

## Entropy production in the quantum walk

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We explore the notion of generated entropy in open quantum systems. We focus on the study of the discrete-time quantum walk on the line, from the entropy production perspective. We argue that the evolution of the coin can be modeled as an open two-level system that exchanges energy with the lattice at some effective temperature that depends on the initial state. The entropy balance shows that there is a positive-entropy production during the evolution, in accordance with the second law of thermodynamics.

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### I. INTRODUCTION

Over the past two decades, interest in the thermodynamic aspects of quantum systems has increased enormously. Very important results have been obtained, which have led to a greater understanding of issues such as the equilibration and thermalization mechanisms [1,2], the canonical typicality of quantum states [3,4], and the possibility of extracting work from quantum systems [5,6], among many other questions. Some reviews on the current state of the discipline can be found in Refs. [7–10].

One of the first questions that is natural to ask is whether the different magnitudes of classical thermodynamics have a counterpart in quantum systems in such a way that the laws of thermodynamics are preserved in the quantum regime. This is not an easy question to answer, given that the inherently statistical character of the macroscopic thermodynamic properties loses its meaning when studying systems with only a few components. In order to shed light on these issues, the approaches to quantum thermodynamics from paradigms such as the quantum mechanics of open systems or from information theory have been very helpful.

With this idea in mind, we explore the concept of generated entropy in quantum systems. Generated entropy is a key concept in classical thermodynamics, since it allows us to establish the degree of irreversibility associated with a thermodynamic process or, equivalently, it can be associated with the work we could have obtained in an ideal process between the same initial and final states, which is lost due to irreversibilities.

For a classical system that undergoes an infinitesimal process, exchanging energy with an environment at temperature  $T$ , one possible statement of the second law of thermodynamics is

$$dS = \frac{\delta Q}{T} + \delta S_{\text{gen}}, \quad \delta S_{\text{gen}} \geq 0, \quad (1)$$

where  $dS$  is the entropy change of the system,  $\delta Q$  is the heat exchanged with the environment,  $\delta S_{\text{gen}} \geq 0$  is the generated entropy associated with the process, and the equality holds for reversible processes.

Some previous works have addressed the study of entropy production, particularly from an information-theoretic point of view [11,12]. The experimental determination of the entropy production rates in quantum systems has been reported recently [13,14]. In this work we analyze the validity of the expression (1) in the paradigmatic model of the discrete-time quantum walk (DTQW) on the line, from a pure thermodynamic approach.

This paper is organized as follows. In Sec. II we describe the DTQW on the line, in particular its evolution when the initial state is a Gaussian-distributed walker on the positions. In Sec. III the coin's degrees of freedom of the walker are considered as a two-level open system, in contact with a thermal bath, associated with the position's degrees of freedom. Our main result, the entropy generation in the quantum walk on the line, is presented in Sec. IV. Finally, some remarks and perspectives are discussed in Sec. V.

### II. DISCRETE-TIME QUANTUM WALK ON THE LINE

The DTQW on the line [15] evolves in the composed Hilbert space  $\mathcal{H}_n \otimes \mathcal{H}_S$ , where  $\mathcal{H}_n$  is the position space spanned by the basis  $\{|n\rangle\}$ , associated with integer positions in the line, and  $\mathcal{H}_S$ , the chirality space described by the basis  $\{|+\rangle, |-\rangle\}$ . The dynamics is given by successive applications of the operator

$$U = \mathcal{T}(I_n \otimes U_\theta), \quad (2)$$

where  $U_\theta$  is a unitary evolution operator in two dimensions, describing the quantum coin and parametrized by the coin bias parameter  $\theta$ ,

$$U_\theta = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix}. \quad (3)$$

Above,  $\mathcal{T}$  is the conditional translation operator

$$\mathcal{T} = \sum_n |n+1\rangle\langle n| \otimes |+\rangle\langle +| + |n-1\rangle\langle n| \otimes |-\rangle\langle -| \quad (4)$$

and  $I_n$  is the identity operator in  $\mathcal{H}_n$ .

Any pure initial state can be expressed as

$$|\psi(0)\rangle = \sum_n |n\rangle \otimes [a_n(0)|+\rangle + b_n(0)|-\rangle], \quad (5)$$

where  $a_n(0)$  and  $b_n(0)$  satisfy the normalization condition  $\sum_n |a_n(0)|^2 + |b_n(0)|^2 = 1$ . After  $t$  applications of  $U$ , the state will be

$$|\psi(t)\rangle = U^t |\psi(0)\rangle = \sum_n |n\rangle \otimes [a_n(t)|+\rangle + b_n(t)|-\rangle]. \quad (6)$$

Since in general the evolution produces entanglement between the systems, the coin will find itself in a mixed state characterized by its reduced density operator

$$\rho_S(t) = \text{tr}_E |\psi(t)\rangle \langle \psi(t)| \quad (7)$$

whose matrix expression in the basis  $\{|+\rangle, |-\rangle\}$  is

$$\rho_S(t) = \begin{pmatrix} \sum_n |a_n(t)|^2 & \sum_n a_n(t)b_n^*(t) \\ \sum_n a_n^*(t)b_n(t) & \sum_n |b_n(t)|^2 \end{pmatrix}. \quad (8)$$

It is well known that for large  $t$ , the expression (8) becomes stationary, so the coin reaches an equilibrium state that depends on the initial state of the global system [16–23]. In what follows we will focus on the coin evolution, considering it as a two-level open system that equilibrates due to interaction with a large environment, composed by the infinite position degrees of freedom of the walker. In order to highlight the interpretation of  $\mathcal{H}_n$  as a thermal bath, we will consider situations in which many sites of the position's Hilbert space are initially occupied. In the case of bipartite systems with a global Hamiltonian without degenerate gaps, this restriction has been proven to be sufficient to ensure the equilibration on average of the system [2]. We must point out that in the case of the DTQW on an infinite line, an equilibrium state is reached even if the walker is initially localized. However, in spite of this singular behavior, as a rule, some kind of thermodynamic behavior can only be expected if many sites of the environment are occupied. Therefore, we will consider this case, which, on the other hand, is the one of interest in quantum computation algorithms [24,25]. In particular, we will consider the family of initial states

$$\begin{aligned} a_n(0) &= \frac{e^{-n^2/4\sigma^2}}{4\sqrt{2\pi}\sigma^2} \cos(\gamma/2), \\ b_n(0) &= \frac{e^{-n^2/4\sigma^2}}{4\sqrt{2\pi}\sigma^2} \sin(\gamma/2)e^{i\varphi} \end{aligned} \quad (9)$$

corresponding to an initially Gaussian walker, distributed around the origin with a width  $\sigma$  and with arbitrary chirality determined by the angles  $\gamma$  and  $\varphi$ . The asymptotic reduced density matrix for the initial state given by Eq. (9) has been obtained in recent works, in the limit  $\sigma \gg 1$  [26,27],

$$\bar{\rho}_S = \frac{1}{2} \begin{pmatrix} 1 + \cos \alpha \cos \theta & \cos \alpha \sin \theta \\ \cos \alpha \sin \theta & 1 - \cos \alpha \cos \theta \end{pmatrix}, \quad (10)$$

where

$$\cos \alpha = \cos \theta \cos \gamma + \sin \theta \sin \gamma \cos \varphi \quad (11)$$

is the cosine of the angle between the initial Bloch vector

$$\vec{B} = (\sin \gamma \cos \varphi, \sin \gamma \sin \varphi, \cos \gamma) \quad (12)$$

and the vector  $\vec{v}$ ,

$$\vec{v} = (\sin \theta, 0, \cos \theta). \quad (13)$$

### III. THE COIN AS AN OPEN SYSTEM

In order to implement an entropy balance, we must analyze the DTQW on the line, which is essentially a mathematical model, from a physical point of view. As it was previously mentioned, we will consider the coin's degrees of freedom as a two-level system in thermal contact with a large bath, described by the position's Hilbert space  $\mathcal{H}_n$ . To complete the physical description, we must identify the local Hamiltonian, whose expectation value will be defined as the internal energy, and the temperature  $T$  of the lattice experienced by the qubit. In Ref. [26] it is shown that for sufficiently wide position distributions the dependence on the initial state in Eq. (10) can be factorized in such a way that the asymptotic reduced density  $\bar{\rho}_S$  can be written in the canonical distribution form

$$\bar{\rho}_S = \frac{e^{-\beta H'_S}}{\text{tr}(e^{-\beta H'_S})} \quad (14)$$

for a fixed Hermitian operator  $H'_S$ , called the entanglement Hamiltonian,

$$H'_S = -\varepsilon \vec{\sigma} \cdot \vec{v}. \quad (15)$$

Here  $\varepsilon$  is an arbitrary factor with units of energy and  $\vec{\sigma}$  the vector whose components are the Pauli matrices.

The initial-state-dependent entanglement temperature  $T_{\text{ent}} = 1/k_B\beta$  is [28]

$$T_{\text{ent}} = \frac{\varepsilon}{k_B \ln[\tan(\alpha/2)]}, \quad (16)$$

where  $k_B$  is the Boltzmann constant. In addition,  $T_{\text{ent}}$  contains all the dependence on the initial state and is a measure of the entanglement produced during the evolution.

We observe that the asymptotic reduced state (14) can be interpreted as the equilibrium state of a two-level system governed by an effective local Hamiltonian  $H'_S$  that equilibrates due to thermal contact with a heat reservoir at temperature  $T_{\text{ent}}$ . In this case, the temperature is not an intrinsic property of the bath, since it also depends on the initial state of the system through the parameter  $\alpha$ . As a consequence, there is no global attractor for all initial states, but a diameter of equilibrium states, one for each value of  $\alpha$ . This implies that all initial states placed on a circumference orthogonal to the vector  $\vec{v}$  on the Bloch sphere evolve to a common equilibrium state, located at the center of the circumference (see Fig. 1).

We should remark that when narrow initial position distributions are considered, the system cannot be modeled under the system-thermal bath paradigm since the equilibrium state cannot be expressed in the form of Eq. (14) for a fixed Hamiltonian [26].

An additional argument that reinforces the idea of taking  $H'_S$  as the local Hamiltonian arises from the analysis of the numerical simulations. Figure 1 shows the evolution of the reduced state in the Bloch sphere for a Hadamard walk

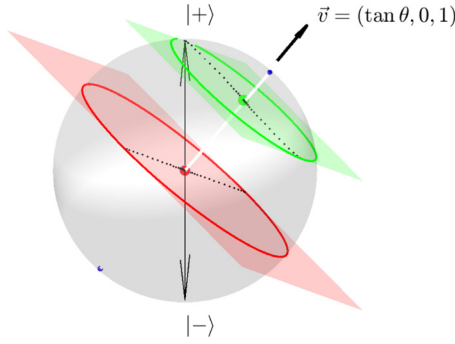


FIG. 1. Time evolution of the Bloch vector associated with the coin state. The initial states considered are Gaussian-distributed walkers with width  $\sigma = 10$  and initial chirality  $|+\rangle$  (green small circle) and  $\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$  (red large circle), respectively. The Bloch vectors are represented by the black dots and converge to the asymptotic state (the center of each circle). The same asymptotic state is reached for all the initial coin states in each circumference.

( $\theta = \pi/4$ ). We notice that for both initial states considered, the Bloch vector at the time  $t + 1$  is very close to the vector that we would obtain by rotating the Bloch vector at time  $t$  an angle  $\eta = \pi$  with respect to the  $\hat{e} = \frac{1}{\sqrt{2}}(1, 0, 1)$  axis. This suggests that the unitary part of the reduced evolution for one step must coincide with such rotation. Recalling the general expression for a rotation operator

$$R_{\eta, \hat{e}} = e^{i\xi} e^{-i(\eta/2)\hat{e}\cdot\vec{\sigma}}, \quad (17)$$

the unitary part of the coin evolution for one step can be obtained by choosing  $\hat{e} = \frac{1}{\sqrt{2}}(1, 0, 1)$ ,  $\eta = -\pi$ , and arbitrary  $\xi$  (in what follows we take  $\xi = 0$  for simplicity),

$$U' = R_{\pi, (1/\sqrt{2})(1,0,1)} = e^{i(\pi/2)H}, \quad (18)$$

where the generator of the rotation  $H$  is the Hadamard operator

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (19)$$

On the other hand, the entanglement Hamiltonian (15) for  $\theta = \pi/4$  is also essentially the Hadamard operator

$$H'_S = -\varepsilon \vec{\sigma} \cdot \vec{v} = -\varepsilon H, \quad (20)$$

which shows that the unitary part of the observed reduced dynamics is generated by the same operator that appears in the expression of the thermal state (14) and supports our argument about considering  $H'_S$  to serve as the local Hamiltonian.

#### IV. GENERATED ENTROPY

Once we have identified the local Hamiltonian and the effective temperature of the thermal bath, we are in a position to implement an entropy balance. We will assume that the entropy of the qubit corresponds to the von Neumann entropy of its reduced state  $\rho_S$ ,

$$S_{vN} = -k_B \text{tr}(\rho_S \ln \rho_S), \quad (21)$$

whose expression in terms of the eigenvalues of  $\rho_S$ ,  $\lambda_{\pm}$ , is [29]

$$S_{vN} = -k_B [\lambda_+ \ln \lambda_+ + \lambda_- \ln \lambda_-]. \quad (22)$$

Defining the internal energy as the expected value of the local Hamiltonian

$$E(t) = \langle H'_S \rangle = -\varepsilon \text{tr}[\rho_S(t)H] \quad (23)$$

and also defining, since there is no work involved, the heat exchanged in one step as the change in the internal energy

$$\delta Q_{t \rightarrow t+1} = E(t+1) - E(t), \quad (24)$$

we will investigate the validity of the expression (1) of the second law of thermodynamics. The entropy generated until step  $t$ , starting from a pure state, which therefore has  $S_{vN}(0) = 0$ , is

$$S_{\text{gen}}(t) = S_{vN}(t) - \frac{Q_{0 \rightarrow t}}{T_{\text{ent}}}, \quad (25)$$

where  $Q_{0 \rightarrow t} = E(t) - E(0)$  is the total heat exchanged during the evolution.

Analyzing the numerical simulations of Fig. 1, we notice that the trajectory defined by the successive nonequilibrium states lies so close to the plane  $\alpha = \text{const}$  that it is not possible to observe them in the figure. This implies that the scalar product of the Bloch vector with the vector  $\vec{v}$  that defines the entanglement Hamiltonian is approximately constant, a fact that, because of the previous definitions, must be interpreted as the approximate conservation of the local energy during the evolution. However, these small energy fluctuations contribute to the generation of entropy in the process, as we will show in the examples below.

In Fig. 2(a) we present the numerical results for the von Neumann entropy as a function of the number of steps, for a Gaussian walker initially centered at the origin, with several values of  $\sigma$ , and the coin initially in the state  $|+\rangle$ . We notice that, in spite of the overall growing trend, the von Neumann entropy oscillates before reaching the asymptotic state. After considering the transport term due to heat flow shown in Fig. 2(b), we notice that the generated entropy [Fig. 2(c)] presents a monotonically increasing behavior. Therefore, whenever the von Neumann entropy of the system decreases, heat is transferred to the environment in an amount such that its increase in entropy exceeds the reduction in the von Neumann entropy.

We note that, although the final value of the entropy does not depend on  $\sigma$ , as long as this width does not take very small values, the evolution to the asymptotic value is faster for small values of  $\sigma$ . This can be understood when the evolution of the occupancy distribution is considered. In Ref. [30] it is shown that the initial Gaussian distribution gradually separates into two Gaussian peaks that move, to the right and to the left, with a velocity that is determined by the parameters of the Hadamard evolution operator. Therefore, the time required for the separation to be complete (within a given approximation) is proportional to the width of the original position distribution. We have verified that when the separation is complete, the entropy stops changing. This explains the slower growth of  $S_{\text{gen}}(t)$  for the larger values of  $\sigma$ .

Numerical simulations show analogous behavior for other nonlocal initial states of the walker, given that many states of the position space are initially occupied. For example, in Fig. 3 we show simulations for the case where the initial state is a uniform superposition of several kets  $|n\rangle$  centered

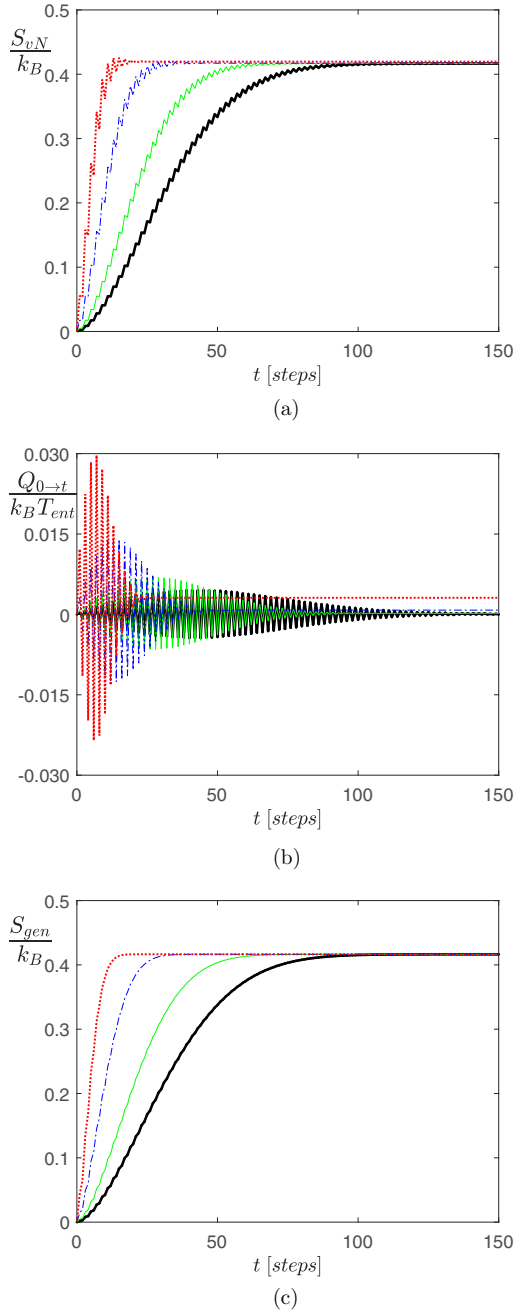


FIG. 2. Dimensionless thermodynamic function for (a) von Neumann entropy, (b) entropy change due to heat transfer, and (c) generated entropy, corresponding to an initially Gaussian-distributed walker, centered at the origin, with  $\sigma = 30$  (black thick line), 20 (green thin line), 10 (blue dot-dashed line), and 5 (red dotted line). The initial chirality is  $|+\rangle$  in all cases.

at the origin. We note that the thermal-state-generated entropy is in good agreement with the one obtained in the previous Gaussian-distributed initial-state case. This supports the use of the same entanglement Hamiltonian in the entropy balance. In Fig. 3 we again notice that the consideration of the entropy flux term corrects the von Neumann entropy oscillations in the evolution towards the asymptotic state. However, in this case, there is a small net contribution from the  $Q_{0 \rightarrow t}/T_{\text{ent}}$  term to the generated entropy.

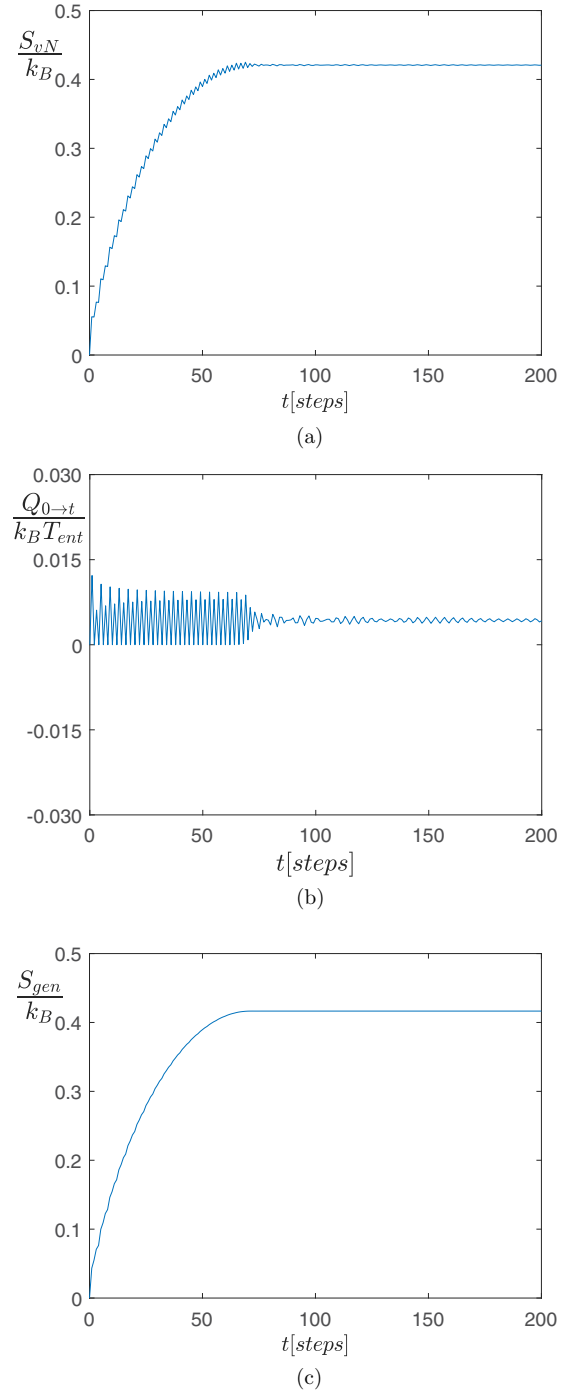


FIG. 3. Similar to Fig. 2 for a walker that starts in a uniform superposition of 101 position states centered at the origin. The initial chirality state is  $|+\rangle$ . The dimensionless thermodynamic function is shown for (a) von Neumann entropy, (b) entropy change due to heat transfer, and (c) generated entropy.

### Consistency with previous work

Reference [12] calculates the entropy generation for open Hamiltonian systems in thermal contact with a large reservoir

$$S_{\text{gen}}(t) = k_B [D(\rho_S(0) || \rho_S^{\text{eq}}) - D(\rho_S(t) || \rho_S^{\text{eq}})], \quad (26)$$

where  $D(\rho || \rho') = \text{tr}(\rho \ln \rho) - \text{tr}(\rho \ln \rho')$  is the relative entropy of the states  $\rho$  and  $\rho'$  and  $\rho_S^{\text{eq}}$  is the equilibrium

state. It is possible to show that the expression (26) is always positive if  $\rho_S^{\text{eq}}$  is a stationary solution of the reduced dynamics. This excludes systems presenting recurrences, but holds for a DTQW evolving on an infinite line.

The consistency between our formalism and Eq. (26) is a direct consequence of the possibility, for initial wide Gaussian position distributions, of writing the equilibrium state in the form of Eq. (14). As an example, note that the asymptotic value of the generated entropy, according to Eq. (26), is

$$S_{\text{gen}}^{\infty} = k_B D(\rho_S(0) || \rho_S^{\text{eq}}). \quad (27)$$

Using the definition of relative entropy and the equilibrium state (14), after some algebra we obtain

$$S_{\text{gen}}^{\infty} = k_B \ln \left[ \frac{2[\tan(\alpha/2)]^{\cos \alpha}}{\sin \alpha} \right]. \quad (28)$$

This coincides with the calculation of the asymptotic value of the von Neumann entropy (22) using the eigenvalues of Eq. (10), as expected since in this case the heat exchanged with the environment  $Q_{0 \rightarrow t}$  is zero, in agreement with the discussion presented in the paragraph following Eq. (25).

For a Hadamard walk with the coin starting in the state  $|+\rangle$ , i.e.,  $\gamma = 0$ , and a Gaussian-distributed walker, Eq. (11) implies that  $\alpha = \pi/4$ . Substituting this value in Eq. (28), we obtain

$$S_{\text{gen}}^{\infty}/k_B = \frac{3}{2} - \frac{\sqrt{2}}{2} \ln(\sqrt{2} + 1) \simeq 0.4165, \quad (29)$$

which coincides with the asymptotic value of Figs. 2(c) and 3(c).

## V. CONCLUSION

The main objective of this work has been the study of the DTQW on the line from the point of view of entropy generation. We considered the chirality degrees of freedom as a two-level system that evolves towards an equilibrium state due to its interaction with a much larger environment, composed by the position degrees of freedom.

It is important to emphasize that the interpretation of  $\mathcal{H}_n$  as a thermal bath could only be established when the initial position occupation level is high. This means that our present study does not include highly localized initial states.

After identifying the local Hamiltonian, we have observed variations in the evolution of its expected value, a fact that can be interpreted as the equivalent of heat transfer with the lattice. This implies, for example, that in optical implementations of quantum walks [31–34], there should always exist energy transfer between the photon and the optical devices. The consideration of the heat transfer term in the entropy balance is of particular importance, since it ensures a monotonic increase in the entropy production during the entire evolution. Since the time-reversed process would imply entropy destruction, our study suggests that, despite being possible due to unitary reversibility, the Gaussian packet narrowing in position space, starting from a highly distributed state, is an extremely unlikely process from the thermodynamic point of view. This is equivalent to saying that, at least in the case of this system, the process of going from a very entangled state to a product state is extremely improbable.

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