XIAMEN UNIVERSITY MALAYSIA

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Prepared by :

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Date Received :

MARKING RUBRICS

No.	Component Title	Mark
1.	Understanding; effort; self-motivation and achievement (7 Marks)	
2.	Report content (6 Marks)	
3.	Presentation and oral exam (7 Marks)	
	TOTAL **(20 Marks)**	

Ong Chong Kim

XIAMEN UNIVERSITY MALAYSIA

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I/We hereby confirm that all the references or sources of citations have been correctly listed or presented and I/we clearly understand the serious consequence caused by any intentional or unintentional misconduct.

This work is not made on any work of other students (past or present), and it has not been submitted to any other courses or institutions before.

Signature: 

Date: 29th June 2025

A. Introduction/ Situation/ Background Information

This assessment offers opportunity for students to build up transferable skills such as master of subject matter and self-learning; critical thinking; scientific methods and problem solving skills and interpersonal communication skills. It complements with tutorial sessions and online lectures.

B. Course Learning Outcomes (CLO) covered

At the end of this assessment, students are able to:

and special relativity

CLO5 Report on current issues or technological advances related to modern physics.

University Policy on Academic Misconduct

1. Academic misconduct is a serious offense in Xiamen University Malaysia. It can be defined as any of the following:
   i. **Plagiarism is submitting or presenting someone else's work, words, ideas, data or information as your own intentionally or unintentionally. This includes incorporating published and unpublished material, whether in manuscript, printed or electronic form into your work without acknowledging the source (the person and the work).**
   ii. **Collusion** is two or more people collaborating on a piece of work (in part or whole) which is intended to be wholly individual and passed it off as own individual work.
   iii. **Cheating** is an act of dishonesty or fraud in order to gain an unfair advantage in an assessment. This includes using or attempting to use, or assisting another to use materials that are prohibited or inappropriate, commissioning work from a third party, falsifying data, or breaching any examination rules.

2. All the assessment submitted must be the outcome of the student. Any form of academic misconduct is a serious offense which will be penalised by being given a zero mark for the entire assessment in question or part of the assessment in question.

If there is more than one guilty party as in the case of collusion, both you and your collusion partner(s) will be subjected to the same penalty.

C. Instruction to Students

Objectives:

- In tutorial assignments and examination, we aim to solving challenging problems. However, you might want to set up your questions and try to solve it all by yourself. You might find some topics more interesting than others and like to know more. The project is to provide an opportunity for you to solve questions asked by you yourself related to the topics taught in the course. A platform to training for creativity, collecting information, organization, analysing and presentation
- It would also provide certain aspect of students self-learning in terms of information gathering, understanding, discussion, presentation and organization of thoughts.
- I would expect the students to be very resourceful in all aspect of the project. You are encouraged to find your information from various sources like internet, published articles in magazines (Scientific American, Science, Nature, Economists), news (newspaper, local and foreign) on science and technologies, websites and etc.
- Everyone have to participate in the project and submit an individual paper.

What do I look for in your paper

- 20 to 30 typed and printed pages long (including figures and graphs). 12 points font and one-and-a-half line spacing.
- Title,abstract, your names and table of contents clearly written on the front page.
- May contain images, figures, graphs and equations to illustrate your points. The images and figures need not be in color as long as features are clearly visible in grayscale.
- Must make proper reference to the sources you used. (Internet, book, published articles, authors and title when available.)
- The paper should summarize your readings and reflect your understanding of the chosen topic.
- Your targeted readers should be your fellow classmates. i.e. you should write it in such a way that your classmates would be able to understand.
- A good report should contain the correct facts, make sound arguments and provide evidence of your own understanding. It should also be clear, original, organized and creative in presentation. References used should also be clearly stated.
- Any innovative ideas (related to your chosen topic) that you have on interesting experiments, techniques and devices will be a plus. (You are not expected to actually do the experiments, but just write down or draw the instrument design of what you think.)

D. Evaluation Breakdown

No.	Component Title	Mark
1.	Understanding; effort; self-motivation and achievement (7 Marks)	
2.	Report content (6 Marks)	
3.	Presentation and oral exam (7 Marks)	
	TOTAL (20 Marks)	

Xiamen University Malaysia

Quantum Random Walks: Theory, Developments, and Open Challenges

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Abstract

Random walks have long been a cornerstone of probability theory and computational sampling. In this report, we trace their journey from simple coin-flip models on the integer lattice to richly structured graph dynamics, then leap into the quantum realm. We begin by reviewing classical discrete- and continuous-time walks on $\mathbb{Z}$ and $\mathbb{Z}^d$, deriving the familiar binomial and heat-kernel approximations, and discussing Pólya's theorem on recurrence versus transience. Next, we introduce the minimal quantum toolbox: Hilbert spaces, Dirac notation, unitary evolution, and projective measurement. We then show how these postulates elevate the classical generator into a Hamiltonian, unifying "coin-flip" and "shift" into a single coherent process.

We then compare discrete-time and continuous-time quantum walks, highlighting how interference drives ballistic spreading ($\sigma \sim t$), in stark contrast to the $\sqrt{t}$ diffusion of classical walks. Drawing on recent literature, we survey advances in multi-target search, hitting-time frameworks, and universal walk-based computation. Finally, we identify open challenges, namely perfect state transfer, uniform mixing on arbitrary graphs, and gate-model compilation of walk algorithms. This outlines a research roadmap that spans quantum algorithmics, spectral graph theory, and experimental implementation.

Contents

1 Introduction

The concept of a "random walk" was formally introduced by Karl Pearson in 1905, which describes a path consisting of a succession of random steps in the mathematical space [1] [2]. However, the foundational ideas underpinning random movements precede Pearson's work, appearing in various mathematical and scientific inquiries. Early investigations of discrete random-walk models trace back to Richard Feynman's "checkerboard" consturction, in which he discussed a checkerboard analog which described the way a spin-$\frac{1}{2}$ particle moved through 1 spatial dimension in discrete time steps [3]. In quantum information theory, similar constructions were rediscovered by John Watrous, who proved that space-bounded quantum Turing machines can efficiently simulate classical random walks on undirected graphs [4].

Mathematically, a random walk, or a Markov chain can effectively sample a distribution since the transition probability between nodes is directly proportional to their correlation strength. Through sufficient steps, the distribution of the position approaches the distribution of the universe we sample from. This aspect quickly found its use in computer science through algorithms like PageRank [5], which assigns a weighting to a webpages to measure its relative importance within the set. This success in web search foreshadows the potential of quantum walks to accelerate analogous graph-based computations.

In 1993, Aharonov et al. [6] officially coined the term quantum random walk and demonstrated that, unlike classical walks whose variance grows linearly ($\sigma^2 \sim n$), quantum walks exhibit quadratic variance growth ($\sigma^2 \sim n^2$) due to quantum interference. Subsequent work by Aharonov et al. [7] generalized discrete quantum walks to arbitrary graphs and established their use in search and element-distinctness algorithms, achieving polynomial or even exponential speedups over classical counterparts.

In addition to theoretical developments, quantum random walks have been implemented in quantum computation. In particular, Childs [8] demonstrated that continuous-time quantum walks can efficiently simulate any quantum circuit, establishing quantum walks as a universal model of quantum computation. On the discrete-time side, [9] introduced a quantum walk algorithm to implement Grover's search, achieving an $O(\sqrt{N})$ runtime on an N-vertex database, while Szegedy's quantization of classical Markov chains provided a systematic method to derive quantum speedups for randomized algorithms on arbitrary graphs [10]. A timeline of different quantum random walk models and their application fields is given in Figure 1.

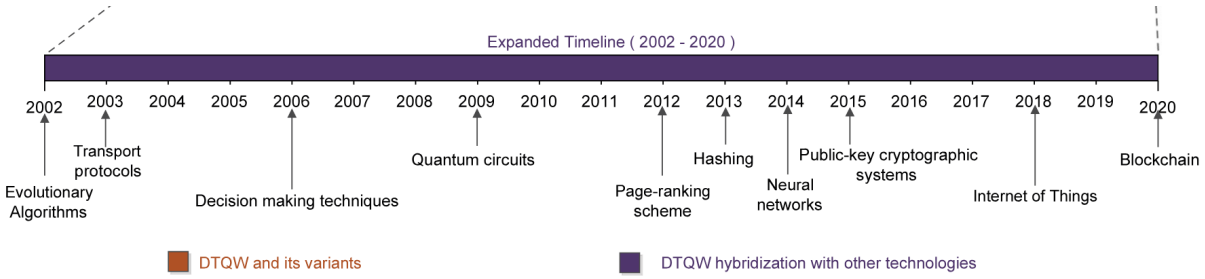


Figure 1: Timeline of applied fields in quantum random walk [11].

This report aims to provide a comprehensive review of random-walk theory. We first review classical random walks, deriving key results such as return probabilities and mixing times. Then, we introduce the Hilbert-space formalism and Dirac notation necessary to understand quantum walks. Next, we present an introduction to discrete and continuous quantum random-walk models, discussing their interference effects and algorithmic advantages. We then survey the applications and open problems of quantum random walks.

2 Classical Random Walks

The work done in this section draws primarily from [12] and [13]. We will introduce the Discrete-Time Random Walk (DTRW) by constructing a probability mass function (PMF) $Prob(x = i)$ that describes the probability that the particle will land at position $x = i$ at the end of its N^{th} step. Then, we will show different approximations of the DTRW, namely via the Gamma function and Heat (or Gaussian) kernel. Lastly, we would generalize into high-dimensional DTRW.

2.1 Discrete Classical Random Walk on a Line

Consider a classical particle initially located at $x = 0$ of the real line. We discretize space and time by defining $x = il$ and $t = N\tau$. Let $N = 0$ at the start of the particle's random walk. At each step, the particle has probability of p_r to step right and $p_l = 1 - p_r$ to step left. In total, the particle takes $N = n_l + n_r$ steps. The total probability that the particle will land at $x = i$ on its N^{th} step is

$$f(n_r) = \binom{N}{n_r} p_r^{n_r}(1 - p_r)^{N-n_r} \tag{2.1.1}$$

In terms of i, using $i = n_r - n_l = 2n_r - N$,

$$Prob(x=i) = \begin{cases} 0 & \text{if } \frac{1}{2}(i+N) \mod 1 \neq 0 \\ f(\frac{1}{2}(i+N)) & \text{otherwise} \end{cases} \tag{2.1.2}$$

where the first constraint is to avoid nonzero probability for half-integer steps.

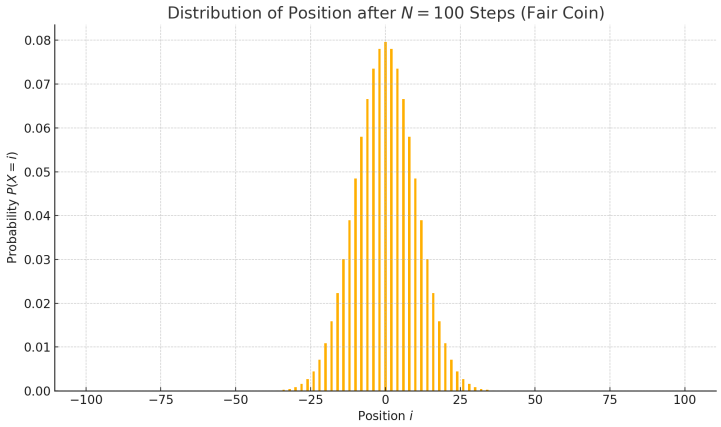


Figure 2: The probability distribution after $N = 100$ steps of a classical random walk on a line.

The expectation and variance of the distribution is follows, and a derivation is provided in [12]:

$$\langle x \rangle = N(p_r - p_l) \tag{2.1.3}$$

$$\sigma^2 = 4Np_rp_l \tag{2.1.4}$$

$$\tag{2.1.5}$$

It is noticed that

$$\sigma \sim \sqrt{N} \tag{2.1.6}$$

which means that the particle in a classical random walk has an expected distance $O\sqrt{N}$ from the origin.

2.2 Continuous Limit of a Classical Random Walk on a Line

We will discuss the two most common approximation methods, namely via the Gamma function (Equation 2.2.2) and the heat-kernel PDE (Equation 2.2.3).

$$P(x,N) = \frac{\Gamma(N+1)}{\Gamma(\frac{x+N}{2}+1)\Gamma(\frac{N-x}{2}+1)} p_r^{\frac{x+N}{2}} (1-p_r)^{\frac{N-x}{2}} \tag{2.2.1}$$

$$\approx \frac{1}{\sqrt{2\pi\, N\, p_r\, p_\ell}} \exp\Big[-\frac{(i-N(p_r-p_\ell))^2}{8\, N\, p_r\, p_\ell}\Big]. \tag{2.2.2}$$

$$P(x,t) = \frac{1}{\sqrt{4\pi\alpha t}} e^{-x^2/(4\alpha t)} \tag{2.2.3}$$

The prior can be simply derived by rewriting the permutation count in gamma functions, $P(n,k) = \frac{\Gamma(n+1)}{\Gamma(n-k+1)}$, and applying Stirling's approximation on each gamma, while the derivation of Equation 2.2.3 will be provided in the Appendix A. The main difference of the two methods is provided in Table 1, and a direct comparison can be seen through the plot in Figure 3.

Table 1: Comparison of Gamma-Function and Heat-Kernel PDE Approximations

Aspect	Gamma-Function	Heat-Kernel PDE
Domain	Discrete lattice ($k \in \mathbb{Z}$)	Continuous ($x \in \mathbb{R}$)
Limit type	Fixed large n	$\Delta x, \Delta t \to 0$
Method	Gamma asymptotics	Taylor-expansion $\to$ PDE
Use case	Precise pointwise PMF approximations	Modeling continuous diffusion

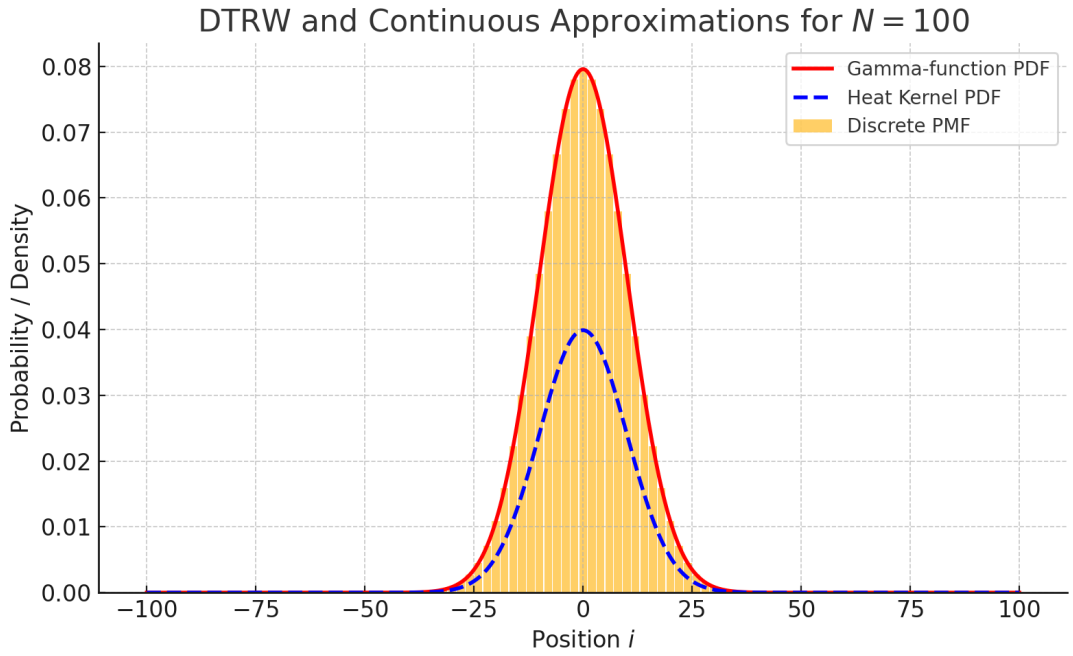


Figure 3: Probability distribution $P(X_n = i)$ for an unbiased discrete-time random walk on $\mathbb{Z}$ after $N = 100$ steps. Yellow bars show the exact PMF at even lattice positions; the solid red curve is the continuous Gamma-function approximation (normalized to the PMF peak); and the dashed blue curve is the Gaussian heat-kernel approximation.

2.3 Classical Random Walk in Higher Dimensions ($\mathbb{Z}^d$)

We now extend the simple symmetric walk on $\mathbb{Z}$ to d spatial dimensions. Let

$$\mathbf{X}_N \;=\; \sum_{n=1}^{N} \mathbf{S}_n,$$

where each increment $\mathbf{S}_n$ is chosen *uniformly* from the $2d$ nearest-neighbour directions

$$\{\pm\mathbf{e}_1, \ldots, \pm\mathbf{e}_d\},$$

with the sample mean

so that

$$P\big(\mathbf{S}_n = +\mathbf{e}_j\big) \;=\; P\big(\mathbf{S}_n = -\mathbf{e}_j\big) \;=\; \frac{1}{2d}, \quad j = 1, \ldots, d.$$

This assumption of equal probability in each direction ensures an unbiased walk.

Here $\{\mathbf{e}_j\}$ denotes the standard basis of $\mathbb{R}^d$. For example, in $d = 2$ we have

$$\mathbf{e}_1 = (1, 0), \quad \mathbf{e}_2 = (0, 1),$$

so the four possible steps are

$$(1, 0),\ (-1, 0),\ (0, 1),\ (0, -1),$$

each occurring with probability $1/4$. With expectation values and covariance matrix:

$$\mathbb{E}[\mathbf{S}_n] = \sum_{j=1}^{d} \Big(P(\mathbf{S}_n = +\mathbf{e}_j)\, \mathbf{e}_j + P(\mathbf{S}_n = -\mathbf{e}_j)\, (-\mathbf{e}_j) \Big) \tag{2.3.1}$$

$$= \sum_{j=1}^{d} \Big(\tfrac{1}{2d}\mathbf{e}_j - \tfrac{1}{2d}\mathbf{e}_j \Big) = \mathbf{0} \tag{2.3.2}$$

$$\mathrm{Cov}(\mathbf{S}_n) = \frac{1}{d} I_d. \tag{2.3.3}$$

Since the random variables are mutually independent and identically distributed (iid), the multivariate Central Limit Theorem then provides

$$\frac{\mathbf{X}_N}{\sqrt{N}} \;\xrightarrow{d}\; \mathcal{N}\Big(\mathbf{0}, \tfrac{1}{d}\, I_d\Big),$$

i.e. for large N, $\mathbf{X}_N$ is approximately an isotropic Gaussian in $\mathbb{R}^d$.

2.4 Pólya's Recurrence Theorem

A drunk man will find his way home, but a drunk bird may get lost forever.

- Shizuo Kakutani

In 1921, Pólya, G proposed the famous Pólya's Recurrence Theorem [14], which states[1]:

Let $\{X_n\}$ be the simple (walker moves exactly one lattice unit) symmetric (unbiased) random walk on $\mathbb{Z}^d$. Then:

1. (Recurrence) When $d = 1, 2$, $P\{\text{the walk ever returns to the origin}\} = 1$. Equivalently,
$$\sum_{n=0}^{\infty} P\{X_{2n} = 0\} = \infty$$
2. (Transience) When $d \geq 3$, $P\{\text{the walk ever returns to the origin}\} < 1$. Equivalently,
$$\sum_{n=0}^{\infty} P\{X_{2n} = 0\} < \infty$$

Pólya's theorem imposes several fundamental consequences for the behavior of random walks. For algorithmns, this implies in low dimensions any sampling scheme based on simple walks will revisit and explore neighborhoods exhaustively; in high dimensions, walks "escape" more quickly, which improves coverage of large graphs at the cost of poor local sampling.

2.5 Classical Continuous Time Markov Chain

Suppose we introduce the graph $G(V, E)$, where V is a set of vertices $\{1, \ldots, v\}$ and the edges E specify which pairs of vertices are connected. To describe how the walker moves between connected vertices we define the **transition matrix**, which is continuous in time. We introduce the jumping rate γ, which is the probability of jumping to any connected vertex in a time ϵ is $p_{\text{jump}} = \gamma\epsilon$, where $\epsilon \to 0$. Thus, our infinitestimal transition matrix is a $d \times d$ matrix M defined as follows:

$$M_{ij} = \begin{cases} k\gamma, & i = j, \text{ where } k = \deg(i) \\ -\gamma, & i \neq j, \ i \text{ and } j \text{ are connected by an edge} \\ 0, & i \neq j, \ i \text{ and } j \text{ are not connected} \end{cases} \tag{2.5.1}$$

[1] A proof of the Pólya's Theorem will not be provided, there are multiple approaches, by formulating it as an electric circuit problem and using Rayleigh's short-cut [15], or the 'potpourri proof' by [16].

The definition is motivated since the jumping rate should be proportional to the basic jumping rate, γ and the number of neighbours, k. Following [17], the probability of being at vertex i and time t is given by

$$\frac{\mathrm{d}p_i(t)}{\mathrm{d}t} = -\sum_j M_{ij}p_j(t) \tag{2.5.2}$$

solving this would give us our probability distribution of being at vertex i. Where the constraint

$$\sum_i p_i(t) = 1 \tag{2.5.3}$$

ensures probability is conserved. This construction of the walk will be extremely useful in the construction of the continuous time quantum walk, demonstrated in Section 4.2.

3 Quantum Formalism

In this section we will study the minimum amount of quantum mechanics: from the mathematical structure to the postulates, in order to understand quantum random walks. If the reader is not satisfied, one should dive into the list of resources [18] [19], which dive into more details than I am able to give here.

3.1 The Hilbert Space

A **Hilbert space**, $\mathcal{H}$ is a vector space with an inner product that is complete (meaning all Cauchy sequeneces converge) and may be viewed as the analogue of the Euclidean space $\mathbb{R}^n$ but built over the complex numbers and possibly infinite dimensional. States are represented as vectors in Dirac notation which we will come to mention.

Definition 3.1.1 (Inner Product). *Let $\mathcal{H}$ be a finite dimensional complex Hilbert space. An inner product on $\mathcal{H}$ is a map $\langle .|. \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ satisfies the following conditions for all $|\phi\rangle, |\psi\rangle, |\mu\rangle \in \mathcal{H}$ and all scalars $\alpha \in \mathbb{C}$*

1. Positivity: $\langle\psi|\psi\rangle = 0, \forall\, |\psi\rangle \in \mathcal{H}$
2. Definiteness: $\langle\psi|\psi\rangle = 0$ if and only if $|\psi\rangle = 0$
3. Additivity: $\langle\psi|\phi + \mu\rangle = \langle\psi|\phi\rangle + \langle\psi|\mu\rangle$
4. Homogeneity: $\langle\psi|\alpha\phi\rangle = \alpha\langle\psi|\phi\rangle$
5. Conjugate Symmetry: $\langle\psi|\phi\rangle = \overline{\langle\phi|\psi\rangle}$

in addition to the above, a Hilbert space requires the additional structure

Definition 3.1.2 (Hilbert Space). *Let $(\mathcal{H}, \langle .|. \rangle)$ be an inner product space. $\mathcal{H}$ is called a Hilbert space if it is complete as a normed space with norm $\|.\|$*

where a complete normed space is defined as follows.

Definition 3.1.3 (Complete normed space). *A normed space $(V, \|.\|)$ is complete if and only if any Cauchy sequence in V is convergent, i.e. If u_n is a sequence in V such that $\|u_n - u_m\| \to 0$ as $n, m \to \infty$ then there exists $u \in V$ such that $\lim_{n\to\infty} \|u_n - u\| = 0$.*

With this framework in mind, let us introduce Dirac notation, which is a crucial tool for quantum theorists and is used throughout quantum mechanics.

3.2 Dirac Notation

We begin by starting in a complex finite dimensional Hilbert space $\mathcal{H} = \mathbb{C}^d$. Within this space we introduce the *ket*, $|.\rangle$, which share a similar structure to d-dimensional row vectors

$$\psi = |\psi\rangle = \begin{pmatrix} a_1 \\ \vdots \\ a_d \end{pmatrix}$$

and for $|\psi\rangle, |\psi_1\rangle, |\psi_2\rangle \in \mathcal{H}$ linearity holds, namely

$$|\psi\rangle = \alpha |\psi_1\rangle + \beta |\psi_2\rangle \in \mathcal{H} \tag{3.2.1}$$

We now introduce the dual space, $\mathcal{H}^*$, which is the space of all continuous linear functionals on $\mathcal{H}$

$$f : \psi \to f(\psi) \in \mathbb{C} \tag{3.2.2}$$

$$f(\alpha\psi_1 + \beta\psi_2) = \alpha f(\psi_1) + \beta f(\psi_2) \tag{3.2.3}$$

where $f \in \mathcal{H}^*$. In simple terms, $\mathcal{H}^*$ is the space of **all linear maps that take a ket to a complex number**. Within this space we introduce the *bra*, $\langle.|$, which has a similar structure to the transposed d-dimensional row vector

$$\psi^\dagger = \langle\psi| = \begin{pmatrix} \bar{a_1} \dots \bar{a_d} \end{pmatrix} \tag{3.2.4}$$

where $\bar{a_d}$ represents the conjugate of a_d. Thus for any $|\psi\rangle \in \mathcal{H}$ we can construct $f_\psi = \langle\psi|.\rangle$ such that

$$f_\psi(\phi) = \langle\psi|\phi\rangle \in \mathbb{C} \tag{3.2.5}$$

where we call $\langle\psi|\psi\rangle$ the "bra-ket". The other properties of the bra-ket simply follows that of a Hilbert space. The inner product is defined by Equation 3.2.5, combining this with the linearity condition 3.2.1 we have

$$\langle\psi|\alpha\phi_1 + \beta\phi_2\rangle = \alpha\langle\psi|\phi_1\rangle + \beta\langle\psi|\phi_2\rangle \tag{3.2.6}$$

and conjugate symmetry

$$\langle\psi|\phi\rangle = \overline{\langle\phi|\psi\rangle} \tag{3.2.7}$$

and thus if $|\phi\rangle = |\psi\rangle$ we define the norm as $\langle\psi|\psi\rangle = \sqrt{\|\psi\|}$.

With this in mind, we can take a look at tensor products, and its application in quantum random walk.

3.3 Orthonormal Basis

In quantum mechanics, we like to deal with orthonromal states as they highlight the mathematical structure of an object. A basis is a set of vectors that are linearly independent and span a d-dimensional space, in our case the Hilbert space $\mathcal{H}$. Though introductory, we shall express orthonormality in Dirac notation.

Definition 3.3.1 (Orthonormality). *Let $\mathcal{H}$ be a Hilbert space. A basis $\{|e_1\rangle \dots |e_d\rangle\}$ of $\mathcal{H}$ is orthonormal if and only if*

$$\langle e_i|e_j\rangle = \delta_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases} \tag{3.3.1}$$

$\forall i, j = 1, \dots, d$

If a set of vectors is not orthonormal, we can make them orthonormal using the Gram-Schmidt procedure. As an immediate consequence, we can write the Fourier decomposition of a state $|\phi\rangle$ as follows

$$|\phi\rangle = \sum_{i=1}^{d} \langle e_i|\phi\rangle\,|e_i\rangle$$

where $\langle e_i|\phi\rangle$ are the Fourier coefficients of $|\phi\rangle$. This can easily be proved by taking the inner product of both sides with $\langle e_k|$ and by Equation 3.3.1:

$$\langle e_k|\psi\rangle = \sum_{i=1}^{d} \langle e_i|\phi\rangle\,\langle e_k|e_i\rangle = \sum_{i} \delta_{ki}\,\langle e_i|\psi\rangle = \langle e_k|\psi\rangle$$

In the elementary Fourier series on the circle, the inner product $\langle e^{in\theta}, f(\theta)\rangle$ pulls out each mode's amplitude. The Dirac-ket version is exactly analogous, where $\langle e_i|\phi\rangle$ "projects" ψ onto the basis vector $|e_i\rangle$.

3.4 Linear Operators

In order to describe the action and dynamics of a quantum mechanical system, we define **linear operators**. Any linear operator on a d-dimensional Hilbert space $\mathcal{H}$ may be represented as a matrix and so folows the mathematical laws associated with matrices.

Definition 3.4.1 (Linear Operators). *Let $(\mathcal{H}, \langle .|. \rangle)$ be a Hilbert space. A linear operator on $\mathcal{H}$ is a map $\hat{A} : \mathcal{H} \to \mathcal{H}$ satisying the linearity condition $\hat{A}(\alpha |\phi\rangle + \beta |\psi\rangle) = \alpha \hat{A} |\psi\rangle + \beta \hat{A} |\phi\rangle$ for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C}$.*

Recall from basic linear algebra that the adjoint of a matrix $A = A_{ij}$ is $A^* = \overline{A^T} = \overline{A_{ji}}$. A matrix that is equal to its adjoin is called self-adjoint and has real eigenvalues. It is important that our operators have real eigenvalues, as the eigenvalues tell us what measurement we are to expect from a given observable. Hence, all observables are represented by self-adjoint operators. Four important linear operators that are used throughout quantum mechanics are the Pauli matrices

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{3.4.1}$$

$\sigma_x, \sigma_y, \sigma_z$ represent the components of spin of a spin-$\frac{1}{2}$ particle.

3.5 Trace

An important matrix function is the trace and has a whole variety of uses throughout quantum mechanics. The trace of a matrix $A \in M_d$ is defined as follows

$$Tr(A) = \sum_i A_{ii}$$

which is basically the sum of the diagonal components.

Definition 3.5.1 (Trace of an Operator). *Suppose $\{|\phi_i\rangle\}$ is a complete, orthonormal basis set in $\mathcal{H}$. Since a linear operator on a d-dimensional Hilbert space can be represented as a matrix with elements $A_{ij} = \langle \phi_i | \hat{A} | \phi_j \rangle$, we can define the trace of an operator as folows*

$$\mathrm{Tr}\left(\hat{A}\right) = \sum_{i=1}^{d} \langle \phi_i | \hat{A} | \phi_i \rangle \tag{3.5.1}$$

Some basic properties of the trace are

1. Linearity: $\mathrm{Tr}\left(\alpha \hat{A} + \beta \hat{B}\right) = \alpha \,\mathrm{Tr}\left(\hat{A}\right) + \beta \,\mathrm{Tr}\left(\hat{B}\right)$
2. Cyclicity: $\mathrm{Tr}\left(\hat{A}\hat{B}\right) = \mathrm{Tr}\left(\hat{B}\hat{A}\right)$

3. Basis free representation: If $\{|\mu_1\rangle, \ldots, |\mu_d\rangle\}$ is another complete orthonormal basis in $\mathcal{H}$ then
$$\mathrm{Tr}\left(\hat{A}\right) = \sum_{i=1}^{d} \langle\phi_i| \hat{A} |\phi_i\rangle = \sum_{i=1}^{d} \langle\mu_i| \hat{A} |\mu_i\rangle$$

4. $\mathrm{Tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$ for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$

Although this object may seem arbitrary at the moment, the trace is the *only* map from operators to numbers that is (1) linear, (2) basis-independent, and (3) recovers the sum of eigenvalues.

3.6 Normal and Unitary Operators

Let us introduce a very important type of linear operator, the unitary operator $\hat{U}$. The unitary operator enables us to describe the evolution of a quantum system, from one state $|\psi\rangle$ to some output state $\hat{U}|\psi\rangle$. An operator $\hat{N}$ is normal if $\hat{N}\hat{N}^\dagger = \hat{N}^\dagger\hat{N}$.

Definition 3.6.1 (Unitary Operators). *A operator $\hat{U}$ is unitary if and only if $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$ where $\hat{U}^\dagger$ is the adjoint of $\hat{U}$. They have the following properties:*

1. The rows and columns of $\hat{U}$ form an orthonormal basis
2. $\hat{U}$ preserves inner products $\left\langle \psi\hat{U} \middle| \hat{U}\phi \right\rangle = \langle\phi| \hat{U}^\dagger\hat{U} |\phi\rangle = \langle\psi|\phi\rangle$
3. The eigenvalues of $\hat{U}$ are all of the form $\exp(i\theta)$
4. Which means $\hat{U}$ can be diagonalized as the following

$$\hat{U} = \begin{pmatrix} e^{i\theta_1} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & e^{i\theta_d} \end{pmatrix}$$

An important example of a unitary operator is the Hadamard, which we will see much of throughout this review. We define the Hadamard as follows

$$\hat{H} = |+\rangle\langle 0| + |-\rangle\langle 1| \tag{3.6.1}$$

where $|+\rangle$ and $|-\rangle$ are the Hadamard basis states which are defined as

$$|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{3.6.2}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle) \tag{3.6.3}$$

in matrix form,

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{3.6.4}$$

We also see that the Hadamard acts on the two basis states $|0\rangle$ and $|1\rangle$ in the following way: $\hat{H}|0\rangle = |+\rangle$ and $\hat{H}|1\rangle = |-\rangle$. This implies that the Hadamard basis states collapses to either $|0\rangle$ or $|1\rangle$ upon measurement with a probability of $\frac{1}{2}$, making it the candidate as our unbiased coin in the context of discrete quantum walks.

3.7 Projectors

Projects play a key role in measurement. Suppose U is k-dimensional subspace of the Hilbert space $\mathcal{H}$, there exists a unique decomposition of a vector $|\psi\rangle \in \mathcal{H}$ in U and $U^{\perp}$, where $U^{\perp}$ is orthogonal complement to U, so that we have

$$|\psi\rangle = |\psi_U\rangle + \left|\psi_U^{\perp}\right\rangle$$

Thus, we define the orthogonal projection onto U by

$$\mathbf{P}_U : |\psi\rangle \mapsto |\psi_U\rangle \tag{3.7.1}$$

basically, it is the linear map that *"keeps" the component in U and throws away the rest.* It has the following nice properties, namely (1) self-adjointness $\hat{P} = \hat{P}^*$, (2) idempotence: $\hat{P}^2 = \hat{P}$ (applying the projection twice does nothing new).

In matrix form, for an orthonormal basis $\{|e_i\rangle\}_{i=1}^{k}$ of U

$$\hat{P} = \sum_{i=1}^{k} |e_i\rangle \langle e_i| \tag{3.7.2}$$

acting on an arbitrary state ψ picks out exactly the parts $\langle e_i|\psi\rangle |e_i\rangle$ that lie within U.

In quantum measurement, projector represents asking a yes/no question: "Is the system in subspace U?". Starting from $|\psi\rangle$, the probability of "yes" is

$$p(m) = \langle\psi| P_m |\psi\rangle \tag{3.7.3}$$

and *collapses* the state to

$$|\psi_m\rangle = \frac{P_m |\psi\rangle}{\sqrt{p(m)}} \tag{3.7.4}$$

3.8 Spectral Decomposition

Spectral decomposition is extremely useful in representing normal operators, as any normal operator may be characterised completely in terms of their eigenvalues and eigenvectors (their spectral data). Recall that eigenvalues λ and the eigenvectors $|i\rangle$ can be found by solving

$$\hat{A}\,|i\rangle = \lambda\,|i\rangle \tag{3.8.1}$$

$$(\hat{A} - \lambda\hat{I}) = 0 \tag{3.8.2}$$

$$\det\left(\hat{A} - \lambda\hat{I}\right) = 0 \tag{3.8.3}$$

where the set of all possible eigenvalues of $\hat{A}$ is called the **spectrum** of $\hat{A}$ and is denoted by $\sigma(\hat{A})$.

Theorem 3.8.1 (Spectral Decomposition). *Let $\hat{A}$ be a normal operator on a d-dimensinoal Hilbert space $\mathcal{H}$. Then there exists an orthonormal basis $\{|\psi_1\rangle, \ldots, |\psi_d\rangle\}$ and a sequence of complex eigenvalues $\{\lambda_1, \ldots, \lambda_d\}$ such that*

$$\hat{A} = \sum_{i=1}^{d} \lambda_i\,|\psi_i\rangle\,\langle\psi_i| \tag{3.8.4}$$

$$= \sum_{i=1}^{d} \lambda_i \hat{P}_{\lambda_i} \tag{3.8.5}$$

An example connecting the ideas of the projector operator and spectral decomposition to quantum mechanics is given in Appendix B.

3.9 Tensor Products

When dealing with several different systems which are part of several different Hilbert spaces, we introduce the tensor product to connect these systems, which essentially acts as a glue to join different systems together.

In a quantum walk we must keep track of two distinct degrees of freedom: a two-level "coin" and a (potentially infinite) "position" register. Mathematically, each lives in its own Hilbert space, and the full system is described by their tensor product. Let us first define the tensor product for matrices

Definition 3.4.1 (Tensor Prouct). *Let $A \in M_{m,n}$ and $B \in M_{k,p}$ be two complex matrices. The tensor product $A \otimes B$ is the $mk \times np$ matrix with the following block structure*

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \cdots & A_{1n}B \\ A_{21}B & A_{22}B & \cdots & A_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1}B & A_{m2}B & \cdots & A_{mn}B \end{pmatrix} \tag{3.9.1}$$

as an example let us take the tensor product of two 2×1 vectors

$$\begin{pmatrix} 2 \\ 8 \end{pmatrix} \otimes \begin{pmatrix} 3 \\ 5 \end{pmatrix} = \begin{pmatrix} 2\begin{pmatrix} 3 \\ 5 \end{pmatrix} \\ 8\begin{pmatrix} 3 \\ 5 \end{pmatrix} \end{pmatrix} = \begin{pmatrix} 6 \\ 10 \\ 24 \\ 40 \end{pmatrix} \tag{3.9.2}$$

It is naturally motivated to make the tensor product space a Hilbert space by defining the inner product of the tensor product:

$$\langle \psi \otimes \phi | \psi' \otimes \phi' \rangle = \langle \psi | \psi' \rangle \langle \phi | \phi' \rangle$$

to a sesquilinear form $\langle . | . \rangle : \mathcal{H}_1 \otimes \mathcal{H}_2 \times \mathcal{H}_1 \otimes \mathcal{H}_2 \to \mathbb{C}$.

We then see how the tensor product acts on linear operators. We define a linear operator $\hat{A} \otimes \hat{B}$ on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ as follows

$$(\hat{A} \otimes \hat{B})(|\psi\rangle \otimes |\phi\rangle) = \hat{A}\,|\psi\rangle \otimes \hat{B}\,|\phi\rangle \tag{3.9.3}$$

3.10 The Postulates

We should now discuss the five basic postulates of quantum mechanics that will bring the framework together. They are by no means "rigorous" laws in the mathematical sense, but are analogous to axioms in a physical sense.

Postulate 1: State. The state space of each quantum system is a Hilbert space $\mathcal{H}$. A state is a normalized vector $|\psi\rangle$ up to a constant phase factor. Equivalently, the state may be described by a one dimensional projection $|\psi\rangle \langle\psi|$. The state vector $|\psi\rangle$ contains all the information we would ever need to know regarding that quantum system.

Postulate 2: Observables. The observables with a state space $\mathcal{H}$ are represented by self-adjoint operators. All self-adjoint operators have real eigenvalues, which means they may be decomposed and written in terms of its spectral data. In general, operators do not commute.

Postulate 3: Unitary Evolution. The evolution of a closed quantum system is described by a unitary transformation of the state space. Mathematically, the state $|\psi(t')\rangle$

of a system at t' is related to the state of the system at an earlier time t by the unitary operator $\hat{U}(t', t)$

$$|\psi(t')\rangle = \hat{U}(t', t)\,|\psi(t)\rangle \tag{3.10.1}$$

The evolution of an isolated system is described by the **Schrödinger Equation**

$$\frac{\partial}{\partial t}\,|\psi(t')\rangle = -\frac{i}{\hbar}\,|\psi(t')\rangle \tag{3.10.2}$$

$$\frac{\partial}{\partial t}\hat{U}(t', t) = -\frac{i}{\hbar}\hat{H}\hat{U}(t', t) \tag{3.10.3}$$

The latter equation (3.10.3) refers to the operator form after we apply Equation 3.10.1, then drop the state vector $|\psi(t)\rangle$. If $\hat{H}$ is not time-dependent we obtain

$$\hat{U}(t', t) = \exp\left(-\frac{i}{\hbar}\hat{H}(t' - t)\right) \tag{3.10.4}$$

which is the unitary that describes the transformation from t to t'.

Before we proceed to the next postulate it is necessary to introduce the projection-valued measure (PVM). One often asks not just "what is the chance of exactly λ_3?" but also compound questions like "what is the chance that the result lies in the set $\{\lambda_2, \lambda_5, \lambda_7\}$?". A PVM handles these kinds of questions

Definition 3.10.1 (PVM). *Let $\mathcal{H}$ be the state space of a quantum system. A **projection valued measure** over a set $\{\lambda_1, \ldots, \lambda_k\}$ is given by a collection of orthogonal projections $\{\hat{P}_{\lambda_1}, \ldots, \hat{P}_{\lambda_k}\}$, with the following properties:*

1. *Orthogonality $\hat{P}_{\lambda_i}\hat{P}_{\lambda_j} = \delta_{ij}\hat{P}_{\lambda_i}$*
2. *Completeness $\sum_{i=1}^{k} \hat{P}_{\lambda_i} = \hat{I}$*

For each subset $E \in \{\lambda_1, \ldots, \lambda_k\}$ we define

$$P(E) = \sum_{\lambda_i \in E} \hat{P}_{\lambda_i}$$

where the projection $P(E)$ is defined as the probability that an event E will occur.

Essentially, PVM behaves like probability that we know and have similar properties like $P(\emptyset) = 0$, $P(\{\lambda_1, \ldots, \lambda_k\}) = I$ and $P(E \cup F) = P(E) + P(F)$ except that it takes values in projection operators rather than real numbers. With this defined, we can formally state the measurement postulate

Postulate 4: Measurement.

1. A quantum measurement with outcomes $\{\lambda_1, \ldots, \lambda_k\}$ on a system with state space $\mathcal{H}$ is described by a PVM $\{\hat{P}_{\lambda_1}, \ldots, \hat{P}_{\lambda_k}\}$ on $\mathcal{H}$.

2. The result of the measurement forms the probability distribution

$$P(\lambda_i) = \left\| \hat{P}_{\lambda_i} |\psi\rangle \right\|^2 = \langle\psi| \hat{P}_{\lambda_i} |\psi\rangle = \mathrm{Tr}\Big\{ |\psi\rangle \langle\psi| \hat{P}_{\lambda_i} \Big\}$$

where $|\psi\rangle$ is the state of the system before measurement.

3. If the measurement outcome is λ_i, the state of the system immediately after the measurement is

$$|\psi'\rangle = \frac{1}{\sqrt{P(\lambda_i)}} \hat{P}_{\lambda_i} |\psi\rangle = \frac{\hat{P}_{\lambda_i} |\psi\rangle}{\left\| \hat{P}_{\lambda_i} |\psi\rangle \right\|}$$

Postulate 5: Composite Systems. The state space of a composite system is the tensor product of the state spaces of the component systems. If the components are numbered 1 to N, and the system number i is prepared in the state $|\psi_i\rangle$ in isolation from others, then the joint state of the total system is

$$|\psi\rangle = |\psi_1\rangle \otimes \cdots \otimes |\psi_N\rangle \tag{3.10.5}$$

4 Quantum Random Walks

We are now in a position to discuss the quantum random walks. We will begin by looking at the discrete case, where the walker moves from position i to $i+1$ on a line via a unitary coin operator $\hat{C}$, followed by a translational shift operator $\hat{S}$. After we have covered the discrete case we shall move on to the continuous quantum random walk, whihc is described by the Schrödinger equation.

4.1 Discrete Quantum Random Walk on The Line

The framework for the discrete quantum walk on the line is described by the tensor product of the coin space $\mathcal{H}_c$ and the position space $\mathcal{H}_p$. Thus the total space is

$$\mathcal{H} = \mathcal{H}_c \otimes \mathcal{H}_p \tag{4.1.1}$$

where $\mathcal{H}_c = \mathrm{span}\{|\uparrow\rangle, |\downarrow\rangle\}$ is the "coin" and $\mathcal{H}_p = \mathrm{span}\{|x\rangle : x \in \mathbb{Z}\}$ is the position. We introduce a unitary shift operator, which enables us to transition between different psoition states. The shift operator acts on $\mathcal{H}$ in the following way:

$$\hat{S} : |\uparrow\rangle \otimes |i\rangle \to |\uparrow\rangle \otimes |i+1\rangle \tag{4.1.2}$$

$$\hat{S} : |\downarrow\rangle \otimes |i\rangle \to |\downarrow\rangle \otimes |i-1\rangle \tag{4.1.3}$$

The shift operator only affects the position space. For the entire walk, we define the shift operator formally as

$$\hat{S} = |\uparrow\rangle\langle\uparrow| \otimes \sum_i |i+1\rangle\langle i| + |\downarrow\rangle\langle\downarrow| \otimes \sum_i |i-1\rangle\langle i| \tag{4.1.4}$$

which runs over all of $\mathbb{Z}$. The shift operator essentially acts as a "move left" or "move right" command according to the results of the coin flip. Interestingly, there is a whole family of unitary coin operators $\hat{C}$ we can use, depending on the behavior we want to observe.

Next, we construct a unitary operator $\hat{U}$, that acts upon the whole $\mathcal{H}$ and describes the evolution of the walk

$$\hat{U} = \hat{S} \cdot (\hat{C} \otimes \hat{I}) \tag{4.1.5}$$

To carry out multiple steps, we must apply $\hat{U}$ t times to some initial state, where t represents the number of steps

$$|\psi(t+1)\rangle = \hat{U}^t |\psi(t)\rangle \tag{4.1.6}$$

after applying the unitary for t steps, we make a measurement $|\psi(t+1)\rangle$ in order to determine the state of the system. To get a feel on how this works, consider the Hadamard coin mentioned in 3.6.1 and the particle in the initial state $|\psi(0)\rangle = |\uparrow, 0\rangle$ and for one step we get the following

$$\begin{aligned}
|\psi(1)\rangle &= \hat{U}^1 |\psi(0)\rangle \\
&= \hat{S}\hat{H}(|\uparrow, 0\rangle) \\
&= \hat{S}\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle\right) \\
&= \left(|\uparrow\rangle\langle\uparrow| \otimes \sum_i |i+1\rangle\langle i|\right)\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle\right) \\
&+ \left(|\downarrow\rangle\langle\downarrow| \otimes \sum_i |i-1\rangle\langle i|\right)\left(\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |0\rangle\right) \\
&= \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle + |\downarrow\rangle \otimes |-1\rangle)
\end{aligned}$$

If we iterate the quantum walk through two more time steps using repeated applications of U on $|\psi_1\rangle$ without making any measurements between the two steps, we get

$$|\psi(2)\rangle = \frac{1}{2}\left[|\uparrow\rangle \otimes |2\rangle - (|\uparrow\rangle - |\downarrow\rangle) \otimes |0\rangle + |\downarrow\rangle \otimes |-2\rangle\right] \tag{4.1.7}$$

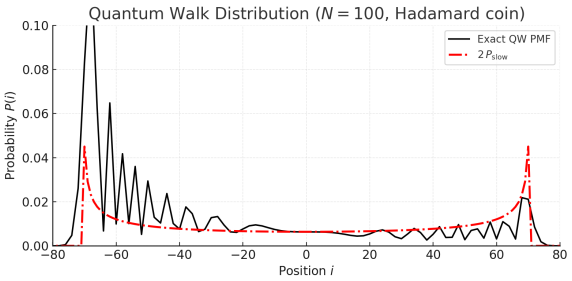
$$|\psi(3)\rangle = \frac{1}{\sqrt{2^3}}\left[|\uparrow\rangle \otimes |3\rangle + |\downarrow\rangle \otimes |1\rangle + |\uparrow\rangle \otimes |-1\rangle - 2\,|\downarrow\rangle \otimes |-1\rangle - |\downarrow\rangle \otimes |-3\rangle\right] \tag{4.1.8}$$

In analysing the equation 4.1.8 we find that the walker can be in multiple positions, each with its own probability. The probability that the walker is in a particular position is given by the following table

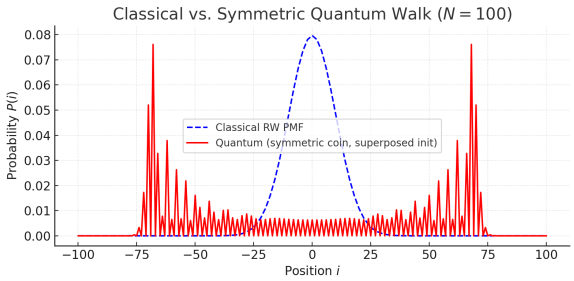
Table 2: Probability $P_n(i)$ of finding the quantum walker at position i after n steps, with initial state $|\Psi_0\rangle = |\downarrow\rangle \otimes |0\rangle$.

$n\backslash i$	-5	-4	-3	-2	-1	0	1	2	3	4	5
0						1					
1					$\frac{1}{2}$		$\frac{1}{2}$				
2				$\frac{1}{4}$		$\frac{1}{2}$		$\frac{1}{4}$			
3			$\frac{1}{8}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		
4		$\frac{1}{16}$		$\frac{5}{8}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{1}{16}$	
5	$\frac{1}{32}$		$\frac{17}{32}$		$\frac{1}{8}$		$\frac{1}{8}$		$\frac{5}{32}$		$\frac{1}{32}$

From table 2 we see that the quantum walk is asymmetric and left-drifting. If we had started in a state $|\psi\rangle = |\uparrow\rangle \otimes |0\rangle$, we would observe a skew to the right. If we were to let the quantum walk run through 100 steps, we would observe the following



(a) Hadamard-walk PMF after $t = 100$, from the initial state $|\downarrow, 0\rangle$. Only even sites are nonzero; the dotted curve is the long-wavelength approximation.



(b) Comparison of the classical (blue dashed) and symmetric quantum (red solid) walks on $\mathbb{Z}$ after $N = 100$ steps, using the balanced coin and initial coin state $(|0\rangle + |1\rangle)/\sqrt{2}$.

Figure 4: (a) Quantum-walk distribution at $t = 100$. (b) Overlay of classical vs. symmetric quantum walk after 100 steps.

In order to get a more symmetrical distribution we can either (1) prepare our initial state in the following way $|\psi(0)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + i\,|\downarrow\rangle) \otimes |0\rangle$ and use the Hadamard coin, or we can introduce the coin operator $\hat{M}$, which is defined as

$$\hat{M} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \tag{4.1.9}$$

From Figures 4a and 4b we can clearly see that the discrete quantum walk on the line has no Gaussian properties, unlike that of the classical case. This implies the statistical

analysis of the discrete quantum random walk much harder. This is because calculating the long term behavior of the walk cannot be done by standard means, since quantum walks do not converge to any stationary distribution. However, it has been shown analytically that the standard deviation of the distribution is t [20]. This is the main reason of the quadratic speed-up of the quantum random walk. From a physical perspective, as long as the walker's position remains unmeasured in intermediate steps, it remains in a superposition of *all* paths. Those many paths can then interfere constructively and destructively, so that the probability amplitude builds up near $\pm n$. Only at the very end when one performs a single position measurement, the superposition collapses and reveals to us a walker that has travelled a distance proportional to n.

4.2 Continuous Quantum Random Walk on Graphs

We shall now construct continuous quantum random walks, which are discrete in space but continous in time. They are fundamentally different from the discrete walks, as continous quantum random walks take place in the position space $\mathcal{H}_p$, as there is no coin space required since no coin flip takes place. Instead, we express the coin and shift operators into a single transition matrix M (Equation 2.5.1). However, it is not unitary. In order to generate norm-preserving, reversible quantum dynamics, we make it unitary by multiplying the matrix by i, the imaginary number [17]. We will see that the transition matrix can be reinterpreted as the quantum Hamiltonian, $\hat{H}$.

In continuous-time quantum walks, the only "rule" is that the time-evolution must be generated by a Hermitian operator H, so that $U(t) = e^{-iHt}$ is automatically unitary. In the classical continuous-time walk we already have the transition matrix M which is real and symmetric (hence Hermitian). It describes exactly how probability "hops" between vertices in the classical case. In quantum mechanics, a Hermitian matrix describes how amplitudes hop, and its exponential gives you a norm-preserving unitary evolution. So we can simply reinterpret our classical M as the quantum Hamiltonian:

$$H = M(\hbar = 1 \text{ units}) \tag{4.2.1}$$

To describe the quantum evolution of the walk in a d-dimensional Hilbert space $\mathcal{H}_p$, according to a given Hamiltonian $\hat{H}$ with matrix elements [2]

$$\langle a| \hat{H} |b\rangle = M_{ab} \tag{4.2.2}$$

where $|a\rangle, |b\rangle$ represent vertices of the graph. Writting the Schrödinger equation in terms of the basis $\{|a\rangle\}$ (by expanding $\hat{I} = \sum_b |b\rangle \langle b|$ on the right hand side and taking $\langle a|$ on both sides) gives:

[2] This is the transition matrix from Section 2.5, except i is now a, and j is now b.

$$i\frac{\mathrm{d}}{\mathrm{d}t}\langle a|\psi(t)\rangle = \sum_b \langle a|\hat{H}|b\rangle\langle b|\hat{H}|\psi(t)\rangle \tag{4.2.3}$$

The Schrödinger equation of this form is almost the same to equation 2.5.2, and it also conserves probability in the same sense

$$\sum_a |\langle a|\psi(t)\rangle|^2 = 1 \tag{4.2.4}$$

except the probabilities are now determined via projection valued measure. Solving the SEQ we gain the following time evolution unitary operator

$$\hat{U}(t) = e^{-i\hat{H}t} \tag{4.2.5}$$

where the time evolution of the walk is defined as

$$|\psi(t)\rangle = \hat{U}(t,0)|\psi(0)\rangle \tag{4.2.6}$$

and the probability distribution given by

$$P(t) = \left|\langle a|\hat{U}(t,0)|\psi(0)\rangle\right|^2 \tag{4.2.7}$$

Let us consider the example of applying the continuous time quantum walk on the line, $k = 2$. This means that our Halmiltonian "transition matrix" is

$$\hat{H}|i\rangle = -\gamma|a-1\rangle + 2\gamma|a\rangle - \gamma|a+1\rangle \tag{4.2.8}$$

Beginning the walk in some initial state $|\psi(0)\rangle = |0\rangle$ and setting $\gamma = \frac{1}{2\sqrt{2}}$, in order to find the state of the walk at any time t, we must find the state vector $|\psi(t)\rangle$. Using the initial state of the walker $|\psi(0)\rangle = |0\rangle$ we write

$$\hat{H}|0\rangle = -\gamma(|-1\rangle - 2|0\rangle + 0|1\rangle) \tag{4.2.9}$$

now for some time t we have the following

$$\hat{H}^t|0\rangle = \gamma^t \sum_t^{a=-t} (-1)^a \binom{2t}{t-a} |a\rangle \tag{4.2.10}$$

where $\binom{2t}{t-a}$ is the binomial coefficient. From this expression we compute $\hat{U}(t,0)|0\rangle$ in terms of two nested sums [21]. We then invert the sums and use the following identity

[20],

$$\exp(-2i\gamma t)J_{|a|}(2\gamma t) = \exp\left(\frac{\pi i}{2}|a|\right)\sum_{j=|a|}^{\infty}\frac{(-i\gamma t)^j}{j!}\begin{pmatrix}2j\\ j-a\end{pmatrix} \tag{4.2.11}$$

where J is the Bessel function of the first kind with interger a. In doing this we find our state for the continuous quantum random walk on the line for any time t to be

$$|\psi(t)\rangle = \sum_{a=-\infty}^{\infty}\exp\left(\frac{\pi i}{2}|a| - 2i\gamma t\right)J_{|a|}(2\gamma t)\,|a\rangle \tag{4.2.12}$$

from which we can deduce the probability distribution to be

$$P(t) = \langle a|\,\hat{U}(t,0)\,|\langle\psi(0)|\psi(0)\rangle\rangle^2 = |J_a(2\gamma t)|^2 \tag{4.2.13}$$

A detailed mathematical derivation for this will not be provided for obvious reasons. It is also worth noting that we can deduce this probability distribution via Laplace transforms as shown in [22], which for some is easier.

5 Recent Developments and Open Problems

Being the quantum analogues of classical random walks, quantum random walks (QRWs) leverage superposition and interference to explore graphs or lattices. In recent years, we have seen significant theoretical progress in understanding QRW dynamics and applications, as well as identifying new uses and challenges. This review summarizes the recent developments of QRW and open problems.

5.1 Discrete-Time Quantum Walks (DTQW) and Continuous-Time Quantum Walks (CTQW)

DTQWs underpin many quantum algorithmns. The Shenvi-Kempe-Whaley (SKW) search algorithm showed how a coined DTQW on a hyperube yields a quadratic speedup (Grover-like) [9] [23]. Building on this, research has focused on generalized search problems, as well as new variants of the walk operator. Recent work has also established general frameworks and even circuit-based models of computation using DTQWs.

Wing-Bocanegra et al. [23] propose a *search-complement* algorithm by perturbing the SKW coin: their modified walk suppresses a target state rather than amplifying it. This "inverse" search flips the behavior of the original walk can be used to initialize states for the Quantum Approximate Optimization Algorithm (QAOA). Besides that, several groups have worked to unify different QRW search approaches. For example, Apers et al. [24] present a general framework that include the "hitting time", MNRS,

and electric network approaches to QW search. This framework not only generalizes previous algorithms but also reveals resource trade-offs: one can interpolate between minimizing walk steps or oracle calls. Moreover, by combining DTQWs with techniques like quantum fast-forwarding and phase estimation, they derive more general bounds and even remove the need for expensive subroutines in some cases. This unification simplifies the landscape of QRW algorithms.

Childs [8] shown that quantum walks are universal for quantum computing. Recent work by Chawla et al. [25] demonstrates a concrete DTQW model for multi-qubit computation on a closed graph. They have showed that a single particle walking on a lattice with an appropriate set of coin shifts can implement a universal gate set, including multi-qubit gates for Grover's algorithm, quantum Fourier transform, and phase estimation. Their scheme even incorporates quantum error-detection and offers an analysis of space-time complexity, highlighting advantages on architectures where walk operations are natural (e.g. photonic lattices.) Such results show that DTQWs can serve as a full computational substrate, not just as subroutines.

For continuous-time quantum walks (CTQWs), the algorithmic uses often mirror DTQW results. It is usually used for quantum simulation, for instance, CTQWs naturally implement quantum analogues of walks on networks, and can encode problems like MAX-CUT (by evolving under an Ising Hamiltonian) [26]. They also form the basis of certain quantum optimization heuristics. Unlike DTQWs, CTQWs do not require periodic coin operations, which can simplify physical interpretation (e.g. in quantum optics or condensed matter).

One of the open problems in CTQWs is perfect state transfer (PST), to achieve probability 1 from one vertex to another at a specific time. Similarly, understanding instantaneous uniform mixing (whether the CTQW ever reaches a uniform distribution) is unresolved except for extremely symmetric graphs. A recent survey, provided by Coutinho and Guo [27] highlights these questions as major open problems in the CTQW theory. They note that PST and mixing properties are deeply linked to algebraic graph properties, and pose it as directions for future study.

5.2 Quantum Walks in Algorithms and Computation

Quantum walks (both DTQW and CTQW) underpin many known quantum algortihms. Notable applications include:

- Grover's search and search generalizations: Grover's algorithm itself can be viewed as a coined DTQW on the complete graph.

- Optimization and Sampling: Several proposals use QRWs for optimization. Slate et al. [28] developed a Quantum Walk Optimization algorithm for portfolio selection,

claiming performance improvements over classical methods. QRWs are also used for network analysis, a notable example is in disease-gene prioritization, which uses a CTQW to rank nodes more flexibly than classical random walks [29]. This applications are growing, though many remain proof-of-concept.

In summary, quantum random walks have proven to be a versatile and strong framework for specific algorithms (search, optimizatoin) and as a computin gmodel. They continiue to inspire new algorithmic ideas, especially in the spatial search domain.

5.3 Open Problems and Future Directions

Despite progress, many theoretical challenges in quantum random walks remain open. Key open problems include (1) Implementation on Genral Hardware, (2) Multi-Target and Dynamic Graphs, (3) Mixing, Hitting Times, and Limit Theorems.

For the hardware side, converting QRW algorithms into gate-model circuits is still incomplete. For example, even the basic SKW search algorithm has no known *efficient* general-purpose quantum-circuit implementation; its realization on a universal quantum computer remains an open problem [23]. Progress in compiling or simulating QRWs as circuits is crucial for near-term testing.

On the other hand, handling multiple or moving marked vertices is still not fully solved. Sahu and Sen [30] propose labeling to track moving targets, but extensions to arbitrary dynamics or continuous target distributions are open. Similarly, quantum walks on time-dependent or dynamics graphs, where edges appear or disappear lack a complete theory.

Finally, classical random walks have well-understood mixing times and central-limit behavior. However, quantum random walks do not mix to a stationary distribution, and their long-time limit theorems can be subtle and hard to detect. Proving general analytic results beyond one-dimensional walks is difficult.

In conclusion, quantum random walks remain a fertile area of research. Recent advances have deepened our theoretical understanding and broadened algorithmic applications, but many directions, especially toward practical implementation and complexity classification await further exploration.

6 Conclusion

In this report, we have traced the development of random-walk theory from its classical origins to its quantum generalizations. Section 2 reviewed how classical random walks on $\mathbb{Z}$ and $\mathbb{Z}^d$ obey diffusive scaling ($\sigma \sim \sqrt{N}$), exhibit recurrence properties in low dimensions (Pólya's theorem), and admit a continuous-time Markov-chain description via the graph Laplacian generator (or for simplicity, the transition matrix), M. In Section

3, we introduced the mathematical machinery of quantum machanics, namely Hilbert spaces, unitary operators, and measurements postulates.

Building on this formalism, Section 4 contrasted discrete-time quantum walks (DTQWs), which employ a separate coin and shift unitary operators, with continuous-time quantum walsk (CTQWs), where the graph generator M itself becomes the Hamiltonian in Schrödinger's equation. We emphasized how quantum interference produces ballistic spreading ($\sigma \sim N$) rather than the diffusive law of classical walks.

In Section 5, we surveyed recent theoretical advances and open challenges in both DTQW and CTQW models, focusing on applications in quantum algorithms. Notable developments include: multi-target and ordered-target DTQW search by Sahu & Sen with auxiliary labels; unified frameworks for hitting-time search algorithms integrating MNRS and Szegedy techniques, and DTQW-based universal computation schemes on closed graphs that implement multi-qubit gates and error-detection codes. These studies further accelerate quantum search beyond classical and standard quantum walks.

Despite this progress, several fundamental questions remain open. Perfect state transfer and instantaneous uniform mixing in CTQWs are understood only for highly symmetric graphs, with no general algebraic criteria known. The design of efficient gate-model compilations for QW algorithms (e.g. the SKW search) is still incomplete, limiting near-term experimental tests. Quantum walks on dynamic or time-dependent graphs, as well as robust handling of decoherence and noise, pose both theoretical and practical challenges. Moreover, long-time limit theorems and mixing-time analogues for QWs beyond one dimension lack the full analytic treatment enjoyed by classical counterparts.

Looking forward, addressing these open problems will deepen our understanding of quantum transport and entanglement propagation on complex networks, refine QW-based algorithmic paradigms, and guide the design of future quantum hardware optimized for walk-based computation. As both discrete and continuous quantum walks continue to reveal new connections between spectral graph theory, quantum information, and complexity theory, they remain a vibrant research frontier at the heart of quantum algorithmics and simulation.

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A Derivation of the Heat-Kernel PDE Approximation

The following derivation is provided by [12]. Starting from the discrete master equation for a one-dimensional walk with step-size ℓ and time-step τ,

$$P(x,t) \;=\; p_r\, P(x-\ell,\; t-\tau) \;+\; p_\ell\, P(x+\ell,\; t-\tau), \tag{27}$$

we divide both sides by τ, subtract $P(x,t-\tau)/\tau$, and use $p_r + p_\ell = 1$ to obtain

$$\frac{P(x,t)-P(x,t-\tau)}{\tau} = p_r\,\frac{P(x-\ell,t-\tau)-P(x,t-\tau)}{\tau} + p_\ell\,\frac{P(x+\ell,t-\tau)-P(x,t-\tau)}{\tau}.$$

We set $p_r = \frac{1}{2}+\varepsilon,\; p_\ell = \frac{1}{2}-\varepsilon$ and take $\varepsilon \to 0$ for the unbiased case.

Next, Taylor-expand in both space and time about (x,t):

$$\begin{aligned} P(x,t-\tau) &= P(x,t) - \tau\,\partial_t P(x,t) + O(\tau^2), \\ P(x\pm\ell,t-\tau) &= P(x,t) - \tau\,\partial_t P(x,t) \pm \ell\,\partial_x P(x,t) + \tfrac{\ell^2}{2}\,\partial_x^2 P(x,t) + O(\ell^3,\tau^2,\ell\tau). \end{aligned}$$

Subtracting and dropping higher-order terms gives

$$\frac{P(x,t)-P(x,t-\tau)}{\tau} = \frac{\ell^2}{2\,\tau}\,\partial_x^2 P(x,t) + O\big(\tfrac{\ell^3}{\tau},\tau\big). \tag{34}$$

Taking the joint limit $\ell,\tau \to 0$ with $\alpha = \frac{\ell^2}{2\tau}$ fixed yields the diffusion (heat) equation

$$\frac{\partial P}{\partial t} = \alpha\,\frac{\partial^2 P}{\partial x^2}, \tag{35}$$

which describes the continuous-space, continuous-time limit of the random walk.

A.1 Solution via Fourier Transform

We introduce the spatial Fourier transform

$$\widehat{P}(k,t) = \int_{-\infty}^{\infty} P(x,t)\, e^{-ikx}\, dx.$$

Applying $\mathcal{F}\{\partial_t P\} = \partial_t \widehat{P}$ and $\mathcal{F}\{\partial_x^2 P\} = -k^2\widehat{P}$, equation (35) becomes the ODE

$$\frac{\partial}{\partial t}\widehat{P}(k,t) = -\alpha\,k^2\,\widehat{P}(k,t),$$

with solution

$$\widehat{P}(k,t) = \widehat{P}(k,0)\, e^{-\alpha k^2 t}.$$

The fact that $\widehat{P}(k,t)$ is a product of two functions of k suggests that it may be solvable

using the convolution theorem of Fourier transforms.

Observe that

$$\widehat{P}(k,t) = \widehat{f}(k)\,\widehat{g}(k,t), \quad \text{where} \quad \widehat{g}(k,t) = e^{-\alpha k^2 t}.$$

By the convolution theorem, $\mathcal{F}^{-1}\{\widehat{f}\,\widehat{g}\} = f * g$, we have

$$P(x,t) = \big(f * g(\cdot,t)\big)(x) = \int_{-\infty}^{\infty} f(\xi)\; g(x-\xi,t)\; d\xi.$$

The inverse transform of $\widehat{g}(k,t)$ is the *heat kernel*:

$$g(x,t) = \mathcal{F}^{-1}\big[e^{-\alpha k^2 t}\big] = \frac{1}{\sqrt{4\pi\,\alpha\,t}}\exp\Big(-\frac{x^2}{4\alpha\,t}\Big).$$

Hence the general solution is

$$P(x,t) = \int_{-\infty}^{\infty} f(\xi)\;\frac{1}{\sqrt{4\pi\,\alpha\,t}}\exp\Big(-\frac{(x-\xi)^2}{4\alpha\,t}\Big)\,d\xi.$$

In particular, for the point-source initial condition $f(x) = \delta(x)$, one obtains the fundamental solution

$$P(x,t) = g(x,t) = \frac{1}{\sqrt{4\pi\,\alpha\,t}}\exp\Big(-\frac{x^2}{4\alpha\,t}\Big).$$

B Spectral Decomposition of the Pauli X Operator

Referring back to the Pauli matrix that represents the spin component of angular momentum of a spin $\frac{1}{2}$ particle in the x-direction, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. The eigenvalues are simply $\lambda_{1,2} = \pm 1$. Solving equation 3.8.1 for λ_1 we find that $\sigma_x \begin{pmatrix} a \\ b \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \end{pmatrix}$, and $a = b$ or $a = -b$ for the respective eigenvalues. Normalizing and setting $a = 1$ we obtain the Hadamard state vectors $|+\rangle$ and $|-\rangle$. To construct the projectors we use equation 3.7.2 and define

$$\hat{P}_+ = |+\rangle \langle +| = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$\hat{P}_- = |-\rangle \langle -| = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

thus we see that the completeness relation is satisfied as $\hat{P}_+ + \hat{P}_- = \hat{I}$ and that the projectors are orthogonal as $\hat{P}_+ \hat{P}_- = 0$ and thus the spectral decomposition of σ_1 is given through the spectral theorem (3.8.4)

$$\sigma_1 = \lambda_1 \hat{P}_+ + \lambda_2 \hat{P}_- = \hat{P}_+ - \hat{P}_- \tag{B.0.1}$$