CHARACTERIZING THE INHERENT RELATIONSHIP BETWEEN UNITARY QUANTUM WALKS AND NON-HOMOGENEOUS RANDOM WALKS ON FINITE GRAPHS

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Dissertação de Mestrado apresentada ao Programa de Pós-graduação em Engenharia de Sistemas e Computação, COPPE, da Universidade Federal do Rio de Janeiro, como parte dos requisitos necessários à obtenção do título de Mestre em Engenharia de Sistemas e Computação.

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Rio de Janeiro
Julho de 2020

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DISSERTAÇÃO SUBMETIDA AO CORPO DOCENTE DO INSTITUTO ALBERTO LUIZ COIMBRA DE PÓS-GRADUAÇÃO E PESQUISA DE ENGENHARIA DA UNIVERSIDADE FEDERAL DO RIO DE JANEIRO COMO PARTE DOS REQUISITOS NECESSÁRIOS PARA A OBTENÇÃO DO GRAU DE MESTRE EM CIÊNCIAS EM ENGENHARIA DE SISTEMAS E COMPUTAÇÃO.

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RIO DE JANEIRO, RJ – BRASIL
JULHO DE 2020

Guedes de Andrade, Matheus

Characterizing the inherent relationship between unitary quantum walks and non-homogeneous random walks on finite graphs/Matheus Guedes de Andrade. – Rio de Janeiro: UFRJ/COPPE, 2020.

IX, 58 p.: il.; 29, 7cm.

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Dissertação (mestrado) – UFRJ/COPPE/Programa de Engenharia de Sistemas e Computação, 2020.

Referências Bibliográficas: p. 54 – 58.

1. Quantum walks. 2. Random walks. 3. Non-homogeneous Markov chains. 4. Quantum computing. I. Ratton Figueiredo, Daniel *et al.* II. Universidade Federal do Rio de Janeiro, COPPE, Programa de Engenharia de Sistemas e Computação. III. Título.

Resumo da Dissertação apresentada à COPPE/UFRJ como parte dos requisitos necessários para a obtenção do grau de Mestre em Ciências (M.Sc.)

CARATERIZAÇÃO DO RELACIONAMENTO INTRÍNSECO ENTRE PASSEIOS QUÂNTICOS UNITÁRIOS E PASSEIOS ALEATÓRIOS NÃO-HOMEGÊNEOS EM GRAFOS FINITOS

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Julho/2020

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Programa: Engenharia de Sistemas e Computação

Passeios quânticos em grafos são ubíquos na Computação Quântica, possuindo uma miríade de aplicações importantes. De forma similar, passeios aleatórios em grafos são fundamentais na descrição de muitos algoritmos com diversas aplicações. Ainda que a relação entre passeios quânticos e passeios aleatórios tenha sido explorada em trabalhos recentes, esta dissertação estabelece uma equivalência entre os dois passeios em grafos finitos, sobre condições gerais dos operadores quânticos e do passeio aleatório. Tal equivalência demanda empoderar passeios aleatórios com heterogeneidade no tempo, de forma que as probabilidades de transição sejam não-uniformes e dependam do instante de tempo. Essa equivalência é obtida ao se igualar, a cada instante e para todos os vértices do grafo, a probabilidade do caminhante clássico estar no vértice com a probabilidade desse mesmo vértice ser resultado da medição do passeio quântico. O resultado apresentado possui duas vertentes similares. A primeira aparece sob a forma de um procedimento para construir a sequência de matrizes estocásticas capaz de gerar um passeio aleatório com a mesma evolução de probabilidade de um dado passeio quântico qualquer, incluindo o cenário de múltiplos caminhantes quânticos que interagem entre si. A segunda vertente apresenta um procedimento na direção oposta, partindo de um aleatório e construindo um passeio quântico equivalente. Nesse contexto, a sequência de matrizes obtida pelo primeiro procedimento permite uma abordagem inédita para a simulação de passeios quânticos onde as amostras da posição do caminhante respeitam a vizinhança dos vértices dando origens a trajetórias quânticas. A convergência da simulação é garantida através da lei dos grandes números, permitindo a amostragem eficiente (em tempo polinomial) de trajetórias quânticas do grafo. Em complemento, a complexidade computacional do procedimento de construção dessas matrizes é discutida para o caso geral.

Abstract of Dissertation presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Master of Science (M.Sc.)

CHARACTERIZING THE INHERENT RELATIONSHIP BETWEEN UNITARY QUANTUM WALKS AND NON-HOMOGENEOUS RANDOM WALKS ON FINITE GRAPHS

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July/2020

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Quantum walks on graphs are ubiquitous in quantum computing finding a myriad of applications. Likewise, random walks on graphs are a fundamental building block for a large number of algorithms with diverse applications. While the relationship between quantum and random walks has been recently discussed in specific scenarios, this work establishes a formal equivalence between the two processes on arbitrary finite graphs and general conditions for shift and coin operators. It requires empowering random walks with time heterogeneity, where the transition probability of the walker is non-uniform and time dependent. The equivalence is obtained by equating the probability of measuring the quantum walk on a given node of the graph and the probability that the random walk is at that same node, for all nodes and time steps. The first result establishes procedure for a stochastic matrix sequence to induce a random walk that yields the exact same vertex probability distribution sequence of any given quantum walk, including the scenario with multiple interfering walkers. The second result establishes a similar procedure in the opposite direction. Given any random walk, a time-dependent quantum walk with the exact same vertex probability distribution is constructed. Interestingly, the matrices constructed by the first procedure allows for a different simulation approach for quantum walks where node samples respect neighbor locality and convergence is guaranteed by the law of large numbers, enabling efficient (polynomial-time) sampling of quantum graph trajectories. Furthermore, the complexity of constructing this sequence of matrices is discussed in the general case.

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Chapter 1

Introduction

Most physicists agree that one of the greatest shifts in the human understanding of nature emerged from the quantum theory of matter. The laws of quantum mechanics are approximately a century old, although, in the sense that quantum phenomena remains counter-intuitive even to experts, its implications are neither completely understood nor diffused within and beyond academia. By these means, it is interesting to start discussing the scope of this dissertation from a more abstract point of view.

At a high level, the main idea behind this work is to address the connections between a classical statistical process and a quantum process, hoping that, at the end of the day, the mathematical statements framing this connection will improve the understanding of the processes in question. Albeit there may be weirdness in connecting classical and quantum processes, specially when the laws of quantum mechanics are taken into account, the very reason of this work is to establish precisely why doing so does not harm any of the principles of quantum theory. Undoubtedly, the central intuition behind this work lies on the fact that the theory of quantum measurements is, in itself, a statistical theory [46].

In a more specific perspective, the scope of this work concerns two processes that have been seen as analogous of each other, and that have been of profound importance on the development of classical and quantum computation: quantum walks and random walks. Its purpose is to formally (mathematically) describe how quantum and random walks are related with each other and to explore the implications of such description. Precisely, it addresses the question of whether it is possible to create a random walk with the exact same vertex distribution of any given quantum walk, and vice-versa. This introduction provides the motivation for this work with a brief narrative and lay out the concrete contributions to the understanding of both quantum and random walks.

1.1 Motivation

Quantum computing is at the imminence of driving a breakthrough on the current state of scientific and technological development. Throughout its short existence, the field of quantum computing has experienced a rapidly evolving atmosphere in both theoretical and experimental realms. During its evolution, it created a myriad of interesting research themes in almost all areas of Computer Science by bringing a completely new framework of computation leveraged by the quantum properties of nature.

Throughout the last five decades, a significant part of the development of classical computers came from the capability of drastically improving the computing power of processors. Particularly, these improvements were mainly driven by a process of consecutive reduction in transistor size. As a direct consequence, such reductions enabled the consecutive increase on the number of transistors that could be put together on a single chip, captured by the celebrated Moore's law for the increase of computing power over time [23].

Albeit the amazing achievements driven by the steep rise on processing capacity, the exponential reduction in size carried with its an intrinsic physical limit. In addition to the problem of heat accumulation, once transistors reached a small enough size the classical laws of physics would not be valid anymore. On the threshold of a few nano-meters, the presence of quantum effects starts to dominate the behavior of transistors and the usual architecture for circuits collapses.

Furthermore, many computational problems have an intrinsic complexity that even the exponential growth predicted by Moore's law was not capable of surpassing. Of particular interest, the simulation of physical systems through the interacting behavior of the fundamental particles of nature with computers. Within this context, the initial idea of a computing machine capable of processing information using quantum properties emerged in a celebrated work by Richard Feynman that addressed the difficulties of classical computers to efficiently describe quantum systems [12].

This novel paradigm started a new field of inquiry, focused on creating a computing device to process information through the laws of quantum mechanics. Quantum computing, as it is currently called, developed as a distinct computing framework that does not rely on the representation of logic through electrical circuits. Instead, it relies on the superposition of quantum states to perform computations.

Quantum computing surpasses the physical limitations of reducing transistor size by being described by the laws of quantum mechanics themselves. In addition, the peculiar dynamics of quantum systems brought efficient solutions (super-polynomial improvements) for problems that are intractable by classical computers, such as the Abelian hidden subgroup problem [8], integer factorization [47] and Hamiltonian simulation [26].

Concerning technological developments, both industry and academia have been fo-

cused on constructing an operational generic quantum computer over the last decades, with a solid expectation for an initial breakthrough within the near future. To analyze the state of practical development of quantum computing, the term quantum supremacy was coined to denote the moment where a quantum computer will be able to perform a task that even the most powerful classical computer will need an unfeasible amount of time to perform [40]. Currently, small and restricted quantum processors can be accessed in the IBM Quantum Experience platform, and even a claim of quantum supremacy has recently been made by Google with the Sycamore quantum processor [5], appearing as some of the important practical landmarks for the development of the field.

As quantum computing matured as a well defined field of research, quantum algorithms appeared as a central part of its theoretical development. Nevertheless, there are few generic strategies that guide the design of quantum algorithms. Quantum walks on graphs are, in this context, one such strategy, being a prominent area of research. In a nutshell, a quantum walk on a graph is a unitary process of diffusion where the edges of the graph are codified as the states of a quantum system.

Quantum walks on graphs were conceived as quantum analogues of classical random walks [1, 2]. They have persistently proven to be an insightful tool for the design of quantum algorithms and drove efficient solutions for problems such as element distinctness [4], marked-vertex searching [27] and Hamiltonian simulation [6]. Among the results obtained for quantum walks, its most amazing capability may be that they form a universal set for quantum computation in both continuous [9] and discrete-time [25] models. Extensive surveys covering multiple aspects of quantum walks can be found in the literature [17, 34, 53].

A few discrete-time models for quantum walks have shown increased community interest over the past years [1, 38, 51]. The coined model works on an extended Hilbert space which codifies both graph vertices and walker direction and has pioneered discrete-time models [1]. The coin space was introduced to allow unitary evolution and represents the degrees of freedom of the walker's movement (outward edges) on the vertices of the graph. The later Szegedy model [51] performs quantization over a bipartite Markov chain. In this model, a reflection based operator is constructed once the transition probabilities to cross the bipartite sets are defined. The operators of the Szegedy model have a well described spectra and its properties are mainly derived from spectral analysis. The staggered model [38] is based on graph tessellations and generalizes the bipartite construction of the Szegedy walk. The partition-based quantum walk framework has recently enabled the analysis of the discrete-time models under the same perspective [22]. This formalism allows one to prove that the two-step coined model, the 2-tessellable staggered model, and the extended Szegedy model for multigraphs are equivalent under unitarity, unifying different models for quantum walks. However, the scope of this dissertation is restricted to the coined model.

The case of multiple walkers has also been investigated in different contexts. As with the single quantum walker, the interacting multi-walker model was also shown to be universal for quantum computing [10]. Non-interacting multi-walker models on arbitrary graphs have been treated generically, and a physical implementation has been proposed [41]. The two-walker case was specifically analyzed, leading to interesting results [48, 49, 56].

In the classical realm, random walks on graphs [24] have been extensively used to drive the design of classical algorithms to solve problems in diverse areas of computing, ranging from sampling [16] to user recommendation [33]. Most applications of random walks assume time homogeneity, which implies that the walker behavior, as it moves on the graph, does not change over time. Time homogeneity favors analytical tractability and important known results have been derived under this restriction, such as conditions for time convergence, i.e mixing time, of the probability distribution [15]. On the other hand, non-homogeneity, or time-dependent behavior, has been explored in particular niches, such as the celebrated Simulated Annealing meta-heuristic for optimization [18].

The connection between quantum and random walks has been investigated and it is clear that homogeneous random walks cannot match quantum walks on arbitrary graphs. However, it has been shown that the evolution of a quantum walk on the infinite line is partially described by time-homogeneous Markovian processes [42]. Its probability evolution can be expressed as a time-independent Markov process with an additional interference term. This separation method was further used to construct a master equation for the global chirality distribution (GCD) of the quantum walk [43], showing a convergence behavior of homogeneous Markovian processes for the GCD.

In addition, a relationship between the walk dimension of both processes was explored through the use of renormalization-group analysis (RG) to evaluate scaling factors of the quantum walk limiting distribution [7]. This analysis allows for the calculation of the walk dimension for quantum walks on some non-trivial graphs and has lead to the conjecture that the number of walk dimensions for the quantum case is half of that of the random walk, a well known result in the case of homogeneous lattices [7].

In the search for their equivalence, a recent work has shown that non-homogeneous random walks can have identical probability behavior to quantum walks on the infinite integer line [29]. In this context, an analysis was carried out to generate a given distribution sequence over the integers with time- and site-dependent discrete-time coined quantum walks and non-homogeneous random walks. The matching is performed by constructing a random walk with time-varying probabilities that has the same distribution sequence of a Hadamard-coined quantum walk on the infinite line.

A different perspective is the Quantum Stochastic Walk (QSW) model, a generalization of both quantum and random walks which accounts for non-unitary transformations [55]. Using the formalism of density matrices, a super operator is constructed to

perform both Hamiltonian (coherent) and stochastic evolution based on the Kossakowski-Lindblad master equation. The walk behavior over a graph is achieved upon connectivity restrictions on the terms that map the states of the system, since the state representing a vertex has to be mapped to neighbors of this vertex. Depending on how such terms are chosen, the behavior of both classical and quantum walks can be obtained, as well as the behavior of a more general quantum stochastic process not captured by either of them. However, QSW has no bearing on the equivalence between random and quantum walks.

1.2 Contributions

The work described in this dissertation formally addresses the connection between unitary discrete-time coined quantum walks and random walks on finite graphs. There are four main contributions to the literature of quantum and random walks.

The first contribution is the demonstration that the vertex probability evolution of any quantum walk can be matched exactly by a time-dependent random walk on the same underlying graph. This connection stems from the locality property of both random and quantum walks and it appears as a recipe to build the time-dependent matrix that drive the random walk dynamics in order to show the same probability distribution sequence of any quantum walk. More precisely, when the random walk evolves according to these matrices, its probability distributions over the vertices are identical to that of the quantum walk. While the sequence of matrices describing the random walk clearly depends on the graph and the quantum walk operators, the procedure is very general and requires mild assumptions, such as unitarity.

In addition, the statistical equivalence is also established for the case of multiple interacting walkers. In the quantum case, the interaction model is taken to be very general, with restrictions solely on the walkers' movement. The equivalence is provided by equating the evolution of the joint probability distribution of the multiple walkers with the joint distribution of the same number of random walkers. The proof for the single-walker case is gracefully extended to the multiple walkers through arguments of unitarity. As with quantum system, the state representation for the random walk has to increase in order to accommodate all possible movements of the multiple walkers. This behavior is captured by constructing a graph in which nodes represent the current position of the walkers. The process can than be viewed as a single random walk on a much larger graph.

The second contribution goes on the opposite direction. It is demonstrated that the vertex probability evolution of any random walk can also be matched exactly by a time-dependent unitary quantum walk on the same underlying graph. In similar ways, the proof appears as a recipe to determine the unitary operators that, when applied to the quantum system, perform the same evolution of vertex probability of that of the given random walk. These two results combined imply that quantum and random walks are statistically

equivalent in terms of vertex probability.

The third contribution of this work is a novel simulation procedure for quantum walks. A direct consequence of the time-dependent matrices that construct an equivalent random walk for a given quantum walk is the possibility to simulate this random walk on the graph. This simulation captures quantum behavior while generating samples that preserve neighbor locality. Different than the commonly used quantum walk simulation procedure, the samples obtained from the random walk simulation are paths of the graph, allowing trajectories driven by the quantum behavior to be sampled.

It is worth noting that quantum walks on graphs resembles Feynman's path integral formulation for quantum mechanics [13] in discrete time and space, in the sense that the probability amplitude of a discrete-time walker at instant t is described by summing up the contributions of all possible paths in the graph with length t connecting the initial and final states. In an essential way, the simulation of trajectories through random walks is a procedure for sampling paths from quantum walks following a trajectory distribution in which, for every instant t, the marginal vertex distribution coalesces to the quantum walk vertex distribution. This provides a powerful tool for efficient simulation of quantum walk trajectories on arbitrary graphs.

Finally, the last contribution is an alternative description of random walks that match the evolution of quantum walks with time-independent evolution operators. The alternative is based on the compact description of the vertex probabilities of a quantum walk using the spectral decomposition of the walk operators. This provides an explicit formula to compute the probability of any given vertex, at any given time, using the eigenvectors and eigenvalues of the walk operator. The explicit formula for the probability also yields verifying the necessary conditions for the walk operators to have a periodic vertex probability evolution [35].

The remainder of this dissertation is structured as follows. The notation for both quantum and random walks, as well as formal definitions, appears in Chapter 2. The demonstration of the equivalence between quantum and random walks from the point of view of the first contribution, including the case of multiple walkers, is addressed in Chapter 3. In Chapter 4, the simulation of graph trajectories from the random walk matrices is addressed together with experimental results and time complexity analysis. The demonstration of the equivalence between the processes in the sense of the second contribution appears in Chapter 5. The dissertation is concluded in Chapter 6, together with the indication of future work.

Chapter 2

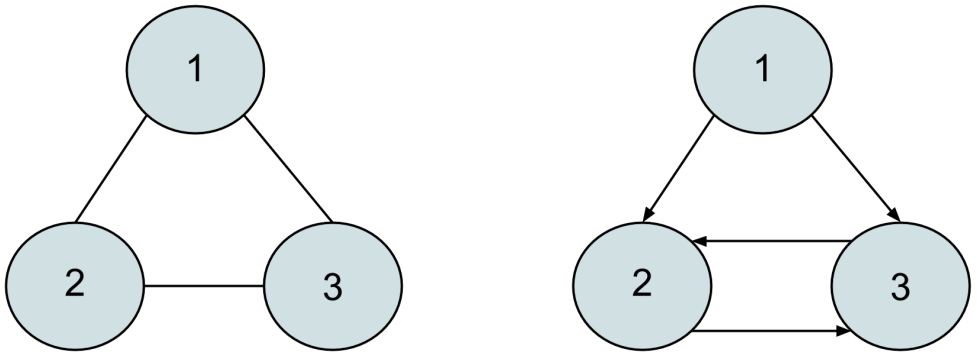
Theoretical background

Graph theory is an important branch of Mathematics and Computer Science that offers the mathematical formalism to represent relationships between pairs of objects [19]. A graph G is a mathematical entity defined by two discrete sets, the vertex set V, that represents the objects, and the edge set E, that represents the relationships among V. In simple terms, V define labels assigned to vertices while E is formed by pairs of these labels. When the relationships represented by the graph are mutual, such that, if u relates to v then v relates to u, the graph is said to be undirected and the edge (u,v) is not ordered. On the other hand, when the relationship is not necessarily mutual, the graph is said to be directed, or called *digraph*, and the edges are ordered pairs, *i.e* $(u,v) \in E$ does not imply $(v,u) \in E$. The edges of directed graphs are also called *arcs*. A visual depiction illustrating the differences between directed and non-directed graphs appear in Figure 2.1.

The vertices that share edges with a given vertex v in a graph G are said to be neighbors of v in G. Throughout this work, for a directed graph G, the sets $N^+(v) \subseteq V$ and $N^-(v) \subseteq V$ respectively denote the sets of outward and inward neighbors of v. In addition, a sequence of vertices $\{u_1,...,u_n\}$ for which $(u_k,u_{k+1}) \in E$, $k \in \{1,...,n-1\}$, is called a *path* of G. In the context of this work, a *trajectory* of G is a path of G.

Furthermore, the relationship represented by the edges of a graph can be weighted under a common numerical basis. To exemplify, imagine that a graph G has its vertices representing cities and its edges representing the distances among them, in such a way that to each edge (u,v) is assigned a real positive number that amounts to the distance between city u and city v measured in kilometers. Graphs with weights on its edges are simply called weighted graphs.

The applicability of graph theory to model and solve important problems on science and engineering is unequivocal. Many famous problems, such as the Traveling-Salesman Problem (TSP) [20] that is usually employed to illustrate the dichotomy between P and NP [14] and the Shortest Path Problem [21] that configures efficient packet routing on the Internet [52], are defined under the formalism of graph theory. In addition, graph algorithms are central to Computer Science, and the technology industry itself, being



(a) An undirected complete graph G_1.

(b) A directed graph G_2.

Figure 2.1: Visual representation of graphs with 3 vertices. The numbered circles represent vertices with labels in the set $V = \{1,2,3\}$. The edges of G_1 are lines and represent mutual relationship among vertices while the edges of G_2 are ordered pairs represented by arrows.

pervasive in various fields. A clear example is the A^* search algorithm [44] that finds applicability in path planning for automated vehicles [54] and in wireless network routing [3].

Finite graphs are the landscape in which the work described in this dissertation unravels. The walk processes to be described within this chapter will be described in finite graphs. It is even more interesting to note that both quantum and random walks can be seen as algorithms with its inner workings respectively explained by the laws of quantum mechanics and the theory of Markov Chains.

From now on, let $G = (V,E)$ be a directed graph obtained from an non-directed graph by introducing two directed edges for each initial one, *i.e* $(u,v) \in E$ if, and only if $(v,u) \in E$. In spite of $N^+(v) = N^-(v)$ for G, the superscript will not be omitted to stress the direction of edges.

2.1 Random walks

A random walk, or more generally a Markov chain, is a stochastic process with numerous applications in Mathematics, Engineering and Physics. Despite its broad applicability, random walks on graphs are extremely simple to describe. Let $\{X(t)\}_{t\geq 0}$ be a sequence of random variables where $X(t) \in V$ for all $t = 0,1,\ldots$. Then, consider the following stochastic process. Assume that $X(k) = v$ for $0 < k < t$ and $v \in V$. The value of $X(k+1)$ is a neighbor u of v with probability p_{vu}.

In abstract terms, the random variable X can be seen as a walker that moves on the graph in a probabilistic fashion. It is clear that if one asks where the walker is at an instant k, the answer has to be a probability distribution over V. In particular, only the neighbors

of the vertex where the walker is at instant $k-1$, *i.e* the value of $X(k-1)$, must have non-zero probability, considering the realization of the stochastic process $\{X(t)\}_{t\geq 0}$.

2.1.1 The assumption of conditional independence

The key principle to understand random walks is the Markovian assumption. As a matter of fact, the simplicity of the description of the walk on the graph was due to the capability of describing $X(t+1)$ by solely knowing the value of $X(t)$. The qualitative behavior of the whole process culminated from the definition of a transition rule that associated the probability p_{vu} to move from vertex u to v.

From this point, is crucial to evaluate the process in formal terms. Since $X(t)$ is a random variable it must have a particular distribution for every time instant t. Hence, completely analyzing the system is to describe a joint probability distribution of X for every possible t. Powerfully, once such description is attained, any possible statistical property of the system can be evaluated. Thus, the joint probability distribution $P[X(0) = v_0, X(1) = v_1, \ldots, X(t) = v_t]$ where $v_k \in V$ for $k = 0, \ldots, t$ is given by the chain rule of conditional probability as

$$P[X(0) = v_0, X(1) = v_1, \ldots, X(t) = v_t] = P[X(t) = v_t | X(t-1) = v_{t-1}, \ldots X(0) = v_0] \\ \ldots P[X(1) = v_1, | X(0) = v_0] P[X(0) = v_0] \quad (2.1)$$

In this context, the Markovian assumption is to assume that $X(t) = v_t$ is conditionally independent from $X(t-2)$ given $X(t-1) = v_{t-1}$, which enables the description of the joint probability as

$$P[X(0) = v_0, X(1) = v_1, \ldots, X(t) = v_t] = P[X(t) = v_t | X(t-1) = v_{t-1}] \\ \ldots P[X(1) = v_1 | X(0) = v_0] P[X(0) = v_0]. \quad (2.2)$$

The power of the Markovian assumption is to replace the joint probabilities in Equation 2.1 with marignal probabilities. In what concerns the description of the walker, this assumption simplified the numerical expression of the joint probability distribution by considering that the walker itself can be explained by such simplification, *i.e* by conditional independence. In a more abstract description a Markovian system can be seen as as a system where the future only depends on the present. All past information that contributes to the future state of the system is contained in the present state.

2.1.2 Non-homogeneous random walks on graphs

The Markovian assumption allows for describing random walks with transition probabilities that vary with time. The intuition built so far concerns the realization of the random

walker variable, as the instantaneous position, *i.e* value of $X(t)$, is key to describe the evolution of the process itself. Albeit, to proceed with the necessary mathematical analysis, random walks will be described in terms of the evolution of the probability distribution on the vertices of G. A non-homogeneous random walk on a directed graph $G = (V, E)$ is, in essence, a diffusion process of a probability distribution over the vertices of V through the edges of E with time-varying transition (conditional) probabilities.

As its most profound implication, the Markovian assumption states that we can define the dynamics of this diffusion by describing how probability flows among the vertices between two adjacent instants in time. For every time step t the probability of a vertex v flows to its neighbors. The amount of probability is defined by transition probabilities that are time-dependent. Trivially, since the vertex probability must sum to one, the total amount of vertex probability is constant in time.

Formally, let $\pi(t) \in \mathbb{R}_+^{|V|}$ denote a probability vector (or a discrete probability distribution) over the set V at discrete time instant t. In particular, $\pi(t) = (\pi_0(t), \pi_1(t), \ldots, \pi_n(t))$ where $n = |V|$ is the number of nodes in V and where $\pi_v(t) = P[X(t) = v]$ for every $v \in V$. Let $p_{vu}(t) \in [0, 1]$ be the transition probability for the walker to step from node u to node v, for which holds the law of total probability

$$\sum_{v \in N^+(u)} p_{vu}(t) = 1, \text{ for all } t, \tag{2.3}$$

and that $p_{vu}(t) > 0$ only if $(u, v) \in E$. The random walk is determined by the evolution of its probability distribution given by

$$\pi_v(t+1) = \sum_{u \in N^-(v)} p_{vu}(t)\pi_u(t). \tag{2.4}$$

Equation 2.4 states that the probability of a vertex at instant $t+1$ is given by a combination of the probabilities of its inward neighbors, on the previous instant t. From this perspective, the sets of transition probabilities can be defined arbitrarily as long as the law of total probability remains valid, implying that the distributions that can be achieved by time evolution are fundamentally constrained by Equation 2.4. This property will be denoted as the *local evolution of probabilities* and is, in fact, the manifestation of the Markovian assumption to the walker system.

In matrix form, Equation 2.4 is represented as

$$\pi(t+1) = P(t)\pi(t), \tag{2.5}$$

where $P(t)$ is a time-dependent column stochastic matrix with entries $p_{vu}(t)$ denoting the transition probability to move from vertex u to vertex v, at instant t. Note that when $\pi_u(t) = 0$, the values of transition probabilities $p_{vu}(t)$ do not contribute to the diffusion

process at further times, *i.e* $p_{vu}(t)$ does not influence $\pi(t+k)$ for $k > 0$.

2.1.3 Homogeneous random walks on graphs

Despite the fact that the non-homogeneous random walk defined in Equation 2.5 is the most general form of a discrete-time random walk on a graph, most of the theory of random walks addresses the case where the transition probabilities are time independent [15]. Taking $p_{vu}(t)$ constant for every t has profound consequences for the dynamics of the system, imposing a clear restriction on the possible evolution of probabilities that can be achieved by random walks.

The constant transition probabilities simplifies the evolution for the diffusion. The fundamental consequence of time homogeneity is that the matrix Equation 2.5, defined as a recursive equation, collapses to a much simpler polynomial matrix equation in time. Since $P(t) = P$, the vertex probability vector at instant $t+1$ is just

$$\pi(t+1) = P^{t+1}\pi(0), \tag{2.6}$$

where $\pi(0)$ is the initial vertex probability distribution.

To describe the impact of this homogeneity, the concepts of *irreducibility* and *aperiodicity* of Markov chains are critical. A random walk is said to be irreducible if, for every pair $u, v \in V$, the probability of traversing from u to v is greater than 0 for some finite time displacement [15].

In addition, let *gcd* denote the greatest common divisor of a set of integers. Let $C(v)$ denote the set of all cycles of G that begins (and ends) in the vertex v. Let $L(c)$ be a function that returns the length of a cycle c in G. A vertex has a period

$$a(v) = gcd\{L(c) : c \in C(v) \text{ and } p(c) > 0\}, \tag{2.7}$$

where $p(c)$ is the probability of c being the path of the walker if the process starts at v, *i.e* $\pi_v(0) = 1$. A random walk is said to be *aperiodic* if $a(v) = 1$ for every $v \in V$ [15]. It then follows the important result on the convergence of $\pi(t)$ [15].

Theorem 1. *Every irreducible and aperiodic random walk converges to a unique stationary probability distribution π, such that*

$$\lim_{t\to\infty} P^t\pi(0) = \pi \tag{2.8}$$

regardless of the initial condition $\pi(0)$.

The convergence stipulated by Theorem 1 represents a state of equilibrium since $\pi(t+1) = P\pi(t)$. Again, from the theory of Markov chains, it is known that this state of

equilibrium is the dominant eigenvector of the left stochastic matrix P. Stochastic matrices have a bounded spectrum, such that the absolute value of its eigenvalues is at most 1. When the Markov chain is aperiodic and irreducible, there exists a unique eigenvector with eigenvalue 1, which becomes a valid probability vector when normalized.

It is fundamental to note once more that this convergence has roots on the homogeneity of transition rules and that such result is not always valid for the generic random walk of Equation 2.5.

2.1.4 Simulation of random walks

The definition of the random variable $X(t)$ implies that the realization of the stochastic process X_t is a path of G. Thus, the random walk can be simulated to sample paths of G. This procedure is, in fact, straightforward. Let v_t denote the realization of the random variable $X(t)$ and $x(t)$ be the sequence $x(t) = (v_0, ..., v_t)$. The random walk is simulated by sampling $x(0)$ according to $\pi(0)$ and, from there on, sampling $x(t+1)$ as a neighbor of $x(t)$ with probability given by the columns of $P(t)$. Since, for $t > 0$, the sample is taken from the neighborhood of $X(t-1) = v_{t-1}$, the sequence $x(t)$ is a path of the graph, which is called *sample path*.

The simulation of random walks finds interesting applications. In spite of the mathematical simplicity to describe random walks, the computational cost associated with the calculation of the evolution of probabilities at a given instant t is $\mathcal{O}(t|V|^2)$, since t matrix-vector multiplications must be performed. When the number of vertices is large, the time to compute all multiplications may be impractical for some applications. In this context, it is possible use the simulation procedure to approximate the value of the probability distribution of random walks. Since, at each time instant, a discrete random variable with support size $\mathcal{O}(|V|)$ is sampled, the time complexity of each simulation step is $\mathcal{O}(|V|)$ and the simulation of a path with t steps is $\mathcal{O}(t|V|)$. The vertex probability can be estimated by generating multiple paths and computing the empiric vertex distribution at every time instant. The simulation procedure is successfully employed to compute the PageRank metric for large graphs [33], as well as to sample more complex probability distributions through the Metropolis-Hastings algorithm [16].

2.2 Quantum walks

Discussing quantum walks in a mathematical framework is fundamental to the goal of this dissertation. As a matter of fact, the usual intuition of a walker that is at a particular vertex of a graph at a specific time instant that motivates the mathematical description of random walks fails in the quantum context. On the other hand, the intuition of a probability diffusion process remains fruitful to guide its description.

Quantum walks are defined in complex vector spaces. The probabilities involved with the process are embedded in the formalism through a postulate that connects the complex vector spaces with the real space of probabilities. For what concerns intuition, quantum walks can be directly described as a diffusion process of a complex quantity, called wavefunction, in a vector space defined by the edges of a graph.

2.2.1 Linear algebra and quantum mechanics

The goal of this section is to address the mathematical background necessary to describe the postulates of quantum mechanics and to define quantum walks on graphs.

Hilbert spaces

The complex vectorial spaces in which quantum systems are described are called *Hilbert spaces*, referred to as $\mathscr{H}$. A Hilbert space is a vector space over the complex field $\mathbb{C}$ with a well-defined inner product operation $(.) : \mathscr{H}, \mathscr{H} \to \mathbb{C}$. Then, let u, v and w be vectors of $\mathscr{H}$. Let a and b be complex numbers and a^* be the complex-conjugate of a. The properties

$$(u,v) = (v,u)^*, \tag{2.9}$$

$$(au + bw, v) = a(u,v) + b(w,v), \tag{2.10}$$

$$(u,u) \geq 0 \text{ with equality only when } u = 0 \tag{2.11}$$

must hold for a function to describe a valid inner product operation and its associated Hilbert space.

The power of abstraction of this algebraic definition is fantastic. For instance, Hilbert spaces can be defined for functions of complex numbers and have infinite dimension, which occurs in the general formalism of quantum mechanics allowing the description of particles in the real world. Nonetheless, the description of quantum walks on finite graphs can be solely described in terms of finite Hilbert spaces. The vectors of the Hilbert spaces in context can be regarded as the usual vectors defined through coordinates. The linear operators that modify these vectors can be regarded as matrices. Finally, the inner product in question is the usual inner product defined for vectors over complex fields such that

$$(u,v) = \sum_k u_k^* v_k.$$

The Bra-ket notation

To enable the fast analysis of quantum systems in algebraic terms, Dirac proposed, in 1939, a notation capable of condensing the description of vectors and operators in Hilbert

spaces [11]. The bra-ket notation, or Dirac's Notation, uses the *ket* symbol $|.\rangle$ to denote a vector in $\mathscr{H}$ and the *bra* symbol $\langle .|$ to represent vectors that lie on the dual space of $\mathscr{H}$. In this context, let $|v\rangle \in \mathscr{H}$ and $|u\rangle \in \mathscr{H}$ be two vectors in a generic Hilbert space $\mathscr{H}$. The inner product of the vectors are represented as $\langle u|v\rangle$ (bra-ket symbol) while the outer product is given by $|u\rangle\langle v|$. As the definitions of linear algebra demands, $\langle u|v\rangle$ is a complex number and $|u\rangle\langle v|$ is a linear operator. The bra-ket notation is powerful and encompasses generic Hilbert spaces of finite and infinite dimensions. Although, since the scope of this work only addresses Hilbert spaces of finite dimensions, is possible to think of $|v\rangle$ as a column vector and $\langle v|$ as a row vector for which the k-th column of $\langle v|$ is the complex conjugate of the k-th row of $|v\rangle$. It is important to note that v is a label for the vector $|v\rangle$.

Linear algebra with the bra-ket notation

At this point, it is fruitful to use the bra-ket notation to describe and state some linear algebra results and definitions that will be essential to this work. Let $A : \mathscr{H} \to \mathscr{H}$ be a linear operator defined on a Hilbert space $\mathscr{H}$. The eigenvectors and eigenvalues of A are, respectively, the set of vectors $\{|\lambda_k\rangle\}$ and set of scalars $\{\lambda_k\}$ for which

$$A\,|\lambda_k\rangle = \lambda_k\,|\lambda_k\rangle\,. \tag{2.12}$$

Note that λ_k is seen as a label, or a bookkeeping variable, for the eigenvector $|\lambda_k\rangle$ and represents a complex number.

Moreover, each operator A has an associated *adjoint* operator $A^\dagger$ for which holds

$$(A^\dagger\,|u\rangle\,,|v\rangle) = (|u\rangle\,,A\,|v\rangle), \tag{2.13}$$

where $(.,.)$ is the inner product operation and $|u\rangle\,,|v\rangle \in \mathscr{H}$ are any pair of vectors in the domain of A. For every pair λ, $|\lambda\rangle$ of eigenvalue and eigenvector of A holds the relation

$$A^\dagger\,|\lambda\rangle = \lambda^*\,|\lambda\rangle\,. \tag{2.14}$$

A *basis* $\{|e_k\rangle\}$ of $\mathscr{H}$ is a set of linearly-independent vectors capable of spanning $\mathscr{H}$: any vector $|u\rangle \in \mathscr{H}$ can be written as a linear combination of the vectors $\{|e_k\rangle\}$ as

$$|u\rangle = \sum_k \langle e_k|u\rangle\,|e_k\rangle\,. \tag{2.15}$$

For a given $\mathscr{H}$, every basis has the same number of linearly-independent vectors, which gives the dimension of the vector space. An *orthonormal basis* is a set of spanning vectors

$\{|u_k\rangle\}$ for which

$$\langle u_k | u_j \rangle = \delta_{kj}, \tag{2.16}$$

where $\delta_{kj} \in \{0,1\}$, $\delta_{kj} = 1 \iff k = j$, is the *Kronecker delta function*. In addition, every basis $\{|e_k\rangle\}$ of $\mathscr{H}$ satisfies the *completeness relation*

$$\sum_k |e_k\rangle\langle e_k| = I, \tag{2.17}$$

where I is the identity operator in $\mathscr{H}$.

The operator A is said to be a normal operator when

$$AA^\dagger = A^\dagger A. \tag{2.18}$$

The spectral theorem concerning normal operators is one of the most important results in linear algebra. It states that for every normal operator A there exists a unique orthonormal basis of $\mathscr{H}$ capable of *diagonalizing* A and that this basis is the set of normalized eigenvectors $\{|\lambda_k\}\rangle$ of A, such that

$$A = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k| . \tag{2.19}$$

Diagonalization means that the matrix representation of operator A is a diagonal matrix in the basis $\{|\lambda_k\}\rangle$. Since $\{|\lambda_k\}\rangle$ is a basis for $\mathscr{H}$, the completeness relation (Equation 2.17) is valid for the eigenvalues of normal operators. In addition, a unitary operator A is a normal operator for which holds

$$A^\dagger A = I. \tag{2.20}$$

Equations 2.14 and 2.20 imply that the eigenvalues of a unitary operator A are all of form

$$\lambda_k = e^{i\theta_k}. \tag{2.21}$$

Unitary operators are *norm preserving* operators since

$$\langle u | A^\dagger A | u \rangle = \langle u | u \rangle \tag{2.22}$$

for every $|u\rangle \in \mathscr{H}$.

The tensor product $\bigotimes : \mathscr{H}_1, \mathscr{H}_2 \to \mathscr{H}_3$ between two vectors is an operation that maps two vectors of arbitrary dimension into a vector of a higher dimension [30]. In precise terms, $dim(\mathscr{H}_3) = dim(\mathscr{H}_1) \times dim\mathscr{H}(2)$. The tensor product allows for the construction of high-dimensional Hilbert spaces by combining spaces of smaller dimensions in an

specific way. In this context, $\mathscr{H}_3$ is the tensor space $\mathscr{H}_1 \bigotimes \mathscr{H}_2$. Formally, $\mathscr{H}$ is a tensor space if

$$\mathscr{H} = \bigotimes_k \mathscr{H}_k. \tag{2.23}$$

A basis for a tensor space $\mathscr{H}$ can be obtained by taking the tensor product among the basis of each subspace $\mathscr{H}_k$. Thus, the dimension of $\mathscr{H}$ is given by the product of the dimensions of its constituent spaces

$$dim(\mathscr{H}) = \prod_k dim(\mathscr{H}_k). \tag{2.24}$$

The tensor product is an abstract operation that can be defined in multiple ways. For this work, the tensor product definition adopted is the *Kronecker product*. Assume that $v \in \mathscr{H}_1$ and $u \in \mathscr{H}_2$ are two column vectors such that $dim(\mathscr{H}_1) = m$ and $dim(\mathscr{H}_2) = n$. The Kronecker product can be visualized as the operation

$$\begin{bmatrix} v_1 \\ . \\ . \\ . \\ v_n \end{bmatrix} \bigotimes \begin{bmatrix} u_1 \\ . \\ . \\ . \\ u_m \end{bmatrix} = \begin{bmatrix} v_1 u \\ . \\ . \\ . \\ v_n u \end{bmatrix}, \tag{2.25}$$

where $v_k u$ on the left side of the Equation represents a multiple of the entire vector u by the k-th entry of v.

The tensor product can also be applied on operators, such that is possible to describe an operator A for the space $\bigotimes_k \mathscr{H}_k$ as

$$A = \bigotimes_k A_k, \tag{2.26}$$

where A_k is a linear operator in $\mathscr{H}_k$. In this case, the visual representation for operators is analogous to Equation 2.25, although the inputs and the output are matrices. A more detailed description of the tensor product and the Kronecker product can be found in [30]. The bra-ket notation has also a simplified form to denote tensor products between vectors. The product $|u\rangle \bigotimes |v\rangle$ is simply referred as $|u\rangle |v\rangle$, or just $|u,v\rangle$. This last form is the one adopted throughout this dissertation.

The last linear algebra result of interest is the Gram-Schmidt procedure, capable of generating an orthonormal basis from a set of linear independent vectors [31, 50]. Given a set of n vectors $\{|v_i\rangle\}$ the Gram-Schmidt procedure constructs an othonormal basis

$\{|u_i\rangle\}$ by taking

$$|u_1\rangle = |v_1\rangle / \||v_1\rangle\|, \tag{2.27}$$

$$|u_k\rangle = \frac{|v_k\rangle - \sum_{j=1}^{k-1} \langle u_{k-j}|v_k\rangle |u_{k-1}\rangle}{\left\||v_k\rangle - \sum_{j=1}^{k-1} \langle u_{k-j}|v_k\rangle |u_{k-1}\rangle\right\|}. \tag{2.28}$$

The postulates of quantum mechanics

The postulates of quantum mechanics are the set of mathematical rules that enable the description of quantum systems. The postulates combined allow for the description of any quantum mechanical system and construct the most accurate known model for describing nature [32]. In essential ways, the postulates of quantum mechanics can be enunciated in more than one form. The version of the postulates presented here were chosen in order to maintain a simple description of discrete-time quantum walk systems on finite graphs.

The first postulate defines that the state of a quantum system is mathematically represented by a unitary vector in a Hilbert space. Albeit, it neither defines which Hilbert space is to be used to represent a certain system, nor explains how to embed the vectors with physical meaning. Those remain to be specified once a system is to be modeled. Thus, let $|\Psi(t)\rangle \in \mathscr{H}$, where $\mathscr{H}$ is any Hilbert space, to represent a generic physical state of some quantum mechanical system. It is a well known fact from linear algebra that any vector in $\mathscr{H}$ can be written as a linear combination of vectors that form a basis to $\mathscr{H}$. Given a basis $\{|e_k\rangle\}$, the generic representation in $\mathscr{H}$ can be expressed as

$$|\Psi(t)\rangle = \sum_k \Psi(e_k,t)\,|e_k\rangle\,, \tag{2.29}$$

where $\Psi(e_k,t)$ is said to be the wavefunction at state $|e_k\rangle$, at instant t. In this generic representation, the system is said to be in a superposition of states that depends on the choice of basis. This simple principle is one of the most beautiful aspects of quantum theory and it usually characterizes the strangeness of quantum phenomena. For example, qubits can be prepared in a superposition of states *zero* and *one*, which is critical for the remarkable improvements in problem solving leveraged by quantum computing such as Shor's algorithm [47]. In addition, the first postulate establishes that systems of more than one particle are represented by the tensor product of the spaces of each particle.

The second postulate defines that a closed quantum mechanical system evolves through the action of a unitary operator $U(t,t') : \mathscr{H} \to \mathscr{H}$ as

$$\big|\Psi(t')\big\rangle = U(t,t')\,|\Psi(t)\rangle\,, \tag{2.30}$$

and such that $U(t,t')$ depends only on the instants t and t'. Since $U(t,t')$ is unitary, the evolution of a closed quantum systems remains closed as $\|\Psi(t)\| = 1$ for all t. Its worth

mentioning that t is not necessarily discrete. Similarly to the first postulate, it does not address which unitary performs time-evolution for a given system, it defines instead the mathematical properties of time-evolution that has to hold for a valid model of a quantum system.

Finally, the last postulate specifies how to associate probabilities with the abstract vectors of $\mathscr{H}$. This association comes from operations defined as *measurements*. A measurement is a procedure that interferes with the system in order to access the value of wavefunction. The quantum theory of measurement is essential to quantum mechanics and is a completely different paradigm than the classical measurement description [46]. The context of this work attains to the subset of measurement theory that addresses projective, or von Neumann, measurement operators. Measurements differs drastically from the postulate of evolution because the action of measurement is itself created by the interaction of a closed system with another system, the measurement device. This interaction causes the wavefunction to collapse, breaking its superposition. Formally, a projective measurement is defined by a set of projective operators $\{M_k\}$ for which holds the completeness relation

$$\sum_k M_k^\dagger M_k = I, \tag{2.31}$$

where I is the identity matrix. After a measurement takes place, the system is postulated to be at the state

$$|\Psi\rangle = \frac{M_k |\Psi(t)\rangle}{\sqrt{\|M_k |\Psi(t)\rangle\|}} \tag{2.32}$$

with probability $\langle\Psi(t)| M_k^\dagger M_k |\Psi(t)\rangle$ [32]. Put in other words, the result of a measurement is probabilistic and the state of the system "jumps" to a given eigenvector of the measurement operator. The probability involved is proportional to the value of the projection of the state vector before measurement into the obtained eigenvector [45].

Quantum computing and the representation of qubits

The usual description of quantum computing and quantum algorithms relies on the representation of qubits, or quantum bits. In order for this dissertation to be self contained, it is necessary to address the computational basis, the usual attribution of vectors of a Hilbert space to represent the state of qubits. A qubit is a two-level quantum system. Hence, the postulate of representation determines that a bi-dimensional Hilbert space $\mathscr{H}_2$ is necessary to describe the system.

The approach used is to represent the values *on* and off of the qubit with two basis vectors of $\mathscr{H}_2$. The computational basis for the qubit is the canonical basis of the bi-

dimensional space $\mathscr{H}_2$. The value 0, or *off*, is represented by the canonical vector $|0\rangle = [1\ 0]^T$, while 1 as the column vector $|1\rangle = [0\ 1]^T$.

In the case where two qubits are to be described, the Hilbert space in question must be four-dimensional. All the possible states (values) that the qubits may asssume are $|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle$, where the bra-ket notation for tensor product is reduced even further, as $|00\rangle = |0\rangle\,|0\rangle$. In consistency with the postulates of quantum mechanics, each of the values must be associated with a basis vector. In order to accommodate them all, the computational basis grows by taking the tensor product of $\mathscr{H}_2$ with itself. Once the Kronecker product is considered, the new basis is simply be the canonical basis for the four-dimensional space $\mathscr{H}_4 = \mathscr{H}_2 \bigotimes \mathscr{H}_2$.

At the end of the day, the dimension of the Hilbert space used to describe a quantum register (a set of qubits) with n qubits is 2^n. Each possible combination between values of qubits is associated with a canonical vector of $\mathscr{H}_{2^n}$. The measurement basis that outputs directly the value of qubits is, in this generic scenario, the canonical basis. A longer description of qubits, together with examples on bi-dimensional quantum systems can be found in the literature [32].

2.2.2 Quantum walks on graphs

With the proper notation and the postulates of quantum mechanics, it is now possible to define quantum walks on graphs. As mentioned in Chapter 1, this work treats discrete-time coined-quantum walks, which are one of the multiple definitions of quantum walks.

A discrete-time coined quantum walk on a graph G is an evolution process of a complex vector in a Hilbert space $\mathscr{H}_w \subseteq \mathscr{H}_v \bigotimes \mathscr{H}_c$ defined by the graph structure [39]. The vertex space $\mathscr{H}_v$ has dimension $|V|$ and codifies the vertices of the graph by assigning to each vertex a basis vector of $\mathscr{H}_v$. In turns, the coin space $\mathscr{H}_c$ denotes the degrees of freedom of the walker movements, with dimension given by the maximum degree of the graph $D = \max\{d(v) : v \in V\}$. In a similar way, the coin space codifies the degrees of movement by assigning each degree to a basis vector of $\mathscr{H}_c$. Precisely, $\mathscr{H}_w$ is $\mathscr{H}_v \bigotimes \mathscr{H}_c$ only when G is a regular graph.

Denoting $\{|c\rangle\}$ and $\{|v\rangle\}$, respectively, as the basis for the spaces $\mathscr{H}_c$ and $\mathscr{H}_v$, and $C_v = \{0, ..., d(v)-1\}$ as the integer set for the number of outward edges of a node v, the basis for $\mathscr{H}_w$ is $\{|v,c\rangle : v \in V, c \in C_v\}$. Assuming $|\Psi(t)\rangle$ is the walker wavefunction at discrete time instant t, the quantum walk evolution is given by the action of two unitary operators $S : \mathscr{H}_w \to \mathscr{H}_w$ and $W : \mathscr{H}_w \to \mathscr{H}_w$ on the system state vector as

$$|\Psi(t+1)\rangle = SW\,|\Psi(t)\rangle\,. \tag{2.33}$$

In this work, we assume that both S and W may vary with time, although the dependence will be omitted in order to simplify notation.

Representation of edges

Precisely, each vector $|v,c\rangle \in \mathscr{H}_w$ refers to one outward edge of v. The value of c is restricted by the number of neighbors of v, which defines the set C_v. In this context, there are $d(v)$ different ways of deciding which edge $(v,u) \in E$ is represented by the vector $|v,c\rangle$. Nonetheless, this mapping is simply a matter of choice that only impacts the definition of the operators S and W by a permutation operation. A broad discussion on the representation of quantum walks can be found in [36].

The coin operator

The coin operator (W) acts on the degrees of freedom of the walker. The most general coin operator is given by

$$W = \sum_{v \in V} |v\rangle\langle v| \bigotimes W_v, \tag{2.34}$$

where W_v is a unitary operator. The coin is responsible for mixing the amplitude of a given state $|v,c\rangle$ with all states $|v,c'\rangle$ such that $c,c' \in C_v$, *i.e* degrees of freedom of the same vertex, through weights $w_{vc'c}$. This mixing behavior is enlightened when one observes the action of W on a generic state vector $|v,c\rangle$

$$W|v,c\rangle = \sum_{j \in C_v} |v,j\rangle\, w_{vjc}. \tag{2.35}$$

For W to be unitary, one must impose conditions on the complex values of w_{vjc}. In particular, once the product $WW^\dagger$ is analyzed, unitarity demands that the operator coefficients obey

$$\sum_{i \in C_v} |w_{vik}|^2 = 1 : v \in V, \text{ and} \tag{2.36}$$

$$\sum_{i \in C_v} \sum_{j \in C_v} \sum_{k \neq j} w^*_{vij} w_{vik} = 0 : v \in V. \tag{2.37}$$

Two coin operators which will be important further ahead are the Hadamard and the Grover operators. The D-dimensional Hadamard operator H_D can be constructed for Hilbert spaces with dimension of the form $D = 2^k$, for $k \in \{1,2,...\}$. Its formal definition is given by

$$H_D = H_{\frac{D}{2}} \bigotimes H_2 \tag{2.38}$$

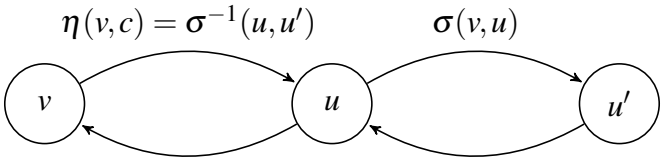


Figure 2.2: Visual depiction of auxiliary functions η and σ. η gives an ordering for the neighbors of v such that, in this case, $\eta(v,c) = u$. σ maps the state $|v,c\rangle$ (edge (v,u)) to the state $|u,\sigma(v,u)\rangle$ (edge (u,u')). The inverse association σ^{-1} connects the state $|u,\sigma(v,u)\rangle$ (edge (u,u')) with state $|v,c\rangle$ (edge (v,u)).

where

$$H_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{2.39}$$

On the other hand, by taking $|c\rangle$ to denote the vectors of the computational basis, the Grover operator can be defined for Hilbert spaces with arbitrary dimension D as

$$G = \frac{2}{D} \sum_{c=0}^{D-1} \sum_{c'=0}^{D-1} |c\rangle\langle c'| - I, \tag{2.40}$$

The shift operator

The shift, or swap, operator (S) acts by moving the mixed amplitudes created by the operator W to outward edges. Let $\eta : V \times C \to V$ be a mapping between outward edges and outward neighbors of every vertex, *i.e* $u = \eta(v,c)$ is the c-th outward neighbor of vertex v; let $\sigma : V \times V \to C$ be a function that maps an inward edge of a vertex with one of its outward edges, such that $\sigma(u,v) = c$ associates the inward edge (u,v) of vertex v with its c-th outward neighbor; and let $\sigma^{-1} : V \times V \to C$ to be the inverse association such that if $v = \eta(u,c')$ and $\sigma(u,v) = c$ than $\sigma^{-1}(u,v) = c'$. The auxiliary functions are abstractly depicted in Figure 2.2, where u is a neighbor of v and u' is a neighbor of u. The action of the shift operator is formally defined as

$$|v,c\rangle \to |u,\sigma(v,u)\rangle, \tag{2.41}$$

where $u = \eta(v,c)$. The flow of wavefunction created by S is depicted in Figure 2.3, where the central figure gives an initial configuration of wavefuction and each adjacent figure shows the outcome of a particular shift operator applied to this initial state.

The functions η and σ can be arbitrarily defined as long as the operator remains unitary and the graph edges are respected. In fact, different definitions for η and σ lead to different state amplitude dynamics. To illustrate their generality, the flip flop shift operator can be simply implemented by taking $\eta(v,c) = u$, $\eta(u,c') = v$, $\sigma(u,v) = c$ and

$\sigma(v,u) = c'$ for all $(u,v) \in e$, and an arbitrary choice for orderings the outward neighbors as shown in Figure 2.3a. Furthermore, the action of SW on a generic state vector

$$|\Psi(t)\rangle = \sum_{v \in V} \sum_{c \in C_v} \Psi(v,c,t)\,|v,c\rangle$$

is given by

$$|\Psi(t+1)\rangle = SW \sum_{v \in V} \sum_{c \in C_v} \Psi(v,c,t)\,|v,c\rangle\,, \tag{2.42}$$

$$|\Psi(t+1)\rangle = S \sum_{v \in V} \sum_{c \in C_v} \sum_{u \in V} \sum_{i,j \in C_u} w_{uji} \Psi(v,c,t-1)(|u\rangle\langle u| \bigotimes |j\rangle\langle i|)\,|v,c\rangle \tag{2.43}$$

$$|\Psi(t+1)\rangle = S \sum_{v \in V} \sum_{j \in C_v} w_{vjc} \sum_{c \in C_v} \Psi(v,c,t-1)\,|v,j\rangle \tag{2.44}$$

$$|\Psi(t+1)\rangle = \sum_{v \in V} \sum_{c \in C_v} \sum_{j \in C_v} w_{vjc} \Psi(v,c,t)\,|\eta(v,j), \sigma(v,\eta(v,j))\rangle\,, \tag{2.45}$$

$$|\Psi(t+1)\rangle = \sum_{v \in V} \sum_{u \in N^-(v)} \sum_{j \in C_u} (\Psi(u,j,t) w_{(u,\sigma^{-1}(u,v),j)})\,|v, \sigma(u,v)\rangle\,. \tag{2.46}$$

Equation 2.46 is obtained by noting that each degree of freedom of a given vertex v corresponds to exactly one outward neighbor of v and by fixing the vertex element of the basis state vector from the summation through a variable substitution from η. A common swap operator which will be mentioned on further sections of this article is the moving-shift operator M for regular graphs depicted in Figure 2.3c, which is simply defined by the relationship

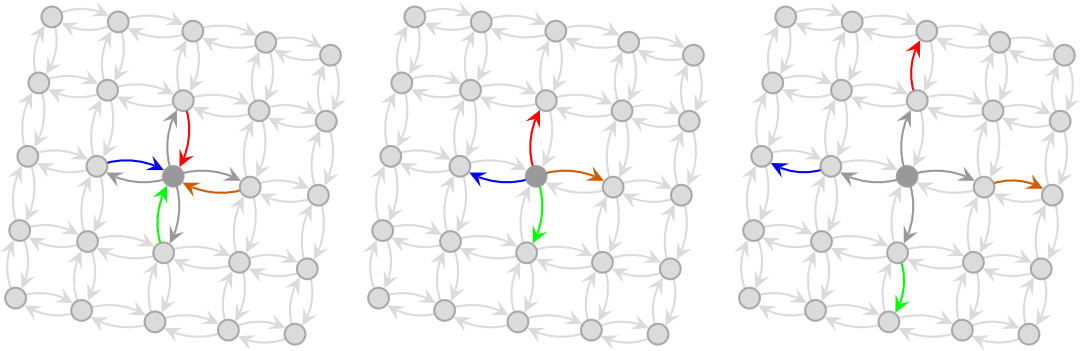
$$M : |v,c\rangle \to |\eta(v,c), c\rangle\,. \tag{2.47}$$

The measurement basis of quantum walks

The given description of quantum walks maps edges of G to basis vectors of $\mathscr{H}_w$. This description is arbitrary and only becomes complete when the measurement basis is defined. Since the goal is to model the behavior of a walk in G, is natural to use the representation basis itself as the basis of measurement. Hence, the measurements operators are simply taken to be the set of operators $|v,c\rangle\langle v,c|$. Then, assuming that $v = \eta(u,c)$, the measurement postulate establishes that the probability of measuring an edge $(u,v) \in E$ is

$$p(u,v) = |\langle v,c|\Psi(t)\rangle|^2. \tag{2.48}$$

The measurement postulate enables the definition of probability density functions for the edges and vertices of G. Let $\rho : V \times C \times \mathbb{N} \to [0,1]$ be the probability density function



(a) Flip-flop operator (b) Initial wavefunction (c) Moving-shift operator

Figure 2.3: Depiction of shift operators on 5-by-5 grid. The central figure shows the initial wavefunction state, where edge color identifies the outward edges of the center vertex. Edges of the same color on different figures are mapped to each other. The left figure depicts the result of the flip-flop operator which maps edge (v,u) to (u,v). The right figure shows the result of the moving-shift operator (Equation 2.47) which maps edges according to directions, *i.e* the left-ward edge of the center vertex is mapped to the left-ward edge of the left-ward neighbor of the center vertex and so on.

of measuring the walker at a given state (outward edge) such that $\rho(v,c,t) = |\Psi(v,c,t)|^2$. Let $\upsilon : V \times \mathbb{N} \to [0,1]$ be the probability density function of measuring vertex v at a given time instant. Since the states form a basis, it follows that

$$\upsilon(v,t) = \sum_{c \in C_v} |\Psi(v,c,t)|^2, \tag{2.49}$$

which combined with Equation 2.46 leads to

$$\upsilon(v,t) = \sum_{u \in N^-(v)} \left| \sum_{j \in C_u} \Psi(u,j,t-1) w_{(u,\sigma^{-1}(u,v),j)} \right|^2. \tag{2.50}$$

It is assumed that the vertex measured in an outward-edge is the source of the edge, *i.e* the vertex outcome of measuring the edge (u,v) is u. The probability distribution in Equation 2.50 encapsulates the statistical properties of the quantum walk in terms of vertices. An alternative description for the dynamics of coined quantum walks can be found in terms of two partition quantum walks is available in [22].

Simulating quantum walks

The interference caused by measurements of quantum systems has strong implications in describing a simulation procedure for quantum walks. These implications are fundamental both in the context of classical computation, as well as when considering the simulation of quantum walks in a quantum computer. In contrast with random walks, samples of quantum walks are taken in an independent fashion. Physically, taking t sam-

ples from a quantum walk in t consecutive time steps means to identically prepare t walker systems with the same initial superposition state, evolve each system independently until a different given time step $k \in \{1,...,t\}$ and than measure each of t systems. In other words, the first prepared system goes through a one-step evolution process and is measured, the second one through a two-step evolution process and measured, and so on until all t measurements are performed.

For simulations on classical computers, the independent measurement scheme means to draw independent samples from the vertex distributions v at the desired time instants. Such independence implies that consecutive samples are not assured to be paths of G.

Chapter 3

The statistical equivalence between quantum and random walks

Early results on quantum walks identified significant differences between quantum and random walks. In particular, initial results show that the wavefunction of quantum walks do not converge to a fixed superposition of states, that the vertex distribution does not necessarily converge, and that the spreading behavior of the probability distribution for quantum walks differ from classical random walks by polynomial factors [1]. Nonetheless, these differences were obtained for time-homogeneous random walks and for quantum walks with time-independent unitary operators S and W.

In contrast with the homogeneous case, the non-homogeneous random walk is not guaranteed to converge and represents a generic process of probability diffusion on the edges of a graph. Furthermore, the intuition behind quantum walks states that the quantum process can be seen as a diffusion process of a complex quantity, the wavefunction, on the edges of a graph. In addition, non-homogeneous random walks and quantum walks were shown to be capable of generating identical probability distributions on the infinite integer line [29]. In this context, the following question arises naturally: is it possible to construct, for any given quantum walk, with unitary operators S and W that may vary with time, a statistically equivalent non-homogeneous random walk in terms of vertex probabilities for an arbitrary finite graph?

In the remainder of this Chapter, a positive answer to this question is presented. Moreover, the solution is extended to the scenario where multiple quantum walkers are allowed to interfere with each other through a generic unitary operator. In spite of its relative simplicity, these results highlight connections between quantum and random walks that were not explicit before and mark the first contribution of this dissertation to the literature of quantum and random walks on finite graphs.

3.1 Quantum walks as non-homogeneous random walks

The law of total probability and Equation 2.4 provide the starting point to establish the equivalence between quantum and random walks. Within this context, let $\pi : \mathbb{N} \to [0,1]^{|V|}$ be the probability vector representing the vertex probability distribution of a quantum walk at a given time instant such that $\pi_v(t) = \upsilon(v,t)$. From this perspective, it is necessary to define the non-homogeneous random walk that matches the evolution of $\pi(t)$, for all t. A sufficient condition is the construction of the time-dependent transition matrix $P(t)$ for which $\pi(t+1) = P(t)\pi(t)$, for all v,t. The existence of such matrices implies the principle of local evolution, in the sense of Equation 2.4, for the full quantum walk operator SW, regardless of initial conditions. Theorem 2 establishes the construction of the time-dependent random walk matrices.

Theorem 2 (Quantum walk local evolution)**.** *For any time instant t, the evolution of the vertex probability of a quantum walk performed by the action of the unitary operator SW is local and equivalent to the Markovian matrix $P(t)$ where*

$$p_{vu}(t) = \begin{cases} \frac{\rho(v,c,t+1)}{\upsilon(u,t)}, & \text{if } \upsilon(u,t) > 0 \text{ and } (u,v) \in E \\ \frac{1}{d(u)}, & \text{if } \upsilon(u,t) = 0 \text{ and } (u,v) \in E \\ 0, & \text{otherwise} \end{cases} \tag{3.1}$$

such that $\pi(t+1) = P(t)\pi(t)$, where $c = \sigma(u,v)$.

Proof. To prove the claim, it is necessary to show that the following three properties hold for P:

1. $0 \leq p_{vu}(t) \leq 1$ for every $u, v \in V$;
2. $\sum_{v \in N^+(u)} p_{vu}(t) = 1$ for each $v \in V$;
3. $\upsilon(v,t+1) = \sum_{u \in N^-(v)} p_{vu}(t)\upsilon(u,t)$ for each $v \in V$.

Whenever $\upsilon(u,t) = 0$, choosing $p_{vu}(t) = \frac{1}{d(u)}$ avoids division by zero and assures the first and the second conditions. Since $p_{vu}(t)\upsilon(u,t) = 0$ for this particular case, the task is to show that the three conditions hold for $\upsilon(u,t) > 0$. Note that $p_{vu}(t)$ could be chosen arbitrarily, as long as the u-th column of P respected conditions 1 and 2. Uniform weights were chosen for simplicity. Using Equation 2.50, and taking $c \in C_v$, $c = \sigma(u,v)$ and $c' = \sigma^{-1}(u,v)$, one has:

$$\rho(v,c,t+1) = \left| \sum_{j \in C_u} \Psi(u,j,t) w_{uc'j} \right|^2 \tag{3.2}$$

$$p_{vu}(t) = \frac{\left| \sum_{j \in C_u} \Psi(u,j,t) w_{uc'j} \right|^2}{\upsilon(u,t)}. \tag{3.3}$$

The numerator on the right-hand side of Equation 3.3 can be thought of as the result of the inner product between the vectors $|\Psi^*(u,t)\rangle$ and $|W_u\rangle$ with j-th coordinates respectively given by $|\Psi^*(u,t)\rangle_j = \Psi^*(u,j,t)$ and $|W_u\rangle_j = w_{uc'j},\ j \in C_u$. By the Cauchy-Schwarz inequality

$$|\langle \Psi^*(u,t) | W_u \rangle|^2 \leq \langle \Psi^*(u,t) | \Psi^*(u,t) \rangle \langle W_u | W_u \rangle . \tag{3.4}$$

Since $\langle W_u | W_u \rangle = 1$ due to the unitarity of W (Equation 2.36),

$$\left| \sum_{j \in C_u} \Psi(u,j,t) w_{(uc'j)} \right|^2 \leq \upsilon(u,t) \tag{3.5}$$

implies that $p_{vu}(t) \leq 1$. As both the numerator and the denominator of Equation 3.3 are positive, $p_{vu}(t) \geq 0$, proving property 1.

Furthermore, the numerator of the sum of conditional probabilities

$$\sum_{v \in N^+(u)} p_{vu}(t) = \frac{\sum_{v \in N^+(u)} \left| \sum_{j \in C_u} \Psi(u,j,t) w_{(u,\sigma^{-1}(u,v),j)} \right|^2}{\upsilon(u,t)} \tag{3.6}$$

is exactly the value of the inner product $\langle \Psi(u,t) | W^\dagger W | \Psi(u,t) \rangle$, with

$$|\Psi(u,t)\rangle = \sum_{i \in C_u} \Psi(u,i,t) \, |u,i\rangle .$$

To see this, note that the correspondence given by the function $\sigma^{-1}(u,v)$ between degrees of freedom is unique, as well as the correspondence between the degrees of freedom of u and its neighbors, yielding

$$\sum_{v \in N^+(u)} \left| \sum_{j \in C_u} \Psi(u,j,t) w_{(u,\sigma^{-1}(u,v),j)} \right|^2 = \sum_{k \in C_u} \left| \sum_{j \in C_u} \Psi(u,j,t) w_{(u,k,j)} \right|^2 . \tag{3.7}$$

Due to the unitarity of W, such inner product is precisely $\upsilon(u,t)$, proving property 2.

Property 3 follows trivially from the definition of the Markovian matrix P in Equation 3.1 and from the orthogonality of the basis states. □

Theorem 2 establishes that any discrete-time coined quantum walk with unitary operators W and S, respectively described by Equation 2.34 and Relation 2.41, is statistically equivalent, from the perspective of vertex probability evolution, to a non-homogeneous random walk over the same graph. Note that Theorem 2 does not require W and S to be time homogeneous, thus they can both depend on time, as long as the graph connectivity restrictions remain valid.

3.2 Generalization for multiple walkers

To extend Theorem 2 to multiple walkers, some additional definitions are needed. In particular, the Hilbert space in which the process unfolds grows to allow for the joint description of the walkers. Let K denote the number of walkers and, again, let $\mathscr{H}_w$ denote the Hilbert space for a single-walker on G. The enlarged space for K walkers is $\mathscr{H}_w^K = \bigotimes_{i=1}^K \mathscr{H}_w$. Let $\boldsymbol{v} = (v_1, ..., v_k)$ denote an ordered sequence of K vertices and $\boldsymbol{c} = (c_1, ..., c_k)$ denotes its associated degrees of freedom such that $c_i \in C_{v_i}$. Let the set $B^K = \{|\boldsymbol{v}, \boldsymbol{c}\rangle\}$ denote a basis for $\mathscr{H}_w^K$ of which elements represents the joint position of the K walkers. Let

$$|\Psi(t)\rangle = \sum_{|\boldsymbol{v},\boldsymbol{c}\rangle \in B^K} \Psi(\boldsymbol{v}, \boldsymbol{c}, t) \, |\boldsymbol{v}, \boldsymbol{c}\rangle$$

denote the state of the system at instant t and $\rho : V^K \times C^K \times \mathbb{N} \to [0,1]$ be the joint probability distribution of states at instant t. Similarly, let $\upsilon : V^K \times \mathbb{N} \to [0,1]$ denote the joint vertex probability distribution of the K walkers at a given instant. Assuming each walker can behave differently, with specific coins and shift operators, let W_i and S_i respectively denote the coin and shift operator for the i-th walker, implying that the full operators are of the form $S = \bigotimes_{i=1}^K S_i$ and $W = \bigotimes_{i=1}^K W_i$. If there is no interaction among the walkers, the system evolves, in the enlarged space, according to Equation 2.33 and the joint distribution of vertices at an instant t is merely

$$\upsilon(\boldsymbol{v}, t) = \prod_{i=1}^{K} \upsilon_i(v_i, t),$$

where $\upsilon_i : V \times \mathbb{N} \to [0,1]$ is the marginal vertex distribution of the i-th walker.

A more interesting scenario appears when the walkers can interact, allowing a dependency among their marginal probability distributions. Let $U : \mathscr{H}_w^K \to \mathscr{H}_w^K$ be a unitary operator defined as

$$U = \sum_{|\boldsymbol{v},\boldsymbol{c}\rangle \in B^K} \sum_{\langle \boldsymbol{v},\boldsymbol{c'}| \in B^{K\dagger}} \theta(\boldsymbol{v}, \boldsymbol{c}, \boldsymbol{c'}) \, \big|\boldsymbol{v}, \boldsymbol{c}\big\rangle\big\langle \boldsymbol{v}, \boldsymbol{c'}\big| \tag{3.8}$$

which accounts for walker interactions, such that the whole system state evolves as

$$|\Psi(t+1)\rangle = SWU\,|\Psi(t)\rangle\,. \tag{3.9}$$

Under constraints of unitarity, the interactions introduced by U can be arbitrarily defined by specifying the values of $\theta(\boldsymbol{v},\boldsymbol{c},\boldsymbol{c'})$. Its inherent restriction resides on the self-mapping of the set of states that represent the vertex position for the K walkers, as $|\boldsymbol{v},\boldsymbol{c}\rangle$ cannot be mapped to $|\boldsymbol{u},\boldsymbol{c'}\rangle$ for $\boldsymbol{u} \neq \boldsymbol{v}$. This mapping implies that U does not move any of the walkers, confining movement to the action of the enlarged shift operator S. Nevertheless, diverse operations are allowed by U, such as generic controlled phase shifts, amplitude mixing and even amplitude shifts within the degrees of freedom of a walker controlled by the position of the others. Within this framework, the connectivity restrictions of the dispersion of the wavefunction are maintained, since amplitudes can only be transmitted through the edges of the graph. Theorem 3 follows as an extension of Theorem 2 for this broader context, in which the movement of K quantum walks is shown to be statistically equivalent to that of K non-homogeneous random walks.

Let $\pi : \mathbb{N} \to [0,1]^{|V|^K}$ be the joint vertex probability vector of the walkers such that that $\pi_{\boldsymbol{v}} = \upsilon(\boldsymbol{v},t)$.

Theorem 3 (Local evolution of multiple interacting walkers)**.** *For any time instant t, the evolution of vertex probabilities for the K walkers performed by the action of the unitary operator SWU is local and equivalent to the Markovian matrix $P(t)$ where*

$$p_{\boldsymbol{vu}}(t) = \begin{cases} \frac{\rho(\boldsymbol{v},\boldsymbol{c},t+1)}{\upsilon(\boldsymbol{u},t)}, & \text{if } \upsilon(\boldsymbol{u},t) > 0 \text{ and } (u_i,v_i) \in E \text{ for all } i \\ \frac{1}{d(\boldsymbol{u})}, & \text{if } \upsilon(\boldsymbol{u},t) = 0 \text{ and } (u_i,v_i) \in E \text{ for all } i \\ 0, & \text{otherwise} \end{cases} \tag{3.10}$$

such that $\pi(t+1) = P(t)\pi(t)$, where $\boldsymbol{c} = \sigma(\boldsymbol{u},\boldsymbol{v})$, $i \in \{1,...,K\}$.

Proof. The random walk dictated by matrix $P(t)$ accounts for the joint movement of the walkers in the sense that an index $\boldsymbol{u}$ of P is a vector of dimension K and denotes the position of the walkers. To formalize, let $G' = (V',E')$ denote a graph with $V' = V^K$ and $E' = E^K$, such that, for all $\boldsymbol{v},\boldsymbol{u} \in V'$ with $\boldsymbol{v} = (v_1,...,v_K)$ and $\boldsymbol{u} = (u_1,...,u_K)$, $e = (\boldsymbol{v},\boldsymbol{u}) \in E'$ if, and only if $(v_i,u_i) \in E$ for all i. Note that $d(\boldsymbol{u}) = \prod_{i=1}^{K} d(u_i)$. In particular, each vertex of G' represents the simultaneous position of all walkers and its edges encodes their joint movements. It must be shown that $P(t)$ indeed represents a non-homogeneous random walk over G' and that its vertex probability evolution matches Equation 3.9.

The three properties which where shown to hold for Theorem 2 are to be demonstrated for this general case, since the requirements for one walker extend to K walkers naturally.

Let

$$|\Psi(\boldsymbol{u},t)\rangle = \sum_{\boldsymbol{c}\in C_{\boldsymbol{u}}} \Psi(\boldsymbol{u},\boldsymbol{c},t)\,|\boldsymbol{u},\boldsymbol{c}\rangle \tag{3.11}$$

denote the overall state of $\boldsymbol{u} \in V'$ such that $\||\Psi(\boldsymbol{u},t)\rangle\|^2 = \upsilon(\boldsymbol{u},t)$. Note that $|\Psi(\boldsymbol{u},t)\rangle \in \mathscr{H}_w^K$, that $\boldsymbol{c} = (c_1,...,c_K)$ is a tuple denoting the degrees of freedom of each walker and that the functions η and σ are now defined for tuples of vertices and degrees of freedom. Assuming that $\boldsymbol{v} = \eta(\boldsymbol{u},\boldsymbol{c'})$ and $\sigma(\boldsymbol{u},\eta(\boldsymbol{u},\boldsymbol{c'})) = \boldsymbol{c}$ for a given $\boldsymbol{c'} \in C_{\boldsymbol{u}}$, the action of SWU gives

$$\frac{\rho(\boldsymbol{v},\boldsymbol{c},t+1)}{\upsilon(\boldsymbol{u},t)} = \frac{\||\boldsymbol{v},\boldsymbol{c}\rangle\langle\boldsymbol{v},\boldsymbol{c}|\,SWU\,|\Psi(\boldsymbol{u},t)\rangle\|^2}{\||\Psi(\boldsymbol{u},t)\rangle\|^2}. \tag{3.12}$$

Since SWU is unitary and $\langle\boldsymbol{v},\boldsymbol{c}|s\rangle \leq 1$ for any unitary $|s\rangle \in \mathscr{H}_w^K$, the inequality

$$0 \leq \frac{\||\boldsymbol{v},\boldsymbol{c}\rangle\langle\boldsymbol{v},\boldsymbol{c}|\,SWU\,|\Psi(\boldsymbol{u},t)\rangle\|^2}{\||\Psi(\boldsymbol{u},t)\rangle\|^2} \leq 1 \tag{3.13}$$

demonstrates property 1.

Simultaneously, the action of SWU also implies that the inequality

$$|\boldsymbol{v},\boldsymbol{c}_v\rangle\langle\boldsymbol{v},\boldsymbol{c}_v|\,SWU\,|\Psi(\boldsymbol{u},t)\rangle \neq 0 \tag{3.14}$$

is only valid for $\boldsymbol{v} \in V$ and $\boldsymbol{c}_{\boldsymbol{v}} \in C_{\boldsymbol{v}}$ if $\boldsymbol{v} = \eta(\boldsymbol{u},\boldsymbol{c})$ and $\boldsymbol{c}_v = \sigma(\boldsymbol{u},\boldsymbol{c})$ for some $\boldsymbol{c} \in C_{\boldsymbol{u}}$. Assuming that $\boldsymbol{v} = \eta(\boldsymbol{u},\boldsymbol{c})$ and $\boldsymbol{c}_{vu} = \sigma(\boldsymbol{u},\boldsymbol{c})$, the last condition gives

$$\sum_{\boldsymbol{v}\in N^+(\boldsymbol{u})} \frac{\||\boldsymbol{v},\boldsymbol{c}_{vu}\rangle\langle\boldsymbol{v},\boldsymbol{c}_{vu}|\,SWU\,|\Psi(\boldsymbol{u},t)\rangle\|^2}{\||\Psi(\boldsymbol{u},t)\rangle\|^2} = 1. \tag{3.15}$$

Due to the fact that SWU is a unitary operator, Equation 3.15 and the orthogonality of the basis states lead to properties 2 and 3. □

Essentially, Theorem 3 constructs a non-homogeneous random walk on G' that matches the evolution of the joint vertex probability distribution of K walkers induced by SWU and, thus, asserts that the vertex probability distribution of the multiple walker interaction model has a local evolution on the vertices of G'. Again, it is worth emphasizing that SWU may vary with time as long as unitarity, graph connectivity and the conditions for the interaction operator U remains valid, since time homogeneity of SWU is not required in the proof of Theorem 3.

Chapter 4

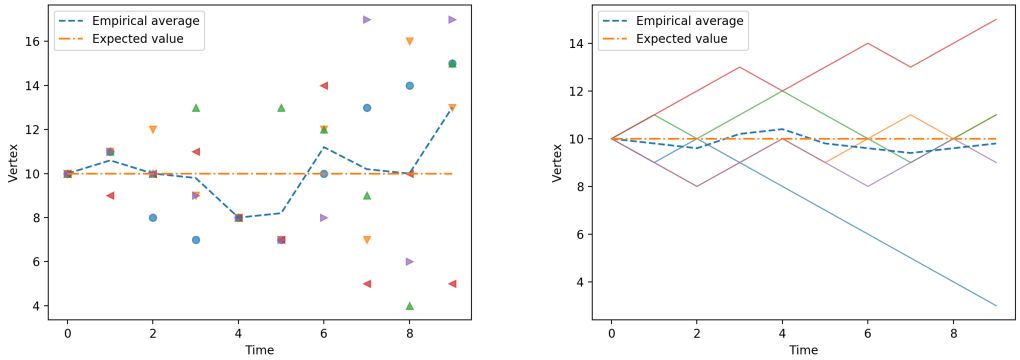
Simulation of trajectories and computational efficiency

The simulation of quantum and random walks have been fundamentally different, as discussed in Chapter 2. However, the demonstration of their statistical equivalence has profound implications on the simulation of quantum walks. In this chapter, a novel simulation procedure motivated by this equivalence is addressed and a numerical analysis is presented. In addition, an explicit formula for the vertex probability of quantum walks with fixed *SW* operator is attained through spectral decomposition. This formula gives a succinct description of υ that can be exploited to make the proposed simulation approach more computationally efficient under certain conditions.

4.1 Simulation of quantum walk trajectories

Theorems 2 and 3 establish respectively the construction procedure for a non-homogeneous random walk that is statistically equivalent to practically any single- and multiple-walker quantum walk. This random walk can be simulated to generate paths on the graph that, by correspondence, also capture the quantum walk statistical dynamics.

As mentioned in Chapter 2, the simulation of a random walk naturally constructs random paths on a graph: at time $t+1$, the walker can only be found in an outward neighbor of vertex v, given that it was in vertex v at time t. Thus, the simulation constructs a sample path that ensures neighbor locality. We denote this sample path as a *quantum walk trajectory*. This procedure is fundamentally different from the usual simulation procedure for quantum walks, where the distribution ρ is sampled independently at each time instant t and graph trajectories are not necessarily constructed. A visual depiction of this divergence is presented in Figure 4.1, where the method of independent sampling is shown on the left and the quantum walk trajectories appears on the right. Note that the samples in the left figure are not trajectories, although the expected vertex value for the



(a) Independent measurements.

(b) Quantum walk trajectories

Figure 4.1: Samples obtained from simulating a Hadamard walk on a cycle with 20 vertices for 10 time steps with initial condition $|\Psi(0)\rangle = \frac{1}{\sqrt{2}}(|10,0\rangle + i|10,1\rangle)$. In the left figure, 5 sequences of 10 independent measurements each are depicted. Points with the same marker style and color represent a sequence of measurements. When consecutive markers of the same style and color differ from more than two points in vertex value (y-axis), the vertices are not neighbors of each other. The right figure shows 5 trajectories sampled with the quantum walk trajectory method. Each colored curve represents a trajectory of length 10.

two sampling procedures is the same (orange dashed line).

Furthermore, the procedure prescribed in Theorem 2 was used to simulate quantum walk trajectories on a 2-D torus with Grover and Hadamard coins, and moving-shift operators, generating the ensembles of trajectories depicted in Figures 4.2 and 4.3, respectively. The figures show the convergence of the probability distribution of quantum walk trajectories to the vertex distribution of quantum walks with the approximation of the vertex expected value (blue dashed lines) by the empirical average over the ensembles (orange dashed lines). Without loss of generality, the following discussion assumes a single-walker.

While one simulated trajectory respects locality, an ensemble of trajectories recover the distribution of the quantum walk for every t. In particular, let $\chi = \{\tau_1, ..., \tau_M\}$ be an ensemble of M independent trajectories. Let $\tau_i(t)$ denote the vertex visited by the walker at instant t in the i-th trajectory. Let $\mathbb{1}(.)$ denote an indicator function activated by its argument condition. Let

$$\hat{p}_u^M(t) = \frac{1}{M}\sum_{i=1}^{M} \mathbb{1}(\tau_i(t) = u) \tag{4.1}$$

denote the fraction of time vertex u was visited by the walker at instant t. Thus, by the law of large numbers, $\hat{p}_u^M(t) \to \upsilon(u,t)$ as $M \to \infty$ and the trajectories recover the vertex distribution of the quantum walk for all t.

Convergence is observed through the decreasing behavior of the total variation dis-

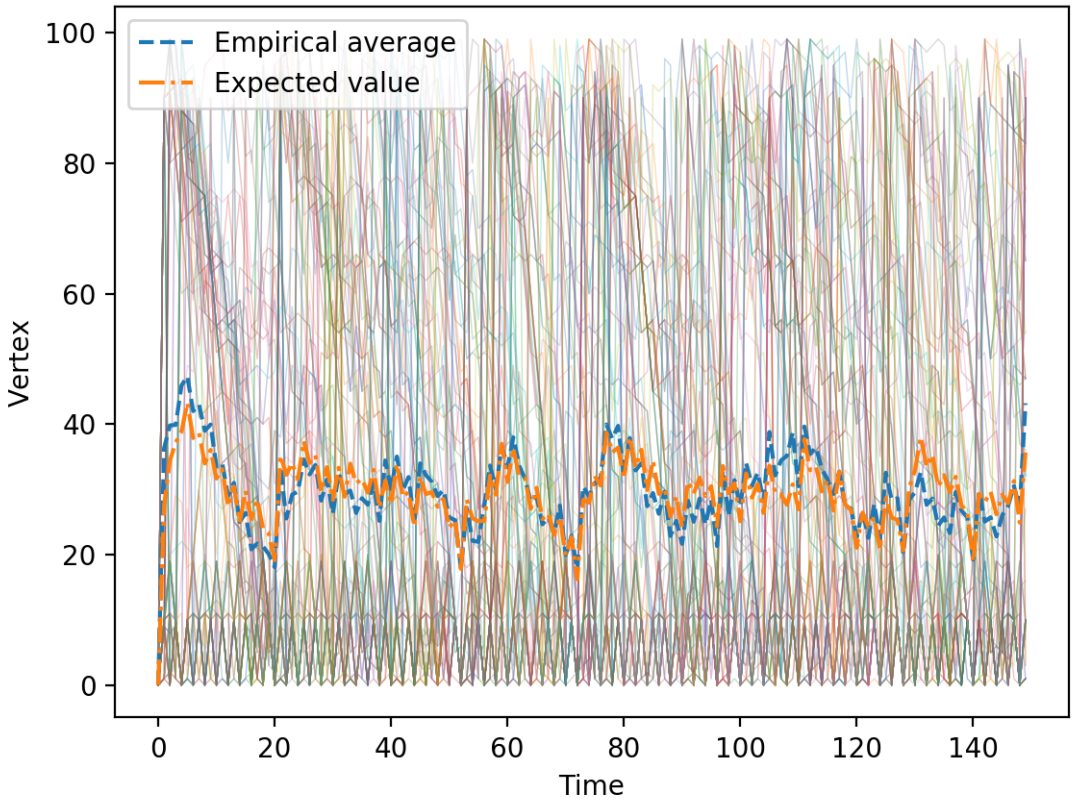


Figure 4.2: Ensemble of 100 trajectories obtained using Theorem 2 for a Grover-coined walk on a 10-by-10 2-D torus with moving shift operators for a localized initial state $|0,0\rangle$ (left edge of the origin). Each one of the solid lines corresponds to an independent trajectory. The blue dashed line represents the empirical average of the vertex random variable for each time instant while the orange point-dashed line represents its expected value.

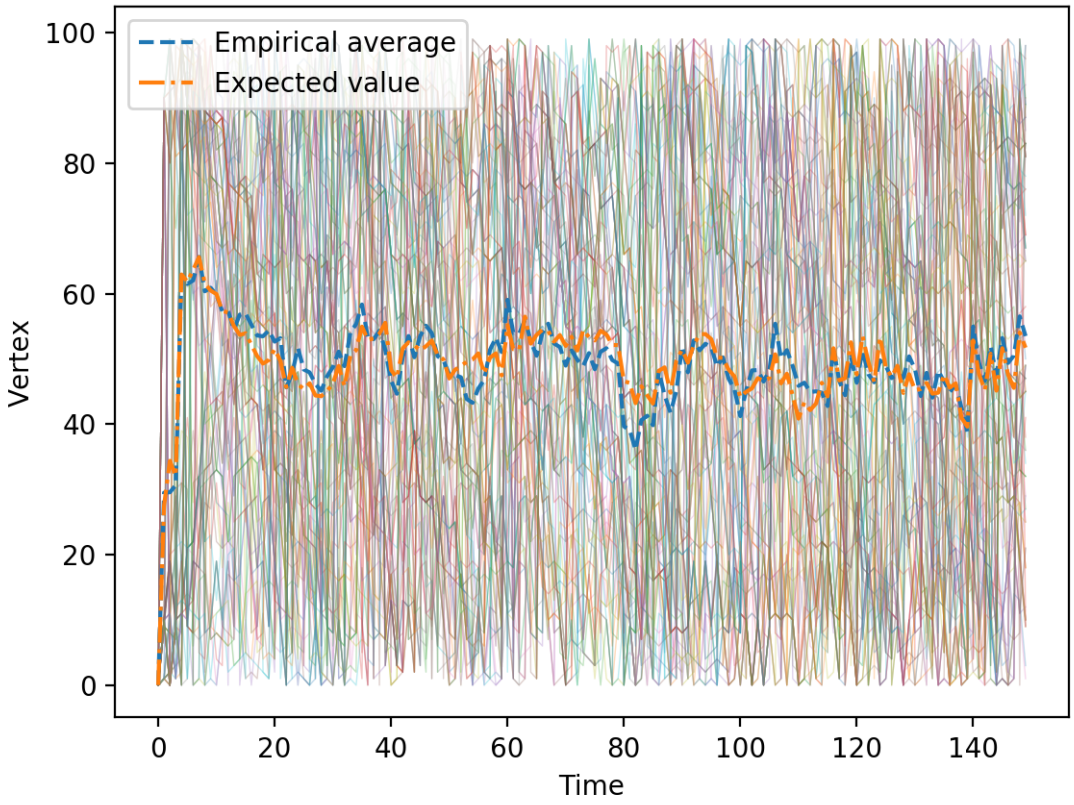


Figure 4.3: Ensemble of 100 trajectories obtained using Theorem 2 for a Hadamard-coined walk on a 10-by-10 2-D torus with moving shift operators for a localized initial state $|0,0\rangle$ (left edge of the origin). Each one of the solid lines corresponds to an independent trajectory. The blue dashed line represents the empirical average of the vertex random variable for each time instant while the orange point-dashed line represents its expected value.

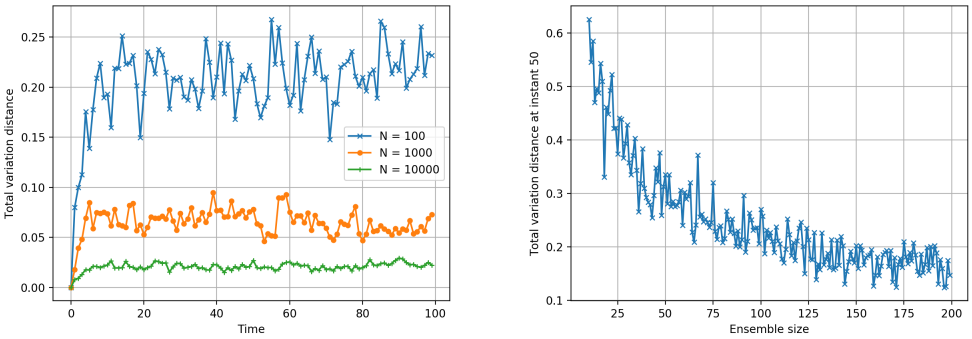


Figure 4.4: Analysis of the total variation distance between the empirical distribution obtained from trajectory sampling and the quantum walk distribution of a Grover-coined walk with moving shift on a 10-by-10 2-D torus. The left figure shows the total variation value for the distribution at each instant, with different curves representing different ensemble sizes. The right figure gives the distance value for a fixed time instant when the ensemble size grows.

tance

$$D_t(\hat{p}, \upsilon) = \frac{1}{2} \sum_v \left| \hat{p}_v^M(t) - \upsilon(v,t) \right| \tag{4.2}$$

between the empirical vertex distribution of the trajectory ensemble and the quantum walk vertex distribution, as it can be seen in Figure 4.4 for a Grover-coined quantum walk on the 2-D torus with moving-shift operator.

The non-homogeneous random walk simulation is a novel perspective for the study of quantum walks as it gives an efficient (polynomial) procedure for sampling trajectories which recover, by the law of large numbers, the vertex probability sequence of any quantum walk. As a matter of fact, measuring quantum walks on a possible physical implementation or independently sampling vertices from the sequence of quantum distributions do not address this question, since samples are obviously independent and there is no guarantee that trajectories (paths) will be generated.

4.2 Limitations of the rejection method for QWT

A possible alternative to sample quantum trajectories on a graph is to consider a rejection method based on the usual simulation of random walks that accepts only sequences of vertices that correspond to paths in the graph. However, the marginal empirical distributions $\hat{p}_v(t)$ within the accepted trajectories would not necessarily match $\rho(v,t)$.

The question in hand is to generate samples of paths of a graph G for which the empirical distribution $\hat{p}(v,t)$ (fraction of instances that the walker is found in vertex v after t hops) converges to $\upsilon(v,t)$, the given vertex distribution of a quantum walk defined on G,

for all $v \in V$, $t \in \{0,...,L-1\}$. Essentially, a path of the graph, or a graph trajectory, of length L is a sequence of vertices $\{v_1,...,v_L\}$ such that $(v_i, v_{i+1}) \in E$ for $i \in \{1,...,L-1\}$.

The usual simulation method for a quantum walk consists in drawing independent samples from distinct time instants. Effectively, assume that one wants to draw a sequence of L samples from a quantum walker system such that the i-th sample is drawn according with the distribution υ at instant i. Note that υ depends on the initial condition. Denoting $V_i = \{v \in V | \upsilon(v,i) \neq 0\}$ as the set of all vertices that can be the outcome of a measurement of the system at instant i, define $\mathscr{X}_L = V_0 \times ... \times V_{L-1}$ as the set of all possible sequences of measurements of length L that can be obtained from the quantum walker system. Simply, the set $\mathscr{X}_L$ is the sample space for the usual simulation procedure of a quantum walk.

Analyzing the set $\mathscr{X}_L$ and considering the general case of initial conditions, it is clear that not every sequence $\tau \in \mathscr{X}_L$ is a valid path of the graph. However, every path of the graph that can be obtained as a quantum walk trajectory belongs to $\mathscr{X}_L$. Thus, this method cannot be directly used to sample quantum walk trajectories as some measured sequences would not be proper paths of the graph.

To overcome this limitation, rejection sampling could be applied where a sample is accepted as a quantum walk trajectory only if it is a valid path on G. In order to address this matter formally, let $\mathscr{T}_L \subset \mathscr{X}_L$ be the set of all sequences of measurements that are paths of length L of G. Let $p(\tau)$ be the probability of obtaining a sequence $\tau = \{\tau_0,...,\tau_{L-1}\} \in \mathscr{X}$ from the independent sampling procedure. Let $\mathscr{X}_L^{v,t} \subset \mathscr{X}_L$ and $\mathscr{T}_L^{v,t} \subset \mathscr{T}_L$ denote the set of all sequences and trajectories of length L in which v appears in position t. It follows trivially from independence that

$$p(\tau) = \prod_{t=1}^{L} \upsilon(\tau_t, t), \tag{4.3}$$

where τ_t denotes the vertex measured at t. In this case, the vertex probability at t is simply,

$$\upsilon(v,t) = \sum_{\tau \in \mathscr{X}_L^{v,t}} p(\tau). \tag{4.4}$$

However, rejecting non-trajectory samples yields the following estimator $\hat{p}(v,t)$ for the probability of finding vertex v at instant t:

$$\hat{p}(v,t) = \frac{\sum_{\tau \in \mathscr{T}_L^{v,t}} p(\tau)}{\sum_{\tau' \in \mathscr{T}_L} p(\tau')}. \tag{4.5}$$

It is not clear whether Equations 4.4 and 4.5 are equal for every possible quantum walk, since the ratio between the probability of generating trajectories with vertex v at position t and the probability of generating any trajectory would have to be $\upsilon(v,t)$, for all $v \in V$

and $t \in \{0, ..., L-1\}$.

Additionally, even for the cases where Equations 4.4 and 4.5 are equal, the expected time to accept a sample in the rejection procedure is precisely the inverse of the probability of generating a trajectory. Although this probability depends on a myriad of factors such as the graph structure, the number of trajectories of a given length L within a graph can be exponentially smaller than the number of possible sequences of measurements. As an example, a D-dimensional torus with V vertices would have VD^{L-1} paths of length L and V^L possible sequences of vertices, which for values of $D \in O(1)$ is exponentially larger than the number of trajectories, suggesting that the expected time to generate a trajectory sample would be unfeasible.

In precise terms, Theorem 2 offers a polynomial time procedure to sample trajectories for any quantum walk. Given the transition matrix $P(t)$, a quantum trajectory of length L can be sampled in time $\mathcal{O}(Ld_{max})$ where d_{max} is the maximum degree of the graph. Moreover, if multiple trajectories are to be generated, then the *alias method* could be used to sample the next neighbor along a trajectory in which case the amortized time complexity for each trajectory is $\mathcal{O}(L)$, and no longer depends on node degrees.

4.3 Complexity of random walk description and simulation

An interesting question which arises once Theorems 2 and 3 are considered is the computational complexity involved in constructing the corresponding random walk matrices $P(t)$. The information required to compute its entries at time instant t are the probability distributions of the quantum walk at times t and $t+1$. Thus, if the state and the vertex distributions for time t and $t+1$ are known, constructing the matrix $P(t)$ has an intrinsic complexity of $\mathcal{O}(|V|^2)$, since each of its entries can be computed in $\mathcal{O}(1)$.

In general, however, the matrix can be computed by using Equation 2.33 to calculate both $|\psi(t)\rangle$ and $|\psi(t+1)\rangle$. Assuming that both S and W may vary with time, the cost for computing the wave function is $\mathcal{O}(t|E|^2)$, since t matrix-by-vector multiplications are performed, each with complexity $\mathcal{O}(|E|^2)$. Computing the vertex distribution from the wavefunction has complexity $\mathcal{O}(|E|)$, since the probability of each outward edge of a vertex must be considered. Hence, the overall complexity is $\mathcal{O}(t|E|^2 + |E| + |V|^2) \in \mathcal{O}(t|E|^2)$.

The computation of the quantum walk wavefunction is the general bottleneck for constructing the random walk matrices, unless the probability distributions of the quantum walk can be computed more efficiently. In terms of complexity, the problem of describing the probability evolution of the non-homogeneous random walk is at least as hard as solving the quantum walk distribution. Nonetheless, specific walker systems can have their

wavefunctions computed by algorithms that are more efficient than direct matrix multiplication. Walker dynamics with known closed-formula expressions for the wavefunction are an interesting case. For example, a generic coined quantum walk on an infinite line for which the walker moves in a single direction or remains on its position at every instant has known explicit probability distribution for all time t [28].

4.4 Dynamic programming for Grover walk on torus

In spite of the general complexity of constructing the transition matrices, the wavefunction and the vertex probability distribution may be computed recursively and more efficiently than the general approach for particular quantum walk operators and graphs.

The Grover-coined (Eq.2.40) walk on a D-dimensional torus with moving-shift operator (Eq.2.47) and purely real initial conditions serves as an example where the probability distribution can be computed by a dynamic programming algorithm that is more efficient than direct matrix multiplication. The number of degrees of freedom within the D-dimensional torus is $2D$. Analyzing the action of the total walk operator MG on a given state

$$\Psi(u,t) = \sum_{c \in C_u} \Psi(u,c,t) \, |(u,c)\rangle$$

and having $\eta(u,c) = v$, the probability $\rho(v,c,t+1)$ is described as

$$\rho(v,c,t+1) = \left| \sum_{c' \in C_u} \Psi(u,c',t) - \Psi(u,c,t) \right|. \tag{4.6}$$

Assuming that $\psi(u,c,t) = \sqrt{\rho(u,c,t)} e^{i \cos \theta_{uct}}$ and noting that $\theta_{uct} = 0$ for every u, c and t whenever purely real initial conditions are considered yields

$$\rho(v,c,t+1) = \left| \sum_{c' \in C_u} \sqrt{\rho(u,c',t)} - \sqrt{\rho(u,c,t)} \right|. \tag{4.7}$$

From Theorem 2, the entries of the random walk matrices for which $\rho(v,c,t) > 0$ are given by

$$\frac{\rho(v,c,t+1)}{\upsilon(u,t)} = \frac{1}{\upsilon(u,t)} \left| \sum_{c' \in C_u} \sqrt{\rho(u,c',t)} - \sqrt{\rho(u,c,t)} \right|. \tag{4.8}$$

Equation 4.8 can be solved through a dynamic programming algorithm in which each time instant has complexity $\mathcal{O}(|V|D^2)$, implying on an overall procedure of complexity $\mathcal{O}(t|V|D^2)$ for all matrices up to time t. The algorithm calculates the value of ρ, since υ is obtained from ρ. The data structure for the dynamic programming is a matrix with $2D|V|$

rows and t columns storing the values of ρ. At each step $k > 0$, the algorithm writes the k-th column of the matrix using the values $\rho(v,c,k-1)$ read from the column with index $k-1$. At each instant, the complexity of writing the column is $\mathcal{O}(D^2|V|)$ since, for each each (u,v) the value of all edges incident to u appears in Equation 4.8 which is evaluated $2D|V|$ times. The algorithm terminates after all t steps were computed, what yields the final time complexity of $\mathcal{O}(t|V|D^2)$.

For $D \in \mathcal{O}(1)$, the algorithm has complexity $\mathcal{O}(t|V|)$, showing a cubic improvement over the generic procedure, since $\mathcal{O}(t|E|^2) \in \mathcal{O}(t|V|^4)$. [1]

4.5 Vertex probabilities and the spectrum of *SW*

In general, it is possible to describe the vertex probability of quantum walks with a time-independent operator *SW* using spectral decomposition. This description is an alternative solution to the sequence of matrix multiplications. However, this analytical formula has the price of computing the eigenvalues and eigenvectors of *SW*.

The spectral theorem establishes a basis of the vector space in which a normal operator is represented in diagonal form (Equation 2.19). Essentially, the spectrum of the evolution operator *SW* contains all information about the evolution of the wavefunction. Thus, it is possible to completely describe the quantum walker system with the eigenvectors of *SW*. Supposing the spectrum of *SW* is known, the walk state expressed on the measurement basis $\{|u,c\rangle\}$ (Equation 2.33) can be re-written in terms of $|\lambda_k\rangle$ from a coordinate transformation, i.e a change of basis, as

$$|\Psi(t)\rangle = \sum_k \phi(k,t)\,|\lambda_k\rangle\,, \tag{4.9}$$

where

$$\phi(k,t) = \sum_{v\in V, c\in C_v} \langle\lambda_k|v,c\rangle\,\Psi(u,c,t). \tag{4.10}$$

The measurement probability associated with each eigenvector is different than the probability associated with measuring a state $|v,c\rangle$. If the measurement basis considered is the eigenvector basis, the probability of having $|\lambda_k\rangle$ as the outcome of a measurement is $\langle\phi(k,t)|\phi(k,t)\rangle$. On the other hand, each eigenstate, or eigenvector, is a linear combination of the states $|v,c\rangle$. This implies that each eigenvector can contribute to the measurement probability of $|u,c\rangle$.

Given that *SW* is unitary, its eigenvalues obey Equation 2.21 such that $\lambda_k = \exp(i\theta_k)$.

[1] D can be at most $|V|$ for the case when the torus degenerates to the complete graph. The overall procedure for this case is in $\mathcal{O}(t|V|D^2) = \mathcal{O}(t|E|D)$, which still represents a linear improvement from the general procedure of matrix multiplication.

Hence, the action of SW on an eigenvector is a shift of its complex phase that preserves its module. The time evolution of the system in terms of the eigenstates is

$$|\Psi(t+1)\rangle = \sum_k \phi(k,t) SW\, |\lambda_k\rangle \tag{4.11}$$

and Equation 2.21 yields

$$|\Psi(t+1)\rangle = \sum_k e^{i\theta_k t} \phi(k,0)\, |\lambda_k\rangle\,. \tag{4.12}$$

Note that Equation 4.12 comes simply from the definition of an eigevector. The last Equation recovers the fundamental fact that the measurement probability of an eigenvector in the eigenvector basis is the same throughout the system evolution. The module of the wavefunction incident into $|\lambda_k\rangle$ does not change because $e^{i\theta_k t}$ has a unitary absolute value.

To understand how the evolution of the eigenstates implies the evolution of probabilities on the basis $\{|v,c\rangle\}$ it is necessary to describe each state $|v,c\rangle$ as a linear combination of the eigenvectors. Even if the representation on the eigenbasis is different from Equation 2.33, the probability distributions ρ and υ must be the same, since the system is the same. Hence, the definition of ρ yields

$$\rho(v,c,t) = \left\| \sum_k e^{i\theta_k t} \langle v,c|\lambda_k\rangle \, \phi(k,0)\, |v,c\rangle \right\|^2 . \tag{4.13}$$

The norm of the vector is simply

$$\rho(v,c,t) = \left| \sum_k e^{i\theta_k t} \langle v,c|\lambda_k\rangle \, \phi(k,0) \right|^2 . \tag{4.14}$$

Note that the only dependence of $\rho(v,c,t)$ in time is the complex exponential $e^{i\theta_k t}$. The values of $\phi(k,0)$ and $\langle v,c|\lambda_k\rangle$ can be computed before hand from the spectrum of SW and the initial condition $|\Psi(0)\rangle$. Finally, υ is achieved by summing up $\rho(v,c,t)$ for all degrees of freedom.

Constructing random walks with the probability description

Equation 4.14 has a direct consequence on the simulation procedure established by Theorems 2 and 3. Without loss of generality, consider the case of a single quantum walker with a given time-independent evolution operator SW. Theorem 2 prescribes the transition

probability for instant t as

$$p_{vu}(t) = \frac{\rho(v,c,t)}{\upsilon(u,t)}, \tag{4.15}$$

where c is defined by the shift operator. Equation 4.14 yields

$$p_{vu}(t) = \frac{\left|\sum_k e^{i\theta_k t+1} \langle v,c|\lambda_k\rangle \phi(k,0)\right|^2}{\sum_{c'\in C_u}\left|\sum_k e^{i\theta_k t} \langle u,c'|\lambda_k\rangle \phi(k,0)\right|^2}. \tag{4.16}$$

The direct benefit of Equation 4.16 for sampling quantum walk trajectories is significant. Describing the transition probability for a time instant t does not depend on having the wavefuction of the system at instants t and $t+1$ entirely computed. More specifically, for any time instant t it is possible to apply Equation 4.16 without any direct knowledge of the wavefunction at instants $k < t$. This behavior implies that it is possible to compute the transition probabilities to leave from vertex v at instant t without computing the entire evolution of the system.

Furthermore, the complexity of simulation is different than the general case. The complexity of evaluating Equation 4.16 for a pair u,v is $\mathcal{O}(|E|)$ since there are $2|E|$ eigenvectors of SW. Sampling a neighbor of u at instant t has a linear complexity on the degree of u. Thus, the total complexity to compute the transition probability and sample the neighbor is $\mathcal{O}(d(u)|E|)$. The worst case scenario is simply $\mathcal{O}(d_{max}|E|)$. Finally, assuming that the spectrum is known, the complexity of generating one quantum walk trajectory of length t is $\mathcal{O}(td_{max}|E|)$ in time, with $\mathcal{O}(|E|^2)$ memory to store all products $\langle u,c|\lambda_k\rangle \phi(k,0)$. If it is necessary to compute the spectral decomposition of SW, simulating the first sample has time complexity $\mathcal{O}(td_{max}|E| + |E|^3)$.

For the general simulation procedure, generating the first quantum walk trajectory of length t has complexity $\mathcal{O}(t|E|^2)$. To sample more trajectories without recomputing the wavefuction for all instants t gives $\mathcal{O}(t|E|)$ memory complexity. If the wavefunction is stored, the time to generate consecutive trajectories is $\mathcal{O}(td_{max})$.

Periodicity conditions for the probabilities of quantum walks

In a parallel direction to simulation, Equation 4.14 brings an important result to the periodicity of both vertex and probability distributions of discrete-time quantum walks.

Theorem 4 (Periodicity of the state probability)**.** *Let SW be a quantum walk operator with eigenvectors $\{|\lambda_k\rangle\}$ and initial condition $|\Psi(0)\rangle = \sum_k \gamma(k) e^{i\phi_k}|\lambda_k\rangle$. The edge probability ρ and the vertex probability υ distributions are periodic if, and only if, $\theta_k \in \mathbb{Q}$ for all k.*

Proof. The probability of finding a state $|v,c\rangle$ is

$$\rho(v,c,t) = \left| \sum_k e^{i\theta_k t} \langle v,c|\lambda_k\rangle \gamma(k) e^{i\phi_k} \right|^2. \tag{4.17}$$

The inner product $\langle v,c|\lambda_k\rangle$ is a complex number. In polar form, the value of the inner product can be written as $\langle v,c|\lambda_k\rangle = \mu_{vck} e^{i\kappa_{vck}}$ and yields

$$\rho(v,c,t) = \left| \sum_k A_{vck} e^{i\omega_{vck}(t)} \right|^2, \tag{4.18}$$

where $A_{vck} = \gamma_k \mu_{vck}$ is the amplitude and $\omega_{vck}(t) = \theta_k t + \phi_k + \kappa_{vck}$ the phase of the complex number. Applying Euller's formula gives

$$\rho(v,c,t) = \left| \sum_k (A_{vck} \cos \omega_{vck}(t) + iA_{vck} \sin \omega_{vck}(t)) \right|^2. \tag{4.19}$$

The complex numbers of Equation 4.19 are in Cartesian form. The definition of the absolute value gives the value of ρ as

$$\rho(v,c,t) = (\sum_k A_{vck} \cos \omega_{vck}(t))^2 + \sum_k (A_{vck} \sin \omega_{vck}(t))^2. \tag{4.20}$$

The functions $\omega_{vck}(t)$ are linear in time and depend on t only by term $\theta_k t$, which comes from the complex phase of the eigenvalues. The value of the probability comes from a finite sum of sines and cosines. Thus, $\rho(v,c,t)$ would always be periodic if t was a real number. Since t only assumes integer values, the sum of the trigonometric functions in question is periodic only if the frequency θ_k is a rational number for all k. □

Corollary 1 (Period of state probability)**.** *Let SW be a periodic quantum walk operator. The period of the state probability ρ induced by SW is the least common multiple of the set $\{\theta_k\}$, where $SW = \sum_k e^{i\theta_k} |\lambda_k\rangle\langle\lambda_k|$.*

Proof. The corollary follows trivially from the trigonometric relation for the period of sums of sines and cosines. □

The results presented in this last section resonates from the power of describing a quantum system in terms of its spectrum. In addition to the conditions for periodicity and the benefits to simulating trajectories, Equation 4.14 shed light on the behavior of quantum walks. The direct description of the probabilities of quantum walks in terms of eigenvectors is helps understanding of the probability evolution of quantum walks [35].

Chapter 5

Constructing quantum walks that are equivalent to random walks

Given Theorems 2 and 3, it is natural to ask if quantum walks can mimic the exact same vertex probability evolution of any given random walk, demonstrating the equivalence in the reverse direction.

Indeed, this problem has a trivial solution if one is allowed to measure a quantum walk at each time instant. It can be shown that the application of a quantum walk operator on the system state after a measurement yields a probability evolution that is compatible with the application of a stochastic matrix. This behavior comes from the destruction of quantum interference caused by the collapse of the wavefunction after measurement [37]. As an example, it is well known that the Hadamard walk on a cycle collapses to the usual uniform random walk on the cycle, i.e the random walk that has a probability of 0.5 to move to the left and to the right, if the walker state is probed at every instant.

Nonetheless, it is interesting to describe a quantum walk operator for which the wavefunction does not have to be measured consistently such that the probabilities of a random walk can be intrinsically embedded in the unitary evolution of a quantum walk. Under the philosophical directive that guides this dissertation, establishing the equivalence between the coherent evolution of quantum walks and the local evolution of random walks indicates a fundamental connection between the two processes. Furthermore, some of the divergences between quantum and random walks mentioned in Chapter 3 were derived under arguments of unitarity [1]. The existence of such a construction procedure establishes that these divergences are not leveraged by unitarity alone, depending also on the time-homogeneity of both processes. For the task at hand, it is reasonable to consider time-dependent quantum walks, since homogeneous quantum walks do not converge in time, and thus are not capable of mimicking the behavior of homogeneous random walks [1].

5.1 The implications of unitarity

In chapter 3, the unitarity of the quantum walk operators was central to guide the demonstration of Theorems 2 and 3. The unitarity of SW imposes constraints to describe quantum walks. In essence, as the definition of local evolution guided the description of the previous theorems, these peculiarities yield an algorithm to construct a quantum walk that is statistically equivalent to any given random walk.

It is fruitful to proceed with an analysis on the vector spaces in which quantum and random walks are defined. This analysis is critical to understanding the intrinsic connections between the two processes. As discussed in Section 2.2.2, the postulate of representation stipulates that quantum walks are described by unitary vectors on $\mathscr{H}_W$. Since the evolution of a quantum system is unitary the wavefuction vector sequence of a quantum walk lies on the unitary complex hyper-sphere of $\mathscr{H}_W$.

For random walks, the probability vectors involved are all real and lie on the positive simplex of dimension $|V|$. To represent the probability vectors of random walks as a state vector of $\mathscr{H}_W$ it suffices to create a map from the probability simplex to the complex hyper-sphere. This ensures the validity of the postulate of representation and enables addressing the random walk probability evolution with the formalism of quantum walks.

Let $\pi : \mathbb{N} \to [0,1]^{|V|}$ denote the probability vector of a random walk, at instant t, as defined in Section 2.1.2. Any state vector $|\Psi(t)\rangle$ for which

$$\sum_{u \in V, c \in C_u} |\langle u, c|\Psi(t)\rangle|^2 = \pi_v(t) \tag{5.1}$$

is a proper quantum state that represents $\pi(t)$, and thus mimic the evolution of the random walk. Since there are infinite possibilities to choose a state for which Equation 5.1 holds, the representation of the random walk state is a matter of choice for the task in hand.

Thus, to complete the understanding on how unitarity affects the description of random walks on the formalism of quantum mechanics, it remains to analyze the probability evolution of random walks. To have a quantum walker capable of matching the time evolution of states respecting Equation 5.1 is to describe a time-dependent unitary operator $Q : \mathscr{H}_W \to \mathscr{H}_W$ with action

$$|\Psi(t+1)\rangle = Q(t)\,|\Psi(t)\rangle$$

and valid decomposition $Q(t) = S(t)W(t)$ for the graph, for every instant t.

From the geometric perspective, unitary evolution is nothing more than a self-mapping of the complex unit hyper-sphere. Unitary operators are norm preserving, performing rotations on the vectors of a given Hilbert space. Since all state vectors compliant with Equation 5.1 are unitary, there has to exist at least one unitary transformation $Q(t)$ that

satisfies the equation above. On the other hand, addressing whether this unitary operator can be properly decomposed as a quantum walk operator demands a deeper algebraic analysis.

5.2 The representation of random walks as quantum walker systems

Initially, it is necessary to define $|\Psi(t)\rangle$. To the task in hand, a good model for the system state is one that simplifies the search for the operators $S(t)$ and $W(t)$. To give intuition on the state representation chosen, consider that the system state is

$$|\Psi(t)\rangle = \sum_{u \in V, c \in C_u} g(u,c,t) e^{i\theta(u,c,t)} \sqrt{\pi_u(t)}\, |u,c\rangle\,, \tag{5.2}$$

where $\theta(u,c,t)$ is an arbitrary complex phase and g respects

$$\sum_{c \in C_u} g(u,c,t)^2 = 1 \text{ for every } u \in V. \tag{5.3}$$

The compliance of the equations above with Equation 5.1 is a direct consequence of the definition of υ (Equation 2.49). Equation 5.2 implies that the value of $\rho(u,c,t)$ is $|\langle u,c|\Psi(u,c,t)\rangle|^2 = g(u,c,t)^2 \pi_u(t)$, while Equation 5.3 assures that the sum over all degrees of freedom of u yields $\upsilon(u,t) = \pi_u(t)$.

The diffusion behavior of the quantum walk leads to the definition of g and θ. Note that W acts by mixing the wavefunction among the edges of a vertex and S creates its flow. Consider a particular instant t of the quantum walk with $W(t) = I$ (the identity matrix), such that the mixing behavior is "turned off" for t and $Q(t) = S(t)$ acts only by creating the flow of the wavefunction. Assuming that $S(t)$ is any valid shift operator and $\eta(u,c) = v$, an inspection of Equation 2.4 indicates that a natural choice for the function $g(u,c,t)$ is

$$g(u,c,t) = \sqrt{p_{vu}(t)}. \tag{5.4}$$

This choice satisfies Equation 5.3 and simultaneously implies that $\upsilon(u,t) = \pi_u(t)$ and $\upsilon(u,t+1) = \pi_u(t+1)$ for all $u \in V$. The first two properties stem directly from the law of total probability (Equation 2.3). The condition for $t+1$ comes from the fact that, in spite of the functions η and σ used to define $S(t)$, for every vertex $v \in V$, all states $|v,c\rangle$ have an incident wavefunction that yields a proper proportion of the probabilities of the

neighbors of v at instant t such that

$$\upsilon(v,t+1) = \sum_{u \in N^-(v)} p_{vu}(t)\pi_u(t). \tag{5.5}$$

The given representation is powerful because it is a valid unitary representation that describes the operator $Q(t)$ as a proper quantum walk operator in the particular scenario considered. This representation gives the intuition for a state representation compatible with the process for every t. If the result of $W(t)\left|\Psi(t)\right\rangle$ is given by the right-hand side of Equation 5.2 for all instant t, $Q(t)$ is properly decomposed into $S(t)W(t)$ for any valid shift operator.

The key aspect is to define the state of the system based on the probabilities of instant $t-1$, instead of using the probabilities of instant t. It is known from the random walk description that the probability of a vertex at instant t is a linear combination of the probability of its neighbors at instant $t-1$. Thus, the following Lemma inspired by Equation 2.4 formalizes the state representation of choice.

Lemma 1 (Quantum representation of random walks)**.** *Let $P(t)$ be a stochastic matrix that defines a random walk on G such that $\pi(t+1) = P(t)\pi(t)$. Let $\sigma^{-1} : V \times V \to C$ be any function that associates an inward edge of a vertex to one of its outward edges defining a valid shift operator for G. For $t > 0$, The probability vector $\pi(t)$ can be represented by a discrete-time coined quantum walk state*

$$\left|\Psi(t)\right\rangle = \sum_{v \in V, c \in C_v} e^{i\theta(u,\sigma^{-1}(u,v),t-1)} \sqrt{p_{vu}(t-1)}\sqrt{\pi_u(t-1)}\left|v,c\right\rangle. \tag{5.6}$$

defined on G, such that $\theta(u,c,t)$ is an arbitrary complex phase, for all $u \in V, c \in C_u$ and $t \in \mathbb{N}$, and with

$$\left|\Psi(0)\right\rangle = \sum_{v \in V, c \in C_v} \sqrt{\frac{\pi_v(0)}{d(v)}}\left|v,c\right\rangle. \tag{5.7}$$

Proof. The proof for $t = 0$ is trivial. Hence, it suffices to show that, for $t > 0$, $\left|\Psi(t)\right\rangle$ is a unitary vector and that $\upsilon(v,t) = \pi_v(t)$, for all $v \in V$. The measurement of state $\left|v,c\right\rangle$ yields that

$$\rho(v,c,t) = \left| e^{i\theta(u,\sigma^{-1}(u,c),t-1)} \sqrt{p_{vu}(t-1)}\sqrt{\pi_u(t)} \right|^2. \tag{5.8}$$

Since $p_{vu}(t)$ and $\pi_u(t)$ are positive reals, $\rho(v,c,t) = p_{vu}(t)\pi_u(t)$. The definition of $\upsilon(v,t)$ gives

$$\upsilon(v,t) = \sum_{u \in N^-(v)} p_{vu}(t-1)\pi_u(t-1) \tag{5.9}$$

Equation 2.4 implies that $\upsilon(v,t) = \pi_v(t)$, for all $v \in V$. Since $\||\Psi(t)\rangle\| = \sum_{v \in V} \upsilon(v,t)$, $|\Psi(t)\rangle$ is clearly unitary and the claim is proved. □

5.3 The complete description of time-evolution

From Lemma 1, any valid shift operator for G can be used to determine the edge maps σ and σ^{-1} to represent the random walk state. In order to simplify both the analysis and the notation used, consider the following shift operator S_{RW}, defined in terms of its auxiliary functions (see Section 2.2.2). Let $\eta : V \times C \to V$ be defined such that the c-th neighbor of v is the neighbor of v with the c-th smallest label. Formally, for all $u \in V$, all $c, c' \in C_u$, $c \neq c'$, it holds

$$\eta(u,c) < \eta(u,c') \iff c < c'.$$

Note that, for each $(u,v) \in E$, there exists a pair $c \in C_u$, $c' \in C_v$ such that $\eta(u,c) = v$ and $\eta(v,c') = u$. Thus, let $\sigma(u,v) = c'$ and $\sigma(v,u) = c$. Furthermore, let $\sigma^{-1}(u,v) = \sigma(v,u)$ and $\sigma^{-1}(v,u) = \sigma(u,v)$. Precisely, S_{RW} maps the edge (u,v) to the edge (v,u) and is well-defined for any graph G of interest. The definitions of η and σ for S_{RW} will be used throughout this section.

The S_{RW} operator yields describing the state of a vertex v at time t as the vector

$$|\Psi(v,t)\rangle = \sum_{u \in N^+} e^{i\theta(u,c,t-1)} \sqrt{p_{vu}(t-1)} \sqrt{\pi_u(t-1)} \left|v,c'\right\rangle, \tag{5.10}$$

where the dependency of c and c' on u and v is omitted, i.e $\eta(u,c) = v$ and $\eta(v,c') = u$. From the analysis of the state representation on the previous section, it is enough to ensure that, for every instant t, the action of $W(t)$ maps

$$|\Psi(v,t)\rangle \to |\Phi(v,t)\rangle, \tag{5.11}$$

where

$$|\Phi(v,t)\rangle = \sum_{c' \in C_v} e^{i\theta(v,c',t)} \sqrt{p_{uv}(t)} \sqrt{\pi_v(t)} \left|v,c'\right\rangle. \tag{5.12}$$

The definition of the coin operator (Equation 2.34) implies that each vertex v has its own independent mixing behavior W_v, where W_v is unitary. In addition, it is a well known result from linear algebra that any operator that changes orthogonal basis can be transformed into a unitary operator. Thus, the following Lemmas respectively provides formal constructions for a set of linearly independent vectors on the coin subspace of a vertex and the coin operator $W(t)$ itself.

Lemma 2 (Linear independent set construction)**.** *Consider the subspace* $\mathscr{H}_{w,d(v)} \subset \mathscr{H}_W$

that represents the coin space $\mathscr{H}_{d(v)}$ of a vertex v. Let $|a\rangle \in \mathscr{H}_{w,d(v)}$ be any vector in the subspace. Let β be the basis $\{|u,c\rangle\}$ for $\mathscr{H}_{w,d(v)}$. The set $A = \{|a\rangle\} \cup \zeta(a,v) \cup B$, where $\zeta(a,v) = \{|v,c\rangle : \langle a|v,c\rangle = 0\}$ and $B \subset \beta \setminus \zeta(a,v)$ is any subset of $\beta \setminus \zeta(a,v)$ with cardinality $|B| = |\beta \setminus \zeta(a,v)| - 1$, is a set of linearly independent vectors.

Proof. It is clear that all vectors from $A \setminus \{|a\rangle\}$ are orthogonal, since they are a subset of the basis β. In the case where $\zeta(a,v) = \{\}$, $\langle a|v,c\rangle > 0$ for all $|v,c\rangle \in \beta$, what implies that exists a c' such that $\langle a|v,c'\rangle > 0$ while $\langle v,c|v,c'\rangle = 0$ for all $|v,c\rangle \in B$. Hence, it is impossible to write $|a\rangle$ as a linear combination of vectors in B, and A is a set of linearly independent vectors.

In the case where $\zeta(a,v) \neq \{\}$ the construction of A implies that the condition of the existence of c' holds because the vectors from $\zeta(a,v)$ are orthogonal to $|a\rangle$ and exactly one of the vectors of the set $\beta \setminus B$ is not a member of $B \cup \zeta(a,v)$. □

Lemma 3 (Coin operators for random walks)**.** *Let $\mathscr{H}_{d(v)}$ denote the Hilbert space defined by the degrees of freedom of a vertex v. Let the sets of vectors α and β be two orthonormal basis for $\mathscr{H}_{d(v)}$, where α_k and β_k are, respectively, the k-th vectors of α and β. Let $\alpha_0 = \frac{1}{\sqrt{\langle\Phi(v,t)|\Phi(v,t)\rangle}}|\Phi(v,t)\rangle$ and $\beta_0 = \frac{1}{\sqrt{\langle\Psi(v,t)|\Psi(v,t)\rangle}}|\Psi(v,t)\rangle$, where $\Psi(v,t)$ and $\Phi(v,t)$ are given by Equations 5.10 and 5.12 respectively. The operator*

$$W_v(t) = \sum_{k=0}^{d(v)-1} |\alpha_k\rangle\langle\beta_k|\,, \tag{5.13}$$

is unitary, inducing a unitary operator $W(t) = \sum_{v\in V} |v\rangle\langle v| \bigotimes W_v(t)$ on $\mathscr{H}_w$.

Proof. Note that $\langle\Psi(u,t)|\Psi(u,t)\rangle = \langle\Phi(u,t)|\Phi(u,t)\rangle$. It follows trivially from the completeness relation (Equation 2.17) that

$$W_v^\dagger(t)W_v(t) = W_v(t)W_v^\dagger(t) = I,$$

what also implies that $W(t)$ is unitary. □

Finally, the following Theorem states that, for any given random walk, a statistically equivalent quantum walk in terms of vertex probabilities can be constructed assuming time-dependent coin operators.

Theorem 5. *Let $P(t)$ be a stochastic matrix that defines the evolution of a random walk on a graph G, such that, for all t, $\pi(t+1) = P(t)\pi(t)$. For every instant t, the quantum walk with state $|\Psi(t)\rangle$ given by Lemma 1, with fixed shift operator $S(t) = S_{RW}$ and coin operator $W(t)$ given by Lemma 3, evolves according to*

$$|\Psi(t+1)\rangle = S_{RW}W(t)\,|\Psi(t)\rangle\,, \tag{5.14}$$

such that $\upsilon(u,t) = \pi_u(t)$ and $\upsilon(u,t+1) = \pi_u(t+1)$ for all $u \in V$.

Proof. For every $u \in V$, the conditions for $\upsilon(u,t) = \pi_u(t)$ and $\upsilon(u,t+1) = \pi_u(t+1)$ are ensured by Lemma 1. As a valid shift operator, S_{RW} is unitary. At instant t, construct two sets of linearly independent vectors $A_{v,1}$ and $A_{v,2}$ by respectively applying Lemma 2 to $|\Phi(v,t)\rangle$ and $|\Psi(v,t)\rangle$ for every vertex v. Use the Gram-Schmidt procedure on the sets $A_{1,v}$ and $A_{2,v}$ to generate the orthonormal basis $\alpha_{k,v}$ and $\beta_{k,v}$ respectively. Take $W(t)$ as the unitary operator defined by Lemma 3 using all basis $\alpha_{v,k}$ and $\beta_{v,k}$. Hence, S_{RW} and $W(t)$ are unitary and well defined for every instant t and the claim is proved. □

It is essential to note that the procedure to construct the quantum walk of Theorem 5 is not unique. In addition to the infinite possibilities of representation that lead to distinct definitions for $S(t)$ and $W(t)$, the operator $W(t)$ can also be defined differently. In fact, the Gram-Schmidt procedure is just one convenient way to define $W(t)$. Nonetheless, there may exist alternative definitions that could be more efficient under specific conditions, such as particular random walks definitions and graphs.

The results of Theorems 2, 3 and 5 reveals that unitary discrete-time coined quantum walks and non-homogeneous random walks are intrinsically related. Knowing the time-dependent stochastic matrix $P(t)$ and the probability vector $\pi(t)$ allows for the construction of a quantum walk operator $S(t)W(t)$ and the state vector $|\Psi(t)\rangle$, and vice-versa.

The random walk considered by Theorem 5 is general and non-homogeneous. Nonetheless, the Theorem can be used to construct a statistically equivalent quantum walk for a time-homogeneous random walk. In this case, the convergence of the vertex probability vector $\pi(t)$ is assured when the random walk is irreducible and aperiodic. In spite of the absence of convergence for the wavefunction caused by unitarity [1], the convergence of the vertex probability does not harm the construction of the equivalent quatnum walk. To illustrate, consider a quantum walk where the wavefunction is permuted among the edges of a vertex perpetually, such that $\Psi(v,c,t) = \Psi(v,c',0)$ for $t > 0$ and $c' \in C_v$. The vetex probability is the same for all t while the wavefuction keeps alternating forever on the edges, and thus does not converge. Note also that a time-homogeneous stochastic matrix $P(t) = P$ does not implies on a time-independent coin operator $W(t) = W$.

Chapter 6

Conclusion

Quantum walks and random walks are fundamental abstractions that find a myriad applications in quantum algorithms and classical algorithms, respectively. While the two processes differ fundamentally, they can both be framed as stochastic processes over the vertices of a graph. Indeed, this work has investigated this connection showing an inherent equivalence between the two processes. In particular, it demonstrated that the evolution of the vertex probability that characterizes quantum and random walks can be matched exactly. Their inherent connection has a statistical nature and the processes cannot be differentiated in terms of their vertex probability distributions, in spite of representing completely different physical systems.

As the central contribution of this work, Theorems 2, 3 and 5 establishes the statistical equivalence between discrete-time coined quantum walks and non-homogeneous random walks on finite graphs in terms of vertex distributions. The procedure prescribed by Theorem 2 allows for the efficient simulation of quantum walk trajectories, paths of the graph that recover the vertex distribution sequence of quantum walks with convergence guaranteed by the law of large numbers. The procedure defined by Theorem 3 extends the simulation of these trajectories to the context of quantum walks with interacting multiple walkers, where trajectories for all walkers are generated simultaneously and convergence remains guaranteed by the law of large numbers. In parallel, Theorem 5 gives a procedure to emulate random walks in a quantum computer through the definition of quantum walk operators that perform unitary evolution. In a nutshell, the Theorems establish a formal correspondence between random and quantum walks on the same graph by showing how the vertex distribution of the two processes can be identical for all time t.

The simulation of quantum walk trajectories can be used to investigate quantum walks from the perspective of vertex locality, as opposed to the simulation of independent samples over time. Since the vertex distribution of quantum walk trajectories converges to the vertex distribution of quantum walks for all time instants, any statistical property of a quantum walk can be analyzed through quantum walk trajectories. The description of quantum walk trajectories allows for establishing a stronger parallel between the theo-

retical properties and concepts of quantum walks with those defined for Markov chains. Specifically, properties of Markov chains such as hitting time, mixing time and dispersion time, were defined for quantum walks in the infinite time limit ($t \to \infty$) [1]. Nonetheless, quantum walk trajectories gives alternative definitions for these properties as the definitions used for random walks, which, in turn, can be calculated from trajectory simulation.

Due to the universality of quantum walks for quantum computation [9, 10, 25], the presented results may have important implications in the development of this larger field. The connections between generic computational processes and time-dependent Markov chains can be explored to guide new interesting research on quantum computing. In particular, the universality implies that any quantum algorithm can be implemented through a sequence of quantum walk circuits. Thus, theorems 2 and 3 can be used to construct a statistically equivalent random walk for any quantum algorithm, a random walk which can be analyzed in the extensive mathematical formalism developed for Markov chains.

Furthermore, one may find that the non-homogeneous random walk prescribed by Theorem 2 is in some sense related to the path integral formulation for quantum mechanics. It is clear that statistical processes have motivated Feynman's celebrated work, in which trajectories play a fundamental role to compute the probability of a particle moving through space [13]. In his formulation, each trajectory that a particle can take to move from point a to point b contributes to the wavefunction in b, and hence, to the probability of finding the particle at b. The resemblance in question lies on the fact that Equation 2.4 implies that the vertex probability at instant t is achieved by summing the contribution of all paths of length $t+1$ on the graph modulated by the initial condition. The contribution of each path in question is the product of the transition probabilities to hop through its vertices. Albeit this resemblance, Theorems 2 and 3 restrict to quantum walks on finite structures.

As one of the philosophical guidelines of this dissertation, the equivalence demonstrated does not harm any of the principles of quantum mechanics. The proofs for the equivalence theorems respect all the rules established by the postulates. Additionally, such statistical equivalence does not enables the use of a classical physical system to compute the probabilities of quantum walks in an efficient way, which emphasizes the need of quantum computers to simulate nature efficiently [12]. The inability of using random walks to compute quantum walk probabilities stems from the necessity of computing the quantum probabilities prior to constructing the matrices prescribed by Theorems 2 and 3.

Finally, in the light of the presented results, the goal of characterizing the connections between quantum and random walk is settled. In contrast with looking at the two processes as analogous of each other, the statistical equivalence firms in formal grounds that quantum and random walks are two distinct forms of describing the same vertex probability evolution, centered on the description of a diffusion process on the edges of a graph.

6.1 Future work

The implications of the results presented brings possible research directions for future consideration.

- The investigation of random walks that are statistically equivalent with quantum walks algorithms. Quantum walks are one of the few generic tools to design quantum algorithms. A direct application of Theorems 2 and 3 is constructing random walks for algorithms based on quantum walks, such as the algorithms for element distinctness [4], sparse-Hamiltonian simulation [6] and marked-vertex searching [27]. From these random walks, it is possible to investigate the behavior of the algorithms in terms of quantum walk trajectories. Also, implementing random walks for quantum algorithms based on quantum oracles may impose interesting challenges on how to represent the results of the functions abstracted by oracles in the probability evolution of random walks.

- Describing random walks with quantum walks implemented by usual quantum gates. A clear difficulty of using Theorem 5 to perform random walks on quantum computers is efficiently implementing the operators $W(t)$ in quantum circuits. The restrictions on the actual technology for quantum circuit size in terms of quantum gates is a clear barrier to perform computations on quantum computing. Each application of a quantum gate can introduce noise causing the system to decohere, *i.e* to collapse the wavefuction annihilating quantum superposition, which introduces errors to the computation. Hence, discussing the size complexity (number of quantum gates) in terms of the random walk matrices and describing the operators $W(t)$ with the smallest possible number of quantum gates is essential to apply Theorem 5 in the near-term prospective of quantum computing.

- Investigating the connections between generic computing procedures and Markov chains. Quantum walks can be employed to perform any type of quantum computation allowed by quantum circuits. Theorems 2 and 3 assure that there exist a random walk that captures the statistical behavior of any computing procedure performed in a quantum computer. Evaluating the computational limits of a stochastic machine capable of performing quantum walk trajectories may shed light on the differences between such a machine and a generic quantum computer. Furthermore, such evaluation may lead to interesting results in areas such as Computing Theory, Complexity Theory and Stochastic Algorithms.

- Investigating the statistical equivalence for continuous time quantum walks. It was emphasized throughout this work that results obtained concerns discrete-time quantum and random walks. A clear extension is to investigate if there exists a version

of the theorems presented for continuous-time, either by taking the continuum limit or by directly defining differential equations for walk probabilities.

- Investigating periodic quantum walks and describing periodicity in terms of the graph structure. Theorem 4 gives sufficient conditions for the periodicity of the quantum walk vertex probability. Nonetheless, the theorem does not address how the graph structure and the coin weights directly affects this periodicity. Investigating how the structure of graphs connects with the spectrum of the operator SW may have profound implications for both fields of Quantum Walks and Graph Theory. In particular, describing if a given quantum walk can be represented by a set of periodic quantum walks would be an amazing result with a strong resemblance to the Fourier expansion of functions that could be used to address graph problems.

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