Quantum Random Walk

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Submitted to the
Institute of Graduate Studies and Research
in partial fulfillment of the requirements for the degree of

Master of Science
in
Physics

Eastern Mediterranean University
February 2023
Gazimağusa, North Cyprus

Approval of the Institute of Graduate Studies and Research

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ABSTRACT

We present an in-depth analysis of the "quantum first detection problem," in other words, quantum renewal equation (QRE) [1] and how it relates to the basic postulates of quantum existence in this thesis. It shows how the Schrödinger equation and projective measurement postulate a guide to the solution of the problem and present equations that describe the system's behavior. The text highlights the surprising features of the problem for closed systems and the sensitivity of the problem to the sampling rate. It also notes that the probability of being eventually detected can be less than unity for finite-sized systems.

Keywords: Quantum Renewal Equation, Schrödinger Equation, Quantum Postulates.

ÖZ

Bu tez, kuantum ilk saptama probleminin (kuantum yenileme denklemi) derinlemesine bir analizini ve bunun kuantum gerçekliğinin temel varsayımlarıyla nasıl bir ilişkisi olduğunu sunar. Schrödinger denklemi ve izdüşümsel ölçüm varsayımının sorunun çözümüne nasıl yol açtığını ve sistemin davranışını tanımlayan denklemleri nasıl sunduğunu gösterir. Kapalı sistemler için problemin şaşırtıcı özelliklerini ve problemin ölçüm hızına olan hassasiyetini vurgulamaktadır. Ayrıca, nihai olarak tespit edilme olasılığının, belirli boyutta sistemler için birim sayıdan daha az olabileceğini de not eder.

Anahtar Kelimeler: Kuantum, Kuantum İlk Saptama Problemi, Schrödinger Denklemi.

... Dedicated to

As I get older, I realize being wrong isn't a bad thing like they teach you in school. It is an opportunity to learn something.

Richard Feynman

ACKNOWLEDGMENTS

I would like to express my deepest appreciation to my advisor Asst. Prof. Dr. Mustafa Rıza would not have been possible without his support. I would also like to extend my deepest gratitude to my family and friends that always supported me through the journey. I'm extremely grateful to have such amazing lecturers along the way. They taught me a lot during my masters degree. I am also grateful to everyone raised and supported me every part of my life.

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LIST OF SYMBOLS

$\|\theta\rangle$	First Detection Wavefunction
$\hat{\mathcal{P}}$	Projection Operator
ψ	Wavefunction of a Quantum Walker
τ	Discrete Time Step
χ	First Detection Amplitude
$\langle n \rangle$	Average Number of Measurement Attemps
$\hat{U}$	Unitary Evolution Operator
A	Connectivity Matrix
F	First Detection Probability
H	Hamiltonian
P	Probability
S	Survival Probability
t	Time
x	Any point in given discrete space
X	Discrete Space

LIST OF ABBREVIATIONS

CRW	Classical Random Walk
CTQW	Continuous Time Quantum Walk
DTQW	Discrete Time Quantum Walk
GF	Generating Function
PDF	Probability Density Function
QM	Quantum Mechanics
QRE	Quantum renewal equation
QRW	Quantum Random Walk
QW	Quantum Walk

Chapter 1

INTRODUCTION

In Quantum mechanics, the conduct of consequence and energy at the atomic and sub-atomic statuses are represented. One of its fundamental precepts is that the momentum and position of a quantum particle generally cannot be calculated simultaneously with incidental exactness. This principle, known as the Heisenberg uncertainty principle, puts a fundamental limit on the ability to track the motion of a quantum particle. That being said, quantum computers can be used to measure the state of quantum particles and, in some cases, track their movement probabilistically. Quantum computing can leverage the precepts of quantum mechanics to manipulate and control quantum systems so that the movement of a quantum particle can be tracked to some period. For example, quantum algorithms such as quantum state tomography, quantum process tomography, and error modification can be used to reconstruct the state of a quantum particle and track its evolution over time. Additionally, quantum machine learning techniques can be used to predict the motion of a quantum particle from a set of observations. Developing techniques for tracking the motion of quantum particles is an active area of research, and new methods and techniques will likely be developed as the field of quantum computing continues to advance. In summary, while it is impossible to track a quantum particle's motion with arbitrarily high precision, quantum computers can be used to measure the state of a quantum particle and track its motion in a probabilistic way. A quantum random walk is a quantum algorithm that affects the spontaneous motion of a quantum particle. It is

a divergence of the classical random walk, a mathematical model of a random process where a particle moves in a specific direction with a certain probability at each step. In a quantum random walk, a quantum particle can exist in multiple states simultaneously, known as superposition. The principle of superposition tells us that before an actual measurement is conducted, the system is accepted to be in all allowed states with a certain probability. The wave function collapses to one of its possible states in the measurement. It stays there with a probability of one until a disorder. Due to the quantum nature of the quantum random walk, all possible paths on a graph are present; therefore, with one single step of the calculation, all paths are incorporated. Additionally, if the particles are entangled, the calculation's complexity may also be decreased. Therefore, the computational complexity of the quantum walk may be significantly lower than its classical counterpart. For example, quantum random walk algorithms can solve specific problems in graph theory, such as discovering the quickest route between two nodes of the graph, and investigation difficulties, like Grover's probe algorithm. QWR is a subject of active research, and new developments are being made in the field. For example, new variations of QW algorithms have been proposed, such as continuous-time and open QW. In summary, QRW is a variation of the CRW that impersonates the spontaneous activity of a quantum particle. A most important feature is that the particle can exist in multiple forms simultaneously, known as superposition, and its motion is represented by the time evolution of its probability distribution. This feature allows quantum random walk algorithms to solve specific problems faster than classical algorithms.

The investigation of QW is a vital research zone with many potential applications. In computer science, it is relevant for designing quantum algorithms quicker than their classical partners, particularly in searching, optimization, and machine learning. In

quantum information science, it allows the development of methods for testing the "quantumness" of appearing technologies for creating QC and sporting quantum communication protocols, quantum cryptography, and quantum error modification [3]. In physics and chemistry, it can be used to study the dynamics of quantum systems, such as quantum walks on lattices and quantum walks in continuous space, and to simulate the dynamics of chemical reactions and understand the behavior of quantum systems at the molecular level.

The classical RW, also known as the straightforward RW, is a well-established concept in probability theory and has been successfully used to develop classical algorithms. On the other hand, QW is the quantum mechanical counterpart of classical RW and has emerged as an effective tool for generating QA. They have been conducted to form a ubiquitous example of QC and evolved into a substantial investigation area with many open problems.

The critical properties of QW are strongly influenced by quantum entanglement, an essential model in QM that represents the correlation between two or more quantum systems [3]. That constructs QW as a helpful mechanism for analyzing the effects of quantum entanglement and its possible applications in QC and transmission. Additionally, QW can sport a comprehensive spectrum of physical systems, such as QT in condensed matter physics and the simulation of quantum chemical reactions.

The representation "quantum random walk" was foremost used by R. P. Feynman [4] in a seminal assignment on quantum mechanical computers, where he proposed that it could be defined as a continuous QW. Nevertheless, that was not until 1993, when a report by Aharonov [5] was publicized, that the notion of QW as a particular subject

from CQW was established.

One of the critical studies of Konno [6] suggested solid mathematical relationships between correlated QW and using the PQRS matrix technique. This technique has been used to demonstrate a more profound acquaintance of the connection between classical and QW and investigate QW's potential applications in computer science.

In summary, the concept of QW as a particular subject from CRW was founded in 1993 by Aharonov. Since then, the relations between CRW and QW and the utility of QW in computer science have evolved into new and novel investigation locations. Konno's study on the PQRS matrix method has significantly contributed to this field, delivering a more in-depth knowledge of the connection between classical and QW and investigating the potential applications of QW in computer science.

Two QW samples have been proposed to comprehend the conduct of a QM system that can move from one position to another. The most prominent, known as discrete-time QW, consists of two QM systems, a walker and a coin, and a development operator that can only be applied to both techniques in discrete time steps. The mathematical structure of this model is based on evolution via a unitary operator. In other words, the system's state at time t_2 is given by the unitary operator involved to the state of the system at time t_1.

Another model, called continuous QW, consists of a walker and a system development (Hamiltonian) operator that can be applied without timing limitations, representing that the walker can drive any time. The mathematical form of this example is based on transition via the Schrodinger equation.

Both discrete and continuous QW representatives have been performed on discrete graphs, mostly due to the widespread use of graphs in computer science. The consequence of quantum algorithms established on QW has been a high-priority movement in this field.

Ambainis et al. represented two comprehensive concepts for analyzing QRW[3]. One is the path-integral technique, and the other is the Schrödinger method. Both approaches have benefits, and the preferred approach will depend on the problem being studied.

Discrete-time quantum random walks (DTQRW) are quantum mechanical systems that are used to generalize discrete classical Markov chains in quantum algorithms. They are represented by a sequence of unitary processes, each with a non-zero evolution amplitude exclusively between graph nodes. Their resemblance of DTQRW to classical Markov chains is a powerful reason for further research into this topic. Furthermore, the discrete qualities of DTQRW permit using robust mathematical instruments from discrete mathematics and computer science, making them versatile tools for studying quantum algorithms.

DTQRW has been applied to a comprehensive spectrum of problems, from inventing new quantum algorithms to analyzing the dynamics of quantum systems. For example, they have been used to develop faster and more efficient quantum algorithms for searching, optimization, and machine learning, as well as for modeling quantum communication protocols, quantum cryptography, and quantum error modification.

The study of DTQRW is an active area of research with many open problems and

potential applications [7]. The ability to design and control DTQRW has important implications for developing quantum technologies such as quantum computers, quantum communication networks, and quantum simulators.

Discrete-time QW on a sequence is a robust mechanism for comprehending QMS and their behavior. Spilling the quantum evolution equation into Markovian and interference terms makes it possible to analyze these walks in great detail. This separation illustrates how the coherence of the quantum evolution affects the variance of the quantum walker's position over time.

It has been shown that the quadratic increase in the conflict of the quantum walker's position with time directly results from the quantum evolution's coherence. In discrepancy to CRW, where the development is decoherent, and the conflict increases linearly with time. This consequence highlights the essential disparity between quantum and classical systems and the essence of coherence in quantum systems.

This thesis [8] on discrete-time QW on a line supplies a more in-depth interpretation of the parcels of QMS and their behavior. It also has important implications for developing quantum technologies such as quantum computers, quantum communication networks, and quantum simulators. The capacity to control and manipulate quantum systems' coherence is crucial for designing and implementing these technologies.

The earliest quantum algorithms based on QW have been informed and have demonstrated impressive speedup approximated to their classical counterparts. These algorithms are based on the indication of a particle inhabiting the set of integers. A

CRW on the line illustrates it. In a CRW, at each time step, the particle carries one unit to the left with possibility p or one unit to the right with probability $q = 1 - p$. Various steps' demands are separate from one another.

CRW can be further classified into continuous time and discrete time RW [6][9]. CTRW affect the probability of completing a move per time unit, while discrete time RW interest represents time-steps.

The quantum interpretation of a discrete-time RW on a ring differs from its classical replica in several methods. In the quantum version, the walker described a quantum state, which allows for superposition and entanglement. This means that a quantum walker can exist in multiple locations simultaneously, and its state can be correlated with other quantum systems.

Compared to classical random walks, the CTQW has provided exponential growth in quickness in graph propagation. The ability of the walker to exist in multiple locations simultaneously and the possibility of quantum interference between different paths. This allows the walker to explore a more significant portion of the graph in less time.

The DTQW is also critical in accelerating a quantum algorithm design for spatial searching [2]. Because the walker can exist in multiple locations simultaneously, the quantum interference between different paths can help the walker encounter the target faster than a classical random walk.

Fig. 1.1 A decision tree is a type of algorithm used in machine learning to classify data into different categories. In the context of quantum random walk, it is used to analyze

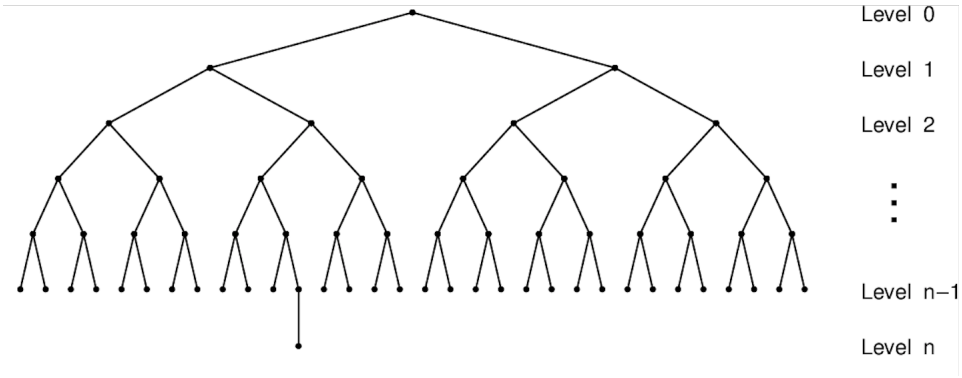

Figure 1.1: This is the decision tree algorithm to show the time steps for a QW [2].

the behavior of a quantum system as it evolves over time.

In a QRW, a quantum particle is placed in a superposition state. Furthermore, it is made to develop according to a unitary operator. At the walk's individual step, proportions are made to determine the particle's position. Finally, the determination tree algorithm is used to analyze the sequence of measurable results and to classify the particle's position into other categories. A decision tree performs by recursively partitioning the data into subsets established on the values of specific components. The algorithm begins with a single node representing the entire dataset and then divides it into smaller subsets founded on the value of a chosen part. Each of these subsets is then split in the same way, creating a tree-like structure with branches describing the various subsets of the data. Each tree leaf node describes a final decision or a data classification. In the context of QRW, the decision tree algorithm can be used to investigate the sequence of measurement results and classify the particle's position into different categories. In addition, the decision tree algorithm can also be used to determine routines in the data and to make predictions about future dimensions established on the sequence of previous dimensions. It is worth noting that the Decision Tree method is a classical machine learning method, and it

does not benefit from the system's quantum nature. Therefore, there are more suitable manners for analyzing a quantum system's behavior, and other methods, such as quantum machine learning algorithms, are more suitable. Suppose a person stood at the beginning of a line, maintaining a coin. They flip the coin, and if it comes up heads, they move to the right; if it comes up tails, they move to the left. They then repeat the procedure, flipping the coin and making movements based on the outcome [10]. After N steps, the probability is $P_N(d)$, of being in position d is

$$P_N(d) = \frac{1}{2^N} \begin{pmatrix} N \\ \frac{d+N}{2} \end{pmatrix}$$

Nd	-4	-3	-2	-1	0	1	2	3	4
0					1				
1				1/2	0	1/2			
2			1/4	0	1/2	0	1/4		
3		1/8	0	3/8	0	3/8	0	1/8	
4	1/16	0	4/16	0	6/16	0	4/16	0	1/16

Consider the quantum version of the walk on a line. The first change we can make is to swap out the coin for a qubit. In this paper, the two levels of the qubit will be represented by the states $|\downarrow\rangle$ and $|\uparrow\rangle$rather than $|0\rangle$ and $|1\rangle$, forming a complete orthonormal set. By application of the Hadamard operator

$$\hat{H} = \frac{1}{\sqrt{2}}(|\uparrow\rangle\langle\uparrow| + |\uparrow\rangle\langle\downarrow| - |\downarrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

on the states $|\uparrow\rangle$ and $|\downarrow\rangle$ gives us the so-called Hadamard states

$$\hat{H}\left|\uparrow\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle\left\langle\uparrow\right| + \left|\uparrow\right\rangle\left\langle\downarrow\right| + \left|\downarrow\right\rangle\left\langle\uparrow\right| - \left|\downarrow\right\rangle\left\langle\downarrow\right|\right)\left|\uparrow\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle - \left|\downarrow\right\rangle\right) = \left|-\right\rangle, \tag{1.1}$$

$$\hat{H}\left|\downarrow\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle\left\langle\uparrow\right| + \left|\uparrow\right\rangle\left\langle\downarrow\right| + \left|\downarrow\right\rangle\left\langle\uparrow\right| - \left|\downarrow\right\rangle\left\langle\downarrow\right|\right)\left|\downarrow\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\right\rangle + \left|\downarrow\right\rangle\right) = \left|+\right\rangle. \tag{1.2}$$

The states $\{\left|+\right\rangle, \left|-\right\rangle\}$ form a complete orthonormal set. [10]

We would get the classical walk described above if we measured the qubit and stepped left or right, relying on the outcome. Rather than someone holding a coin, consider a particle whose movement is limited to one dimension. Now, we consider the particle a quantum system and perform the quantum walk as demonstrated below. We involve the Hadamard operation during each iteration, pursued by the operation that steps right if the qubit is down and left if the qubit is up. So, we employ the operator

$$\hat{U} = e^{i\hat{p}\hat{\sigma}_z}\hat{H}$$

where $\hat{\sigma}_z$ is the Pauli-z operator [10] operating on the qubit and $\hat{p}$ is the momentum operator of the particle confined to one dimension. As a result, the system's state after the N steps is

$$\left|\psi_N\right\rangle = (e^{i\hat{p}\hat{\sigma}_z})^N \left|\psi_0\right\rangle \tag{1.3}$$

Chapter 2

1D QUANTUM WALK

2.1 First Detection Probability

The first detection wave function, also known as the first path wave function, is an essential notion in investigating QRW. It represents the probability amplitude of the system for the first time a quantum walker is detected at a specific location.

The first detection wave function is crucial because it allows us to study the quantum walk's temporal conduct and the QW's effects. For example, it can be used to calculate the probability and expected time of first detection at a specific location, which can be used to understand the sensitivity of the QW to initial conditions and measurement parameters.

Similarly, the first detection wave function can be used to investigate the statistical properties of QRW, such as the probability distribution of the QW's appointment, the position's contention, and the survival probability of the walker in the system. In addition, these quantities can be used to understand the differences between quantum and CRW, such as the emergence of interference patterns, the suppression of diffusive conduct, and the presence of the Zeno effect.

However, it can also be used to study the localization properties of the quantum walker's probability of trapping or the required behavior of the QW. These developments can be used to comprehend the essential difference between quantum

and CRW and the potential application of QRW in quantum computing, quantum communication, and quantum simulation.

2.2 Discrete Time Quantum Walk

The discrete-time QW needs a Hamiltonian for the particle. Then, after applying a development operator, we can make calculations and even measures to find probabilities for detecting the particle in a given space.

The evolution of the state of a particle is described through the time-dependent Schrödinger equation:

$$i\hbar\partial_t |\psi\rangle = H |\psi\rangle$$

with

$$|\psi(t=0)\rangle] |\psi(0\rangle .$$

as the initial condition.

Assuming the resulting eigenstates are elements of the complete set of discrete states

$$X = \{|x\rangle\},$$

where according to the tight-binding approach, only changes to the next neighbors are allowed, i.e. $|x\rangle \to |x+1\rangle$ and $|x\rangle \to |x-1\rangle$.

The time-independent tight-binding Hamiltonian governing the next neighbor approach yields to

$$H = \gamma \sum_{x \in X} |x\rangle \langle x+1| + |x+1\rangle \langle x| .$$

This Hamiltonian describes the motion on a one-dimensional discrete path. In general,

the size of the set X is infinite. Employing periodic boundary conditions,

$$|n\rangle \rightarrow |0\rangle$$

reduces the size of the set to n. In the special case for $n = 6$, which can be arranged in form of a hexagonal ring, the set X reduces to

$$X = \{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle\}.$$

$|\psi(0)\rangle = |x'\rangle$ defines that initially particle is detected at lattice in the state $|x'\rangle$. Measurement on the subset is done after passing the time interval $\Delta\tau = \tau$ at distinct times, i.e. at

$$\tau, \tau + \Delta\tau, ..., \tau + (n-1)\Delta\tau.$$

The first attempt to detect the state of the system is done at the times τ and $\tau + \Delta\tau$[1][11][12] These measurements may have two outcomes, either the detected state $|x\rangle$ is element of the the set of discrete states X or not, i.e.

$$x \in X \text{ or } x \notin X$$

Let us first consider the measurement at $t = \tau$, by approaching from the left, the wave function becomes

$$\lim_{\varepsilon \to 0} |\psi(\tau + \varepsilon)\rangle = \hat{\mathcal{U}}(\tau) |\psi(0)\rangle, \tag{2.1}$$

with $\hat{\mathcal{U}}(t)$ being the wellknown time-evolution operator in Quantum Mechanics.

$$\hat{\mathcal{U}}(t) = \exp\left\{\frac{iHt}{\hbar}\right\}.$$

The time evolution operator [1] plays a prominent role in a QRW. It represents how the state of a quantum system transforms over time according to the Schrödinger equation. The time evolution operator is unitary, meaning that it conserves the state vector's normalization and the wave function's probability understanding. In the case of QRW,

the time evolution operator is used to evolve the system's initial state at time t=0 to the system's state at a later time t. This evolution of the system's Hamiltonian represents the system's energy levels and changes. The time evolution operator can be used to calculate the probability of discovering the QW in a specific position at a given time and the typical values of various observables, such as position and momentum. In addition, the time evolution operator can be used to analyze the temporal behavior of the QW , such as the probability distribution and the variance of the position of the QW. These quantities can be used to understand the contrasts between quantum and classical RW, such as the emergence of interference patterns and the suppression of diffusive behavior in QRW.

Probability to find the particle in subspace X at time τ is

$$P_1 = \lim_{\varepsilon \to 0} \sum_{x \in X} |\langle x|\psi(\tau - \varepsilon)\rangle|^2 \, [1] \tag{2.2}$$

The probability of detecting the particle at the time $t_f = \tau$ is P_1, wheras the probability of not detecting the particle at $t_f = \tau$ is evidently $1 - P_1$. If the particle is not detected, the time-evolution will resume, otherwise it will stop, as the wave function collapses to a state $|x\rangle \in X$. Any trial of detecting the particle at later time will fail, i.e. the probability will be identical to zero, which can be represented by the so-called null state.

A measurement at a later time can be linked as following

$$\lim_{\varepsilon \to 0} |\psi(\tau + \varepsilon)\rangle = \lim_{\varepsilon \to 0} N \left(1 - \sum_{x \in X} |x\rangle \langle x| \right) |\psi(\tau - \varepsilon)\rangle \tag{2.3}$$

The measurement of the particle is conducted using the principle of projective

measurement. For the projective measurement, we need the projection operator.

$$\hat{\mathcal{P}} = \sum_{x \in X} |x\rangle \langle x| .$$

So,

$$\lim_{\varepsilon \to 0} |\psi(\tau+\varepsilon)\rangle = \lim_{\varepsilon \to 0} N(1-\hat{\mathcal{P}}) |\psi(\tau-\varepsilon)\rangle$$

Probability of finding the particle at the second measurement becomes:

$$P_2 = \lim_{\varepsilon \to 0} \sum_{x \in X} \left| \langle x| \hat{\mathcal{U}}(\tau) |\psi(\tau+\varepsilon)\rangle \right|^2$$

$$P_2 = \sum_{x \in X} \left| \langle x| \hat{\mathcal{U}}(\tau) \frac{1}{\sqrt{1-P_1}} (1-\hat{\mathcal{P}}) |\psi(0)\rangle \right|^2$$

Probability of finding the particle at the third measurement:

$$P_3 = \lim_{\varepsilon \to 0} \sum_{x \in X} \left| \langle x| \hat{\mathcal{U}}(\tau) |\psi(2\tau+\varepsilon)\rangle \right|^2$$

$$|\psi(2\tau+\varepsilon)\rangle = \frac{1-\hat{\mathcal{P}}}{\sqrt{1-P_2}} \left|\psi(2\tau^-)\right\rangle = \frac{1-\hat{\mathcal{P}}}{\sqrt{1-P_2}} \hat{\mathcal{U}}(\tau) |\tau+\varepsilon\rangle = \frac{1-\hat{\mathcal{P}}}{\sqrt{1-P_2}}$$

$$P_3 = \sum_{x \in X} \left| \langle x| \hat{\mathcal{U}}(\tau) \frac{1}{\sqrt{(1-P_1)(1-P_2)}} [(1-\hat{\mathcal{P}}) \hat{\mathcal{U}}(\tau)]^2 |\psi(0)\rangle \right|^2$$

Therefore we can measure the probability to find the particle at any given point of state by [11]:

$$P_n = \frac{\sum_{x \in X} \langle x \ \hat{\mathcal{U}}(t)(1 \quad \hat{\mathcal{P}})^n \ ^1 \hat{\mathcal{U}}(t) \ \psi(0)\rangle \Big|^2}{(1 \quad P_1)(1 \quad P_2) \cdots (1 \quad P_n \ _1)} \tag{2.4}$$

First detection wave function can be described as [1]:

$$|\theta_n\rangle = \hat{\mathcal{U}}(t)[(1-\hat{\mathcal{P}})\hat{\mathcal{U}}(t)]^{n-1}|\psi(0)\rangle \tag{2.5}$$

$$|\theta_1\rangle = \hat{\mathcal{U}}(\tau)|\psi(0)\rangle$$

$$|\theta_n\rangle = [(1-\hat{\mathcal{P}})\hat{\mathcal{U}}(t)]^{n-1}|\theta_1\rangle \tag{2.6}$$

$$P_n = \frac{\langle\theta_n|\hat{\mathcal{P}}|\theta_n\rangle}{\prod_{j=1}^{n-1}(1-P_j)} \tag{2.7}$$

First detection on the n^{th} measurement probability is F_n. Detection and not detection are determined by coin tossing concept using a uniform random number generator (discrete time steps). After $t-2\tau$ we toss a coin and if the particle is not detected we calculate P_2 at $t=2\tau$ then we toss a coin again, and if the particle is not detected we calculate P_3.

$$F_n = (1-P_1)(1-P_2)...(1-P_n-1)P_n \tag{2.8}$$

$$F_n = \prod_{j=1}^{n-1}(1-P_j)\frac{\langle\theta_n|\hat{\mathcal{P}}|\theta_n\rangle}{\prod_{j=1}^{n-1}(1-P_j)} \tag{2.9}$$

$$F_n = \langle\theta_n|\hat{\mathcal{P}}|\theta_n\rangle \tag{2.10}$$

$$S_n = 1-\sum_{n=1} F_n$$

is the probability of not detecting the particle after n measurements (survival probability).

2.3 First Detection Amplitude

In this part, the time problem will be solved according to only one detection site (i.e. applying measurement only at one point). Single detection at site 0, labelled $x=0$, then the projection operator is $\hat{\mathcal{P}} = |0\rangle\langle 0|$

Amplitude at first detection

$$\chi_n = \langle 0|\theta_n\rangle, F_n = |\,\chi_n\,|^2$$

$$\chi_1 = \langle 0|\theta_1\rangle = \langle 0|\,\hat{\mathcal{U}}(t)\,|\psi(0)\rangle$$

$$\chi_2 = \langle 0|\theta_2\rangle = \langle 0|\,\hat{\mathcal{U}}(t)(1-\hat{\mathcal{P}})\hat{\mathcal{U}}(t)\,|\psi(0)\rangle$$

$$= \langle 0|\,U(2t)\,|\psi(0)\rangle - \sum_{x\in X}\langle 0|\,\hat{\mathcal{U}}(t)\,|x\rangle\,\langle x|\psi(\tau^-)\rangle$$

$$\vdots = \vdots$$

in this case as $\hat{\mathcal{P}} = |0\rangle\langle 0|$ only

$$\langle x|\psi(\tau^-)\rangle = \langle 0|\,\hat{\mathcal{U}}(t)\,|\psi(0)\rangle = \chi_1 \tag{2.11}$$

$$\chi_2 = \langle 0|\,U(2t)\,|\psi(0)\rangle - \chi_1\,\langle 0|\,\hat{\mathcal{U}}(t)\,|0\rangle \tag{2.12}$$

$$\chi_3 = \langle 0|\theta_3\rangle = \langle 0|\,\hat{\mathcal{U}}(t)[(1-\hat{\mathcal{P}})\hat{\mathcal{U}}(t)]^2\,|\psi(0)\rangle \tag{2.13}$$

$$\vdots = \vdots$$

$$\chi_n = \langle 0|\,U(n\tau)\,|\psi(0)\rangle - \sum_{j=1}^{n-1}\chi_j\,\langle(|\,0)\,\hat{\mathcal{U}}((n-j)\tau)\,|0\rangle \tag{2.14}$$

proof by induction is easily carried out. is the QRE [1]. The quantum first-detection problem, also known as the QRE, is a concept in QM that represents a quantum system's behavior when it is constantly measured. Other than classical systems, which follow a deterministic behavior, quantum systems can exhibit random and probabilistic behavior. QRW represents how the probability of detecting a typical outcome changes over time as more measurements are taken. The equation considers the system's quantum state, the proportions operators, and the time between proportions. The first part of the equation (2.12) is the probability amplitude of the particle being at the origin at time $n\tau$ in the absence of measurement. The second part is the particle's probability amplitude to return to the source in the time interval

$(j\tau, n\tau)$. If we assume that the initial condition is $|\psi(0)\rangle = |0\rangle$ and use the fact that

$$\hat{\mathcal{U}}^n = \hat{\mathcal{U}}(n\tau)$$

$$\hat{\mathcal{U}}(0) = \mathbb{I} \Rightarrow \chi_1 = \langle 0| \hat{\mathcal{U}}(\tau) |0\rangle = 1$$

Now we can calculate the first detection amplitude for any step as follows:

$$\chi_1 = \langle 0| \hat{\mathcal{U}}(\tau) |0\rangle = 1 \tag{2.15}$$

$$\chi_2 = \langle 0| \hat{\mathcal{U}}^2 |0\rangle - \langle 0| \hat{\mathcal{U}}^1 |0\rangle^2 \tag{2.16}$$

$$\vdots \tag{2.17}$$

$$\Rightarrow \chi_n = \sum_{i=1}^{n} \sum_{m_1, m_2, \ldots, m_i} (-1)^{i+1} \langle 0| \hat{\mathcal{U}}^{m_i} |0\rangle \ldots \langle 0| \hat{\mathcal{U}}^{m_i} |0\rangle \tag{2.18}$$

n tuple of positive integers $[m_1, m_2, \ldots, m_i]$ satisfying $m_1 + m_2 + \ldots + m_i = n$

$$n = 5, i = 1 \Rightarrow 5$$

GF is simply the discrete Laplace transform of χ_n [1][13].

$$\hat{\chi}(z) = \sum_{n=1}^{\infty} z^n \chi_n \tag{2.19}$$

$$\hat{\chi}(z) = \sum_{n=1}^{\infty} \langle 0| z^n \hat{\mathcal{U}}^n |\psi(0)\rangle - \sum_{n=0}^{\infty} \sum_{j=1}^{n=1} \chi_j z^j \langle 0| z^{n-j} \hat{\mathcal{U}}^{n-j} |0\rangle \tag{2.20}$$

$$\hat{U}(z) = \sum_{n=1}^{\infty} z^n \hat{\mathcal{U}}^n = \sum_{n=1}^{\infty} e^{\frac{-iHn\tau}{\hbar}} z^n = \frac{1}{1 - ze^{\frac{-iH\tau}{\hbar}}} - 1 \tag{2.21}$$

$$\frac{1}{1 - ze^{\frac{-iH\tau}{\hbar}}} - 1 = \frac{1 - 1 + ze^{\frac{-iH\tau}{\hbar}}}{1 - ze^{\frac{-iH\tau}{\hbar}}} = \frac{ze^{\frac{-iH\tau}{\hbar}}}{1 - ze^{\frac{-iH\tau}{\hbar}}}$$

$$|\theta_n\rangle = (\hat{\mathcal{U}}(\tau)(1 - \hat{\mathcal{P}})^{n-1} \hat{\mathcal{U}}(\tau) |\psi(0)\rangle \tag{2.22}$$

If we combine the GF of χ_n and the first detection wave function we can get GF for the first detection wave amplitude which is going to allow us to include Hamiltonian of the particle in the measurement.

$$|\theta_n\rangle = \hat{\mathcal{U}}(n\tau)\,|\psi(0)\rangle - \sum_{k=1}^{n-1} \hat{\mathcal{U}}^{n-k}\hat{\mathcal{P}}\,|\theta_k\rangle \tag{2.23}$$

$$|\theta_{n+1}\rangle = \hat{\mathcal{U}}(\tau)(1-\hat{\mathcal{P}})\,|\theta_n\rangle = \hat{\mathcal{U}}((n+1)\tau)\,|\psi(0)\rangle - \sum_{k=1}^{n-1} \hat{\mathcal{U}}^{n-k+1}\hat{\mathcal{P}}\,|\theta_k\rangle \tag{2.24}$$

$$|\theta(z)\rangle = \sum_{n=1}^{\infty} z^n\,|\theta_n\rangle = \sum_{n=1}^{\infty} z^n[\hat{\mathcal{U}}^n(\tau)\,|\psi(0)\rangle - \sum_{k=1}^{n-1} \hat{\mathcal{U}}^{n-k}\hat{\mathcal{P}}\,|\theta_k\rangle] \tag{2.25}$$

$$|\theta(z)\rangle = \hat{U}(z)\,|\psi(0)\rangle - \sum_{n=1}^{\infty}\sum_{k=1}^{n-1} z^n\,\hat{\mathcal{U}}^{n-k}(\hat{\mathcal{U}}(1-\hat{\mathcal{P}}))^{k-1}\,\hat{\mathcal{U}}\,|\psi(0)\rangle \tag{2.26}$$

It is not easy to figure out a way to measure on an infinite line mathematically. Therefore we created an infinite environment by putting the particle on a closed ring with discrete steps. In order to have measurements on the ring we need to focus on the following.

Relationships between $\chi(z)$ *and* $\chi_n, S_\infty, and, \langle n\rangle$

$$\chi_n = \frac{1}{(n!)}\frac{d^n}{dz^n}\hat{\chi}(z)|_{z=0} \quad \text{or} \quad \chi_n = \frac{1}{2\pi i}\oint_C \hat{\chi}(z)z^{-n-1}dz \tag{2.27}$$

where C is anticlockwise path including origin and also the radius of $\hat{\chi}(z)$. We can also relate the measurement probability to the $\hat{\chi}(z)$ by

$$1 - S_\infty = \sum_{n=1}^{\infty} F_n = \sum_{n=1}^{\infty} |\chi_n|^2 \tag{2.28}$$

$$= \frac{1}{2\pi}\int_0^{2\pi} |\hat{\chi}(e^{i\theta})|^2 d\theta \tag{2.29}$$

Similarly,
$$\langle n\rangle = \sum_{n=1}^{\infty} F_n = \frac{1}{2\pi}\int_0^{2\pi} [\hat{\chi}(e^{i\theta})]^*(-i)\hat{\chi}(e^{i\theta})d\theta \tag{2.30}$$

[14] This is the main equation we are going to use for probability calculation of the measurements.

2.4 Hexagonal Ring Model

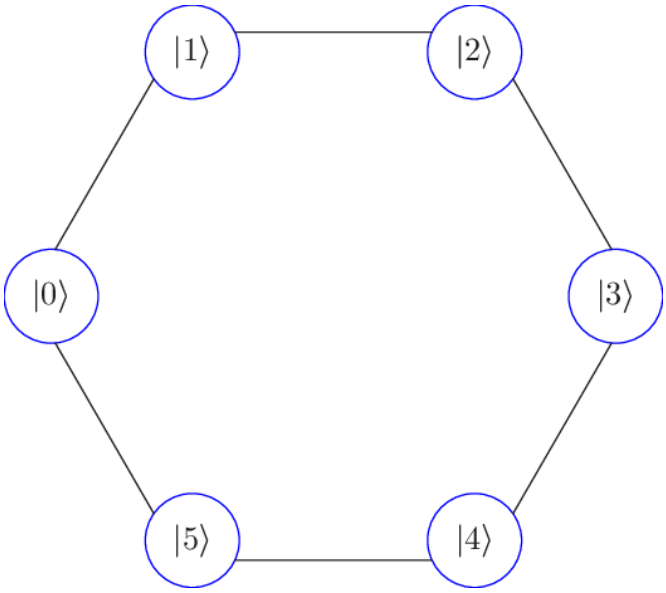

Figure 2.1: Hexagonal Ring for QW model Ref. [1]

This is the model of a hexagonal (benzene) ring. We perform measurements on site labelled $|0\rangle$, which we assume initial position, with variety of initial conditions depending on the Hamiltonian.

First Detection $(1, e^{i\theta_k}, e^{i2\theta_k}, e^{i3\theta_k}, e^{i4\theta_k}, e^{i5\theta_k})/\sqrt{6})^T$ with

$$\theta_k = \frac{\pi}{3}k$$

Hence, the coefficients $|C_k|^2 = |\langle E_k|0\rangle|^2 = 1/6$, reflects the hexagonal structure of the problem [1].

When $\tau \to 0 \exp\{-iH\tau\} = 1$ and we can simplify evolution operator to $\hat{\mathcal{U}}(z) = z/(1-z)$ using

$$\lim_{\tau\to 0} \chi(z) = z\langle 0|\psi(0)\rangle$$

This equation allows us to find the probability amplitude of finding the particle at the origin initially, i.e. at $t = 0$.

Using 2.21 to find a time-independent Hamiltonian

$$\langle E_m | \hat{\mathcal{U}}(z) | E_i \rangle = [z^{-1} \exp\{iE_m\tau\} - 1]^{-1} \delta_{mj}$$

the evolution operator is diagonal in the energy representation. $|E_i\rangle$ is a stationary eigenstate of the Hamiltonian H for the eigenenergy E_i. Expanding $|0\rangle = \sum_k C_k |E_k\rangle$ where $C_k = \langle E_k|0\rangle$. Including the Hamiltonian in the GF (see chapter 4) can be done by replacing the time evolution operator $\hat{\mathcal{U}}(t)$ in the GF with the time-dependent Schrödinger equation, which describes the time evolution of the system under the Hamiltonian.

Chapter 3

MATRIX APPROACH

Two different techniques can guide us to the last result, which is the average probability of detection. The first one is the matrix approach. The transition of the matrix will analyze the probability of the detection. One state to another by providing initial conditions. First of we need to set a matric for a network.

Connectivity Matrix for a Network of N nodes [15]

$$A_{kj} = \begin{cases} f_j & \text{for } k = j \\ -1 & \text{if } k \text{ and } j \text{ are connected and } A_{kj} = A_{jk} \\ 0 & \text{else} \end{cases}$$

f_j is the number of nodes eminating from node j

Properties of A:

1. A is real and symmetric
2. All eigenvalues of A are real and $\gamma_n > 0$
3. A has a single smallest eigenvalue

For a ring network of N nodes

$$A = \begin{pmatrix} 2 & -1 & 0 & ... & -1 \\ -1 & 2 & -1 & ... & . \\ 0 & . & . & . & . \\ . & . & . & . & 0 \\ . & . & . & . & -1 \\ -1 & ... & 0 & -1 & 2 \end{pmatrix}$$

Specifically for $N = 6$, $A = 6 * 6$ matrix

$$A = \begin{pmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & 0 & -1 & 2 \end{pmatrix}$$

in Dirac Notation: $$A = \sum_{l-1}^{N} 2\left|l\right\rangle\left\langle l\right| - \left|l-1\right\rangle\left\langle l\right| - \left|l+1\right\rangle\left\langle l\right|$$

Transition probability from $j \to k$ is $p_{kj}(t)$ Initial condition $\langle k|j\rangle = p_{kj}(0) + \varepsilon T_{kj} = \delta_{kj} + \varepsilon T_{kj}$ where $T_{kj} = \left\langle k\right| T \left|j\right\rangle$ transfer matrix

Markovian process holds (assumption)

$$\frac{d}{dt} P_{kj}(t) = \sum_{l} T_{kl} P_{kj}(t)$$

If all bonds are equal $\gamma = \gamma_{kj}$ $$T = -\gamma A$$

The formal solution of (χ) is $$P_{kj}(t) = \langle k| e^{-\gamma A t} |j\rangle$$

with $\{|q_n\rangle\}$ being the eigenstates of A

A can be diagonalised $$A = \sum_n |q_n\rangle e^{-\gamma t \lambda_n} \mathbb{I} \langle q_n|$$

$$P_{kj}(t) = \sum_n e^{-\gamma t \lambda_n} \langle k|q_n\rangle \langle q_n|j\rangle$$

Eigenvalues for Benzene ring [15]:

$\lambda_1 = 4, \lambda_2 = 3, \lambda_3 = 3, \lambda_4 = 1, \lambda_5 = 1, \lambda_6 = 0$

$$\vec{v}_1 = \begin{pmatrix} -1 \\ 1 \\ -1 \\ 1 \\ -1 \\ 1 \end{pmatrix}, \vec{v}_2 = \begin{pmatrix} -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \end{pmatrix}, \vec{v}_3 = \begin{pmatrix} -1 \\ 1 \\ 0 \\ -1 \\ 1 \\ 0 \end{pmatrix}, \vec{v}_4 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ -1 \\ 0 \\ 1 \end{pmatrix}, \vec{v}_5 = \begin{pmatrix} -1 \\ -1 \\ 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \vec{v}_6 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$$

$P_{kj}(t) \to 0$ as $\lambda_n > 0$ except one $\lambda = 0$

Only the eigenvector $|q_1\rangle = \frac{1}{N} \sum_l |l\rangle$ survives [15]

Ground state dominance: in quantum mechanics the nodes span a Hilbert space $\{|j\rangle\}$ is an orthonormal complete set where $\langle k|j\rangle = \delta_{kj}$, $\sum_j |j\rangle \langle j| = \mathbb{I}$ [15]

Dynamics is governed by a Hamiltonian

$$\frac{d}{dt}\alpha_{kj}(t) = -i\sum_l H_{kl}\alpha_{lj}(t), \text{ with } \alpha_{kj}(t) = \langle k| e^{-iHt} |j\rangle$$

Transition Probability

$$\Pi_{kj}(t) = |\alpha_{kj}(t)|^2$$

$p_{kj}(t)$ represents transition probability $\alpha_{kj}(t)$ represents transition probability amplitude

$$H = -T$$

This allows us to compare classical transport with Quantum mechanical transport on the same network topology $H = \gamma A$ Eigenvalues of H are E_n, and eigenstates are $|\psi_n\rangle$

$$\Pi_{kj}(t) = \left|\sum_n e^{-iE_n t} \langle k|\psi_n\rangle \langle \psi_n|j\rangle\right|^2$$

long time average

$$\begin{aligned}
\chi_{kj} &= \lim_{T\to\infty} \frac{1}{T}\int_0^T dt \pi_{kj}(t) \\
&= \lim_{T\to\infty} \frac{1}{T}\int_0^T dt \sum_n e^{-iE_n t} \langle k|\psi_n\rangle \langle \psi_n|j\rangle \sum_m e^{iE_m t} \langle \psi_n|k\rangle \langle j|\psi_m\rangle \\
&= \lim_{T\to\infty} \frac{1}{T}\sum_{n,m} \frac{e^{(E_n-E_m)t}}{i(E_n-E_m)}\Bigg|_0^T \langle k|\psi_n\rangle \langle \psi_n|j\rangle \langle \psi_m|k\rangle \langle j|\psi_m\rangle \\
&= \sum_{n,m} \lim_{T\to\infty} \frac{e^{(E_n-E_m)T}-1}{i(E_n-E_m)T} \langle k|\psi_n\rangle \langle \psi_n|j\rangle \langle \psi_m|k\rangle \langle j|\psi_m\rangle \\
\chi_{kj} &= \sum_{n,m} \delta_{E_n,E_m} \langle k|\psi_n\rangle \langle \psi_n|j\rangle \langle \psi_m|k\rangle \langle j|\psi_m\rangle \qquad (3.1)
\end{aligned}$$

For a Discrete Ring we need to find the Bloch States

Ring of N nodes $\rightarrow |N+1\rangle = |1\rangle$

Bloch States

$$|\psi_0\rangle = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\theta j} |j\rangle$$

$$H|\psi_0\rangle = \gamma \sum_{l=1}^{N} (2|l\rangle\langle l|j\rangle - |l-1\rangle\langle l|j\rangle - |l+1\rangle\langle l|j\rangle) \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\theta j} |j\rangle$$

$$\begin{aligned}
H|\psi_0\rangle &= \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} (2|l\rangle\langle l|j\rangle - |l-1\rangle\langle l|j\rangle - |l+1\rangle\langle l|j\rangle) \\
&= \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} (2|l\rangle - |l-1\rangle\delta_{lj} - |l+1\rangle\delta_{lj}) \\
&= \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} (2|j\rangle - |j-1\rangle - |j+1\rangle) \\
&= \gamma(2 - (e^{i\theta} + e^{-i\theta})) \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} |j\rangle \\
&= \gamma(2 - 2\cos\theta) \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} |j\rangle
\end{aligned}$$

$$|j\rangle = \frac{\gamma}{\sqrt{N}} \sum_{l=1}^{N} \sum_{j=n}^{N} e^{ij\theta} |\psi_0\rangle$$

$$\alpha_{kj}(t) = \frac{1}{N} \sum_{\theta,\theta'} \langle\psi_\theta| e^{-ik\theta} e^{-iHt} e^{ij\theta} |\psi_\theta\rangle$$

$$= \frac{1}{N} \sum_{\theta} e^{itE_\theta} e^{-i\theta(k-j)}$$

periodic boundary condition $\theta_n = 2\pi n/N$

$$\alpha_{jk}(t) = \frac{e^{-2it}}{N} \sum_{n} e^{i2t\cos 2\pi n/N} e^{-i2\pi n(k-j)/N} \tag{3.2}$$

$$P_{jk}(t) = \alpha^*_{jk}(t)\alpha_{jk}(t)$$

$$= \frac{e^{2it}}{N}\sum_n e^{-2it\cos 2\pi n/N} e^{i2\pi n(k-j)/N} * \frac{e^{2it}}{N}\sum_m e^{-2it\cos 2\pi m/N} e^{i2\pi m(k-j)/N}$$

$$P_{jk} = \frac{1}{N^2}\sum_{n,m} \exp\left\{2it\left(\cos\frac{2\pi m}{N} - \cos\frac{2\pi n}{N}\right)\right\} \exp\left\{i\frac{2\pi}{N}(k-j)(n-m)\right\}$$

Chapter 4

TIME EVOLUTION OF HAMILTONIAN

4.1 Next Neighbour Model

We will investigate the sum of all positions that quantum walker can be measured. So, we need to calculate the Hamiltonian and the time evolution.

$$e^{-x} = \sum_{n=0}^{\infty} \frac{(-x)^n}{n!}$$

Hamiltonian of the walker is given as:

$$H = \gamma(|x\rangle \langle x+1| + |x+1\rangle \langle x|) \text{ [15]}$$

$$H^2 = \gamma^2 (|x\rangle \langle x+1| + |x+1\rangle \langle x|)(|x\rangle \langle x+1| + |x+1\rangle \langle x|)$$

$$= \gamma^2 |x\rangle \langle x+1|x\rangle + |x\rangle \langle x+1|x+1\rangle \langle x| + |x+1\rangle \langle x|x\rangle \langle x+1| + |x+1\rangle \langle x|x+1\rangle \langle x|$$

$$= \gamma^2 (|x\rangle \langle x| + |x+1\rangle \langle x+1|)$$

$$H^3 = \gamma^3 (|x\rangle \langle x+1| + |x+1\rangle \langle x|)$$

$$H^3 = \gamma^2 H$$

since $H = \gamma(|x\rangle \langle x+1| + |x+1\rangle \langle x|)$

$$H^{2n} = \gamma^{2n} (|x\rangle \langle x| + |x+1\rangle \langle x+1|)$$

$$H^{2n+1} = \gamma^{2n+1} (|x\rangle \langle x+1| + |x+1\rangle \langle x|) = \gamma^{2n} H$$

Therefore, time evolution can be shown as:

$$e^{-iH\tau/\hbar} = \sum_{n=0}^{\infty} \frac{iH\tau/\hbar^4}{h!}[15]$$

$$= \sum_{n=0}^{\infty} \left(|x\rangle\langle x| + |x+1\rangle\langle x+1|\right) \frac{-i\tau/\hbar^{2n}}{(2n)!} + iH\frac{-\tau/\hbar^{2n+1}}{(2n+1)!}$$

$$= |x\rangle\langle x| + |x+1\rangle\langle x+1| \left(\cos\left(\frac{\tau\gamma}{\hbar}\right) + \frac{1}{\gamma} iH \sin\left(\frac{\tau\gamma}{\hbar}\right)\right)$$

4.2 New Time Evolution Model: Next Neighbour and Preserving Position

This time Hamiltonian is changed into

$$H = \gamma(|x\rangle\langle x+1|x\rangle\langle x| + |x+1\rangle\langle x| + |x+1\rangle\langle x+1|),$$

meaning the walker now has an option stay at the same site after one time step τ.

$$H^2 = \gamma H$$
$$H^3 = \gamma^2 H$$
$$H^n = \gamma^{n-1} H$$

$$e^{-iH\tau/\hbar} = \sum_{n=0}^{\infty} \frac{-iH\tau/\hbar^n}{n!} = \sum_{n=0}^{\infty} \frac{-i\tau/\hbar^n}{n!}\gamma^{n-1}H$$
$$= \frac{H}{\gamma}\sum_{n=0}^{\infty} \frac{-i\gamma\tau/\hbar^n}{n!}$$
$$= \frac{H}{\gamma}e^{-i\gamma\tau/\hbar} = \frac{H}{\gamma}\left(\cos\gamma\tau/\hbar - i\frac{H}{\gamma}\sin\gamma\tau/\hbar\right)$$

Chapter 5

GENERATING FUNCTION APPROACH

5.1 First Detected Passage Time Problem

This chapter is the second approach, in which we are going to consider the GF and use it together with the survival probability in order to be able to integrate over a ring. That will help us calculate the average number of detection attempts performed on a single site. After that, it will be approximated to some specific detection time values to analyze the behavior of the particle on a ring system.

The GFs [1] are a robust mathematical tool used in various fields, including probability theory, combinatorics, and physics. In the context of QRW, GFs are used to study the walk's statistical properties and simplify the system's investigation.

The GF of a QRW is a complex-valued function that encodes the probability amplitudes of the walker being in different positions at different times. By investigating the effects of the GF, it is possible to understand the behavior of the QW over time, such as the probability distribution, the variance of the position, and the survival probability.

$$\hat{\chi}(z) = \sum_{n=1}^{\infty} \langle 0| z^n \hat{\mathcal{U}}^n |\psi(0)\rangle - \sum_{n=1}^{\infty} \sum_{j=1}^{n-1} \chi_j z^j \langle 0| z^{n-j} \hat{\mathcal{U}}^{n-j} |0\rangle \tag{5.1}$$

$$\hat{\chi}(z) = \frac{\langle 0| \hat{U}(z) |\psi(0)\rangle}{1 + \langle 0| z^n \hat{U}(z) |0\rangle} \tag{5.2}$$

$$\sum_{n=1}^{\infty} \langle 0| z^n \hat{\mathcal{U}}^n |\psi(0)\rangle = \langle 0| \sum_{n=1}^{\infty} z^n \hat{\mathcal{U}}^n |\psi(0)\rangle = \langle 0| \hat{U}(z) |\psi(0)\rangle \tag{5.3}$$

$$\hat{\chi}(z) = \sum_{n=1}^{\infty} \chi_n z^n \tag{5.4}$$

$$\chi_n = \langle 0| U(n\tau) |\psi(0)\rangle - \sum_{j=1}^{n-1} \chi_j \langle (|\,0) U[(n-j)\tau] |0\rangle \tag{5.5}$$

$$\hat{U}(z) = \sum_{n=1}^{\infty} z^n \hat{\mathcal{U}}^n \tag{5.6}$$

[16]

$$\hat{\chi}(z) = \langle 0| z^n \hat{\mathcal{U}}^n |\psi(0)\rangle - \sum_{n=1}^{\infty} \sum_{j=1}^{n-1} \chi_j z^n \langle 0| \hat{\mathcal{U}}^{n-j} |0\rangle$$

$$\hat{\chi}(z) + \langle 0| \hat{U}(z) |0\rangle \hat{\chi}(z) = \langle 0| \hat{U}(z) |\psi(0)\rangle$$

$$\hat{\chi}(z) = \frac{\langle 0| \hat{U}(z) |\psi(0)\rangle}{1 + \langle 0| \hat{U}(z) |0\rangle} \tag{5.7}$$

[1]

Using GFs is that they allow to convert a problem involving a sequence of probability amplitudes into an algebraic problem involving polynomials. This simplifies the calculation of the statistical properties of the walk.

$$\sum_{n=1}^{\infty} \sum_{j=1}^{n-1} \chi_j z^j \langle 0| z^{n\ \ j} \hat{\mathcal{U}}^{n\ \ j} 0\rangle$$

$$n=2 \qquad \chi_1 z \langle 0| zU |0\rangle$$

$$n=3 \qquad \chi_1 z \langle 0| z^2 \hat{\mathcal{U}}^2 |0\rangle + \chi_2 z^2 \langle 0| zU |0\rangle$$

$$n=4 \qquad \chi_1 z \langle 0| z^3 \hat{\mathcal{U}}^3 |0\rangle + \chi_2 z^2 \langle 0| zU |0\rangle + \chi_3 z^3 \langle 0| zU |0\rangle$$

$$\sum_{n=1}^{\infty} \chi_1 z \langle 0| z^n \hat{\mathcal{U}}^n |0\rangle + \sum_{n=1}^{\infty} \chi_2 z^2 \langle 0| z^n \hat{\mathcal{U}}^n |0\rangle + ... + \hat{\chi}(z) \langle 0| \hat{U}(z) |0\rangle$$

$$\chi_n = \frac{1}{n!} \frac{d^n}{dz^n} \hat{\chi}(z) \tag{5.8}$$

$$\chi_n = \frac{1}{2\pi i} \oint_C \hat{\chi}(z) z^{-n-1} dz \tag{5.9}$$

By studying the large-n limit of the GF, it is possible to understand the behavior of the walk in the long-time limit, such as the emergence of interference patterns.

Adding the Hamiltonian in the GF allows analyzing how the Hamiltonian affects the statistical properties of the walker, such as the probability distribution, the variance of the position, and the survival probability. It can also be used to investigate the effects of the energy levels and transitions on the walker's behavior, such as the emergence of interference patterns, the suppression of diffusive behavior, and the presence of the Zeno effect [1] .

$$1 - S_\infty = \sum_{n=1}^{\infty} F_n = \sum_{n=1}^{\infty} |\chi_N|^2 = \sum_{n=1}^{\infty} \left| \frac{1}{2\pi i} \oint_C \hat{\chi}(z) z^{-n-1} dz \right|^2$$

$r = 1$ circle $\rightarrow C \rightarrow re^{i\theta} = e^{i\theta} \qquad dz \rightarrow d\theta$

$$\begin{aligned} 1 - S_\infty &= \sum_{n=1}^{\infty} \left(\frac{1}{2\pi} \int_0^{2\pi} \hat{\chi}(z) e^{i\theta} d\theta \right) \left(\frac{1}{2\pi} \int_0^{2\pi} \hat{\chi}(z) e^{i\theta} d\theta \right) \\ &= \frac{1}{2\pi} \int_0^{2\pi} \sum_{n=1}^{\infty} \chi_k e^{ik\theta} \left(\sum_{l=1}^{\infty} \chi_l e^{ikl} \right)^* d\theta \\ &= \frac{1}{2\pi} \int_0^{2\pi} \left| \hat{\chi}(e^{i\theta}) \right|^2 d\theta \end{aligned}$$

$$\hat{\chi}(z) = z^4 H(\frac{1}{z})/H(z)$$

It should be noted that this analysis is based on the Hamiltonian is the time-independent and coherent of the system is long enough to keep the Hamiltonian's effects.

$$H(z) = z^3(2\cos\gamma\tau + \cos 2\gamma\tau) - z^2(3 + 6\cos\gamma\tau\cos 2\gamma\tau) + z(4\cos\gamma\tau + 5\cos 2\gamma\tau) - 3$$

$$\hat{\chi}(e^- i\theta)\chi(e^- i\theta) = 1 \tag{5.10}$$

$$H(z) = az^3 + bz^2 + cz + d \tag{5.11}$$

$$\chi_n = \frac{1}{2\pi i}\oint \chi(z) z^{-n-1} dz \tag{5.12}$$

$$\gamma(\theta) - 1 - e^{i\theta}, \gamma'(\theta) = ie^{i\theta} \tag{5.13}$$

$$\chi_n = \frac{1}{2\pi i}\int_0^{2\pi} \chi(e^i\theta) e^{-(n+1)i\theta} ie^{i\theta} d\theta \tag{5.14}$$

$$= \frac{1}{2\pi i}\int_0^{2\pi} \chi(e^i\theta) e^{-in\theta} d\theta \tag{5.15}$$

$$= \frac{1}{2\pi i}\int_0^{2\pi} \frac{e^{4i\theta}\left(ae^{-3i\theta} + be^{-2i\theta} + ce^{i\theta} + d\right)}{ae^{3i\theta} + be^{2i\theta} + ce^{i\theta} + d} e^{-ni\theta} d\theta \tag{5.16}$$

$$\tag{5.17}$$

The average number of detections $\langle n \rangle$ in a QRW can be calculated using the survival probability and the GF [1]. The survival probability is that the QW has not been detected at a specific location after a specific number of steps.

One method to calculate the average number of detections is to use the following connection [1]:

$$\langle n\rangle = \sum_{n=1}^{\infty} nF_n = \frac{1}{2\pi}\int_0^{2\pi}\Big(\chi(e^{i\theta})\Big)^*\left(-i\frac{\partial}{\partial\theta}\chi(e^{i\theta})\right)d\theta \tag{5.18}$$

$$\langle n\rangle = \frac{1}{2\pi}\int_0^{2\pi}\frac{e^{-i4\theta}H(e^{i\theta})H(e^{-i\theta})}{H(e^{-i\theta})}\frac{\partial}{\partial\theta}\frac{e^{4i\theta}H(e^{-i\theta})}{H(e^{i\theta})}d\theta \tag{5.19}$$

$$= \frac{1}{2\pi}4i\int_0^{2\pi}\left(1+\frac{H(e^{i\theta})}{H(e^{-i\theta})}\frac{\partial}{\partial\theta}\frac{H(e^{-i\theta})}{H(e^{i\theta})}\right) \tag{5.20}$$

$$= 4+\frac{1}{2\pi}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln\frac{H(e^{-i\theta})}{H(e^{i\theta})}d\theta \tag{5.21}$$

$$= 4+\frac{1}{2\pi}\int_0^{2\pi}\frac{\partial}{\partial\theta}\Big(\ln H(e^{-i\theta})-\ln H(e^{i\theta})\Big)d\theta \tag{5.22}$$

$$= 4-\frac{1}{\pi i}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln\Big(H(e^{i\theta})\Big)d\theta \tag{5.23}$$

$$H(z) = a(z-z_1)(z-z_2)(z-z_3) = a\prod_{j=1}^{3}(z-z_j) \tag{5.24}$$

$$\ln H(z) = \sum_{j=1}^{3}\ln(z-z_j)+\ln a \tag{5.25}$$

$$= 4-\frac{1}{\pi i}\sum_{j=1}^{3}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln\Big(e^{i\theta}-z_j\Big)d\theta \tag{5.26}$$

$$= 4-\frac{1}{\pi i}\sum_{j=1}^{3}\ln\Big(e^{i\theta}-z_j\Big)\Big|_0^{2\pi} \tag{5.27}$$

$$\gamma\tau = \pi/2 \tag{5.28}$$

$$H(z) = (2\cos(\pi/2)+\cos\pi)z^3-(3+6\cos(\pi/2)\cos\pi)z^2+(4\cos(\pi/2)+5\cos\pi)z-3 \tag{5.29}$$

$$= -2z^3-3z^2-5z-3 \tag{5.30}$$

$$= a(z+1)(z+1+i\sqrt{2})(z+1-i\sqrt{2}) \tag{5.31}$$

$Z_1 = -1$, $Z_2 = -1-i\sqrt{2}$, $Z_3 = 1+i\sqrt{2}$

Combining $H(z)$ and $\langle n\rangle$

$$\langle n\rangle = 4-\frac{1}{i\pi}\left(\ln\Big(e^{i\theta}+e^{2\pi i}\Big)+\ln\left(e^{i\theta}+2(\frac{1}{2}+\frac{1}{\sqrt{2}}i)\right)\right)$$

Here it should be noted that besides the exceptional sampling times $\langle n\rangle$ should be equal to 4. Using equation (4.24) we can show that

$$\langle n\rangle = 4 - \frac{1}{i\pi}\sum_{j=1}^{3}\int_0^{2\pi}\frac{\partial}{\partial\theta}\ln\left(e^{i\theta}-z_j\right)d\theta$$

writing simply

$$\langle n\rangle = 4 - 2\alpha - \beta$$

where $\alpha(or\beta)$ is number of zeros on the unit circle of $H(z)$ for z. For exceptional sampling times we find $\alpha > 0$,

$$\alpha = \begin{cases} 1, & \gamma\tau = \frac{1}{2}\pi + k\pi \\ 2, & \gamma\tau = \frac{2}{3}\pi + 2k\pi, \pi + 2k\pi, \gamma\tau = \frac{4}{3}\pi + 2k\pi \\ 3, & \gamma\tau = 2k\pi \\ 0, & \text{otherwise.} \end{cases}$$

In order to estimate the average number of detection attempts, one can first calculate the GF, then calculate the probability of detection at each site and sum these probabilities over all sites. The calculation depends on the assumption that GF has been calculated for a large enough number of steps and that the initial state of the walker is normalized.

$$\chi(z) = \frac{f(z)}{1+f(z)}$$
$$\chi^{'}(z) = \frac{f^{'}(z)(1+f(z)) - f(z)f^{'}(z)}{(1+f(z))^2} = \frac{f^{'}(z)}{(1+f(z))^2}$$
$$f(z) = \frac{1}{3}\left(Re\left(\frac{1}{\frac{e^{2i\gamma\tau}}{z}-1}\right) + 2Re\left(\frac{1}{\frac{e^{i\gamma\tau}}{z}-1}\right)\right)$$

Then the function needs to be simplified in order to obtain an equation that can easily

be integrated over and over again (for example 1000 times) to get the average number of detections.

let $x = \gamma\tau$

$$\begin{aligned} f(z) &= \frac{1}{3} Re\left[\frac{z}{e^{2ix}-z} + \frac{2z}{e^{i}x-z}\right] \\ &= \frac{1}{3} Re\left[\frac{z(e^{-2ix}-z)}{(e^{2ix}-z)(e^{-2ix}-z)} + \frac{2z(e^{-ix}-z)}{(e^{i}x-z)(e^{-ix}-z)}\right] \\ &= \frac{1}{3} Re\left[\frac{z(\cos 2x - i\sin 2x - z)}{1-z(e^{2ix}+e^{-}2ix)+z^2} + \frac{2z(\cos x - i\sin x - z)}{1-z(e^{ix}+e^{-ix})+z^2}\right] \\ &= \frac{1}{3}\left[\frac{z(\cos x - z)}{1-2z\cos 2x+z^2} + \frac{2z(\cos x - z)}{1-2z\cos x+z^2}\right] \end{aligned}$$

Introducing a new function $g(\lambda, z) = \dfrac{z(\cos\lambda x - z)}{1-2z\cos\lambda x+z^2}$

Now we obtain $f(z) = \dfrac{1}{3}(g(2,z) + 2g(1,z))$

$$\begin{aligned} g(\lambda,z)' &= \frac{(\cos\lambda x - 2z)(1-2z\cos\lambda x+z^2) - z(\cos\lambda x - z)(-2\cos\lambda x + 2z)}{(1-2z\cos\lambda x+z^2)2} \\ &= \frac{(\cos\lambda x - 2z)(1-2z\cos\lambda x+z^2) + 2z(\cos\lambda x - z)^2}{(1-z\cos\lambda x+z^2)^2} \\ g(\lambda,z) &= \frac{z(\cos\lambda x - z)}{\sin^2\lambda x + (\cos\lambda x - z)^2} = \frac{z\chi(z)}{\sin^2\lambda x + \chi(z)^2} \\ g(\lambda,z)' &= \frac{(\chi(z) + z\chi'(z))(\sin^2\lambda x + \chi(z)^2) - z\chi(z)2\chi(z)\chi'(z)}{(\sin^2\lambda x + \chi(z)^2)^2} \\ &= \chi(z)\sin^2\lambda x + \chi(z)^3 + z\chi'(z)\sin^2\lambda x - z\chi'(z)\chi(z)^2 \end{aligned}$$

where $\chi(0) = \cos\lambda x$, $\chi'(0) = -1$

$$g(\lambda,0) = \frac{(\cos\lambda x - z)(\sin^2\lambda x + \cos^2\lambda x) - 0}{(\sin^2\lambda x + \cos^2\lambda x)^2} = \cos\lambda x$$

$$f'(z) = \frac{1}{3}(\cos 2x + 2\cos x)$$

$$f(0) = 0$$

Now we are going to use the new functions created ($f(z)$ and $g(\lambda, z)$) to run the simulation on Mathematica and see the results for the detection attemps.

Chapter 6

ANALYSIS AND RESULTS

$$\hat{\chi}(z,\gamma\tau) = \frac{\frac{1}{3}\left(Re\begin{bmatrix} 1 \\ \frac{1}{exp(2i\gamma\tau)} & 1 \\ z & \end{bmatrix} + 2Re\begin{bmatrix} 1 \\ \frac{1}{exp(i\gamma\tau)} & 1 \\ z & \end{bmatrix}\right)}{1+\frac{1}{3}\left(Re\begin{bmatrix} 1 \\ \frac{exp(2i\gamma\tau)}{z} & 1 \end{bmatrix} + 2Re\begin{bmatrix} 1 \\ \frac{exp(i\gamma\tau)}{z} & 1 \end{bmatrix}\right)} \tag{6.1}$$

We use this to calculate the integral in limit:

$$\hat{\chi}(n,\gamma\tau) = N\frac{1}{n!}\lim_{z\to 0}\left(\frac{\partial^n}{\partial z^n}\chi(z,\gamma\tau)\right) \tag{6.2}$$

Remembering the survival probability S_∞, which will give 0 if we integrate (2.26) over θ, describes the behavior in the classical definition, meaning the walker will always be detected at some point. However, this is not the point for the quantum counterpart. Thus, we created a system that will measure at the same site (see figure **??**) but differs in the initial position. For example, if we take site $|1\rangle$ to start and measure at $|0\rangle$, we should perform this measurement for every site taken as initial position on full periods, which will result in not detecting the particle at some points. That is the expected scenario because, for a quantum particle, the survival probability does not necessarily vanish when you take many measurements, i.e., $n \to \infty$. In order to get rid of any issues, we set special measurement times, which we call the exceptional sampling times $\gamma\tau = 0, \pi/2, 2\pi/3, \pi, ...$

As mentioned before, $\langle n\rangle$ is some integer which is $\langle n\rangle = 4$ except for the sampling times. The figure below shows how $\langle n\rangle$ varies against $\gamma\tau$ during measurements.

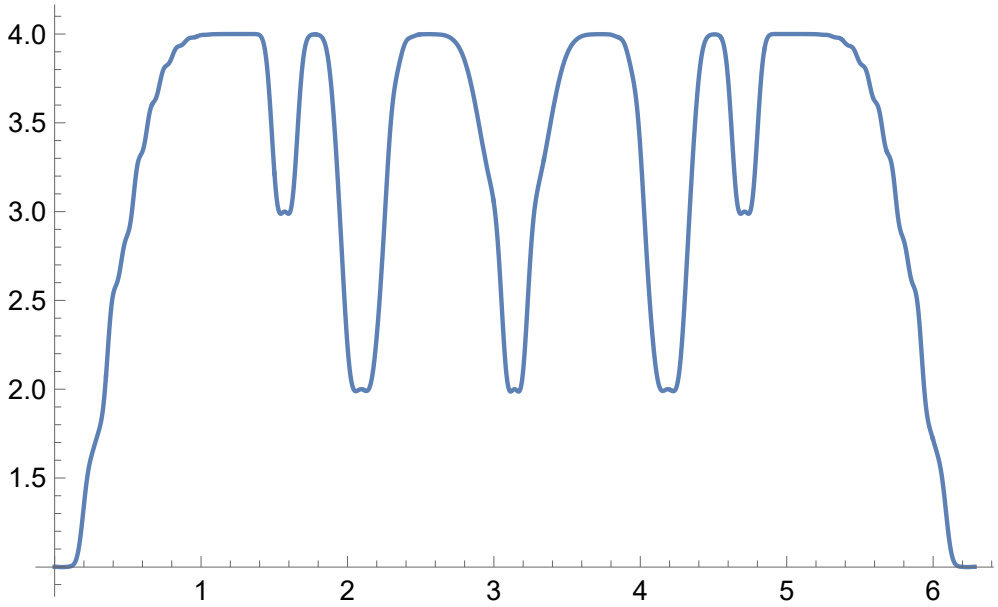

Figure 6.1: Average number of detection attemps on a benzene ring N=10

Fig. 6.1 The average number of detection attemps $\langle n \rangle$ on benzene ring. As we can see except for the sampling times, $\langle n \rangle = 4$. Only at points $\gamma\tau = 0, \pi/2, 2\pi/3, \pi, 3\pi/2, 4\pi/3, 2\pi$ we have distinct spikes for $\langle n \rangle$ being $\langle n \rangle = [1,3,2,2,2,3,1]$. There is an interesting symmetry in the results.

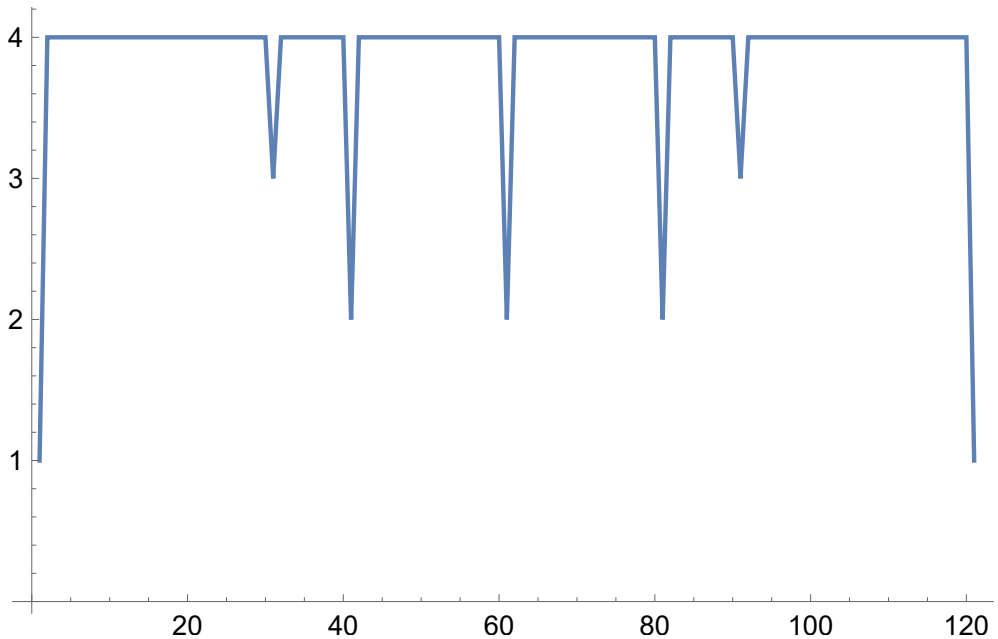

Figure 6.2: Average number of detection attemps on a benzene ring for N=100

As we see in Fig. 6.2 increasing the number of detections, results in sharper spikes giving more analytical results.

Looking at the graphs to investigate the QRW around a benzene ring, given that the detection at the first site has the highest probability, while the probabilities at other sites are equal, it could indicate several things:

1- Symmetry in the ring: One possible explanation for this outcome is that the hexagonal ring has a high degree of symmetry, which leads to the probability of detection being highest at the first site and the same for all other sites. That would indicate that the structure of the ring, precisely the hexagonal shape, plays a significant role in determining the probability of detection.

2 - Initial condition: Another possibility is that the initial condition of the walker is chosen such that the highest probability of detection is at the first site. For example, if the initial state of the walker is chosen to be localized at the first site, it would have a higher probability of being detected at that site.

3 - The Zeno effect: The Zeno effect can also play a role in this result as the QW is being continuously measured, and the measurement rate is high enough that the walker may be "frozen" at the first site, resulting in a higher probability of detection there.

Chapter 7

SUMMARY AND CONCLUSION

The quantum first-detection problem is an essential area of investigation that aims to understand how the fundamental postulates of QM, such as the Schrödinger equation, lead to the solution of the problem of detecting a QW for the first time. The QRE and the Z-transforms equations give a relationship between the amplitude of first-detection and the system's wave function free of measurement. The problem of first detection can be reduced to solving the Schrödinger equation and determining the energy spectrum of the system.

The QRE shows behaviors that are different from classical systems. However, similarities remain, such as the power-law decay of the first-passage probability density function. In addition, the quantum problem also exhibits wealthy behaviors, such as oscillations of the GF superimposed on the power-law decay, the Zeno effect, and critical slowing down. These results are essential for understanding the sensitivity of quantum systems to the sampling rate and initial conditions and the difference between quantum and classical systems.

The sensitivity of quantum systems to the sampling rate and initial conditions is crucial in practical scenarios where the coherence time of the system is limited. The difference between quantum and classical systems should be considered when designing quantum algorithms and protocols. The results of the quantum first-detection problem could have potential applications in quantum computing,

quantum communication, and quantum simulation. Further research on the quantum first-detection problem could lead to a deeper understanding of quantum mechanics and its implications on the physical world.

It's also important to note that this conclusion is based on the assumption that the initial state of the walker is normalized and the coherence time of the system is long enough to maintain the Hamiltonian's effects.

In summary, the quantum first-detection problem is a complex and essential area of research that aims to understand how the fundamental postulates of quantum mechanics lead to the solution of the QRE. The problem can be reduced to solving the Schrödinger equation and determining the energy spectrum of the system. The results of this problem exhibit wealthy behaviors that are very different from classical systems, but some similarities remain. These outcomes are essential for understanding the sensitivity of quantum systems to the sampling rate and initial conditions and the difference between quantum and classical systems. The potential applications of the results of this problem include quantum computing, quantum communication, and quantum simulation, and further research could lead to a deeper understanding of QM and its implications on the physical world.

REFERENCES

[1] Harel Friedman, David A Kessler, and Eli Barkai. Quantum walks: The first detected passage time problem. *Physical Review E*, 95(3):032141, 2017.

[2] Colm A Ryan, Martin Laforest, Jean-Christian Boileau, and Raymond Laflamme. Experimental implementation of a discrete-time quantum random walk on an nmr quantum-information processor. *Physical Review A*, 72(6):062317, 2005.

[3] Salvador Elías Venegas-Andraca. Quantum walks: a comprehensive review. *Quantum Information Processing*, 11(5):1015–1106, 2012.

[4] Richard P Feynman. Simulating physics with computers. In *Feynman and computation*, pages 133–153. CRC Press, 2018.

[5] Yakir Aharonov, Luiz Davidovich, and Nicim Zagury. Quantum random walks. *Physical Review A*, 48(2):1687, 1993.

[6] Norio Konno. A new type of limit theorems for the one-dimensional quantum random walk. *Journal of the Mathematical Society of Japan*, 57(4):1179–1195, 2005.

[7] Neil Shenvi, Julia Kempe, and K Birgitta Whaley. Quantum random-walk search algorithm. *Physical Review A*, 67(5):052307, 2003.

[8] Alejandro Romanelli, AC Sicardi Schifino, Ricardo Siri, Gonzalo Abal, Adriana Auyuanet, and Raúl Donangelo. Quantum random walk on the line as a

markovian process. *Physica A: Statistical Mechanics and its Applications*, 338(3-4):395–405, 2004.

[9] Norio Konno. Quantum random walks in one dimension. *Quantum Information Processing*, 1(5):345–354, 2002.

[10] Ben C Travaglione and Gerald J Milburn. Implementing the quantum random walk. *Physical Review A*, 65(3):032310, 2002.

[11] Shrabanti Dhar, Subinay Dasgupta, Abhishek Dhar, and Diptiman Sen. Detection of a quantum particle on a lattice under repeated projective measurements. *Physical Review A*, 91(6):062115, 2015.

[12] Eric Bach, Susan Coppersmith, Marcel Paz Goldschen, Robert Joynt, and John Watrous. One-dimensional quantum walks with absorbing boundaries. *Journal of Computer and System Sciences*, 69(4):562–592, 2004.

[13] Frank LH Brown. Generating function methods in single-molecule spectroscopy. *Accounts of chemical research*, 39(6):363–373, 2006.

[14] Sidney Redner. *A guide to first-passage processes*. Cambridge University Press, 2001.

[15] Oliver Mülken and Alexander Blumen. Continuous-time quantum walks: Models for coherent transport on complex networks. *Physics Reports*, 502(2-3):37–87, 2011.

[16] F Alberto Grünbaum, Luis Velázquez, Albert H Werner, and Reinhard F Werner. Recurrence for discrete time unitary evolutions. *Communications in Mathematical Physics*, 320(2):543–569, 2013.