Temperature and entanglement of the three-state quantum walk

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Abstract

In the present work, the evolution of a three state quantum walk without decoherence is investigated. Despite being a closed quantum system under unitary evolution, its Hilbert space can be divided in two subspaces, which enables the analysis of the subsystems (the coin or the walker) as an open system in contact with a reservoir. We calculate the asymptotic reduced density matrix of the coin space of the three-state quantum walk in an infinite line, and use that result to analyze the entanglement between the chirality, and position space. We calculate the von Neumann entropy and the entanglement temperature per mean energy of the system in the asymptotic limit.

1. Introduction

Quantum walks are a wide group of dynamical systems that represent the time evolution of a walker on a graph. Those are divided in discrete-time quantum walks and continuous time quantum walks. In this work, we are interested in discrete-time quantum walks on a one-dimension position space, that is, on the lattice sites (vertices) of a line. The study of quantum walks started as a generalization of the classical random walks to quantum systems. However, some of their properties have attracted the attention of researchers to the possibility of using them as a mathematical tool to build quantum algorithms. Among those properties, we can cite: (i) the quantum walk in one dimension spreads ballistically, i.e., quadratically faster than the random walk. (ii) The amount of time taken to reach the limiting distribution of a quantum walk is quadratically faster than its classical counterpart. (iii) It has been proved that quantum walks, under particular conditions, can be used to implement a model of universal computation [1, 2]. (iv) The quantum walk can be used to simulate analogous systems, such as relativistic quantum mechanical systems [3].

The three-state quantum walk is a generalization of the usual Hadamard walk, where the probability of the walker to stay still (in the same vertex of the graph) in a time step of the dynamics of the system is also taken into account. In the classical case, this additional consideration does not add much difference to the behavior of the system. On the other hand, for the quantum case, the addition of one degree of freedom in the chirality space causes a huge difference on the evolution of the position probability distribution. The probability amplitude of staying in the same vertex can generate a localization on the initial position. This property has been analyzed previously in [4–6]. The analysis of evolution of partial Hilbert spaces in quantum walks has a close connection to the evolution of quantum open systems, when the walker Hilbert space acts as a reservoir for the coin (chirality subspace), which tends to reach equilibrium in the asymptotic regime with the former. This dynamical process of equilibration clearly motivates one to question whether it is possible or not for it to be described as thermalization, in which case a definition of temperature for the walker subsystem must be defined. It was previously proposed [7–12] that the entanglement between the position and chirality space allows one to define a so called 'entanglement temperature', which in some specific situations may correspond to the Gibbs temperature.

This paper has two significant contributions. The first one is the calculation of the steady state reduced density matrix, which was done for a specific coin but can be easily extended to other types of the
dimensional coins using the same method. The second one is the extension of the calculation of the entanglement entropy and temperature for the three state quantum walk. An informational, and thermodynamic analysis of the two state quantum walk has been approached by other works recently [7–12], as well as the lazy quantum walk [4–6, 13]. The paper connects these two studies, analyzing the three state quantum walk from a thermodynamic perspective. We analyze the entanglement between the position and chirality space in the asymptotic limit of the three-state quantum walk using the tools defined in references [7, 11, 12]. We obtain an expression for the asymptotic coin density matrix as a function of the initial conditions. With that, we calculate the entanglement entropy and derive a concept of temperature, assuming that the system achieves the Gibbs state in the asymptotic limit, when it thermalizes with the bath.

The paper is organized as follows. Firstly, in section 2, we introduce the notation making an overview of the three-state quantum walk on the infinite line. Then, in section 3, we use the results of [6] to calculate the asymptotic reduced density matrix of the three-state quantum walk. In section 4 we present our results concerning the thermodynamics of the three-state quantum walk, i.e., the values of entropy and temperature depending on the initial condition. Finally, in section 5, we present the last remarks and conclusions.

2. Three-state quantum walk

The principle behind the three-state quantum walk—also known as the lazy quantum walk—on a line is similar to the two-state one-dimension quantum walk [14]. Therefore the approach we employ to the analysis in this and in the following section is analogous to the one used to characterize the chirality space and thermodynamics of the two-state quantum walk [7]. The main difference between the two and three-state walks is that in the second case the chirality space has three dimensions, therefore, besides the possibility of going to the left or right, the probability of staying in the same site (vertex) is also taken into account. One can interpret this as a walk with a three-sided ‘coin’. Figure 1 illustrates the possible steps of a walk at the nth site of the lattice.

Mathematically speaking, the joint system is composed by two subsystems, with Hilbert space given by

$$\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C,$$

where $\mathcal{H}_P$ is the position Hilbert space with infinite dimension, and $\mathcal{H}_C$ is the ‘coin’ Hilbert space with dimension 3. The state of the system, denoted as $|\psi(t)\rangle$, evolves according to a unitary evolution that can be recast in a sequence of two operators—one responsible for the flip of the ‘coin’ (C) and the other for the conditioned shift of the walker in the sites of the lattice (Sh)

$$|\psi(t + 1)\rangle = U|\psi(t)\rangle = (\text{Sh}(\mathbb{I} \otimes C))|\psi(t)\rangle.$$  

The operator we will consider here to represent the action of the ‘coin’ toss is

$$C = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix},$$

known as Grover coin [6], spanned in terms of the basis \{|L\}, |S\}, |R\} representing, respectively, left, stay, and right chirality. This specific operator was chosen since it generates the generalized version of the Hadamard walk on a line [4]. The shift of the walker, conditioned on the coin state is given by

$$\text{Sh} = \sum_{n=-\infty}^{\infty} |n-1\rangle \langle n| \otimes |L\rangle \langle L| + \sum_{n=-\infty}^{\infty} |n\rangle \langle n| \otimes |S\rangle \langle S| + \sum_{n=-\infty}^{\infty} |n+1\rangle \langle n| \otimes |R\rangle \langle R|.$$  

The state of the system at time $t$ can be written as

$$|\psi(t)\rangle = U^t|\psi_0\rangle = \sum_{n=-\infty}^{\infty} \left( \begin{array}{c} a_n(t) \\ b_n(t) \\ c_n(t) \end{array} \right) |n\rangle,$$

where the action of the ‘coin’ and shift operators can be summarized in the following recurrence relations
Figure 1. Diagram of the three-state quantum walk. The coefficients \( a_n, b_n \) and \( c_n \) correspond to the left (L), no movement (S) and right (R) chiralities, respectively.

\[
a_n(t+1) = \frac{1}{3}(-a_{n+1}(t) + 2b_{n+1}(t) + 2c_{n+1}(t)),
\]

\[
b_n(t+1) = \frac{1}{3}(2a_n(t) - b_n(t) + 2c_n(t)),
\]

\[
c_n(t+1) = \frac{1}{3}(2a_{n-1}(t) + 2b_{n-1}(t) - c_{n-1}(t)).
\]

Equation (6)

Therefore, defining the global chirality probabilities (GCP) of the walk in an analogous way to the two-state walk [15],

\[
P_L(t) = \sum_{n=-\infty}^{\infty} |a_n(t)|^2,
\]

\[
P_S(t) = \sum_{n=-\infty}^{\infty} |b_n(t)|^2,
\]

\[
P_R(t) = \sum_{n=-\infty}^{\infty} |c_n(t)|^2.
\]

Equation (7)

One can use equation (6) to find the recurrence relation of the GCP

\[
\begin{pmatrix}
P_L(t+1) \\
P_S(t+1) \\
P_R(t+1)
\end{pmatrix}
= \frac{1}{9}
\begin{pmatrix}
1 & 4 & 4 \\
4 & 1 & 4 \\
4 & 4 & 1
\end{pmatrix}
\begin{pmatrix}
P_L(t) \\
P_S(t) \\
P_R(t)
\end{pmatrix}
- \frac{\Re[Q_1(t)]}{9}
\begin{pmatrix}
4 \\
4 \\
-8
\end{pmatrix}
- \frac{\Re[Q_2(t)]}{9}
\begin{pmatrix}
4 \\
-8 \\
4
\end{pmatrix}
- \frac{\Re[Q_3(t)]}{9}
\begin{pmatrix}
4 \\
4 \\
4
\end{pmatrix},
\]

Equation (8)

where the terms \( Q_1(t), Q_2(t) \) and \( Q_3(t) \), are given by

\[
Q_1(t) = \sum_{n=-\infty}^{\infty} a_n(t)b_n^*(t);
\]

\[
Q_2(t) = \sum_{n=-\infty}^{\infty} a_n(t)c_n^*(t);
\]

\[
Q_3(t) = \sum_{n=-\infty}^{\infty} b_n(t)c_n^*(t),
\]

Equation (9)

which are responsible for the interference effects of the walk, and consequently for its quantum behavior. For comparison, the presence of decoherence would cause the terms appearing in (9) to vanish and therefore, instead of (8) we would have

\[
\begin{pmatrix}
P_L(t+1) \\
P_S(t+1) \\
P_R(t+1)
\end{pmatrix}
= \frac{1}{9}
\begin{pmatrix}
1 & 4 & 4 \\
4 & 1 & 4 \\
4 & 4 & 1
\end{pmatrix}
\begin{pmatrix}
P_L(t) \\
P_S(t) \\
P_R(t)
\end{pmatrix},
\]

Equation (10)

which describes the evolution of the GCPs as a classical Markovian process. This map can then be solved analytically to obtain the vector of probabilities as function of the initial condition after \( k \) time steps.
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Figure 2. Distribution after 100 time steps. Two different initial conditions were considered—one that generates localization, $|\psi_0\rangle = \frac{1}{\sqrt{2}}(i, 0, 1)^T|0\rangle$, in light gray (red) and one that does not, $|\psi_0\rangle = \frac{1}{\sqrt{6}}(1, -2, 1)^T|0\rangle$, in black.

\[
\begin{pmatrix}
    P_L(kt) \\
    P_S(kt) \\
    P_R(kt)
\end{pmatrix} = M \begin{pmatrix}
    P_L(0) \\
    P_S(0) \\
    P_R(0)
\end{pmatrix},
\]

(11)

where

\[
M = \frac{1}{3} \begin{pmatrix}
    1 + 2 \left(\frac{-1}{3}\right)^k & 1 - \left(\frac{-1}{3}\right)^k & 1 - \left(\frac{-1}{3}\right)^k \\
    1 - \left(\frac{-1}{3}\right)^k & 1 + 2 \left(\frac{-1}{3}\right)^k & 1 - \left(\frac{-1}{3}\right)^k \\
    1 - \left(\frac{-1}{3}\right)^k & 1 - \left(\frac{-1}{3}\right)^k & 1 + 2 \left(\frac{-1}{3}\right)^k
\end{pmatrix}.
\]

(12)

The asymptotic limit of this process gives equal probabilities for each chirality independent of the initial conditions, i.e.,

\[
\lim_{n \to \infty} \begin{pmatrix}
    P_L(kt) \\
    P_S(kt) \\
    P_R(kt)
\end{pmatrix} = \begin{pmatrix}
    1/3 \\
    1/3 \\
    1/3
\end{pmatrix}.
\]

(13)

If this stationary state could be seen as a thermalization process, the final distribution of chiralities would indicate that the system is coupled to a bath of infinite temperature. The meaning of this and comparisons with the quantum case will be addressed in the next sections.

Returning to the full description of the quantum walk as given by (8), the simple unitary evolution of the quantum walk considering interference effects can be easily simulated. Figure 2 shows the probability distribution of positions of the three-state quantum walk after 100 time steps. We consider that the walker starts at position 0. Depending on specific chirality initial conditions, a peak in the distribution is observed at the initial location of the walker, indicating localization. This happens due to the fact that one of the eigenvectors of the evolution operator of the Fourier space of the system is constant, as it will be further explored in the next section.

To calculate the distributions presented in figure 2 we have to perform a partial trace over the chirality space. The aim of this work, however, is to analyze the entanglement between both—chirality and position—spaces and this can be done by tracing over any space, as the joint system state is pure. Since the chirality space has a lower dimension, choosing to work with its reduced density matrix will make the calculations less laborious. The chirality reduced density matrix is given by

\[
\rho_c(t) = \begin{pmatrix}
    P_L(t) & Q_1(t) & Q_2(t) \\
    Q_1^*(t) & P_S(t) & Q_3(t) \\
    Q_2^*(t) & Q_3^*(t) & P_R(t)
\end{pmatrix}.
\]

(14)
3. Asymptotic limit

We are interested in equilibrium solutions of the evolution. Therefore, we consider the asymptotic reduced state of the walk,

$$\rho_{c, \infty} = \lim_{t \to \infty} \rho_c(t).$$  \hspace{1cm} (15)

Throughout our calculations, we consider a localized initial condition in the position space, which means that the chirality components can take any value, but the initial space component is $|0\rangle$:

$$|\psi_0^n\rangle = \begin{pmatrix} a \\ b \\ c \end{pmatrix} |0\rangle.$$  \hspace{1cm} (16)

A method similar to the one used in reference [16] to calculate the asymptotic state of the two-state quantum walk is applied. Considering the Fourier transform of the wave function of the system, $\tilde{\Psi}(k, t)$, the equation describing the dynamics of the walk is

$$\tilde{\Psi}(k, t) = \tilde{M}^t \tilde{\Psi}(k, 0),$$  \hspace{1cm} (17)

where, in its diagonal form, the matrix $\tilde{M}$ has two time dependent eigenvalues ($\lambda_2$, $\lambda_3$) and a constant one ($\lambda_1 = 1$) [4, 6]. The constant eigenvalue is responsible for the main difference in the behavior of the two and three-state quantum walk, because it causes a localization around the walker’s initial position. The localization will depend on the action of the matrix of eigenvectors of $\lambda_1$ in the initial condition. Using its diagonal form, the evolution operator $\tilde{M}$ can be decomposed as

$$\tilde{M}^t = \tilde{M}_1 + \lambda_2 \tilde{M}_2 + \lambda_3 \tilde{M}_3.$$  \hspace{1cm} (18)

The matrices $\tilde{M}_1$, $\tilde{M}_2$ and $\tilde{M}_3$ are composed by the eigenvectors of $\tilde{M}$. The state vector is obtained performing the inverse Fourier transform. A more detailed explanation of this procedure can be found on [6], where the asymptotic limit distribution was calculated with the matrices $U_1$, $U_2$ and $U_3$, defined in such a way that in the limit of $t \to \infty$ the state vector is

$$|\psi_\infty^n\rangle = (U_1(n) + U_2(n) + U_3(n))|\psi_0^n\rangle.$$  \hspace{1cm} (19)

To obtain the asymptotic reduced density matrix of the three-state quantum walk, we used the numerical calculations presented in the supplementary material of [6], where the matrices $\tilde{M}_1$, $\tilde{M}_2$ and $\tilde{M}_3$ were obtained using the saddle point method. Those results suggest that to calculate the asymptotic density matrix, $\rho_{c, \infty} = \sum_n |\psi_\infty^n\rangle \langle \psi_\infty^n|$, the cross terms—terms that involve different $U$ matrices—should not be considered. This is due to the fact that the functions $\langle \psi_0^n|U_1|U_2 + U_3\rangle + (U_2 + U_3)^\dagger U_1 |\psi_0^n\rangle$ and $\langle \psi_0^n|U_2^T U_3 + U_3^T U_2 |\psi_0^n\rangle$ are not nonnegative quantities, hence cannot be interpreted as probabilities and both functions oscillate and average to zero (see [6]). Therefore

$$\rho_{c, \infty} = \sum_n |\psi_\infty^n\rangle \langle \psi_\infty^n| = \sum_n U_1|\psi_0^n\rangle \langle \psi_0^n|U_1^\dagger + U_2|\psi_0^n\rangle \langle \psi_0^n|U_2^\dagger + U_3|\psi_0^n\rangle \langle \psi_0^n|U_3^\dagger.$$  \hspace{1cm} (20)

The analytical form of $\rho_{c, \infty}$ is too large to be displayed here. However, we present it in appendix A. The confirmation of our results, by comparing the evolution of the state and the asymptotic result is provided in the appendix B.

4. Entanglement entropy and temperature

Figure 3 shows values for the norm of the asymptotic generalized Bloch vector for all possible initial conditions of the type

$$|\psi_{G, 0}^0\rangle = \begin{pmatrix} \cos \theta \\ 0 \\ \sin \theta e^{i\phi} \end{pmatrix} |0\rangle.$$  \hspace{1cm} (21)

We see that $|B_\infty| < 1$, meaning that although the initial chirality state is pure, as the evolution occurs, it goes to a mixed state. This behavior is due to the entanglement between position and the chirality spaces, which can be quantified by the entanglement entropy, or von Neumann entropy

$$S = - \text{Tr}(\rho_c \log \rho_c).$$  \hspace{1cm} (22)
The entanglement entropy can be calculated at any time step, since our goal here is to analyze the asymptotic limit of the three-state quantum walk, we present the entropy after 400 time steps and the asymptotic entropy of the walk for initial conditions of the type (21), without any loss of generality, figure 4. One can see that the symmetries of the colormap of the norm of the Bloch vector are preserved in the colormap of the asymptotic values of entropy. This is due to the fact that both variables are connected, i.e., if a state has a Bloch vector of size 1 it is pure ($S = 0$), as the norm of $B$ decreases the state becomes mixed and entropy increases. We see that the minimum values of the entropy in the asymptotic limit are achieved around ($\phi = 0, \theta = 3\pi/2$) and ($\phi = \pi, \theta = \pi/2$) and the maximum around ($\phi = \pi, \theta = 3\pi/2$) and ($\phi = 0, \theta = \pi/2$). After 400 time steps the asymptotic pattern has begin to form and the minimums are the same as for $t = \infty$. 

Figure 3. Norm of the asymptotic generalized Bloch vector.

Figure 4. Entropy of the three-state quantum walks with initial condition of the type (21) after $t = 400$ time steps (upper panel) and in the asymptotic limit (lower panel).
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One important aspect to notice at this point is that the localization generated by the walk, i.e., the probability of the walker being at position 0 in the asymptotic limit, is given by \[ P(0, t = \infty) = (a^* \ b^* \ c^*) U_1^d U_1 b^* c^* \]

\[ = (5 - 2\sqrt{6}) \left[(2a + b)a^* + (a + b + c)b^* + (b + 2c)c^* \right], \tag{23} \]

where \(a, b\) and \(c\) are the initial chirality components. Therefore, all initial conditions of the type (21) have localization \(10 - 4\sqrt{6} \approx 0.2\). This means that, although both features depend on the initial condition, there is no direct connection between the localization of the walk and its entanglement entropy.

A variable called entanglement temperature \(T_E\) can be defined with the help of the von Neumann entropy [12]. The main idea is to apply the definition from classical thermodynamics,

\[
\frac{1}{T} = \frac{\partial S_{\text{class}}}{\partial E},
\tag{24}
\]

where \(S_{\text{class}}\) stands for the equilibrium thermodynamic entropy. Since the von Neumann entropy is the quantum extension of the statistical entropy—besides a \(k_B\) factor—we extend this definition to the quantum case by considering the equivalence of both. To simplify the calculation, we consider \(k_B = 1\). This definition was used in [12] to calculate the entanglement temperature of the two-state discrete-time quantum walk, so, in principle we could also use it to calculate the entanglement temperature of the three-state quantum walk,

\[
\frac{1}{T_E} = \frac{\partial S}{\partial E}.
\tag{25}
\]

The problem in calculating the entanglement temperature in the case of the three-state quantum walk is that the mean value of another observable, besides the energy, is required to be used as a constraint [11]. This means that, unlike the two-state case, we will not be able to calculate the entanglement temperature at an arbitrary time. In the asymptotic limit, however, this restriction is surpassed if we note that system converges to an equilibrium distribution. Assuming the asymptotic state to be a Gibbs state provides a third constraint, and the process can be analyzed as a thermalization. We also performed the reverse calculation, i.e., we used the resultant expression of temperature to find the entropy definition (25). This was already known to be true, but the exercise of calculating it from the temperature is relevant to confirm that there are no inconsistencies in our results.

Let us start by writing the eigenvalues of the density matrix when the system (chirality) achieves equilibrium with the bath (walker)

\[
\tau_j = \frac{e^{-\beta \epsilon_j}}{Z} = \frac{e^{-\beta \epsilon_1}}{e^{-\beta \epsilon_1} + e^{-\beta \epsilon_2} + e^{-\beta \epsilon_3}}, \tag{26}
\]

where \(\epsilon_j\) and \(\tau_j\) are the energies and probabilities of being in each level, and the index \(j\) stands for 1, 2 or 3. The Gibbs temperature per difference of energy can be obtained dividing any two of the three eigenvalues as

\[
\frac{T_G}{\epsilon_j' - \epsilon_j} = \frac{1}{\log \left( \frac{\tau_j'}{\tau_j} \right)}. \tag{27}
\]

In the two-state quantum walk, the temperature per difference of energy is well defined. In the present case, however, since there are three different ways of defining the temperature per difference of energy, it is more convenient to define the Gibbs temperature per mean energy. To derive this definition we set \(H\) to be traceless, which is the same as choose the energy spectrum to be measured from the zero energy level.

Using the fact that the mean energy is given by

\[
E = \text{Tr}[H \rho_0] = \epsilon_1 \tau_1 + \epsilon_2 \tau_2 + \epsilon_3 \tau_3, \tag{28}
\]

and that, we chose to define \(H\) such that the sum of the three eigenenergies is null,

\[
\epsilon_1 + \epsilon_2 + \epsilon_3 = 0. \tag{29}
\]

Dividing expressions (26) of \(\tau_1\) by the other two eigenvalues we find

\[
\frac{\tau_1}{\tau_2} = e^{-\beta (\epsilon_1 - \epsilon_2)} = e^{-\beta (2\epsilon_1 + \epsilon_3)},
\]

\[
\frac{\tau_1}{\tau_3} = e^{-\beta (\epsilon_1 - \epsilon_3)}, \tag{30}
\]

\[
\frac{\tau_2}{\tau_3} = e^{-\beta (2\epsilon_1 + \epsilon_3)}.
\]

\[
\tau_1 = \tau_2 = \tau_3 = 0.
\]

\[
\frac{\tau_1}{\tau_2} = e^{-\beta (\epsilon_1 - \epsilon_2)} = e^{-\beta (2\epsilon_1 + \epsilon_3)},
\]

\[
\tau_1 = \tau_2 = \tau_3 = 0.
\]

\[
\tau_1 = \tau_2 = \tau_3 = 0.
\]
where we used that \(1 = \tau_1 + \tau_2 + \tau_3\) in the first line. Then, multiplying both expressions we get

\[
\frac{\tau_1^2}{\tau_2 \tau_3} = e^{-\beta E_1} \Rightarrow \epsilon_1 = -\frac{T_G}{3} \log \left( \frac{\tau_1^2}{\tau_2 \tau_3} \right).
\] (31)

Following an analogous procedure, we obtain the expressions of the other eigenenergies

\[
\begin{align*}
\tau_2 \epsilon_2 &= -\frac{T_G}{3} \tau_2 \log \left( \frac{\tau_2^2}{\tau_1 \tau_3} \right), \\
\tau_3 \epsilon_3 &= -\frac{T_G}{3} \tau_3 \log \left( \frac{\tau_3^2}{\tau_1 \tau_2} \right).
\end{align*}
\] (32)

Now the mean energy (28) can be written as a function of the temperature and the eigenvalues of the density matrix only,

\[
E = -\frac{T_G}{3} \left[ \tau_1 \log \left( \frac{\tau_1^2}{\tau_2 \tau_3} \right) + \tau_2 \log \left( \frac{\tau_2^2}{\tau_1 \tau_3} \right) + \tau_3 \log \left( \frac{\tau_3^2}{\tau_1 \tau_2} \right) \right],
\] (33)

which leads to the final expression for the temperature per mean energy

\[
T = \frac{T_G}{E} = -3 \left[ \tau_1 \log \left( \frac{\tau_1^2}{\tau_2 \tau_3} \right) + \tau_2 \log \left( \frac{\tau_2^2}{\tau_1 \tau_3} \right) + \tau_3 \log \left( \frac{\tau_3^2}{\tau_1 \tau_2} \right) \right]^{-1}. \] (34)

Figure 5 shows the result of \(|T|\) for two types of initial conditions, namely

\[
|\psi_{0_1}^0\rangle = \left( \begin{array}{c} \cos \theta \\ \sin \theta e^{i\phi} \end{array} \right) |0\rangle, \quad \text{and} \quad |\psi_{0_2}^0\rangle = \left( \begin{array}{c} \cos \theta / \sqrt{2} \\ 1 / \sqrt{2} \sin \theta e^{i\phi} \end{array} \right) |0\rangle.
\] (35)

For the first initial condition, which is the same as the one used to generate the colormaps of \(B_\infty\) and \(S_\infty\), we see that the symmetry is preserved again. This is due to the connection between the entropy and \(T\) that will be derived further (39). The second set of initial conditions generates a colormap that differs from the first one in many aspects, but have some of the minimums and maximums at the same place.

Manipulating expression (33) we can write \(E\) as a function of the von Neumann Entropy and of the partition function, \(Z = \text{Tr}[e^{-\beta H}]\). To do that, we first isolate the energy

\[
E = -\frac{T_G}{3} \left[ \tau_1 \log(\tau_1^2) - \tau_1 \log(\tau_2 \tau_3) + \tau_2 \log(\tau_2^2) - \tau_2 \log(\tau_1 \tau_3) + \tau_3 \log(\tau_3^2) - \tau_3 \log(\tau_1 \tau_2) \right],
\] (36)

then substituting the entropy \(S = -\sum_{j=1}^{3} \tau_j \log(\tau_j)\), we find

\[
E = -\frac{T_G}{3} \left[ -2S - \tau_1 \log(\tau_2 \tau_3) - \tau_2 \log(\tau_1 \tau_3) - (1 - \tau_2 - \tau_1) \log(\tau_1 \tau_2) \right],
\] (37)

which leads to

\[
E = -\frac{T_G}{3} \left[ -3S + \log \left( \frac{1}{\tau_1 \tau_2 \tau_3} \right) \right].
\] (38)

Finally, substituting the eigenvalues by the Gibbs probabilities we conclude that the von Neumann entropy is

\[
S = \frac{E}{T_G} + \log(Z),
\] (39)

and, consequently, the definition (25) is valid for the Gibbs temperature.

\[
\frac{\partial S}{\partial E} = \frac{1}{T_G} \Rightarrow T_k = T_G.
\] (40)

This was already expected, since we started by using the Gibbs distribution to describe the system after it equilibrates with the bath, and is in accordance with [17]. In the appendix B we give an independent proof of this argument.
5. Conclusions

It is clear that the evolution of the chirality space of the two and three-state quantum walk is an equilibration process. Under certain conditions [18], such a process can also describe thermalization. Here we analyzed the subsystem of the coin of a three-state quantum walk from the point of view of the theory of quantum open systems. In references [8, 12] it was shown that for the two-state case the coin state converges to a thermal state. Here we considered that for the three-state quantum walk the equilibrium state is also thermal and used the canonical ensemble to derive a definition of temperature per mean energy.

First, we calculated the asymptotic reduced density matrix for the three-state quantum walk using the saddle point method. Then the von Neumann entropy was calculated for different initial conditions and different times, including the asymptotic limit. In opposition to the case of the Hadamard walk, the temperature of the three-state quantum walk can only be defined in the asymptotic limit. We calculated the expression for this temperature as a function of the eigenvalues of the asymptotic reduced density matrix, which depends on the initial conditions. We then see that, in contrast with the three-state random walk that always equilibrates with equal chirality probabilities—which would correspond to $T = \infty$ if the process could be described as a thermalization—the three-state quantum walk temperature depends on the initial condition.

The paper relies on the hypothesis that in the asymptotic limit the state achieves equilibrium with the bath (position space). The Hamiltonian of this process is an effective Hamiltonian. This assumption was motivated by previous references for the two-state quantum walk [7–9], and was reinforced by the fact that the dimension of the position subspace is large in comparison to the coin subspace, and the chirality distribution has well defined asymptotic values.

The validity of this hypothesis can be questioned and might be the subject of future work. We also remark that the asymptotic matrix, as well as the entropy and generalized Bloch values do not rely on that hypothesis. The entanglement entropy, and the generalized Bloch vector are relevant variables to the
quantification of the entanglement caused by the dynamics of the process (specifically the shift operator). The asymptotic matrix, on the other hand, can be used in any analysis of the asymptotic behavior of the coin subspace of this system. Furthermore, the expression derived for the temperature per mean energy was not derived explicitly for the three-state quantum walk only, but for any three-level system that achieves thermal equilibrium with a reservoir, therefore it can be used in other works where this assumption is valid.

The results obtained in the paper make room to the view of the three-state quantum walk as a thermodynamic system giving space to other ideas and analyses emerge, e.g., the entanglement analysis of the system under decoherence.

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Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

Appendix A. Asymptotic reduced density matrix

Here we present the asymptotic reduced density matrix of the three-state quantum walk calculated with Wolfram Mathematica, with the help of the complement material of [6]. This matrix was used to calculate the asymptotic results of the three-state quantum walk sections 3 and 4.

Considering an initial condition of the type (16) the reduced density matrix has the following form

$$\rho_{\infty} = \begin{pmatrix}
\rho_{\infty,11} & \rho_{\infty,12} & \rho_{\infty,13} \\
\rho_{\infty,21} & \rho_{\infty,22} & \rho_{\infty,23} \\
\rho_{\infty,31} & \rho_{\infty,32} & \rho_{\infty,33} 
\end{pmatrix}, \quad (A1)
$$

where the matrix elements are presented in equation (A2).

$$\rho_{\infty,11} = \frac{1}{48} \left((48 - 11\sqrt{6})a + 6(-8 + 3\sqrt{6})b + (-48 + 19\sqrt{6})c) \right) a^*$$
$$+ 2(3(-8 + 3\sqrt{6})a + \sqrt{6}(3b + c)) b^* + ((-48 + 19\sqrt{6})a + \sqrt{6}(2b + 5c)) c^* \right),$$

$$\rho_{\infty,22} = \frac{1}{24} \left((3\sqrt{6}a + 24b - 10\sqrt{6}b + 48c - 19\sqrt{6}c) a^*$$
$$+ 2((12 - 5\sqrt{6})a - 3(-4 + \sqrt{6})b + (12 - 5\sqrt{6})c) b^*$$
$$+ (48a - 19\sqrt{6}a + 24b - 10\sqrt{6}b + 3\sqrt{6}c) c^* \right),$$

$$\rho_{\infty,33} = \frac{1}{48} \left((5\sqrt{6}a + 2\sqrt{6}b - 48c + 19\sqrt{6}c) a^* + 2(\sqrt{6}a + 3\sqrt{6}b - 24c + 9\sqrt{6}c) b^*$$
$$+ ((-48 + 19\sqrt{6})a + 6(-8 + 3\sqrt{6})b + (48 - 11\sqrt{6})c) c^* \right),$$

$$\rho_{\infty,12} = (\rho_{\infty,21})^* = \frac{1}{24} \left((3(-8 + 3\sqrt{6})a + 96b - 39\sqrt{6}b + 144c - 59\sqrt{6}c) a^*$$
$$+ (3\sqrt{6}a + 24b - 10\sqrt{6}b + 48c - 19\sqrt{6}c) b^* + \sqrt{6}(a - b + c) c^* \right),$$

$$\rho_{\infty,13} = (\rho_{\infty,31})^* = \frac{1}{48} \left(\left((-48 + 19\sqrt{6})a + 288b - 118\sqrt{6}b + 576c - 235\sqrt{6}c) a^*$$
$$+ 2(\sqrt{6}a + 48b - 19\sqrt{6}b + 144c - 59\sqrt{6}c) b^* + (5\sqrt{6}a + 2\sqrt{6}b - 48c + 19\sqrt{6}c) c^* \right),$$

$$\rho_{\infty,23} = (\rho_{\infty,32})^* = \frac{1}{24} \left((\sqrt{6}a + 48b + 19\sqrt{6}b + 144c - 59\sqrt{6}c) a^*$$
$$- (\sqrt{6}a + 24b + 10\sqrt{6}b - 96c + 39\sqrt{6}c) b^* + (\sqrt{6}a + 3\sqrt{6}b - 24c + 9\sqrt{6}c) c^* \right). \quad (A2)
As expected, the matrix is Hermitian and

\[ \text{Tr}(\rho_{c,\infty}) = |a|^2 + |b|^2 + |c|^2 = 1. \]

**Appendix B. Thermalization and evolution of the Bloch vector**

Let us consider that the reduced coin system can be modeled by the quantum Brownian motion as in the reference [7]. Thus, the quantum Liouville equation can be reduced to the following master equation (for a more detailed demonstration we refer to [19])

\[ \frac{\partial \rho_c}{\partial t} = -\frac{i}{\hbar}[H_c, \rho_c] + \Gamma \rho_c, \tag{B1} \]

where \( H_c \) is an effective Hamiltonian of the reduced system and \( \Gamma \) is a Liouvillian representing the fluctuation and dissipation effects exerted effectively by the interaction of the coin and the walker as a noise exerted on \( \rho_c \). The Hamiltonian can be associated to a parameter, \( v \), and must be written as \( H_c = -v \cdot \lambda \).

By definition, if the system achieves equilibrium in the asymptotic limit, \( \frac{\partial \rho_{c,\infty}}{\partial t} = 0 \). However [19], (pg 88) also showed that if the asymptotic state is the Gibbs state, then \( \Gamma \rho_{c,\infty} = 0 \) as well. Since the reduced space has three dimensions we will use the Gell-Mann matrices [20, 21], \( \lambda = (\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6, \lambda_7, \lambda_8) \) and the identity, \( I \) as a basis. Therefore, the reduced density matrix can be written as

\[ \rho_{c,\infty} = \frac{1}{3} (I + \sqrt{3} \mathbf{B} \cdot \lambda), \tag{B2} \]

where \( \mathbf{B} \) is a generalized Bloch vector. Hence,

\[ 0 = [H_c, \rho_{c,\infty}] = -\frac{\sqrt{3}}{3} [v \cdot \lambda, \mathbf{B} \cdot \lambda] = -\frac{1}{\sqrt{3}} \sum_{ij} [v_i \lambda_j, B_j \lambda_i] \]

\[ = -\frac{1}{\sqrt{3}} \sum_{ij} v_i B_j [\lambda_i, \lambda_j] = -\frac{2i}{\sqrt{3}} \sum_{ijk} v_i B_j f_{ijk} \lambda_k, \tag{B3} \]

where \( f_{ijk} \) are structure constants. Since the Gell-Mann matrices are linearly independent, equation (B3) leads to a system of eight equations, for which \( v \propto \mathbf{B} \) is a solution. This suggests that in equilibrium the generalized Bloch vector is parallel to the parameter \( v \) associated with the Hamiltonian.

To show that the asymptotic limit was calculated correctly, we compare the generalized Bloch vector, \( \mathbf{B} \), with the asymptotic value obtained by us, \( \mathbf{B}_{\infty} \), for different initial conditions—figure 6 shows the norm of the difference between both vectors. To obtain the generalized Bloch vector at time \( t \), we simulate the walk using the recurrence relations (6), calculate the reduced density matrix, \( \rho_c(t) \), and use (B2). The results of figure 6 suggest that the Bloch norm is indeed approaching the asymptotic value calculated using the asymptotic reduced density matrix and expression (B2). Besides that, after obtaining our results, we became aware of two other papers that also analyze the limits of the three-state quantum walk [22, 23]. Specifically, if one calculates the off-diagonal terms of the reduced density matrix using lemma A.1 of [22] with \( r = 0 \).
the results are equal to the ones we obtained in the appendix. This is another confirmation that the asymptotic density matrix of the chirality space is correct.

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