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In [1] the Quantum Walk was used to discuss the possibility of introducing the concept of temperature for an isolated quantum system that evolves in a composite Hilbert Space. Concomitantly, because of its large application on the development and optimization of quantum algorithms, new types of Quantum Walks have been studied. Here we discuss the meaning of temperature and thermodynamic equilibrium for Discrete Quantum Walks with 2 and 3-sided coins.

1 Introduction

Quantum Walks are a wide group of dynamic systems that represent the time evolution of a walker on a graph. Those are divided on discrete-time Quantum Walks and continuous time Quantum Walks. On this work the main interest is on discrete-time Quantum Walks on a one-dimension position space, that is, on the lattice points of a line.

The study of Quantum Walks started as a generalization of classical random walks to quantum systems, however some of its properties, such as having a ballistic behavior ($\sigma^2 \propto t^2$), called the attention of researchers to the possibility of using it as a mathematical tool to build quantum algorithms. It has been proved that Quantum Walks, under particular conditions, can be used to implement a model of universal computation [2, 3].

The three-state Quantum Walk is a generalization of the usual Hadamard Walk, where the probability of the walker to stay still on a time step of the dynamics of the system is also taken in to account. On the classical case this additional consideration does not add much difference to the behavior of the system, the evolution of the position probability distribution is just slowed. On the other side, for the quantum case, the addition of one degree of freedom on the chirality space causes a huge difference on the evolution of the position

probability distribution. The probability amplitude of staying in the same place generates a localization the initial position. This property has been analyzed in [4–6].

In the present work we analyze the entanglement between the position and chirality space on the asymptotic limit of the three-state Quantum Walk using the tools defined on [1,7–10]. Firstly, we introduce notation making an overview of the two-state Quantum Walk on the line and summarizing the calculation of the temperature and entropy of that system. Then, we explain the basics of three-state Quantum Walk and, in section 3.2, we present our results concerning the thermodynamics of the three-state Quantum Walk. At last, in section 4 we point the last remarks and conclusions.

2 Two State Quantum Walk on the line

2.1 Overview

The Quantum Walk on the line is the quantum version of the simple random walk. The system is composed by a coin and a walker, therefore its Hilbert space is written as $\mathcal{H} = \mathcal{H}_C \otimes \mathcal{H}_P$, where $\mathcal{H}_C$ is the coin Hilbert space and $\mathcal{H}_P$ the Hilbert Space associated with the positions of the walker. The state of the system can be described as a spinor

$$|\psi(t)\rangle = \sum_{n=-\infty}^{\infty} \begin{pmatrix} a_n(t) \\ b_n(t) \end{pmatrix} |n\rangle \,, \tag{1}$$

where a_n and b_n are the wave components correspondent to left and right chirality, respectively.

As in its classical counterpart, each time step of the Quantum Walk dynamics is composed by two operations. A rotation on the coin (chirality) space (C), followed by a shift (S) operation. Using the variable θ to determine the bias of the coin, the first operator can be written as

$$C = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}. \tag{2}$$

If $\theta = \pi/4$ the coin is unbiased and we call it the Hadamard Walk. On the other side the shift operator is

$$\mathrm{Sh} = \left(\sum_{n=-\infty}^{\infty} |n-1\rangle \langle n| \otimes |L\rangle \langle L| \right) + \left(\sum_{n=-\infty}^{\infty} |n+1\rangle \langle n| \otimes |R\rangle \langle R| \right). \tag{3}$$

Therefore, using this two unitary operators the dynamics can be summarized to

$$|\psi(t)\rangle = (\mathrm{Sh}(C \otimes I))^t \, |\psi(0)\rangle \,, \tag{4}$$

where I stands for the identity on position space. The asymptotic limit distribution of the two-state quantum walk on the line can be found using the Fourier space and stationary phase method [11].

On [12] the global left (or right) chirality probabilities (GCP) were defined as the probability that, if measured, the state is found with chirality left (or right) in any position, i.e,

$$\begin{aligned} P_L(t) &= \sum_{n=-\infty}^{\infty} |a_n(t)|^2, \\ P_R(t) &= \sum_{n=-\infty}^{\infty} |b_n(t)|^2. \end{aligned} \tag{5}$$

Evolving the system using equation (4) and applying definitions (5) the dynamics of the GCP is found,

$$\begin{pmatrix} P_L(t+1) \\ P_R(t+1) \end{pmatrix} = \begin{pmatrix} \cos\theta^2 & \sin\theta^2 \\ \sin\theta^2 & \cos\theta^2 \end{pmatrix} \begin{pmatrix} P_L(t) \\ P_R(t) \end{pmatrix} + \mathbb{R}\mathbf{e}[Q(t)] \sin 2\theta \begin{pmatrix} 1 \\ -1 \end{pmatrix}, \tag{6}$$

where $Q(t) = \sum_{n=-\infty}^{\infty} a_n(t) b_n^*(t)$ is a interference term. If this term is left out a classical Markovian Process [13] is recovered.

2.2 Temperature of two sate Quantum Walk

It was shown on [12] that the global distribution of chirality has stationary long-time limit that depend only on the initial conditions. Therefore, asymptotic limits of the GCP and the interference term can be defined as [1]

$$\begin{aligned} \Pi_L &= \lim_{t\to\infty} P_L(t), \\ \Pi_R &= \lim_{t\to\infty} P_R(t), \\ Q_0 &= \lim_{t\to\infty} Q(t). \end{aligned} \tag{7}$$

Since the system follows a unitary evolution, if the initial conditions define a pure state, the state remains pure during the time evolution. This means that the von Neumann entropy of the system is zero. However the shift operation generates entanglement between chirality and position. Such an entanglement can be quantified calculating the entropy of the reduced density operator. The reduced density operator of the coin space in the limit where $t \to \infty$ is

$$\rho_c(t) = \begin{pmatrix} \Pi_L & Q_0 \\ Q_0^* & \Pi_R \end{pmatrix}, \tag{8}$$

and the entropy limit is

$$S(\rho) = -\lambda_+ \log \lambda_+ - \lambda_- \log \lambda_-, \tag{9}$$

where λ_+ and λ_- are the eigenvalues of (8).

Now, to define an entanglement temperature of the system, it is necessary to connect the eigenvalues of the density operator with its associated Hamiltonian, H. In the stationary state $[H, \rho] = 0$, therefore there is a basis in witch H and ρ

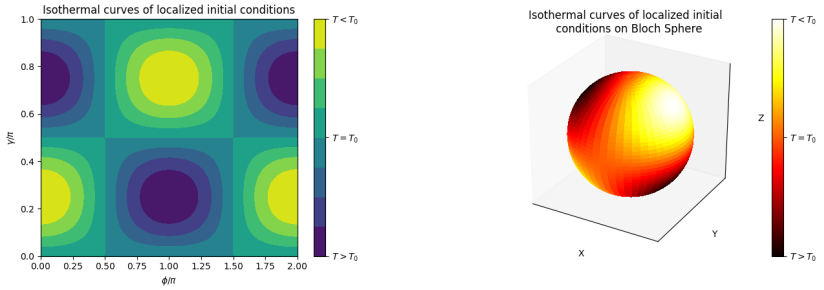

Figure 1: Temperature is displayed as a function of initial conditions θ and ϕ. Both figures present the same result, but on the right one, for a better visualization, the initial conditions are shown on the Bloch sphere. $T_0 \approx 2.27$ is a characteristic parameter.

can be written on a diagonal form. Since only the gap between the eigenvalues of H are relevant for us, we call them $\pm\varepsilon$. The explicit dependence between the eigenvalues of both operators depend on the ensemble constructed. Assuming canonical ensemble,

$$\lambda_{\pm} = \frac{e^{\pm\beta\varepsilon}}{e^{\beta\varepsilon} + e^{-\beta\varepsilon}}, \tag{10}$$

where $\beta = 1/T$ is the temperature inverse. Thus, inverting the expression the temperature is obtained

$$T = \frac{2\varepsilon}{\log\left(\frac{\lambda_+}{\lambda_-}\right)}. \tag{11}$$

Therefore, to see this result with clarity the bias of the walk was fixed on $\theta = \pi/4$ (Hadamard walk) and the temperature per unit of ε was calculated for the initial condition (12) for values of γ from 0 to π and ϕ from 0 to 2π. The isotherms corresponding the results are displayed on figure (2.2), where T_0 is a characteristic temperature

$$|\psi(0)\rangle = \begin{pmatrix} \cos(\gamma/2) \\ e^{i\phi}\sin(\gamma/2) \end{pmatrix} |0\rangle. \tag{12}$$

3 Three-State Quantum Walk on the Line

3.1 Overview

The principle of the three-state Quantum Walk is similar to the regular one-dimension Quantum Walk explained above. The main difference is that on this case the chirality state space has three dimensions, therefore besides the

possibilities of going to left or right, a probability of staying in the same place is also accounted. Hence the state of the system on time t is written as

$$|\psi(t)\rangle = \sum_{n=-\infty}^{\infty} \begin{pmatrix} a_n(t) \\ b_n(t) \\ c_n(t) \end{pmatrix} |n\rangle \,, \tag{13}$$

where the coefficients a_n, b_n and c_n corresponds to the left (L), no movement (S) and right(R) chiralities respectively. The coin operator analog to the Hadamard operator is

$$C = \frac{1}{3} \begin{pmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{pmatrix}, \tag{14}$$

and the shift operator is

$$\mathrm{Sh} = \left(\sum_{n=-\infty}^{\infty} |n-1\rangle \langle n| \otimes |L\rangle \langle L| \right) + \left(\sum_{n=-\infty}^{\infty} |n\rangle \langle n| \otimes |S\rangle \langle S| \right) + \left(\sum_{n=-\infty}^{\infty} |n+1\rangle \langle n| \otimes |R\rangle \langle R| \right). \tag{15}$$

On this walk the Global chirality probabilities are defined on analogous way to the two-state walk, eq. (5)

$$\begin{aligned} P_L(t) &= \sum_{n=-\infty}^{\infty} |a_n(t)|^2, \\ P_S(t) &= \sum_{n=-\infty}^{\infty} |b_n(t)|^2, \\ P_R(t) &= \sum_{n=-\infty}^{\infty} |c_n(t)|^2. \end{aligned} \tag{16}$$

Therefore, recurrence relation of the GCP is easily obtained from eq. (4)

$$\begin{aligned} \begin{pmatrix} P_L(t+1) \\ P_S(t+1) \\ P_R(t+1) \end{pmatrix} &= \frac{1}{9} \begin{pmatrix} 1 & 4 & 4 \\ 4 & 1 & 4 \\ 4 & 4 & 1 \end{pmatrix} \begin{pmatrix} P_L(t) \\ P_S(t) \\ P_R(t) \end{pmatrix} + \frac{\mathbb{R}\mathbf{e}[Q_1(t)]}{9} \begin{pmatrix} -4 \\ -4 \\ 8 \end{pmatrix} \\ &\quad + \frac{\mathbb{R}\mathbf{e}[Q_2(t)]}{9} \begin{pmatrix} -4 \\ 8 \\ -4 \end{pmatrix} + \frac{\mathbb{R}\mathbf{e}[Q_3(t)]}{9} \begin{pmatrix} -8 \\ -4 \\ -4 \end{pmatrix}, \end{aligned} \tag{17}$$

where the interference terms are

$$\begin{aligned} Q_1(t) &= \sum_{n=-\infty}^{\infty} a_n(t) b_n^*(t), \\ Q_2(t) &= \sum_{n=-\infty}^{\infty} a_n(t) c_n^*(t), \\ Q_3(t) &= \sum_{n=-\infty}^{\infty} b_n(t) c_n^*(t). \end{aligned} \tag{18}$$

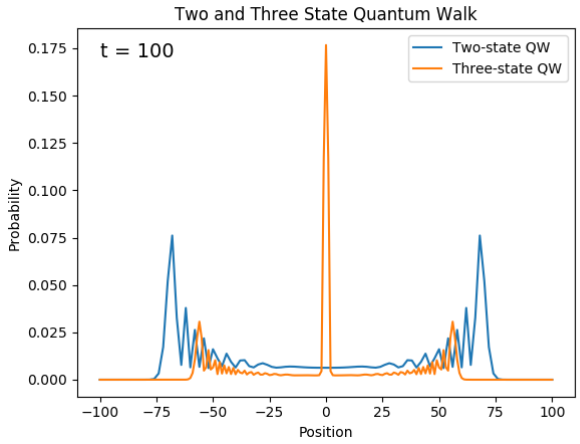

Figure 2: Probability distributions of the two and three state Quantum Walk after 100 time steps

Considering the Fourier transform of the wave function of the system, $\tilde{\Psi}(k,t)$, the equation describing the dynamics of the walk is

$$\tilde{\Psi}(k,t+1) = \tilde{M}^t \tilde{\Psi}(k,0), \tag{19}$$

where in its diagonal form $\tilde{U}$ has two time dependent eigenvalues (λ_2, λ_3) and a constant one ($\lambda_1 = 1$) [4, 6]. The constant eigenvalue is responsible for the main difference in behavior of two and three state Quantum Walk, because it causes a localization around its initial position. Figure 2 shows the probability distributions of the two and three state Quantum Walk after 100 time steps. Therefore using its diagonal form the evolution operator $\tilde{M}$ can be written as follows

$$\tilde{M}^t = \tilde{M}_1 + \lambda_2^t \tilde{M}_2 + \lambda_3^t \tilde{M}_3. \tag{20}$$

Then 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 on such a way that on the limit of $t \to \infty$ the state vector is

$$|\psi_n^\infty\rangle = (U_1 + U_2 + U_3)\,|\psi_0^0\rangle\,, \tag{21}$$

where

$$|\psi_0^0\rangle = \begin{pmatrix} a_n(0) \\ b_n(0) \\ c_n(0) \end{pmatrix} |0\rangle\,,$$

is the initial state of the walker. To perform the inverse Fourier transform on the time dependent parts of $\tilde{M}$ the method of stationary phase was used.

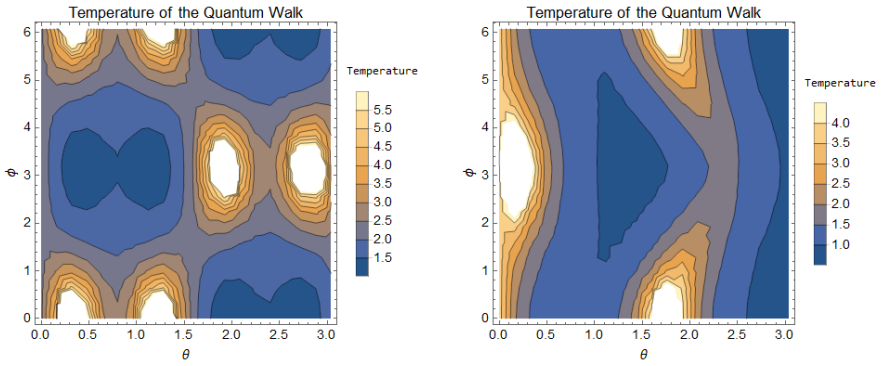

Figure 3: Temperature is displayed as a function of initial conditions. The left figure has initial condition $|\psi_0^0\rangle = (\cos\theta, 0, e^{i\phi}\sin\theta)^T |0\rangle$, while on the right figure the initial condition is $|\psi_0^0\rangle = (\cos\theta/\sqrt{2}, 1/\sqrt{2}, e^{i\phi}\sin\theta/\sqrt{2})^T |0\rangle$. The parameters $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$ vary keeping the condition that the initial condition is normalized.

3.2 Temperature of Three-State Quantum Walk

To obtain the temperature of three-state Quantum Walks the results of [6] were strongly used to calculate the density matrix of the asymptotic state of the walk, then following the procedure established by [1] the canonical ensemble was used to define the a temperature.

The results of [6] suggested that the cross terms of eq. (21) should not be considered on the calculation of the asymptotic density matrix, i.e,

$$\rho_\infty = |\psi_n^\infty\rangle\langle\psi_n^\infty| \approx U_1 |\psi_0^0\rangle\langle\psi_0^0| U_1^\dagger + U_2 |\psi_0^0\rangle\langle\psi_0^0| U_2^\dagger + U_3 |\psi_0^0\rangle\langle\psi_0^0| U_3^\dagger. \tag{22}$$

Therefore the eigenvalues of ρ_∞ can be associated with the following probabilities

$$\lambda_j = \frac{e^{\beta\varepsilon_j}}{e^{\beta\varepsilon_1} + e^{-\beta\varepsilon_2} + e^{-\beta\varepsilon_3}}, \tag{23}$$

where $j = 1,2,3$ and ε_j are the energy eigenvalues of the of the common basis of ρ_∞ and the Hamiltonian. Thus the temperature is defined with respect to the energy difference between two of the eigenvalues. Any pair of eigenvalues could be used, here we chose

$$T = \frac{\varepsilon_1 - \varepsilon_2}{\log\left(\frac{\lambda_1}{\lambda_2}\right)}. \tag{24}$$

Figure 3.2 shows the temperature in units of energy difference as a function of initial conditions.

The asymptotic entanglement entropy was also calculated using expression

$$S(\rho) = -\lambda_1 \log\lambda_1 - \lambda_2 \log\lambda_2 - \lambda_3 \log\lambda_3. \tag{25}$$

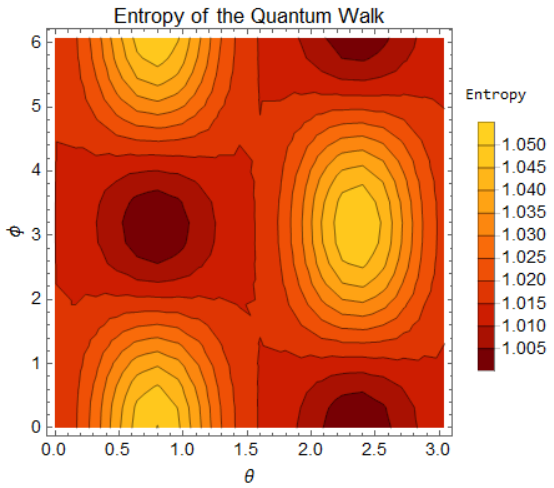

Figure 4: Entanglement entropy for initial conditions $|\psi_0^0\rangle = (\cos\theta, 0, e^{i\phi}\sin\theta)^T |0\rangle$, with $\theta \in [0,\pi]$ and $\phi \in [0,2\pi]$.

The result obtained for the initial condition $|\psi_0^0\rangle = (\cos\theta, 0, e^{i\phi}\sin\theta)^T |0\rangle$ is displayed on Figure 4.

4 Conclusions

Using the definitions proposed by [1] for thermodynamic variables and the methods used by [6], to find the asymptotic wave function, we were able to calculate entropy and temperature per unit energy for different initial conditions. This investigation together with a deep analysis of the possible correlation between these thermodynamic variables and localization will be analyzed elsewhere.

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