Exploring Graph Dynamics and Transport Properties with Staggered Quantum Walks

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Abstract

Quantum walks provide a versatile framework for quantum algorithms and transport properties within graph-encoded structures. In this study, we investigate the staggered quantum walk model, incorporating angle decoherence and alterations in graph structure through tessellation. These modifications may entail disruptions in connections or shifts in operator orders. Additionally, we analyze various transport properties, including mean, standard deviation, inverse participation ratio, and localization. Through computational simulations, we shed light on the intricate interplay between quantum walk dynamics and graph evolution, offering insights into the fundamental properties of quantum systems and their potential applications in quantum computing and transport phenomena.

1 Introduction

The exploration of quantum walks, quantum analogs of random walks, has garnered significant attention in both physics and computer science, mainly due to the advancements in quantum computation. Unlike their classical counterparts, quantum walks take advantage of quantum coherence, enabling interference effects that lead to the ballistic spreading of the walker. This unique characteristic has proven invaluable in various applications, from designing quantum search algorithms [27, 20] and implementing communication protocols [26, 11] to achieving universal quantum computation [16, 9]. Moreover, quantum walks are versatile tools for simulating diverse physical phenomena, including quantum phase transitions [7, 29], interacting particles [10, 23], rogue waves [5, 6], and nonlinear dynamics [17, 3]. Their effectiveness in these applications underscores their potential as powerful environments for developing quantum algorithms and intuitive frameworks for studying and exploring quantum systems. However, harnessing the full capabilities of quantum walks necessitates a profound understanding of the underlying dynamics, particularly in designing and controlling these quantum processes over extended periods.

Quantum walks are generally categorized into continuous- and discrete-time versions, each exhibiting distinct characteristics. Continuous-time quantum walks involve a unitary time evolution dictated by a Hamiltonian, providing the walker's dynamics in continuous time within a discrete spatial framework [12]. In discrete-time quantum walks, the evolution of the walker occurs in discrete steps, often relying on internal degrees of freedom and sequential application of quantum operators to dictate its dynamics. Two of the most well-known versions are the coined [1] and the

Szegedy [28] models. The essential feature of the coined quantum walk lies in utilizing an internal state to dictate the potential directions the particle may traverse. During each step, the walker undergoes an operation involving the sequential application of the coin operator, which controls state changes, and the shift operator, which determines the feasible directions for particle movement. On the other hand, Szegedy's quantum walk arises as a coinless quantization of classical Markov chains following a transition matrix. This model combines evolution and mixing operators through a unitary operation, providing a versatile framework for quantum walk dynamics.

Staggered quantum walks represent a recent approach in discrete-time quantum walks, offering a distinctive framework for investigating quantum dynamics on graph structures [19, 22]. Unlike traditional quantum walks, which proceed straightforwardly from one vertex to another, staggered quantum walks introduce a partitioning scheme that divides arbitrary graphs into tessellations. Such a tessellation-based approach provides a structured framework for the evolution of quantum states, enabling the exploration of complex graph structures with enhanced versatility and precision [8, 15]. This model encompasses a substantial portion of the subclass of discrete-time quantum walks, including the coined and Szegedy's models [22, 18, 21].

Recent advancements have introduced extensions enabling physical realizations of quantum walk dynamics using time-independent Hamiltonians [21, 14], presenting exciting opportunities for investigating quantum phenomena in well-controlled experimental setups. However, it's essential to acknowledge that implementing quantum systems is prone to decoherence, which can significantly impact the performance of quantum walks [13, 4, 2, 25]. Therefore, understanding how decoherence influences the transition from quantum to other regimes is paramount and requires further exploration, particularly in staggered quantum walks. The effect of breaking polygons and vertices has been investigated on a two-dimensional grid of 4-cliques, revealing a loss of quantum behavior [24]. Furthermore, the authors have shown that resilience against decoherence can be improved by expanding the intersection of tessellations within the graph. Considering that fault-tolerant architectures are constructed based on a thorough understanding of each potential component, we explore here the inhomogeneity in tessellations as the main agent affecting the staggered quantum walk dynamics.

2 Staggered Quantum Walk Model

Jaime: Isto ainda é um copy paste rudimentar da minha dissertaçao, vou ainda adaptar para o nosso paper.

The staggered quantum walk (SQW) model disperses transition probabilities across neighboring vertices in discrete time steps, leveraging the concept of adjacency through cliques. Initially, the graph is partitioned into cliques in a process called *tessellation*. In tessellation $\mathscr{T}$, an element is termed a polygon if its vertices are in the same $\mathscr{T}$'s clique. These polygons must collectively encompass all graph vertices, while the tessellation set $\{\mathscr{T}_1, \mathscr{T}_2, ..., \mathscr{T}_k\}$ should cover all edges.

Operators $H_1, H_2, ..., H_k$ are constructed to propagate probability amplitudes locally within each polygon. The state for each polygon in the k^{th} tessellation is represented as:

$$\left|u_j^k\right\rangle = \frac{1}{\sqrt{|\alpha_j^k|}} \sum_{l \in \alpha_j^k} |l\rangle \,, \tag{1}$$

where α_j^k denotes the j^{th} polygon. Associated with each tessellation is a unitary, local, and Hermitian operator H_k, defined in [21] as

$$H_k = 2\sum_{j=1}^{p} \left| u_j^k \right\rangle \left\langle u_j^k \right| - I, \tag{2}$$

The evolution operator, solving the time-independent Schrödinger equation for H_k, is given by

$$U = e^{i\theta_k H_k} \cdots e^{i\theta_1 H_1}, \tag{3}$$

where each term $e^{i\theta_k H_k}$ simplifies to $\cos(\theta_k)I + i\sin(\theta_k)H_k$, leveraging $H_k^2 = I$. This highlights H_k as a reflection operator, enabling local operation through Taylor series expansion.

2.1 SQW on the line

The simplest use case of this quantum walk model is the one-dimensional lattice, where the minimum tessellations are

$$\mathscr{T}_\alpha = \{\{2x, 2x+1\} \colon x \in \mathbb{Z}\}, \tag{4}$$

$$\mathscr{T}_\beta = \{\{2x+1, 2x+2\} \colon x \in \mathbb{Z}\}. \tag{5}$$

Each element of the tessellation has a corresponding state, as can be seen in figure 1, and the

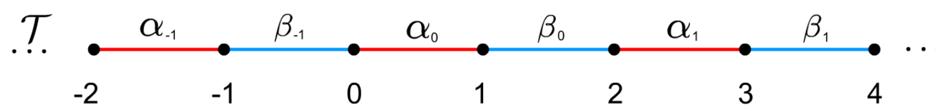


Figure 1: Tessellation of a line graph.

uniform superposition of these states is

$$|\alpha_x\rangle = \frac{|2x\rangle + |2x+1\rangle}{\sqrt{2}}, \tag{6}$$

$$|\beta_x\rangle = \frac{|2x+1\rangle + |2x+2\rangle}{\sqrt{2}}. \tag{7}$$

We can now define Hamiltonians H_α and H_β as

$$H_\alpha = 2\sum_{x=-\infty}^{+\infty} |\alpha_x\rangle\langle\alpha_x| - I, \tag{8}$$

$$H_\beta = 2\sum_{x=-\infty}^{+\infty} |\beta_x\rangle\langle\beta_x| - I. \tag{9}$$

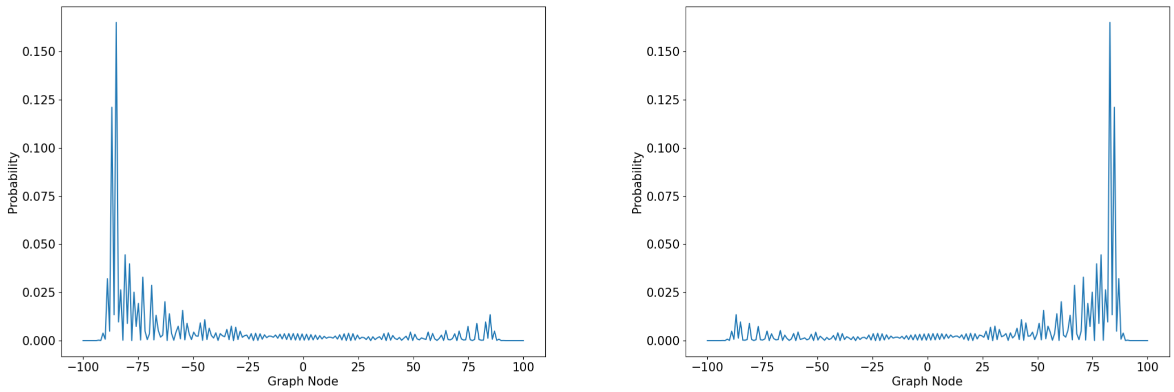
The Hamiltonian evolution operator reduces to

$$U = e^{i\theta H_\beta} e^{i\theta H_\alpha}, \tag{10}$$

and applying it to an initial condition $|\psi(0)\rangle$ results in the time evolution operator

$$U\,|\psi(t)\rangle = U^t\,|\psi(0)\rangle\,. \tag{11}$$

Defining the time evolution operator allows for the coding of the quantum walk with specific initial conditions and a chosen θ value, to observe the spread of the probability distribution over



(a) $|\psi(0)\rangle = |0\rangle$

(b) $|\psi(0)\rangle = |1\rangle$

Figure 2: Probability distributions for the staggered quantum walk on a line after 50 steps, for different initial conditions.

time. The quantum walk's outcomes, as depicted in figure 2, reveal that starting with $|\psi(0)\rangle = |0\rangle$ or $|\psi(0)\rangle = |1\rangle$ produces asymmetric probability distributions. Specifically, the former initial condition favors a peak on the left side, whereas the latter results in a peak on the right side.

When the initial condition is a uniform superposition of $|0\rangle$ and $|1\rangle$, varying θ helps explore its effect on the quantum walk, as illustrated in figure 7. Although the probability distribution's general structure remains consistent across different θ values, the likelihood of the walker being farther from the origin increases with the angle.

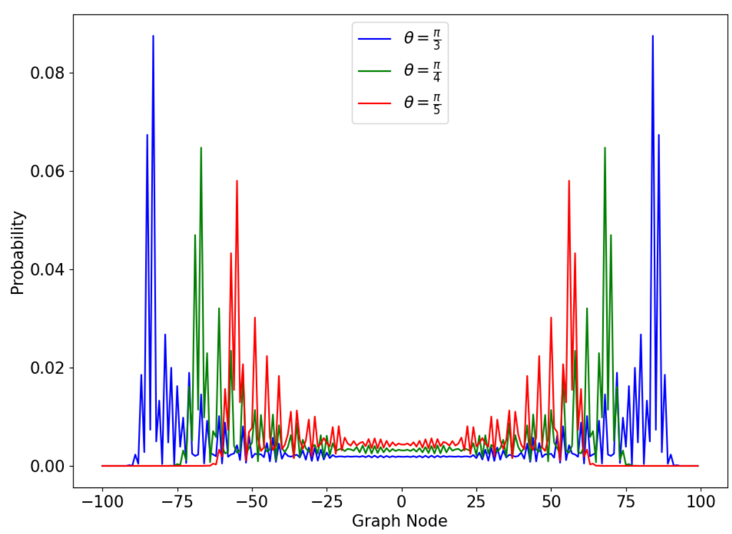


Figure 3: Probability distribution for the staggered quantum walk on a line after 50 steps, with initial condition $|\psi(0)\rangle = \frac{|0\rangle+|1\rangle}{\sqrt{2}}$, for multiple values of θ.

2.2 Noisy Staggered Quantum Walk Model

$$U = \prod_j U_j(T_j(t), \theta_j(t)) \tag{12}$$

3 Computational Simulations

- Figure 1 - Temporal evolution of the standard deviation and return probability, considering the scenario without disorder and disordered. Well-known results for the case without disorder. With disorder, we must find a standard deviation saturating at a fixed value after some time of evolution. The return probability must also saturate at a finite value.
- Figure 2 - Probability distribution. We can evaluate the distribution in the first stages of temporal evolution and the scenario where the localization (saturation of σ) is already well established. I believe that the exponentially localized profile will be dominant in this last scenario.
- Figure 3 - Evaluate the initial transient time as a function of the disorder degree, considering the standard deviation. In figure (a), we can show examples, and in figure (b), a graph of "saturation time" vs. "disorder degree." I believe that the saturation time is inversely proportional to the disorder width.
- Figure 4 - Considering using a certain tessellation in all previous figures, we can try to generalize the study, considering other tessellation relationships (equivalent to changing the θ). Another possibility is to apply these considerations to a well-known algorithm, such as search or hitting time. In the search, unless I'm mistaken, there is an optimal value to retrieve the optimal number of steps $O(\sqrt{N \ln N})$ and the success probability $O(1/\ln N)$. How does our model impact this performance? Anyway, there are two possible itineraries to conclude our article. What do you think is most viable?.

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4 Anotações

Pessoal, acabo de ver os experimentos na seção seguinte. Pelo que pude entender, foi estabelecido $\theta = \pi/3$ em todos os cenários, entretanto, tive dificuldade em entender a diferença entre as configurações das figuras 5, 6, e 7. Entendi que a figura 4 considera um sistema sem desordem e possivelmente as outras possuem. Sobre este ponto, gostaria de salientar para o caso de sensibilidade e tempo de evolução. Possivelmente, nesta largura de desordem, precisaremos de 2000 steps ou mais para perceber uma influência efetiva. Outro ponto é sobre o número de amostras. Com ≈ 5 amostras teremos um ensaio sobre o perfil do caminhante, bem como sua medida de desvio quadrático médio minimamente confiável.

5 Experimentos

5.1 Dinâmica Simples

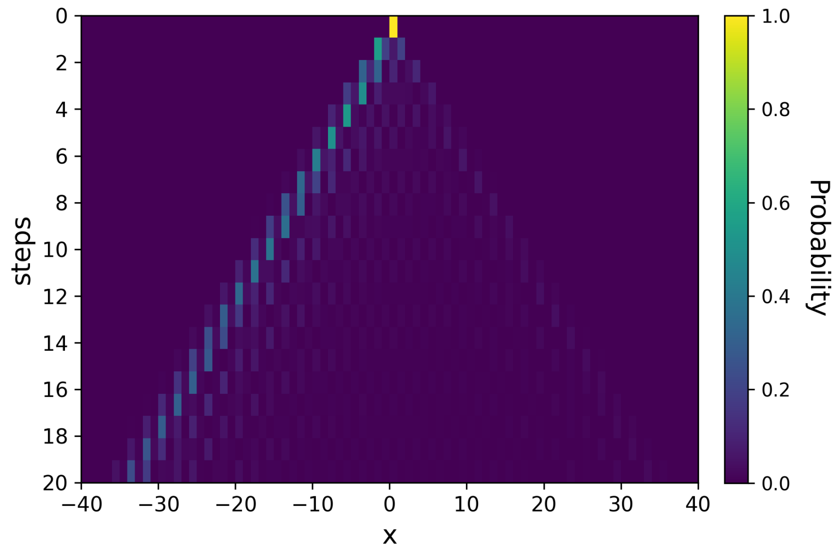

Figure 4: Probability distribution for the staggered quantum walk on a line after 20 steps, with initial condition $|\psi(0)\rangle = |50\rangle$, and $\theta = \pi/3$

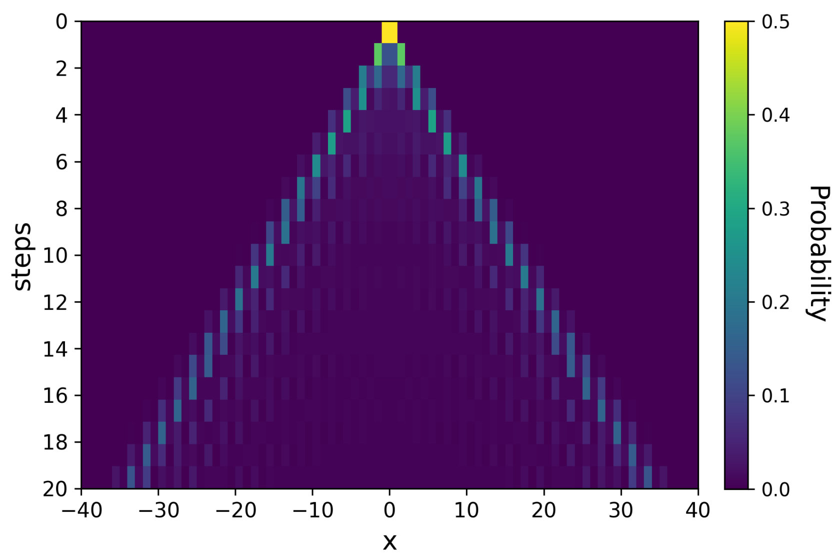

Figure 5: Probability distribution for the staggered quantum walk on a line after 20 steps, with initial condition $|\psi(0)\rangle = |50\rangle$, and $\theta = \pi/3$, and angles with deviation of 0.4

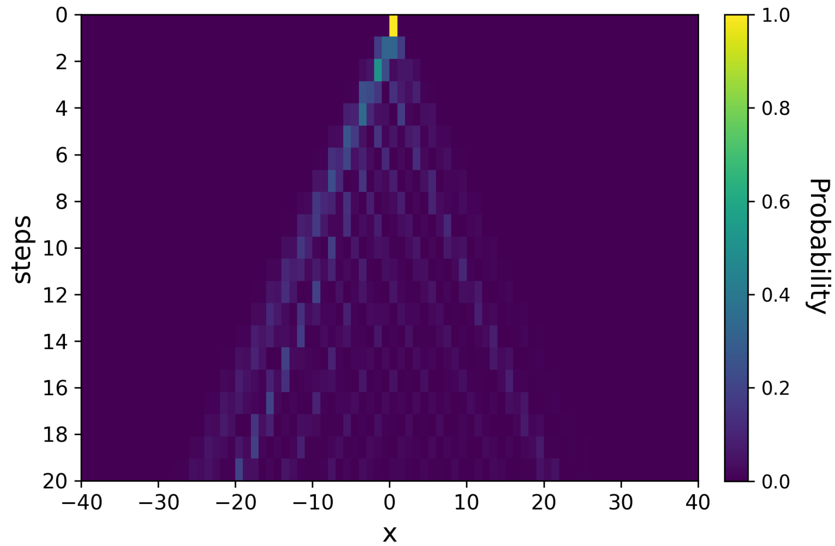

Figure 6: Probability distribution for the staggered quantum walk on a line after 20 steps, with initial condition $|\psi(0)\rangle = |50\rangle$, and $\theta = \pi/3$, and angles with deviation of 0.4

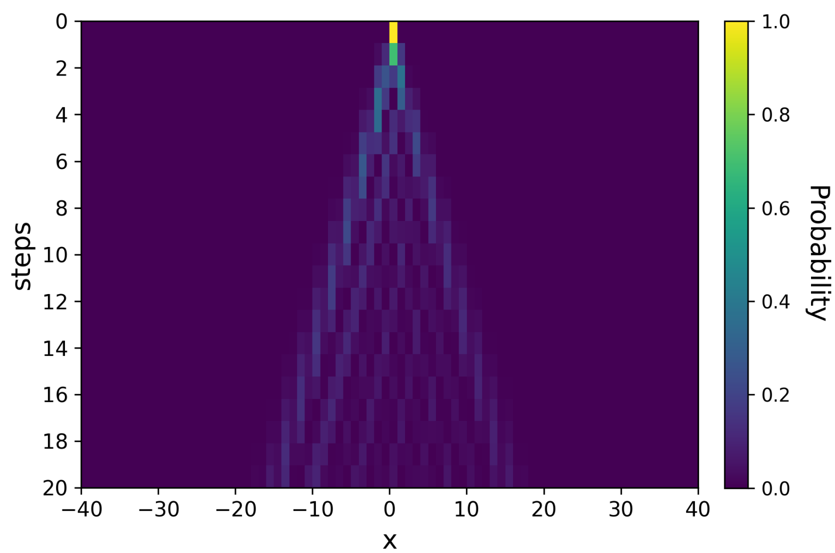

Figure 7: Probability distribution for the staggered quantum walk on a line after 20 steps, with initial condition $|\psi(0)\rangle = |50\rangle$, and $\theta = \pi/3$, and angles with deviation of 0.4