possible values of the entanglement energy. This interpretation agrees with the fact that Λ_s is the probability that the system is in the eigenstate $|\Phi_s\rangle$.

To construct this connection, we note that Eq. (36) together with $\Lambda_s \geqslant 0$ implies that $0 \leqslant \Lambda_s \leqslant 1$, therefore making it possible to associate a Boltzmann-type probability with each Λ_s. In other words, it is possible to associate, with each Λ_s, a virtual level of energy ϵ_s. The precise dependence between Λ_s and ϵ_s is determined by the type of ensemble we construct. We propose in the present work that this equilibrium can be made to correspond to a quantum canonical ensemble. To do this, we define the relation

$$\Lambda_s \equiv \frac{e^{-\beta\epsilon_s}}{\mathbb{Z}}, \tag{38}$$

where $\mathbb{Z}$ is the partition function of the system, that is,

$$\mathbb{Z} \equiv \sum_{s=1}^{2N} e^{-\beta\epsilon_s}, \tag{39}$$

and the parameter β can be put into correspondence with an entanglement temperature

$$T \equiv \frac{1}{\kappa\beta}, \tag{40}$$

where κ is the Boltzmann constant. Since only the relative difference between energy eigenvalues has physical significance, we consider the eigenvalues in decreasing order and, without loss of generality, set

$$\epsilon_1 = \epsilon, \tag{41}$$

$$\epsilon_{2N} = -\epsilon. \tag{42}$$

The value of ϵ can be determined from Eqs. (38), (41), and (42):

$$\epsilon = \frac{1}{2\beta} \log \frac{\Lambda_{2N}}{\Lambda_1}. \tag{43}$$

The energy eigenvalues for the remaining values of s, $s = 2,3\ldots,2N-1$, are, again using Eq. (38),

$$\epsilon_s = \epsilon - \frac{1}{\beta} \log \frac{\Lambda_s}{\Lambda_1}. \tag{44}$$

Therefore the asymptotic density matrix of Eq. (35) can be thought as the density matrix of the canonical ensemble,

$$\varrho = \frac{1}{\mathbb{Z}} \begin{pmatrix} e^{-\beta\epsilon_1} & 0 & 0 & . & . & 0 & 0 \\ 0 & e^{-\beta\epsilon_2} & 0 & . & . & 0 & 0 \\ 0 & 0 & e^{-\beta\epsilon_3} & . & . & 0 & 0 \\ . & . & . & . & . & . & . \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & . & e^{-\beta\epsilon_{2N-1}} & 0 \\ 0 & 0 & 0 & . & . & 0 & e^{-\beta\epsilon_{2N}} \end{pmatrix}. \tag{45}$$

Starting from the partition function of the system given by Eq. (39), it is possible to build the thermodynamics for the QW entanglement. In particular, the Helmholtz free energy A is given by

$$A \equiv -\frac{1}{\beta} \log \mathbb{Z} = -\frac{1}{\beta} \log \sum_{s=1}^{2N} e^{-\beta\epsilon_s}, \tag{46}$$

and the internal energy U is given by

$$U \equiv -\frac{1}{\mathbb{Z}} \frac{\partial \mathbb{Z}}{\partial \beta} = \frac{1}{\mathbb{Z}} \sum_{s=1}^{2N} \epsilon_s e^{-\beta\epsilon_s}. \tag{47}$$

Thus, the asymptotic entanglement entropy as a function of the eigenvalues Λ_s is

$$S = -\sum_{s=1}^{2N} \Lambda_s \log \Lambda_s. \tag{48}$$

Substituting Eq. (38) into Eq. (48), after straightforward operations using Eqs. (46) and (47), we obtain the following expression for the asymptotic entanglement entropy:

$$S = \beta(U - A). \tag{49}$$

As should be expected, the latter equation agrees with the thermodynamic definition of the entropy.

Of course, in Eq. (43), 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 the chirality degrees of freedom. Note that while the temperature makes sense only in the mentioned equilibrium state, the entropy concept can be introduced without such a restriction. For all practical purposes we take $\epsilon = \kappa$; then the entanglement temperature is determined by

$$T = \frac{2}{\log(\Lambda_{2N}/\Lambda_1)}, \tag{50}$$

and the energy eigenvalues by

$$\epsilon_s = 1 - 2\frac{\log(\Lambda_s/\Lambda_1)}{\log(\Lambda_{2N}/\Lambda_1)}. \tag{51}$$

IV. INITIAL CONDITIONS

We now discuss the consequences of choosing different initial conditions on the thermal evolution of the system. We are interested in characterizing the long-time coin-position entanglement generated by the evolution of the N-dimensional QW. We consider the case of a separable coin-position initial state. More specifically, we take initial chirality conditions of the form

$$|\psi_{\mathbf{x},0}\rangle = \xi_{\mathbf{x},0}|\chi\rangle, \tag{52}$$

where $\xi_{\mathbf{x},0}$ is a generic position wave function and

$$|\chi\rangle = \cos(\gamma/2)|Z_+\rangle + e^{i\varphi}\sin(\gamma/2)|Z_-\rangle, \tag{53}$$

with

$$|Z_\pm\rangle \equiv \frac{1}{\sqrt{N}}\sum_{\alpha=1}^{N}|\,\alpha_\pm\rangle. \tag{54}$$

The two parameters $\gamma \in [0,\pi]$ and $\varphi \in [0,2\pi]$ define the initial point on the generalized Bloch's sphere. The DFT of Eq. (52) is

$$|\tilde{\psi}_{\mathbf{k},0}\rangle = \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}}|\psi_{\mathbf{x},0}\rangle = \sum_{\mathbf{x}} e^{-i\mathbf{k}\cdot\mathbf{x}}\xi_{\mathbf{x},0}|\chi\rangle. \tag{55}$$

In order to obtain a closed equation for Λ_s we consider in detail the simple case where the amplitudes $\xi_{\mathbf{x},0}$ have an isotropic Gaussian position distribution multiplied by the plane waves $e^{i\mathbf{k_0}\cdot\mathbf{x}}$; that is,

$$\xi_{\mathbf{x},0} \propto e^{i\mathbf{k_0}\cdot\mathbf{x}}\frac{1}{\sigma^{N/2}}\exp\left(-\frac{\mathbf{x}\cdot\mathbf{x}}{\sigma^2}\right), \tag{56}$$

where $\sigma > 0$ is a characteristic width and $\mathbf{k_0}$ is a particular initial momentum that characterizes the initial condition. We deal with a sufficiently large value of σ for the Gaussian so as to make possible the connection of the DFT with the continuous limit. Then, for these values of σ, Eq. (55) can be written as

$$|\tilde{\psi}_{\mathbf{k},0}\rangle \propto \sigma^{N/2}\sum_{\mathbf{x}} e^{-\frac{\sigma^2}{2}(\mathbf{k}-\mathbf{k_0}+2\pi\mathbf{x})^2}|\chi\rangle \tag{57}$$

(see the Appendix). If we want to simulate an uniform initial distribution for the N-dimensional QW, we can take $\sigma \mapsto \infty$ in Eq. (57). In this case we can use the following mathematical property for the Dirac δ:

$$\lim_{\sigma\mapsto\infty}\left(\frac{\sigma}{\sqrt{\pi}}\right)^N e^{-\sigma^2(\mathbf{k}-\mathbf{k_0}+2\pi\mathbf{x})^2} \equiv \delta^N(\mathbf{k}-\mathbf{k_0}+2\pi\mathbf{x}). \tag{58}$$

Equation (57) can then be expressed as

$$|\tilde{\psi}_{\mathbf{k},0}\rangle \propto \left[\sum_{\mathbf{x}}\delta^{N/2}(\mathbf{k}-\mathbf{k_0}+2\pi\mathbf{x})\right]|\chi\rangle. \tag{59}$$

We now assume that the components of $\mathbf{k_0}$ belong to the interval $(-\pi,\pi)$; then in the sum of Eq. (59) the only term that survives is the one for $\mathbf{x} = \mathbf{0}$. This is due to the facts that all components of $\mathbf{k}$ lie within the interval $[-\pi,\pi]$ and that the vector $\mathbf{x}$ has only discrete components. Then using Eq. (24), Eq. (59), and the normalization condition, we have

$$\left|\tilde{f}_{\mathbf{k}}^{(s)}\right|^2 = (2\pi)^N\delta^N(\mathbf{k}-\mathbf{k_0})\left|\langle\phi_{\mathbf{k}}^{(s)}|\chi\rangle\right|^2. \tag{60}$$

Therefore in this case, from Eq. (34), it is straightforward to obtain the eigenvalues for the asymptotic density matrix,

$$\Lambda_s = \left|\langle\phi_{\mathbf{k_0}}^{(s)}|\chi\rangle\right|^2, \tag{61}$$

and their respective eigenfunctions,

$$|\Phi_s\rangle = \left|\phi_{\mathbf{k_0}}^{(s)}\right\rangle. \tag{62}$$

As a second example, we consider a nonseparable coin-position initial state. In particular, we take

$$|\psi_{\mathbf{x},0}\rangle = \int\frac{d^N\mathbf{k}}{(2\pi)^N}\exp[i(\mathbf{k}\cdot\mathbf{x})]|\tilde{\psi}_{\mathbf{k},0}\rangle, \tag{63}$$

with

$$|\tilde{\psi}_{\mathbf{k},0}\rangle = \cos(\gamma/2)\frac{1}{\sqrt{N}}\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(s)}\right\rangle + e^{i\varphi}\sin(\gamma/2)\frac{1}{\sqrt{N}}\sum_{s=N+1}^{2N}\left|\phi_{\mathbf{k}}^{(s)}\right\rangle, \tag{64}$$

and then

$$\left|\tilde{f}_{\mathbf{k}}^{(s)}\right|^2 = \left|\langle\phi_{\mathbf{k}}^{(s)}|\tilde{\psi}_{\mathbf{k},0}\rangle\right|^2 = \frac{1}{N}\begin{cases}\cos^2(\gamma/2) & \text{for} \quad s = 1,2,\ldots,N,\\ \sin^2(\gamma/2) & \text{for} \quad s = N+1,N+2,\ldots,2N.\end{cases} \tag{65}$$

Therefore the eigenvalues Λ_s are the eigenvalues of the matrix associated with the following operator [see Eq. (34)]:

$$\frac{1}{N}\int\frac{d^N\mathbf{k}}{(2\pi)^N}\left\{\cos^2(\gamma/2)\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(s)}\right\rangle\left\langle\phi_{\mathbf{k}}^{(s)}\right| + \sin^2(\gamma/2)\sum_{s=N+1}^{2N}\left|\phi_{\mathbf{k}}^{(s)}\right\rangle\left\langle\phi_{\mathbf{k}}^{(s)}\right|\right\}. \tag{66}$$

As a third example, we take

$$|\tilde{\psi}_{\mathbf{k},0}\rangle = \cos(\gamma/2)\frac{1}{\sqrt{N}}\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(2s)}\right\rangle + e^{i\varphi}\sin(\gamma/2)\frac{1}{\sqrt{N}}\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(2s-1)}\right\rangle, \tag{67}$$

and then

$$\left|\tilde{f}_{\mathbf{k}}^{(s)}\right|^2 = \left|\langle\phi_{\mathbf{k}}^{(s)}|\tilde{\psi}_{\mathbf{k},0}\rangle\right|^2 = \frac{1}{N}\begin{cases}\cos^2(\gamma/2) & \text{for } s \text{ even},\\ \sin^2(\gamma/2) & \text{for } s \text{ odd}.\end{cases} \tag{68}$$

Finally, using Eq. (34), the eigenvalues Λ_s are the eigenvalues of the matrix associated with the operator

$$\frac{1}{N}\int \frac{d^N\mathbf{k}}{(2\pi)^N}\left\{\cos^2(\gamma/2)\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(2s)}\right\rangle\left\langle\phi_{\mathbf{k}}^{(2s)}\right| + \sin^2(\gamma/2)\sum_{s=1}^{N}\left|\phi_{\mathbf{k}}^{(2s-1)}\right\rangle\left\langle\phi_{\mathbf{k}}^{(2s-1)}\right|\right\}. \quad (69)$$

V. APPLICATION TO THE 2D QUANTUM WALK

In this section we illustrate the general treatment introduced above in the special case of the 2D QW. References [6] and [36] introduced a one-parameter family of QW models in two dimensions as a generalization of Grover's model by specifying the corresponding matrix $C_{\mathbf{k}}$ [see Eq. (20)] as

$$C_{\mathbf{k}} = \begin{pmatrix} -pe^{ik_1} & qe^{ik_1} & \sqrt{pq}e^{ik_1} & \sqrt{pq}e^{ik_1} \\ qe^{-ik_1} & -pe^{-ik_1} & \sqrt{pq}e^{-ik_1} & \sqrt{pq}e^{-ik_1} \\ \sqrt{pq}e^{ik_2} & \sqrt{pq}e^{ik_2} & -qe^{ik_2} & pe^{ik_2} \\ \sqrt{pq}e^{-ik_2} & \sqrt{pq}e^{-ik_2} & pe^{-ik_2} & -qe^{-ik_2} \end{pmatrix}, \quad (70)$$

where the parameter $p \in [0,1]$, $q = 1-p$, and $\mathbf{k} = (k_1,k_2)$ is the quasimomentum vector. If $p = q = 1/2$, we have the Grover coin. Henceforth we take this to be the case.

Equation (70) has four eigenvalues λ_s, $s = 1, 2, 3, 4$,

$$\lambda_1 = 1, \quad \lambda_2 = -1, \quad \lambda_3 = e^{i\omega(k_1,k_2)}, \quad \lambda_4 = e^{-i\omega(k_1,k_2)}, \quad (71)$$

where

$$\cos\omega(k_1,k_2) = -\tfrac{1}{2}(\cos k_1 + \cos k_2). \quad (72)$$

The eigenvectors corresponding to the eigenvalues are given by the column vectors

$$\left|\phi_{\mathbf{k}}^{(s)}\right\rangle = \frac{1}{\mathcal{N}_{\mathbf{k}}^{(s)}}\begin{pmatrix} \left(1+e^{-ik_1}\lambda_{\mathbf{k}}^{(s)}\right)^{-1} \\ \left(1+e^{+ik_1}\lambda_{\mathbf{k}}^{(s)}\right)^{-1} \\ \left(1+e^{-ik_2}\lambda_{\mathbf{k}}^{(s)}\right)^{-1} \\ \left(1+e^{+ik_2}\lambda_{\mathbf{k}}^{(s)}\right)^{-1} \end{pmatrix}, \quad (73)$$

where the normalization factors $\mathcal{N}_{\mathbf{k}}^{(s)}$ are given by

$$\mathcal{N}_{\mathbf{k}}^{(1)} = \sqrt{\frac{1}{1+\cos k_1}+\frac{1}{1+\cos k_2}},$$
$$\mathcal{N}_{\mathbf{k}}^{(2)} = \sqrt{\frac{1}{1-\cos k_1}+\frac{1}{1-\cos k_2}}, \quad (74)$$
$$\mathcal{N}_{\mathbf{k}}^{(3)} = \mathcal{N}_{\mathbf{k}}^{(4)} = \sqrt{2\,\frac{4-(\cos k_1+\cos k_2)^2}{(\cos k_1-\cos k_2)^2}}.$$

From Eq. (71), we see that the first two eigenvalues $\lambda_1 = 1$ and $\lambda_2 = -1$ do not depend on k, and the last two eigenvalues are complex conjugates of each other. Equation (72) is a dispersion relation of the system. The frequency $\omega(k_1,k_2) \in [0,2\pi]$, and when $k_1 = 0$ and $k_2 = 0$ the system has a degeneracy because the three eigenvalues $\lambda_2 = \lambda_3 = \lambda_4 = -1$ [see Eqs. (71) and (72)]. Then, due to this degeneracy the frequencies $\pm\omega(k_1,k_2)$, as a function of k_1 and k_2, has a diabolo shape. These degenerate points are called "diabolical points" [19].

A. Quantum-walk temperature for a separable coin-position initial state

In order to calculate Λ_s, Eq. (61), we select the diabolical point $\mathbf{k_0} = \mathbf{0}$, and we must be very careful, because the calculation of the eigenvectors, Eq. (73), has indeterminacies. The eigenvectors of the 2D Grover walk matrix are given by Eq. (73). Whenever $\mathbf{k}$ is not close to a diabolical point these eigenvectors vary smoothly around $\mathbf{k}$. However, we want to study the behavior of the eigenvectors close to the diabolical point at $\mathbf{k} = \mathbf{k}_0 \equiv (0,0)$. We find it convenient to use polar coordinates $(k_1,k_2) = (k\cos\theta, k\sin\theta)$. Performing the limit of (73) for $k \to 0$ we find

$$\left|\phi_{\mathbf{k_0}}^{(1)}\right\rangle = \frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \quad (75)$$

$$\left|\phi_{\mathbf{k_0}}^{(2)}\right\rangle = \frac{i}{\sqrt{2}}\begin{pmatrix}-\sin\theta\\+\sin\theta\\-\cos\theta\\+\cos\theta\end{pmatrix}, \quad (76)$$

$$\left|\phi_{\mathbf{k_0}}^{(3)}\right\rangle = \frac{i}{2\sqrt{2}}\begin{pmatrix}1-\sqrt{2}\cos\theta\\1+\sqrt{2}\cos\theta\\-1+\sqrt{2}\sin\theta\\-1-\sqrt{2}\sin\theta\end{pmatrix}, \quad (77)$$

$$\left|\phi_{\mathbf{k_0}}^{(4)}\right\rangle = \frac{i}{2\sqrt{2}}\begin{pmatrix}-1-\sqrt{2}\cos\theta\\-1+\sqrt{2}\cos\theta\\1+\sqrt{2}\sin\theta\\1-\sqrt{2}\sin\theta\end{pmatrix}. \quad (78)$$

Taking the 2D expression of $|\chi\rangle$ [see Eq. (53)] in its matrix shape,

$$|\chi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}\cos(\gamma/2)\\e^{i\varphi}\sin(\gamma/2)\\\cos(\gamma/2)\\e^{i\varphi}\sin(\gamma/2)\end{pmatrix}, \quad (79)$$

we can evaluate Λ_s [see Eq. (61)]; that is,

$$\Lambda_1 = \tfrac{1}{2}(1+\sin\gamma\cos\varphi), \quad (80)$$

$$\Lambda_2 = \tfrac{1}{4}(1+\sin 2\theta)(1-\sin\gamma\cos\varphi), \quad (81)$$

$$\Lambda_3 = \Lambda_4 = \tfrac{1}{8}(1-\sin 2\theta)(1-\sin\gamma\cos\varphi). \quad (82)$$

Figure 1 shows the dependence of Λ_s, $s = 1,2,3,4$, with the initial conditions given through the parameter

$$x \equiv \sin\gamma\cos\varphi. \quad (83)$$

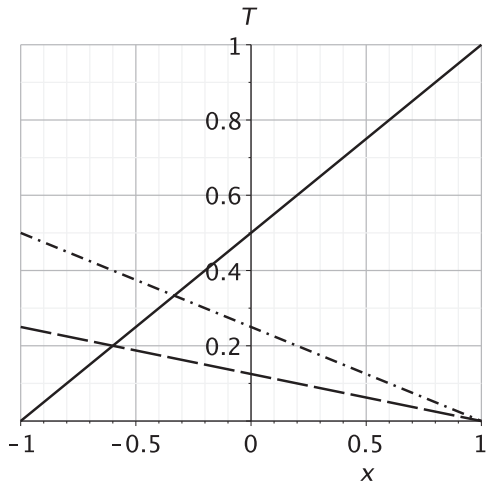

FIG. 1. Eigenvalues of the reduced density matrix [Eqs. (80), (61), and (82)] as a function of the parameter $x = \sin\gamma\cos\varphi$, with $\theta = \pi$. Λ_1, solid line; Λ_2, dashed line; and Λ_3, dot-dashed line.

From Eq. (50), the entanglement temperature in the diabolical point is

$$T = 2/\log\left(\frac{\Lambda_{\max}}{\Lambda_{\min}}\right), \tag{84}$$

where $\Lambda_{\max}$ and $\Lambda_{\min}$ are, respectively, the maximum and minimum value of Λ given by Eqs. (80)–(82).

Equation (84) shows that the QW initial conditions γ, φ, and θ ($\mathbf{k_0}$) determine the entanglement temperature, and for a fixed θ the isothermal lines as a function of the initial conditions are determined by the equation

$$x = \sin\gamma\cos\varphi = \mathcal{C}, \tag{85}$$

where $\mathcal{C}$ is a constant.

In Fig. 2 we see that the temperature as a function of x increases from $T = 0$ for $x = -1$, to the constant value $T_0 = 2/\log 2$ in the x interval $[-3/5, -1/3]$, and then decreases gradually, reaching $T = 0$ at $x = 1$. The isotherms are the intersections of the Bloch sphere with the planes $x =$ constant.

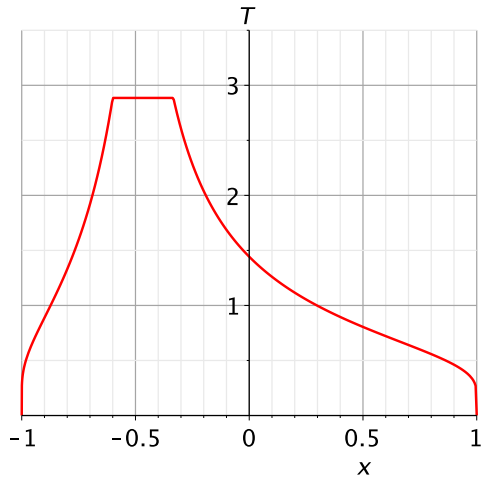

FIG. 2. (Color online) Entanglement temperature [see Eq. (84)] as function of the dimensionless parameter $x = \sin\gamma\cos\varphi$, with $\theta = \pi$.

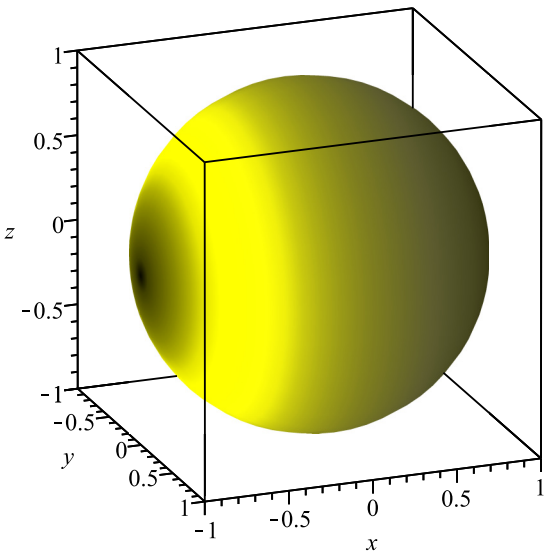

FIG. 3. (Color online) Isotherms on the Bloch sphere. $|Z_+\rangle$ and $|Z_-\rangle$ are the North and South Pole, respectively. The two black points ("cold points," corresponding to $T = 0$) on the sphere are the points $\frac{1}{\sqrt{2}}(|Z_+\rangle + |Z_-\rangle)$ and $\frac{1}{\sqrt{2}}(|Z_+\rangle - |Z_-\rangle)$. The light (yellow) zone is the "hot zone," $T = T_0$.

Figure 3 shows the isotherms for the entanglement temperature as a function of the QW initial position, defined on the Bloch sphere. The figure shows three regions: two dark zones, left and right, corresponding to temperatures $0 < T < T_0$, and a light one, corresponding to the constant temperature $T = T_0$.

B. Quantum-walk temperature for nonseparable coin-position initial state I

Taking the initial state given by Eqs. (63) and (64) and adding Eq. (66), it is easy to show that $\widehat{\varrho}$ reduces to

$$\widehat{\varrho} = \frac{1}{4}\begin{pmatrix} 1 & a & b & b \\ a & 1 & b & b \\ b & b & 1 & a \\ b & b & a & 1 \end{pmatrix}, \tag{86}$$

where

$$a = (1 - 4/\pi)\cos\gamma, \tag{87}$$

$$b = (1 - 2/\pi)\cos\gamma. \tag{88}$$

The eigenvalues of Eq. (86) are

$$\Lambda_1 = [1 - \cos\gamma]/4, \tag{89}$$

$$\Lambda_2 = [1 - (3 - 8/\pi)\cos\gamma]/4, \tag{90}$$

$$\Lambda_3 = [1 - (1 - 4/\pi)\cos\gamma]/4 \tag{91}$$

$$\Lambda_4 = \Lambda_3. \tag{92}$$

The entanglement temperature, Eq. (50), is thus given by

$$T = \frac{2}{\left|\ln\frac{1+(\frac{4}{\pi}-1)\cos\gamma}{1-\cos\gamma}\right|}. \tag{93}$$

Figure 4 shows that the temperature as a function of γ increases from $T = 0$ for $\gamma = 0$, to infinity for $\gamma = \pi/2$, and then decreases gradually to $T = 2/|\ln(1 - 2/\pi)|$ at $\gamma = \pi$. In order

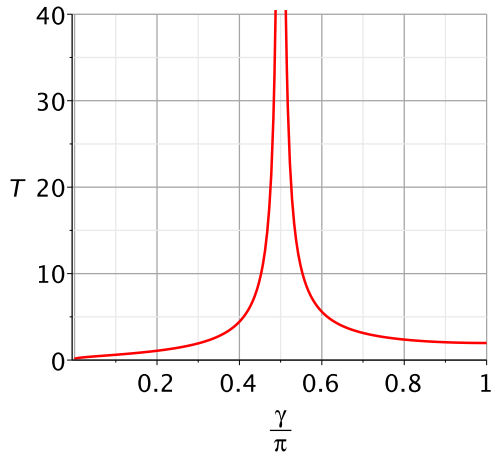

FIG. 4. (Color online) Entanglement temperature [see Eq. (93)] as a function of the dimensionless parameter γ.

to take the initial condition on the generalized Bloch sphere, we redefine

$$|Z_+\rangle \equiv \frac{1}{\sqrt{N}} \sum_{s=1}^{N} |\phi_{\mathbf{k}}^{(s)}\rangle, \tag{94}$$

$$|Z_-\rangle \equiv \frac{1}{\sqrt{N}} \sum_{s=N+1}^{2N} |\phi_{\mathbf{k}}^{(s)}\rangle. \tag{95}$$

Then the initial state, Eq. (64), takes the form

$$|\tilde{\psi}_{\mathbf{k},0}\rangle = \cos(\gamma/2)|Z_+\rangle + e^{i\varphi} \sin(\gamma/2)|Z_-\rangle, \tag{96}$$

where γ and φ define a point on the unit Bloch sphere. In this case the isotherms have a rotation symmetry around the axis defined by the points $|Z_+\rangle$ and $|Z_-\rangle$, the North and South Poles, respectively. Therefore the isotherms are the parallels $z =$ constant on the Bloch sphere. In the northern hemisphere the temperature of the isotherms increases from $T = 0$ at the North Pole to infinity at the Equator, and in the southern hemisphere the temperature of the isotherms decreases from infinity at the Equator to the finite value $T = 2/|\ln(1 - 2/\pi)|$ at the South Pole.

C. Quantum-walk temperature for nonseparable coin-position initial state II

For the 2D case, taking the initial state given by Eq. (67), after some straightforward operations, we can evaluate Λ_s and they satisfy

$$\Lambda_s = \tfrac{1}{4} \quad \text{for} \quad s = 1, 2, 3, 4, \tag{97}$$

which, according to Eq. (50), indicates that the temperature is infinite all over the Bloch sphere, representing a degenerate case. The symmetries of the Grover coin seem to point out that $\widehat{\varrho} = \frac{\hat{I}}{2N}$ for $N > 2$ when we use the initial condition, Eq. (67).

VI. CONCLUSION

During the last 30 years, several technological advances have made it possible to construct and preserve quantum states. They also have increased the possibility of building quantum computing devices. Therefore, the study of the dynamics of open quantum systems becomes relevant for the development of these technologies and of the algorithms that will run on those future quantum computers. The QW has emerged as a useful theoretical tool to study many fundamental aspects of quantum dynamics. It provides a frame to study, among other effects, the entanglement between its degrees of freedom, in a simple setting that often allows for a full analytical treatment of the problem. The study of this kind of entanglement is important in order to understand the asymptotic equilibrium between its internal degrees of freedom.

In this paper we have studied the asymptotic regime of the N-dimensional QW. We have focused on the asymptotic entanglement between chirality and position degrees of freedom and have shown that the system establishes a stationary entanglement between the coin and the position that allows the development of a thermodynamic theory. Then we were able to generalize previous results, obtained in Refs. [15] and [37]. The asymptotic reduced density operator was 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 particle coupled to an infinite bath, the $|x\rangle$ position states. It was shown that the QW initial condition determines the system's temperature, as well as other thermodynamic functions. A map of the isotherms was analytically built for arbitrary localized initial conditions. 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. Thus, if one only had information related to the chirality degrees of freedom, it would be very difficult 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 act on only one subspace could camouflage the unitary character of the global evolution.

The development of experimental techniques has made possible the trapping of samples of atoms using resonant exchanges in momentum and energy between atoms and laser light. However, it is not yet possible to prepare a system with a particular initial chirality. Therefore, the average thermodynamical functions could have more meaning when considered from an experimental point of view. It is interesting to point out that for a given family of initial conditions, such as that given by Eq. (53), the explicit dependence of thermodynamic functions with the initial position on the Bloch's sphere, γ and φ, can be eliminated if we take the average of Λ_s over all initial conditions. Then each family could be characterized by a single asymptotic average temperature.

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APPENDIX

Here we derive Eq. (57). We employ the well-known Poisson summation formula

$$\sum_{n=-\infty}^{n=\infty} g(n) = \sum_{n=-\infty}^{n=\infty} \int_{-\infty}^{\infty} g(x) e^{-i2\pi nx}\, dx, \tag{A1}$$

which, together with Eqs. (55) and (56), leads to

$$\begin{aligned}\sum_{\mathbf{x}} e^{-i(\mathbf{k}-\mathbf{k_0})\cdot\mathbf{x}} \exp\left(-\frac{\mathbf{x}\cdot\mathbf{x}}{2\sigma^2}\right) &= \sum_{\mathbf{x}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-i(\mathbf{k}-\mathbf{k_0})\cdot\mathbf{y}} \exp\left(-\frac{\mathbf{y}\cdot\mathbf{y}}{2\sigma^2}\right) e^{-i2\pi\mathbf{x}\cdot\mathbf{y}} \mathbf{dy} \\ &= \sum_{\mathbf{x}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} e^{-i(\mathbf{k}-\mathbf{k_0}+\mathbf{2\pi x})\cdot\mathbf{y}} \exp\left(-\frac{\mathbf{y}\cdot\mathbf{y}}{2\sigma^2}\right) \mathbf{dy}. \end{aligned} \tag{A2}$$

The last integrals can be evaluated using

$$\int_{-\infty}^{\infty} e^{-p^2x^2 \pm qx}\, dx = \frac{\sqrt{\pi}}{p} \exp\left(-\frac{q^2}{2p^2}\right), \tag{A3}$$

where $p \geqslant 0$. In this way we obtain

$$\sum_{\mathbf{x}} e^{-i\mathbf{t}(\mathbf{k}-\mathbf{k_0})\cdot\mathbf{x}} \exp\left(-\frac{\mathbf{x}\cdot\mathbf{x}}{2\sigma^2}\right) = (\sqrt{2\pi}\sigma)^N \sum_{\mathbf{x}} e^{-\sigma^2(\mathbf{k}-\mathbf{k_0}-\mathbf{2\pi x})^2}. \tag{A4}$$

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