DECOHERENCE EFFECTS IN QUANTUM RANDOM WALKS

KUANTUM RASGELE YÜRÜYÜŞTE EŞ-EVRESİZLİK ETKİLERİ

ARASH SALIMI KIA

PROF. DR. YİĞİT GÜNDÜÇ

Supervisor

Submitted to Graduate School of Science and Engineering of Hacettepe University

as a Partial Fulfilment to the Requirement

for the Award of the Degree of Master of Science

in Physics

2016

This work named "**Decoherence Effects in Quantum Random Walks**" by **ARASH SALIMI KIA** has been approved as a thesis for the degree of **MASTER OF SCIENCE IN PHYSICS** by the below mentioned Examining Committee Members.

Prof. Dr. Ali ULVİ YILMAZER
Head
.....

Prof. Dr. Yiğit GÜNDÜÇ
Supervisor
.....

Prof. Dr. Metin ÖNDER
Member
.....

Prof. Dr. Sadi TURGUT
Member
.....

Doç. Dr. Ahmet Mecit ÖZTAŞ
Member
.....

This thesis has been approved as a thesis for the Degree of **MASTER OF SCIENCE IN PHYSICS** by Board of Directors of the Institute for Graduate School of Science and Engineering.

Prof. Dr. Salih Bülent ALTEN
Director of the Institute of Graduate School of Science and Engineering

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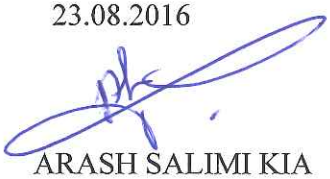

ARASH SALIMI KIA

ABSTRACT

DECOHERENCE EFFECTS IN QUANTUM RANDOM WALKS

Arash SALIMI KIA

Master of Science, Department of Physics Engineering

Supervisor: Prof. Dr. Yiğit GÜNDÜÇ

August 2016, 73 page

Quantum particles exhibit similar behavior with a classical particle on a lattice. Their behavior resembles random walk. Due to the deep differences between quantum and classical mechanics, it is expected that the similarities can not go far. Nevertheless, at the classical limit, a quantum system must exhibit classical behavior. Because of the probability nature of quantum mechanics, the quantum correlations and the origin of randomness are different in comparison with classical random walks. For this reason, quantum walk exhibits different behavior than its classical counterpart. The wave function of a quantum mechanical particle explains its motion, the wave function also contains relevant information on the state of the quantum mechanical system. Generally, an isolated particle does not exist. Hence interaction with its environment must also be considered. The wave function of the quantum mechanical system must include all particles or parts of the quantum system. In such a quantum system parts of the system interact with each other creating correlations which make the parts as a whole quantum system. Quantum correlations including entanglement are correlations that have no classical interpretations. If the wave function possesses a quantum correlation which is named entanglement, the particle, and environment are correlated in such a way that there is no classical analogue . However, in general, the system may interact with the other parts of the environment, which results in losing the quantum coherence that exists in the system. This phenomenon is called decoherence. Decoherence may appear in different ways, for example, as a change in Hamiltonian of the interacted systems.

The quantum particles moving in a structure may be similar with a classical particle, which moves randomly. In the classical case, the motion of the particle is governed by an external influence. In the quantum case, the probabilistic nature of the quantum system inherits the probability distribution. The probabilities in quantum walk is related with the quantum correlation between the spin and position spaces. Entanglement is the one which measures purely quantum correlations exist between the spin and position spaces. If the system interacts with the environment the system loses its quantum nature and become classical. The types of interaction which leads to the loss of quantum correlation are interesting for both scientific and technological applications.

The main goal of this thesis work is to discuss entanglement in quantum random walks and the effects of the decoherence and to show that the decoherence may be used to tune the system and hence it may be useful in some specific applications.

After the brief introduction of classical random walks, quantum walks have been derived by using two different methods, the position space, and the momentum space. Then decoherence has been explained and results derived for a special case called coin decoherence. Finally, a brief discussion on the effects of the decoherence is given. It is shown that tuning method of setting specific decoherence may be used to control the decoherence and it may be used in technological applications.

Keywords: Classical Random Walks, Quantum Random Walks, Laplace Equation, Decoherence, Momentum space, Useful Decoherence.

ACKNOWLEDGEMENTS

I would like to thank my supervisor, Prof. Dr. Yiğit GÜNDÜÇ, for the patient guidance, encouragement and advice he has provided throughout my time as his student. I have been extremely lucky to have a supervisor who cared so much about my work, and who responded to my questions and queries so promptly.

I must express my gratitude to Masiha, my wife, for her continued support and encouragement. I was continually amazed by the patience of my mother, father, sister and brother who experienced all of the ups and downs of my research.

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1.INTRODUCTION

The random walk is one of the most crucial topics of both science and computation. On one hand it explains the propagation of particles in physical media and on the other hand it describes the propagation of information in computational modes. This knowledge is the base of the motivation for studies on quantum walks. In physical systems, motion of single atoms or photons is a good example of quantum random walks. Quantum walks, like classical counterpart, have been the underlying structure for several new quantum algorithms.

Despite the fact that the quantum random walk studies are relatively new, growing interest on the quantum walks is due to the expectation that the quantum random walks are similar to their classical counterpart, namely classical random walks. Its origin can be traced back as early as the introduction of path integral formalism of quantum mechanics by Feynman [1]. Quantum diffusion dynamics was one of the earliest well-studied phenomena in the literature based on the quantum walk. Feynman's idea that quantum mechanical systems can only be simulated on the quantum computers has been the starting initiative for the search of quantum algorithms and methods of quantum computation. Early studies of particles moving on regular lattices with discrete time steps appeared in late 1980s and such formulations are named "quantum random walk". The early works on quantum random walk are due to Gudder [2] , Grossing and Zeilinger [3]. Aharonov applied the quantum walk ideas onto applications of quantum optics [4], while Meyer [5] studied similar systems to formulate quantum cellular automata.

The relation between the concepts of quantum information processing and quantum walk started with Farhi and Gutmann [6]. Their first approach was based on solving time evolution equation in continuous time. Discrete time quantum walks, which emerged immediately after the continuous time quantum walks, resemble more to classical random walks since they require coin for calculation of the probabilities. They are shown to be more useful for new quantum algorithms [7], Ambainis et al. and Nayak and Vishwanath [8].

When a quantum mechanical system is formed, two types of correlations may appear. The first is the correlations that may appear in classical particle systems, the second type is the one which can only be seen in quantum systems. Quantum correlations are phenomena which have no classical analogue. Entanglement is a type of quantum correlation that is strikingly different from the experiences in the classical world. Quantum random walk exhibits entanglement. The quantum correlations between the coin and position is the source of entanglement. In quantum random walk the initial state consists of two parts, the coin and the position. Repetitive application of a unitary time evolution operator creates correlations between coin and the spatial lattice which cannot be separated from each other. If this system is an isolated system correlations in the system grow as the walk continues. If it is not an iso-

lated system, it interacts with the environment. The interactions between the system and the environment result in the decrease or total loss of the quantum correlations. This phenomena is called decoherence in the quantum systems. Decoherence is unavoidable aspects of the quantum systems. When a quantum system is in isolation, without any observation made on it, retains all quantum and classical correlations. In fact there exist no such system that can be totally isolated from the environment. When an experiment is designed, the effects of decoherence must be taken into consideration. The effect of the decoherence is to change a quantum system to a classical system. Hence it is important to understand the tools to control decoherence. Moreover, such tools provide a better control over the quantum systems, create more opportunities for various applications. The decoherence in the quantum random walk can be studied both analytically and numerically. Hence quantum random walk with decoherence is an interesting laboratory for both the studies of physical phenomena and the quantum information.

In this thesis work, the classical random walk will be reviewed in order to set the terminology which will be used in the discussions of the quantum walks. Following the classical random walk chapter, chapter 3 is devoted to the definition of the quantum walk in real space. Quantum walk is different in nature. Dominating effect on quantum walk is quantum correlation. In general spatial distribution of the walk is not symmetric. Both coin and the shift operator are responsible from the width and the Form of the probability distribution. In chapter 3, creation of quantum correlations, starting from separable coin and spatial spaces, and the origin of the asymmetry of quantum walks are shown by using simple analytical calculations. Analytical studies of the quantum walk is extended in chapter 4. In this chapter quantum walk is analytical treatment using momentum space representation. Chapter 5 includes studies of the added effects of decoherence. Decoherence can simply be described as any effect that reduces the quantum correlations. In quantum walk both the coin and the spatial components of the system may be under the influence of the external disturbances. Here, in this thesis, the effects of the decoherence on the coin space is discussed using numerical techniques. The last section is the discussions section. In the discussions the methods of controlling the decoherence and its effects on the quantum algorithms are discussed.

2. CLASSICAL RANDOM WALKS

Introduction

Random walk can be described as a succession of steps that are random both in size and direction in each discrete, equal time step. One dimensional random walk is the simplest example. In one dimensional random walks the particle is constrained to move on a line. At every time step, particle moves right or left from present spatial position. The decision of choices right or left moves are random. The randomness of this choice can be obtained by toss of a coin. If the coin is head or tail particle moves one unit to right or left respectively. One dimensional random walk is the the simplest case of a vast number of random walk examples in the literature. To keep track of such a random motion is not easy and after a couple of steps one cannot exactly determine the position of the particle. Despite the difficulty of keeping trace of each move of the particle, mathematics indicate the most probable location of the particle.

In order to make a formal definition of random walk, consider a set of independent random variables, $x_1, x_2, \ldots$. At each time step the random variable may change its value by Δx or $-\Delta x$ with 50 percent probability,

$$S_0 = 0, \quad S_n = \sum_{j=1}^{n} x_j. \tag{2.1}$$

which S_0 is the initial point of the walk where S_n indicates position of the particle after n steps. The series S_n is called the *simple random walk* on $\mathbb{Z}$. This series (the sum of the sequence of $-\Delta x$'s and Δx's) gives the distance walked.

Since the random walk is based on random variables, one can study two quantities, the expectation value and the standard deviation. The expectation value $E(S_n)$ of S_n can be defined as,

$$E(S_n) = \frac{1}{n} \sum_{j=1}^{n} x_j \tag{2.2}$$

which vanishes as the number of coin flips, n, increase. For a truly random walk, $E(S_n) = 0$. As one considers head and tails +1 and -1 representations the mean of all coin flips approaches zero due to the finite additive property of expectation. Hence the expectation value doesn't show the *expected translation distance* after n steps.

Despite the fact that the average of the random variables vanishes, they exhibits a distribution around the mean value. In order to estimate this distribution one can calculate the standard deviation of the random variables. By definition, standard deviation is the root mean square

of variance. By the fact that,

$$E(x_n^2) = 1/n(\sum x_n^2) = \Delta x^2 \tag{2.3}$$

and hence,

$$E(S_n^2) = \sum_{j=1}^{n} E(x_j^2) = n\Delta x^2. \tag{2.4}$$

So the expected translation distance after n steps should be of the order of $\sqrt{n}\Delta x$. This is the most crucial result of classical random walk. This result sets a limit on the speed of information propagation for stochastic processes.

The probability distribution for a classical walk is symmetric and it is a Gaussian function around the origin or initial point of walker figure (2.1). Some properties of one dimensional random walk can be derived from Pascal's triangle Table (2.1) since there is a close relation between steps of the walk and Pascal triangle. If one considers a random walk where the walker starts from the origin, 0, and takes a distance of one unit length at each time step, in the first time step, the particle can be at either $+1$ or -1. At the second step, the particle is either at the position $+1$ or -1. If it is at the position $+1$ it can move backward or forward one step ending at either 0 or 2. If on the contrary the particle is at the position -1, at the next move it can be either at -2 or 0. Hence after two time steps there are two chances for walker to be at the position 0 (the starting point). The particle has no chance to be at $+1$ and -1 and there is one chance to be at the positions $+2$ or -2 at the end of the second time step.

Table 2.1: Pascal triangle.

$n = 0$:				1				
$n = 1$:			1		1			
$n = 2$:		1		2		1		
$n = 3$:	1		3		3		1	
$n = 4$:	1		4		6		4		1

Markov-chains

Markov-chains is the name of a random process that changes the state of a system from one state to another in the domain of an state space. Each state is only dependent on the previous state and it is independent from the earlier states.

Consider there is a set of states called $S = \{s_0, s_1, s_2, ...\}$, Suppose system is in state s_i after a random process, system jumps to the state s_j. Each jump is called a step. Probability of transition between the states$i$ and j is P_{ji} and is called transition probability. This probability is time independent and also independent from the previous steps.

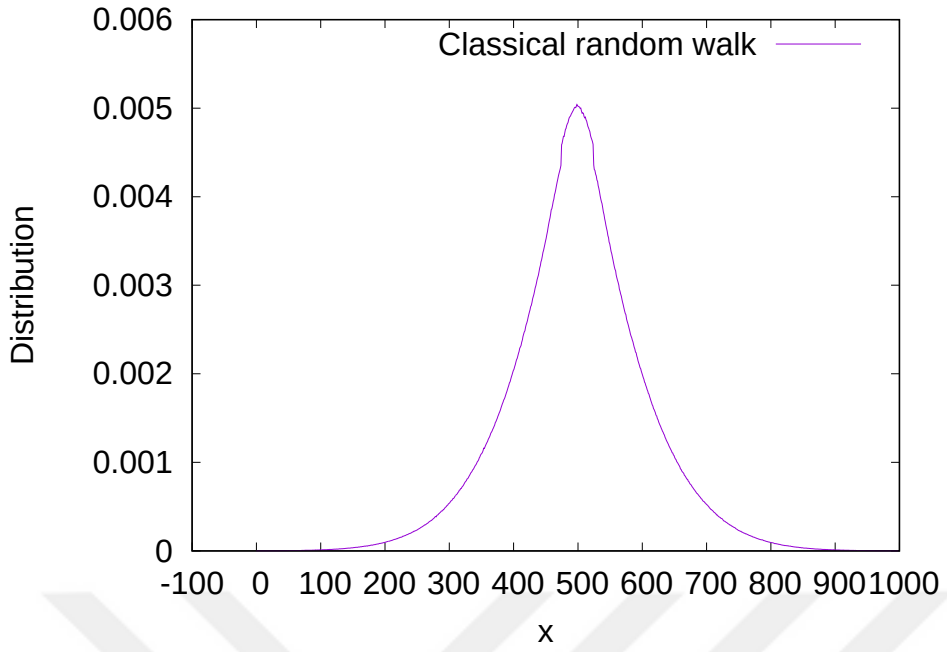


Figure 2.1: Distribution of one dimentional random walk

Solving Laplace equation using Markov chains

Classical random walk plays a very important role in numerical analysis. It is the mathematical base of wide range of algorithms. Solving the partial differential equations is one of the important application areas of classical random walk. This methodology is used in solving the Laplace equation[9].

Problem is to find a solution of Laplace's equation,

$$\nabla^2 V = 0. \tag{2.5}$$

In two dimensions the equation becomes,

$$\frac{\partial^2 V}{\partial x^2} + \frac{\partial^2 V}{\partial y^2} = 0. \tag{2.6}$$

The problem is solved by using two dimensional walks so two dimensional surface have been divided into equal distance points or nodes just like a 2D regular lattice. Values of potential V sets the boundary conditions. Differential equation will be simplified to finite difference equations by using the method of successive displacement called Gauss-Shield method [37].

Suppose the area is divided as in figure (2.2) and the value of potential V ar the point $M(x_0, y_0)$ is required. Starting from M, walker is constrained to move on the mesh choosing one of four directions, up, down, right or left. Process is repeated until the walker reaches a point on the boundary. Suppose the Value of the potential in reached boundary is V_i. Repeating this process starting from M generates a set of V_i's. It can be shown that the value of potential in

point M is:

$$V_M = \lim_{n \longrightarrow \infty} \frac{\sum_{i=1}^{n} V_i}{n}, \tag{2.7}$$

which n is number of repeated process (see ref. [37]).

Choosing the direction of motion is random with some probability provided by the transition probability matrix.

Transition probability matrix is a rectangular matrix that changes the state of the system when it is applied on the state matrix of the system. Elements of this matrix consist of transition probabilities among the points or nodes. A transition probability matrix is related with the walker. By using boundary conditions in the form of potentials that they can absorb the walker, the value of the unknown nodes can be calculated.

The transition probability, P_{ji} contains all the probabilities of transitions. Markov-chain describes the dynamics using these probabilities of the particle at time t to the time $t+1$:

$$\mathbf{P} S_t = S_{t+1} \tag{2.8}$$

S_t defines the particle at step t.

Here the transition matrix is equal to:

$$\mathbf{P} = \begin{pmatrix} P_{00} & P_{01} & P_{...} \\ P_{10} & P_{11} & P_{...} \\ P_{...} & P_{...} & P_{...} \end{pmatrix}. \tag{2.9}$$

Stochastic matrix,P, consist of all probabilities. Sum of a row, $(\sum P_{ij} = 1)$, is equal to unity,

remember that the nodes are the states of the system.

Surface is gridded by nodes. Some nodes are supposed to be non absorbing nodes called n, they don't absorb walker. It means that no potential acts on the particle at those nodes, but the other absorbing nodes absorb the walker. Total number of nodes are $n + a$. Then the transition matrix is:

$$\mathbf{P} = \begin{pmatrix} I & 0 \\ P^{na} & P^{nn} \end{pmatrix}. \tag{2.10}$$

The transition matrix in block diagonal form consist of four different matrices. The first matrix is a unit matrix, I which is square $a \times a$ matrix and , 0 is an $a \times n$ and it means that $(P^{an} = 0)$, P^{na} is an $n \times a$ matrix and it is related with probabilities of moving between non-absorbing to absorbing points. P^{nn} also is an $n \times n$ matrix and represents probabilities of moving between non-absorbing points. The elements of P^{nn} and P^{na} are $1/4$ if there is a direct connection between the points, otherwise it is zero.

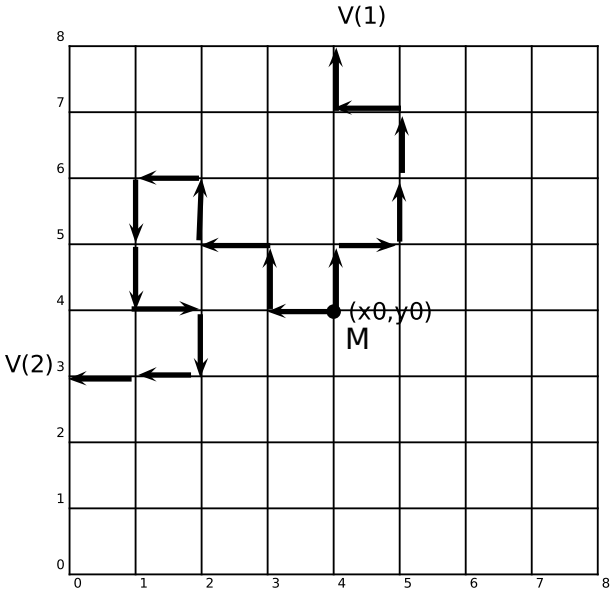


Figure 2.2

The probability matrix P' can be separated from transition matrix P in a way that:

$$P' = \begin{pmatrix} P^{na} & P^{nn} \end{pmatrix}. \tag{2.11}$$

In which P_{ji} is the probability that walker starting at point i will end the walk at point j. P' is an $n \times (n + a)$ matrix. Therefore

$$V_n = P'V_a \tag{2.12}$$

In which V_n and V_a are potentials in non-absorbing and absorbing points respectively. This equation will give us all potentials in non-absorbing nodes.

Example

The above mentioned will be clarified with an example. In this simple example 5 points or nodes are considered. This system consist of one non-absorbing point at the center and four absorbing points around. The aim is to determine the value of potential at center, where the non-absorbing point. Length of sides of each square is 1/2 unit.

Boundary conditions are presented in figure (2.3) as:

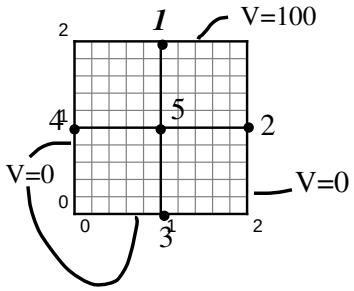


Figure 2.3

$$\begin{aligned} V(0,1) &= V(1,y) \\ &= V(x,0) \\ &= 0 \end{aligned} \tag{2.13}$$

$$V(x,1) = 100. \tag{2.14}$$

The transition probability matrix is as follows:

$$\mathbf{P} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ 1/4 & 1/4 & 1/4 & 1/4 & 0 \end{pmatrix}, \tag{2.15}$$

therefore $P^{nn} = 0$ and $P^{na} = \begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix}$ so:

$$P' = \begin{pmatrix} P^{na} & P^{nn} \end{pmatrix} \tag{2.16}$$

$$= \begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 & 0 \end{pmatrix} \tag{2.17}$$

and according to equation (2.12):

$$V_5 = \begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 & 0 \end{pmatrix} \begin{pmatrix} V_1 \\ V_2 \\ V_3 \\ V_4 \\ V_5 \end{pmatrix} \tag{2.18}$$

$$U_5 = \begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 & 0 \end{pmatrix} \begin{pmatrix} 100 \\ 0 \\ 0 \\ 0 \\ V_5 \end{pmatrix} \tag{2.19}$$

$$V_5 = 1/4(100 + 0 + 0 + 0) = 25. \tag{2.20}$$

Separation of variables solution of the laplace equation is obtained,

$$V(x, y) = \frac{400}{\pi} \sum_{m=1}^{\infty} \frac{sin(\frac{n\pi x}{a}) sinh(\frac{n\pi y}{a})}{n sinh(n\pi)}, \qquad n = 2m - 1. \tag{2.21}$$

In this example the value of $V_5 = V(1/2, 1/2)$ was calculated as 25. Solution for $V(1/2, 1/2)$ using the equation (2.21), is exactly as the same as Markov-chains method.

This was a simple example representing one of the applications of classical Markov-Chains. However, quantum walk based algorithms have many interesting properties, including faster hitting times with respect to their classical counterpart. In next chapter, one dimensional quantum random walks will be introduced.

3.1-DIMENSIONAL QUANTUM RANDOM WALK

Introduction

Quantum analog of classical random walks are called as quantum walks [4, 10]. Quantum and classical systems have subtle differences. In classical random walk the probabilities that govern the dynamics of the walk comes as an external parameter. On the contrary the probabilistic nature of the quantum world, inherently contain the probability information in the wave function of the particle. This information is used to govern the dynamics of quantum mechanical particles [4]. For this reason quantum random walk may simply be called quantum walk.

Quantum walk like all quantum phenomena can be studied in real space or momentum space. In this chapter of the thesis work the quantum random walk in real-space will be reviewed. The quantum walk, like its classical counterpart, continuous and discrete time versions of the quantum walk can be studied.

In continuous time the solution is based on time evolution equations [6, 11]. In this form of the quantum walk, the wave function and hence the probabilities change continuously in time. Hence, definition of the walk on the coordinate space does not require a coin operator . In the discrete model however, Introduction of quantum coin operator is necessary [12]. The coin which provides the probability information of the walk is an artifact necessary when the time is discretized. The similarity of both continuous and discrete time solutions is shown [6]. Nevertheless, the coin degrees of freedom enable one to increase control on dynamics. For this reason the discrete time quantum walk is more widely studied and it is more powerful than the continuously-time quantum walk in some cases [13].

Our focus in this thesis will be around the discrete time quantum random walks and their decoherence. The present chapter will start with a brief discussion on the dynamics of continuous time walks. Following this introductory section, the dynamics of discrete time quantum walks need to be discussed in more detail.

A detailed analytical example of one dimensional coined quantum random walks is discussed will be given next. In these analytical calculations the state vector of the particle in position space and the probabilities of being in certain point of space will be presented for 4 steps of walk.

Continuous time quantum walks

Continuous time walks were first introduced by Farhi and Gutmann in 1998 [6, 11]. The quantum walk, as classical counterpart, is defined for a particle or particles that reside at

the vertices on connected graphs. Before explaining continuous time quantum walk, it is convenient to explain classical Markov-chains. Supposing that a gragh $G = (V, E)$, has V vertices (points or nodes) and E edges that connect the vertices. For this purpose we need to define two matrices **A** and **G**. The first matrix **A**,which is called adjacency matrix, is the matrix that defines the connections on the graph. The adjacency matrix is a $V \times V$ square matrix and its non-vanishing elements represent connections between vertices i and j. The elements of adjacency matrix are unity if there is a connection between$i$ and j else, they are zero. zero.

$$A_{ij} = \begin{cases} 1 & \text{if i and j have been connected} \\ 0 & \text{Else} \end{cases} \tag{3.1}$$

In this approach it is assumed that the walker can only use the connection between the two neighboring vertices. The second matrix, G_{ij}, is called generator matrix. The generator matrix governs time evolution of systems. Elements of the generator matrix, G_{ij} define the probability of moving or transforming from vertex i to j per unit time.

The matrix elements of the generator matrix are given by,

$$G_{ij} = \begin{cases} \gamma d_i & \text{if } i = j \\ -\gamma & \text{if } i \neq j \\ 0 & \text{if there is no connection} \end{cases} \tag{3.2}$$

where γ is a fixed time independent constant that represents the probability of a particle moving from the site i to site j per unit time. Coefficient, d_i, is degree of vertex i . γ transforms the system continuously in time and it represents the speed of evolution of the system or simply the rate of jumping.

The probability of a particle being at a vertex at a given time t is $P_i(t)$. The rate of change of probability of being at site i is obtained by applying the generator matrix to the probabilities:

$$\frac{dP_i(t)}{dt} = -\sum_k \mathbf{G}_{ik} P_k(t). \tag{3.3}$$

This equation is a classical continuous Markov-Chain equation and its solution gives the time dependent probability relation for the site i,

$$P_i(t) = e^{-Gt} P_i(0). \tag{3.4}$$

So far these arguments are valid for the classical dynamics. The wave function $|\psi(t)\rangle$ describes the quantum mechanical particle at time t. Hence, the quantum analogue of the clas-

sical Markov-Chain equation, (Eq. 3.3) can be obtained using the idea of the wave function . The quantum mechanical analogue of the classical Markov-Chain can be obtained by considering the probabilities in quantum mechanics which can be calculated using the wave function of the particle. The only missing component in this analogy is fixed by considering that the Hamiltonian, which is the generator of time evolution operator for quantum mechanics Hamiltonian is related with the time derivative of the wave function. Replacing the time dependent probability $P_i(t)$, and the generator matrix, **G** by the wave function, $\psi_i(t)$ and the Hamiltonian **H** of system respectively the similarity between the classical Markov-Chain and the Schrödinger equation becomes apparent.

The Hamiltonian operator is $\mathbf{H} = i\hbar\frac{d}{dt}$. Hence multiplying left hand side of the classical Markov-Chain equation (Eq. 3.3) by $i\hbar$, is necessary to obtain the correct form of the Schrödinger equation:

$$i\hbar\frac{d}{dt}\psi_i(t) = -\sum_k H_{ik}\psi_k(t) \tag{3.5}$$

or in Dirac notation the form of the Schrödinger equation becomes,

$$i\hbar\frac{d}{dt}\left|\psi\right\rangle_i = \mathbf{H}\left|\psi\right\rangle_i \tag{3.6}$$

and the solution is:

$$\left|\psi_i\right\rangle = e^{-iHt/\hbar}\left|\psi_i(t=0)\right\rangle . \tag{3.7}$$

The classical random walk in continuous time propagate according to diffusion equation (Eq. 3.3). Schrödinger equation is the quantum version of the same equation. Both equations are first order equations with respect to time. The major difference is that Schrödinger equation is a wave equation (without absorbing potential terms) while the Markov Chain equation is a diffusion equation. Therefore, this primary difference makes quantum walks quadratically faster than its classical peer.

In the following section discrete-time quantum walk will be reviewed.

Discrete time quantum walk in 1-dimension

The idea of discrete time quantum walk is based on a quantum mechanical translation operator. In quantum mechanics, momentum is the generator of translation. It means that the motion of the particle, representing a step of size l is given by shift operator $U_l = \exp(-ipl/\hbar)$. Therefore

$$U_l\left|\psi_{x_0}\right\rangle = \left|\psi_{x_0+l}\right\rangle . \tag{3.8}$$

The probabilistic nature of the translations can be added into this unitary operator by adding a new component which decides on the direction of the walk. An immediate consideration may be to use a new degree of freedom namely spin. Assuming that the particle has spin quantum number, $s = 1/2$, the action of the third component of spin operator is given as,

$$\begin{aligned} \mathbf{S}_z \left|\uparrow\right\rangle &= \hbar/2 \left|\uparrow\right\rangle \\ \mathbf{S}_z \left|\downarrow\right\rangle &= -\hbar/2 \left|\downarrow\right\rangle . \end{aligned}$$

With the help of the spin operators, the translation operator (Eq. 3.8), can be modified to include the spin degrees of freedom attached to the quantum mechanical particle. This modified form of the translation operator,

$$U_l = \exp(-2iS_z \otimes pl)/\hbar^2 \tag{3.9}$$

The operator **U** defines motion of the particle in term of internal parameters. The total wave function consist of both position and spin wave functions. If the initial spin state is $|\uparrow\rangle$ the conditional translation operator, Eq. 3.9, shifts the position wave function to right, $|\uparrow\rangle \otimes |\psi_{x_0+l}\rangle$. Similarly, spin down case the particle position wave function will be shifted left, $|\downarrow\rangle \otimes |\psi_{x_0-l}\rangle$. Initially the particle is located at the origin. When the initial spin state is superposition of both up and down states,

$$|\psi_{in}\rangle = (\alpha^{\uparrow} |\uparrow\rangle + \alpha^{\downarrow} |\downarrow\rangle) \otimes |\psi_{x_0}\rangle . \tag{3.10}$$

At each time step, the operator **U** will create superposition of different components of position dependent wave function. Here operators acting on spin space can be considered as a kind of coin operator which modifies the probability of the moves.

$$U |\psi_{in}\rangle = \alpha^{\uparrow} |\uparrow\rangle \otimes |\psi_{x_0+l}\rangle + \alpha^{\downarrow} |\downarrow\rangle \otimes |\psi_{x_0-l}\rangle \tag{3.11}$$

At this point, if a measurement is performed on the spin, the state will be

$$|\uparrow\rangle \otimes |\psi_{x_0+l}\rangle . \tag{3.12}$$

The probability of being of the particle in position $x_0 + l$ is given by $p_{\uparrow}$. The other possible state,

$$|\downarrow\rangle \otimes |\psi_{x0-l}\rangle , \tag{3.13}$$

which indicates the particle sitting at the position $x_0 - 1$ with probability $P_{\downarrow}$. This selective move of the particle indicates that the spin degrees of freedom plays the role of the coin for

quantum walk[12]. The coin degrees of freedom is not an external parameter in quantum walk case. The quantum mechanical probability due to the definition of the wave function of the particle is modified by using a time evolution operator. Moreover, since this coin is quantum mechanical coin, it does not only take up or down state, but it can be in superposition of up and down states simultaneously. Repeated application of the shift operator attribute different probability values to different discrete spatial space points. If one defines different unitary coin operators, which give the probability relations for the moves of the particle, different probability distributions can be attained for different coin operators. Despite the fact that the operators are unitary such probability distribution resembles a random walk on the spatial space.

In the next section the dynamics of quantum walk will be explained by analytical calculations in position space using Dirac's notation.

Dynamics of quantum walks in position space

The present subsection is devoted to studies of 1-dimensional motion of a quantum mechanical particle. The wave function, $|\psi_0\rangle$ which is a vector in an n-dimensional abstract complex vector space, describes The particle, initially localized around the position x_0. The Hilbert space of this particle consist of direct product space of two Hilbert spaces, namely, $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_c$. Here, $\mathcal{H}_P$ and $\mathcal{H}_c$ are the spatial and coin (spin) Hilbert spaces respectively.

Discrete time quantum walk has two components. The first component, the coin, is related with the decision on the direction the particle. The second realize the actual movement. The coin operator acts on spin space. The requirement of physical system determines the form of the coin operator. As long as it is unitary, the choice of the coin operator is arbitrary. The most general coin operator can be defined as a general unitary matrix[12].

SU(2) coin operator optimization and it's combination with the shift operator S

constructed using SU(2) group element with three complex parameters. 2×2 matrix elements of the group must have following properties:

$$C = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} = \begin{pmatrix} a_1 + ia_2 & b_1 + ib_2 \\ -b_1 + ib_2 & a_1 - ia_2 \end{pmatrix} \tag{3.14}$$

and

$${a_1}^2 + {a_2}^2 + {b_1}^2 + {b_2}^2 = 1.$$

In equation (3.14) a and b's are real numbers or functions. This is the most general form of a SU(2) quantum coin. A simpler form of this coin operator that satisfies the requirements in

equation (3.14) can be written by using Euler angles, named:

$$C = \begin{pmatrix} e^{i\alpha}\cos(\gamma) & e^{i\beta}\sin(\gamma) \\ e^{-i\beta}\sin(\gamma) & -e^{-i\alpha}\cos(\gamma) \end{pmatrix}. \tag{3.15}$$

For $\alpha = \beta = 0$:

$$C = \begin{pmatrix} \cos(\gamma) & \sin(\gamma) \\ \sin(\gamma) & -\cos(\gamma) \end{pmatrix}. \tag{3.16}$$

In the literature there exist various widely used coin operators all of which corresponds to a set of parameter values of the most general definition of the coin operator. The most popular of all is the Hadamard operator. For $\gamma = \frac{\pi}{4}$ Hadamard coin is derived:

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

.

Quantum shift operator

The coin acts on the spin space, the actual move of the walker requires a shift operator which realizes the move of the particle as a function of coin operator outcome.The following operator describes the conditional translation of the system:

$$\mathbf{S} = |\uparrow\rangle\langle\uparrow| \otimes \sum_n |n+1\rangle\langle n| + |\downarrow\rangle\langle\downarrow| \otimes \sum_n |n-1\rangle\langle n|. \tag{3.17}$$

First coin operator is applied. After that, the shift operator **S** translates the particle both left and right with some probabilities. Both the coin and the shift operators together constitute actual quantum walk (time evolution) operator **U**,

$$\mathbf{U} = \mathbf{S}\,\mathbf{C}. \tag{3.18}$$

This operator is a unitary operator. This operator acts on the state vector,

$$|\Psi\rangle = |\psi_p\rangle \otimes |\psi_c\rangle \tag{3.19}$$

where $|\psi_p\rangle$ and $|\psi_c\rangle$ are the wave function of the particle defined on spatial and coin spaces. Together with the coin operator initial coin state plays an important role in quantum walk. The most general initial coin state can be a unit vector in coin space,

$$|\Psi_c\rangle = cos(\gamma)\ |\uparrow\rangle + ie^{i\phi} sin(\gamma)\, |\downarrow\rangle \tag{3.20}$$

where γ is the angle between the unit vector and the z axis, and ϕ is the angle between x axis and the projection of the unit vector on the $x-y$ plane, which x,y and z are Cartesian coordinates. The importance of the choices of the parameters γ and ϕ, will be discussed in the following section.

The following section is devoted to application of the quantum walk with a specific choice of the coin operator, namely Hadamard coin.

Quantum walk with Hadamard coin

In this section the quantum walk will be studied on an explicit example. A specific value of $\gamma = \frac{\pi}{2}$ in equation (3.16), corresponds to the most widely used coin operator which is called Hadamard coin [12]:

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{3.21}$$

The Hadamard coin acts on the eigenstates of S_z operator. The action of the Hadamard coin on the eigenstate of the $\mathbf{S}_z$ operator can be represented as:

$$|\uparrow\rangle \longrightarrow \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \tag{3.22}$$

$$|\downarrow\rangle \longrightarrow \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle). \tag{3.23}$$

These relations exhibit a very different choices than those can be made by using the classical coin. In the classical coin case, the walker moves according to the state which is determined by the application of the coin operator. In the quantum walk, the direction in general, is a superposition of the eigenstates of the chosen operator. It makes the particle move left and right simultaneously with probabilities given by the form of the quantum coin.

The parameter value of the general coin is an important component. As an example, for the Hadamard walk in general the probability distribution is not symmetric. It will move to the right with higher probability. If the initial state vector has spin up, the particle will move to left with higher probability.

After the initial state is set, the time development of the walk is governed by the action of a unitary operator **U**. The following steps depend on the translation operator **U** and the current state of the walker. As in the classical case, the next position of the walker depends only on the current state of the walker and is independent of the previous steps.

Starting from the present state $|\psi(t)\rangle$, the state of the walker at the next time step is obtained by applying the unitary operator **U**, and it is written as:

$$|\psi(t+1)\rangle = \mathbf{U}\,|\psi(t)\rangle\,. \tag{3.24}$$

Quantum walk on the position space can be illustrated by using Hadamard coin and a spin up particle placed at the origin, where $|\psi(t=0)\rangle = |\uparrow\rangle_c \otimes |0\rangle_p$. Here the indices c and p, indicate coin and position space kets. In the following, the position and the coin indices will be omitted in order to avoid further complications in writing the time evolved state functions.

The application of the Hadamard operator on the $|\uparrow\rangle$ mixes up and down states:

$$H\,|\psi(0)\rangle = H\,|\uparrow\rangle \otimes |0\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \otimes |0\rangle\,.$$

Since the initial spin state is simply up state, the coin state at the fist application of the coin operator is a mixture of the both up and down states. The time evolution of the quantum walk is completed by the action of the shift operator, **S**:

$$S(H\,|\psi 0\rangle) = \frac{1}{\sqrt{2}}\,|\uparrow\rangle\,\langle\uparrow|\uparrow\rangle \otimes \sum_n |n+1\rangle\,\langle n|\,0\rangle$$

$$+\frac{1}{\sqrt{2}}\,|\uparrow\rangle\,\langle\uparrow|\downarrow\rangle \otimes \sum_n |n+1\rangle\,\langle n|\,0\rangle$$

$$+\frac{1}{\sqrt{2}}\,|\downarrow\rangle\,\langle\downarrow|\uparrow\rangle \otimes \sum_n |n-1\rangle\,\langle n|\,0\rangle$$

$$+\frac{1}{\sqrt{2}}\,|\downarrow\rangle\,\langle\downarrow|\downarrow\rangle \otimes \sum_n |n-1\rangle\,\langle n|\,0\rangle\,.$$

Second and third terms of right hand side of the above equation vanish, resulting state vector of the quantum mechanical walker at the time step, $t = 1$,

$$|\psi(1)\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle) + \frac{1}{\sqrt{2}}(|\downarrow\rangle \otimes |-1\rangle). \tag{3.25}$$

The particle will be on the lattice sites 1 or -1 with equal probabilities. This equation also indicates entanglement between the particle's position and its spin. Probabilities of being in points $+1$ and -1 is calculated as follows:

$$\langle 1|\ \psi(1)\rangle = \frac{1}{\sqrt{2}}$$

$$\langle -1|\ \psi(1)\rangle = \frac{1}{\sqrt{2}}$$

$$|\langle 1|\ \psi(1)\rangle|^2 = \frac{1}{2} \tag{3.26}$$

$$|\langle -1|\ \psi(1)\rangle|^2 = \frac{1}{2}. \tag{3.27}$$

The second step is obtained by applying the time evolution operator **U** onto $|\psi(1)\rangle$. The equation (3.25) contains two terms. By applying the coin operator, **H** to the first term,

$$H\frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle) = \frac{1}{2}(|\uparrow\rangle + |\downarrow\rangle) \otimes |1\rangle$$

sets the new coin state while the shift operator **S** sets the final probabilities for the particle by,

$$S \otimes H\,|\psi(1)_1\rangle = \frac{1}{2}\,|\uparrow\rangle\,\langle\uparrow|\uparrow\rangle \otimes \sum_n |n+1\rangle\,\langle n|\ 1\rangle$$

$$+\frac{1}{2}\,|\uparrow\rangle\,\langle\uparrow|\downarrow\rangle \otimes \sum_n |n+1\rangle\,\langle n|\ 1\rangle$$

$$+\frac{1}{2}\,|\downarrow\rangle\,\langle\downarrow|\uparrow\rangle \otimes \sum_n |n-1\rangle\,\langle n|\ 1\rangle$$

$$+\frac{1}{2}\,|\downarrow\rangle\,\langle\downarrow|\downarrow\rangle \otimes \sum_n |n-1\rangle\,\langle n|\ 1\rangle$$

completes the time evolution of the first term,

$$|\psi(2)_1\rangle = \frac{1}{2}(|\uparrow\rangle \otimes |2\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |0\rangle). \tag{3.28}$$

Similarly the time evolution operator $U(t)$ changes the second term, of the equation (3.25) result in,

$$|\psi(2)_2\rangle = \frac{1}{2}(|\uparrow\rangle \otimes |0\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |-2\rangle). \tag{3.29}$$

The equations (3.28) and (3.29) sums up to the state vector of the particle at the second step of the walker:

$$|\psi(2)\rangle = \frac{1}{2}(|\uparrow\rangle \otimes |2\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |0\rangle) + \frac{1}{2}(|\uparrow\rangle \otimes |0\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |-2\rangle). \tag{3.30}$$

It is clear that probabilities are symmetric with respect to the origin:

$$|\langle 2|\ \psi(2)\rangle|^2 = \frac{1}{4} \tag{3.31}$$

$$|\langle 0|\ \psi(2)\rangle|^2 = \frac{1}{2} \tag{3.32}$$

$$|\langle -2|\ \psi(2)\rangle|^2 = \frac{1}{4}. \tag{3.33}$$

Equations above are the probabilities of being at the spatial points 2, 0, and -2 respectively. The probabilities of finding particle at points 1 and -1 are zero. Up the the second step, the probabilities are symmetric in the position space. This is similar with the classical walk. This similarity ends after the second time step. For Hadamard coin and initial $|\uparrow\rangle$ initial coin state, the observed symmetry up to second time slice ends and a preferred direction appears after the third time step.

Applying the same rules as shown above, the state ket after the third time step is given as,

$$|\psi(3)\rangle = \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |3\rangle) + \frac{1}{2\sqrt{2}}(|\downarrow\rangle \otimes |1\rangle) + \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle) - \frac{1}{2\sqrt{2}}(|\downarrow\rangle \otimes |-1\rangle)$$

$$+ \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |-1\rangle) - \frac{1}{2\sqrt{2}}(|\uparrow\rangle \otimes |-1\rangle) + \frac{1}{2}(|\downarrow\rangle \otimes |-3\rangle) \tag{3.34}$$

and again probabilities of finding particle in space has been calculated as follows:

$$|\langle 3|\ \psi(3)\rangle|^2 = \frac{1}{8} \tag{3.35}$$

$$|\langle -1|\ \psi(3)\rangle|^2 = \frac{1}{8} \tag{3.36}$$

$$|\langle 1|\ \psi(3)\rangle|^2 = \frac{5}{8} \tag{3.37}$$

$$|\langle -3|\ \psi(3)\rangle|^2 = \frac{1}{8}. \tag{3.38}$$

The probabilities of being at the points $+3$, -1, $+1$, -3 are respectively $\frac{1}{8}, \frac{1}{8}, \frac{5}{8}, \frac{1}{8}$ It is clear that the symmetry observed up to the third step is broken and particle has a preferred direction after this step.

By using results in equations (3.26),(3.27),(3.31),(3.32),(3.33),(3.35),(3.36),(3.37) and (3.38), one can draw a table similar to Pascals triangle in classical random walk.

Table 3.1: The probabilities of finding particle at the position n after 4 steps. Symmetric probability distribution is lost after the third step of the walk.

Step $t=0$:					1			
Step $t=1$:				1/2		1/2		
Step $t=2$:			1/4		1/2		1/4	
Step $t=3$:		1/8		1/8		5/8		1/8
Step $t=4$:	1/16		1/8		1/8		5/8		1/16

.

Further steps can be done by using Monte-Carlo sampling. Figure (3.1) represents probability distribution for 150 steps with the given initial wave function and Hadamard coin. As it is clear this distribution is strikingly differs from its classical form. Calculations show that the symmetry break depends on coin or particles initial state. In our calculations by Hadamard coin, symmetry breaking comes from walkers initial state.

One way of obtaining a symmetric distribution is to start by a superposition state like $\frac{1}{\sqrt{2}}(|\uparrow\rangle + i\,|\downarrow\rangle \otimes |0\rangle)$. another way to obtain a symmetric distribution is to use a symmetric coin, namely

$$Y = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}. \tag{3.39}$$

Symmetric distribution is shown in figure: (3.2).

It is clear that analytical calculation of the time evolution on the real space is extremely cumbersome. It is very difficult to continue calculating the probabilities for a particle observed for a long time duration. In the following chapter the momentum space representation of the quantum random walk will be presented. Since the transition probability matrix of the quantum walk in the Fourier transformed form is diagonal, it is easier to go steps far above a few of initial steps.

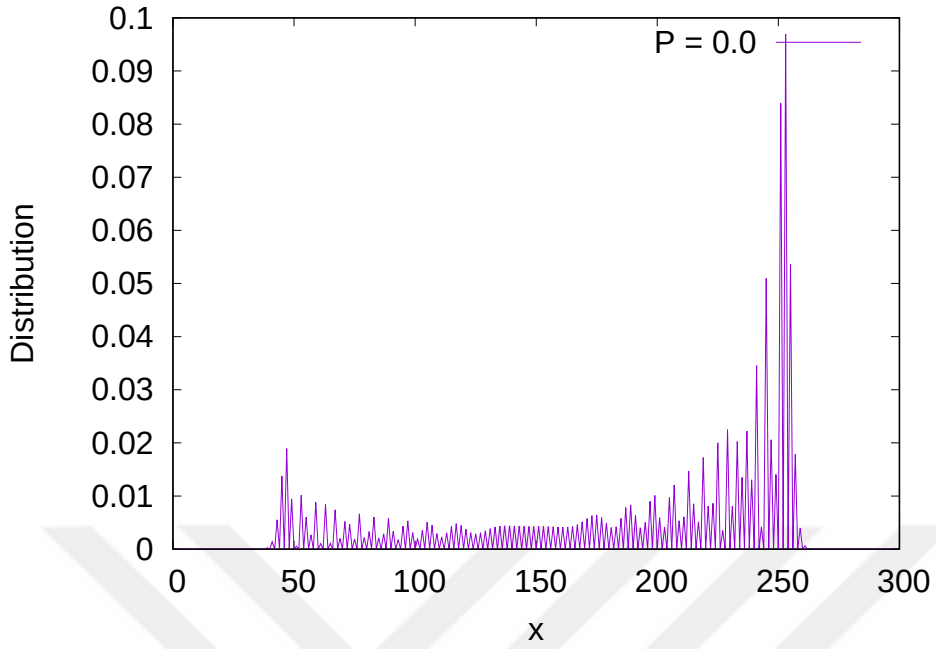


Figure 3.1: Probability distribution of quantum walk on a line with Hadamard coin for 150 steps. Initial state is $|\uparrow\rangle \otimes |0\rangle$.

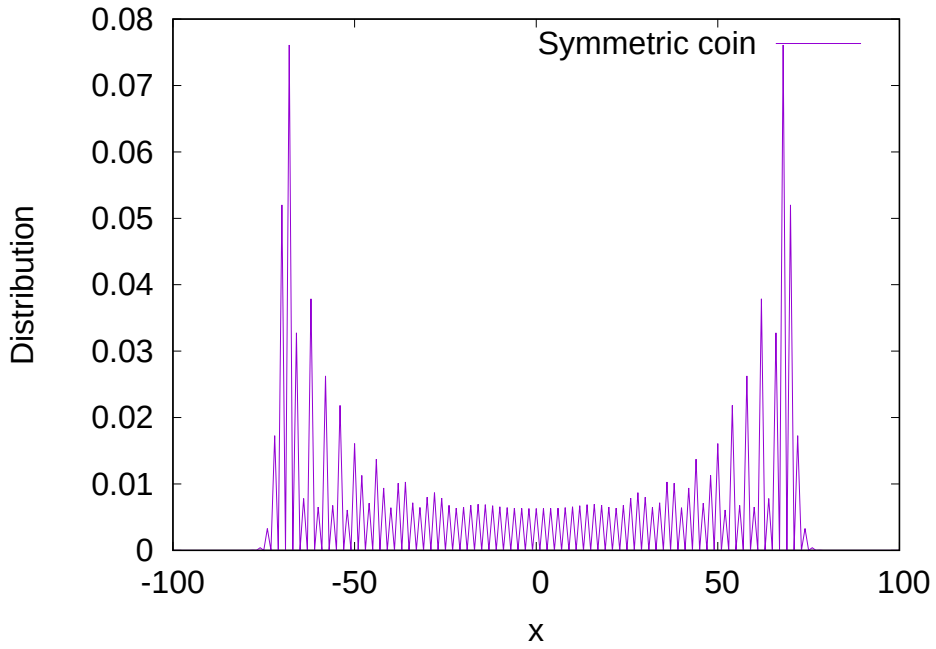


Figure 3.2: Probability distribution of quantum walk with a symmetric coin for 150 steps. Initial state is $|\uparrow\rangle \otimes |0\rangle$. *THis probability distribution can also be derived by Hadamard coin with symmetric initial state (*$\frac{1}{\sqrt{2}}(|\uparrow\rangle + i\,|\downarrow\rangle \otimes |0\rangle$*).*

4. QUANTUM WALKS ON ALINE USING MOMENTUM SPACE

Introduction

First mathematical formulations of quantum walks on a line is done directly in position space. This method is explained in the previous chapter and results are presented for four steps of quantum walk. Another approach for calculating quantum walk is to formulate it using momentum space or fourier transformations of the real space quantum walk. This chapter is devoted to the second approach, in which the wave function of the particle, written in coordinate space, is transformed to momentum space. An important advantage of this method is that matrices and the operators in momentum space are diagonal and hence it is easy to apply them to wave functions written in momentum space.Therefore, it can facilitate mathematical calculation and develops a method in which diagonalized operators generate an analytical formalism to find general form of wave function in any quantum walk with arbitrary number of steps. In short the momentum space quantum walk method provides a formalism in which a general form to quantum walk can be generated. In this chapter the details of formalism of quantum walk in momentum space is reviewed. By the end of this chapter a fairly general notation for quantum walk on a line is provided to be used in the following chapter for the case with decoherence.

Generating quantum walk operators in momentum space

In the previous chapter, quantum walks generated by the spatial shift operator S. This operator makes conditional translation of the system by applying to the wave function. The present section is devoted to derivation of the quantum walk in momentum space. To generate the momentum space representation of S, it is convenient to start with completeness relations in momentum and position spaces [21]:

$$\int |p\rangle \langle p| \, dp = 1 \tag{4.1}$$

$$\sum_n |n\rangle \langle n| = 1 \tag{4.2}$$

The definition below shows relation between momentum and position spaces:

$$\langle n| \, p\rangle = \frac{e^{-ipn/\hbar}}{\sqrt{2\pi\hbar}}. \tag{4.3}$$

To calculate integrals, the definition of the Dirac delta function in both position and momentum spaces are necessary,

$$\langle n| \, m\rangle = \delta_{n,m} \tag{4.4}$$

$$\langle p|\ p\prime\rangle = \delta(p - p\prime). \tag{4.5}$$

Hence by using equations (4.1) and (4.4), is calculated that:

$$\int \langle n|\ p\rangle \langle p|\ m\rangle\, dp = \delta_{n,m}$$

$$\int \frac{e^{-ipn/\hbar}}{\sqrt{2\pi\hbar}} \frac{e^{+ipm/\hbar}}{\sqrt{2\pi\hbar}} dp = \delta_{n,m}.$$

Using equation (4.3):

$$\int\ e^{-ip(n-m)/\hbar} dp = (2\pi\hbar)\ \delta_{n,m} \tag{4.6}$$

and from equations (4.2), (4.3) and (4.5) it is written as:

$$\sum_n\ e^{-i(p-p\prime)n/\hbar} dp = (2\pi\hbar)\ \delta(p - p\prime). \tag{4.7}$$

These seven equations form a set of relations necessary to obtain momentum space representation of unitary operator S:

$$S = |\uparrow\rangle \langle\uparrow| \otimes \sum_n |n+1\rangle \langle n| + |\downarrow\rangle \langle\downarrow| \otimes \sum_n |n-1\rangle \langle n|. \tag{4.8}$$

It is convenient to separate space part of the equation (4.8) in two parts called T_+ and T_- operators as follows:

$$T_+ = \sum_n |n+1\rangle \langle n|$$

and

$$T_- = \sum_n |n-1\rangle \langle n|.$$

By using equation (4.1) twice, T_+ can be written as:

$$T_+ = \int dp \int dp\prime\, |p\rangle \langle p|\, T_+(n)\, |p\prime\rangle \langle p\prime|\,.$$

By using equation (4.4) it is:

$$T_+ = \iint dp\, dp\prime\, |p\rangle \langle p\prime| \sum_n \langle p|\ n+1\rangle \langle n|\ p\prime\rangle =$$

$$\iint dp\, dp\prime\, |p\rangle\, \langle p\prime|\, \frac{1}{2\pi\hbar} \sum_n e^{+ip(n+1)/\hbar} e^{-ipn/\hbar} =$$

$$\iint dp\, dp\prime\, |p\rangle\, \langle p\prime|\, \frac{1}{2\pi\hbar} \sum_n e^{-ipn(p\prime - p)/\hbar} e^{ip/\hbar}.$$

From equation (4.3) :

$$T_+ = \iint dp\, dp\prime\, |p\rangle\, \langle p\prime|\, \frac{1}{2\pi\hbar} (2\pi\hbar)\, \delta(p\prime - p) e^{ip/\hbar}$$

and finally one can get a simple form for T_+ as:

$$T_+ = \int dp\, |p\rangle\, \langle p|\, e^{ip/\hbar}. \tag{4.9}$$

In the same way one can work out that $T_-(p)$ has following form:

$$T_- = \int dp\, |p\rangle\, \langle p|\, e^{-ip/\hbar}. \tag{4.10}$$

To represent operator S in momentum space, it is conveniently expressed spin the matrix representation of part of the operator in the equation (4.8). Base vectors in 2-dimensional coin Hilbert space can be define as follows:

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

and

$$|\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Therefore coin related parts of the S operator are equal to:

$$|\uparrow\rangle\, \langle\uparrow| = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, |\downarrow\rangle\, \langle\downarrow| = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.11}$$

By putting equations above in equation (4.8) it turns out to be [21]:

$$S = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \int dp\, |p\rangle\, \langle p|\, e^{ip/\hbar} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes \int dp\, |p\rangle\, \langle p|\, e^{-ip/\hbar}.$$

Finally by adding two terms of this equation, S appear in momentum space as:

$$S = \int dp \begin{pmatrix} e^{ip/\hbar} & 0 \\ 0 & e^{-ip/\hbar} \end{pmatrix} \otimes |p\rangle\, \langle p|\, . \tag{4.12}$$

Equation (4.12) is the new form for equation (4.8) in momentum space. It is obvious that in

this form, the matrix is diagonal and it is simpler than its counterpart in position space.

The most general SU(2) operator,C, must be multiplied to S to get U operator as $U = SC$ in momentum space. From equations (3.16) and (4.12) **U** is equal to:

$$\mathbf{U} = \int dp \begin{pmatrix} e^{ip/\hbar}cos(\gamma) & e^{ip/\hbar}sin(\gamma) \\ e^{-ip/\hbar}sin(\gamma) & -e^{-ip/\hbar}cos(\gamma) \end{pmatrix} \otimes |p\rangle \langle p| . \tag{4.13}$$

In the specific case, the Hadamard coin operator is used. The unitary time evolution operator, **U**(p) for Hadamard walk can be written as:

$$\mathbf{U} = \frac{1}{\sqrt{2}} \int dp \begin{pmatrix} e^{ip/\hbar} & e^{ip/\hbar} \\ e^{-ip/\hbar} & -e^{-ip/\hbar} \end{pmatrix} \otimes |p\rangle \langle p| \tag{4.14}$$

which creates a one step $|\psi(t+1)\rangle = \mathbf{U}\,|\psi(t)\rangle$ Hadamard walk in momentum space. **U(p)** will be used to generate quantum walk in momentum space by.

U(p) contains a matrix which act on both coin space and momentum space. We call this matrix as C(p) since it resembles the coin operator while contains the momentum information.

$$C(p) = \begin{pmatrix} e^{ip/\hbar} & e^{ip/\hbar} \\ e^{-ip/\hbar} & -e^{-ip/\hbar} \end{pmatrix}. \tag{4.15}$$

Generating Hadamard walk in momentum space

Equation (4.14) is the time evolution operator of one step quantum walk in momentum space. As in the previous chapter the quantum walk can be generated by applying this operator to each step of walk and hence one can calculate probability distributions in momentum space. Remembering that the particle's wave function in position space is represented by a wave function $|\psi\rangle$. The wave function of the walker could be expanded by the aid of position base vectors $|n\rangle$'s or momentum space base vectors $|p\rangle$'s like as:

$$|\psi\rangle = \sum_n |n\rangle \langle n|\, \psi\rangle$$

$$|\psi\rangle = \int dp\, |p\rangle \langle p|\, \psi\rangle .$$

Similar to expansion coefficients $\langle n|\, \psi\rangle$ in position space, the expansion coefficients $\langle p|\, \psi\rangle$ in momentum space can also be derived starting the walk on a space position with a particle of definite spin wave function. Deriving $\langle p|\, \psi\rangle$'s in momentum space is easier than position space since in momentum space matrices are diagonal as seen in equation (4.14). The relation

between spatial and momentum space coefficients can be derived by using equation (4.1):

$$|\psi\rangle = \int dp\, |p\rangle \langle p|\ \psi\rangle$$

$$\langle n|\ \psi\rangle = \int dp\, \langle n|\ p\rangle \langle p|\ \psi\rangle$$

and from the equation (4.4) :

$$\langle n|\ \psi\rangle = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{-ipn/\hbar} \langle p|\ \psi\rangle\,. \tag{4.16}$$

Quantum walk of a particle is calculated by iterative application of the operator **U** onto the wave function $|\psi\rangle$ in the current time step:

$$|\psi(t+1)\rangle = \mathbf{U}\, |\psi(t)\rangle\,. \tag{4.17}$$

The discrete time parameter t, in the equation (4.17) corresponds to steps in random walk or in other words the steps can be interpreted as a discrete time. At this point, all relevant expressions to calculate $\langle p|\ \psi\rangle$s are obtained. Therefore equation (4.17) will be multiplied by $\langle p|$ from the left side as follows:

$$\langle p|\ \psi(t+1)\rangle = \langle p|\, \mathbf{U}(p)\, |\psi(t)\rangle\,. \tag{4.18}$$

Suppose that a particle with spin $|\uparrow\rangle$ is placed at the origin initially. The initial wave function of the particle can be written as:

$$|\psi(0)\rangle = |0\rangle \otimes |\uparrow\rangle\,. \tag{4.19}$$

substituting the initial state into the equation (4.14), the walk of the particle with degrees of freedom placed at the origin starts. after the first step, $|\psi(1)\rangle$ represents the wave function of the particle. Hence $\langle p|\ \psi(1)\rangle$ is obtained from:

$$\langle p|\ \psi(1)\rangle = \frac{1}{\sqrt{2}} \int dp\prime\, \langle p|\ p\prime\rangle \langle p\prime|\ 0\rangle \otimes \begin{pmatrix} e^{ip\prime/\hbar} & e^{ip\prime\prime/\hbar} \\ e^{-ip\prime/\hbar} & -e^{-ip\prime/\hbar} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Using delta Dirac functions definition in equation (4.4), it becomes:

$$\langle p|\ \psi(1)\rangle = \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}} \int dp\prime \delta(p-p\prime) e^{ip\prime n/\hbar} \otimes \begin{pmatrix} e^{ip\prime/\hbar} & e^{ip\prime/\hbar} \\ e^{-ip\prime/\hbar} & -e^{-ip\prime/\hbar} \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

which will lead to the simple form of,

$$\langle p|\ \psi(1)\rangle = \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}} \begin{pmatrix} e^{ip/\hbar} \\ e^{-ip/\hbar} \end{pmatrix}.$$

This vector can be expanded in term of base vectors of spin Hilbert space as,

$$\langle p|\ \psi(1)\rangle = \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}}(e^{ip/\hbar} \begin{pmatrix} 1 \\ 0 \end{pmatrix} + e^{-ip/\hbar} \begin{pmatrix} 0 \\ 1 \end{pmatrix}). \tag{4.20}$$

The expansion coefficients of the wave function after one iteration in momentum space which corresponds to $|\uparrow\rangle$ and $|\downarrow\rangle$ spins are:

$$\langle p|\ \psi\rangle_{\uparrow} = \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}} e^{ip/\hbar} \tag{4.21}$$

$$\langle p|\ \psi\rangle_{\downarrow} = \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}} e^{-ip/\hbar}. \tag{4.22}$$

These coefficients can be compared with the position space counterparts by taking inverse Fourier transformations. equation (4.16) with equations (4.21) and (4.22) gives:

$$\langle n|\ \psi\rangle_{\uparrow} = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{-ipn/\hbar}\, \langle p|\ \psi\rangle_{\uparrow}$$

$$\langle n|\ \psi\rangle_{\uparrow} = \frac{1}{\sqrt{2\pi\hbar}} \int dp\, e^{-ipn/\hbar} \frac{1}{\sqrt{2}\sqrt{2\pi\hbar}} e^{ip/\hbar} = \frac{1}{2\pi\hbar}\frac{1}{\sqrt{2}} \int dp\, e^{-ip(n-1)/\hbar}.$$

From delta Dirac relation in equation (4.6):

$$\langle n|\ \psi\rangle_{\uparrow} = \frac{1}{2\pi\hbar}\frac{1}{\sqrt{2}}(2\pi\hbar)\ \delta_{n.1}.$$

The probability of finding particle at position n=1 is:

$$|\langle +1|\ \psi\rangle_{\uparrow}|^2 = \frac{1}{2}. \tag{4.23}$$

In the same manner one can find the probability of having a particle at the point n=-1:

$$|\langle -1|\ \psi\rangle_{\downarrow}|^2 = \frac{1}{2}. \tag{4.24}$$

As it is expected, these results are the same as the previous results obtained in position space approach.

At this point is useful to generate a general form for the quantum walk on the momentum space. According to equation (4.17):

$$|\psi(1)\rangle = \mathbf{U}\,|\psi(0)\rangle$$

and

$$|\psi(2)\rangle = \mathbf{U}\,|\psi(1)\rangle$$

so

$$|\psi(2)\rangle = (\mathbf{U}(p))^2\,|\psi(0)\rangle\,.$$

After t steps one can obtain the particle wave function from the initial state function by applying $\mathbf{U}$ t times,

$$|\psi(t)\rangle = (\mathbf{U})^t\,|\psi(0)\rangle\,. \tag{4.25}$$

Powers of equation (4.14) must be found, and for generating step 2 we need to square power as follows:

$$\iint dp\,dp\prime\,|p\prime\rangle\,\langle p\prime|\,p\rangle\,\langle p|\,C(p\prime)C(p) =$$

$$\iint dp\,dp\prime\,|p\prime\rangle\,\delta(p-p\prime)\,\langle p|\,C(p\prime)C(p) =$$

$$\mathbf{U}^2 = \int dp\,|p\rangle\,\langle p|\,C(p)^2. \tag{4.26}$$

All that it needs to be done is to find powers of 2×2 matrix in equation (4.15) which is called C(p) and square of it:

$$C(p)^2 = \frac{1}{2}\begin{pmatrix} e^{ip/\hbar} & e^{ip/\hbar} \\ e^{-ip/\hbar} & -e^{-ip/\hbar} \end{pmatrix}\begin{pmatrix} e^{ip/\hbar} & e^{ip/\hbar} \\ e^{-ip/\hbar} & -e^{-ip/\hbar} \end{pmatrix} =$$

$$\frac{1}{2}\begin{pmatrix} e^{2ip/\hbar}+1 & e^{2ip/\hbar}-1 \\ 1-e^{-2ip/\hbar} & 1+e^{-2ip/\hbar} \end{pmatrix}. \tag{4.27}$$

Now by acting $\mathbf{U}^2$ just on initial state step 2 would be generated directly without using results of step 1. This is th main reason why it is better to use momentum space method rather direct position space method. $\mathbf{U}^2$ applied as follow:

$$\begin{aligned}\langle p\prime|\,\mathbf{U}^2\,|\psi(0)\rangle = & \\ & \langle p\prime|\,\mathbf{U}^2\,|0\rangle\otimes|\uparrow\rangle \\ & = \int dp\,\langle p\prime|\,p\rangle\,\langle p|\,0\rangle\,\frac{1}{2}\begin{pmatrix} e^{2ip/\hbar}+1 & e^{2ip/\hbar}-1 \\ 1-e^{-2ip/\hbar} & 1+e^{-2ip/\hbar} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix}. \\ & = \frac{1}{2}\frac{1}{2\pi\hbar}\int dp\,\delta(p-p\prime)\begin{pmatrix} e^{2ip/\hbar}+1 \\ 1-e^{-2ip/\hbar} \end{pmatrix}\end{aligned} \tag{4.28}$$

Again as in the step 1 result can be studied separately to two components of the spin. Hence there are two terms which are for spin up:

$$\langle p|\ \psi(2)\rangle_{\uparrow} = \frac{1}{2}\frac{1}{2\pi\hbar}(e^{2ip/\hbar}+1) \tag{4.29}$$

And the other is for spin down:

$$\langle p|\ \psi(2)\rangle_{\downarrow} = \frac{1}{2}\frac{1}{2\pi\hbar}(1-e^{-2ip/\hbar}). \tag{4.30}$$

Now the equation (4.16) can be readily lined to find coefficients in position space as follows:

$$\langle n|\ \psi\rangle = \frac{1}{2}\frac{1}{2\pi\hbar}\int dp\, e^{-ipn/\hbar}(e^{2ip/\hbar}+1)$$

$$= \frac{1}{2}\frac{1}{2\pi\hbar}\int dp e^{-ip(n-2)/\hbar} + \frac{1}{2}\frac{1}{2\pi\hbar}\int dp e^{-ipn/\hbar}$$

$$= \frac{1}{2}\frac{1}{2\pi\hbar}(2\pi\hbar)\ \delta_{n,2} + \frac{1}{2}\frac{1}{2\pi\hbar}(2\pi\hbar)\ \delta_{n,0}$$

$$\langle n|\ \psi\rangle = \frac{1}{2} \qquad n=2 \tag{4.31}$$

$$\langle n|\ \psi\rangle = \frac{1}{2} \qquad n=0 \tag{4.32}$$

$$\langle n|\ \psi\rangle = \frac{1}{2}\frac{1}{2\pi\hbar}\int dp\, e^{-ipn/\hbar}(1-e^{-2ip/\hbar})$$

$$= \frac{1}{2}\frac{1}{2\pi\hbar}\int dp e^{-ipn/\hbar} + \frac{1}{2}\frac{1}{2\pi\hbar}\int dp e^{-ip(n+2)/\hbar}$$

$$= \frac{1}{2}\frac{1}{2\pi\hbar}(2\pi\hbar)\ \delta_{n,0} + \frac{1}{2}\frac{1}{2\pi\hbar}(2\pi\hbar)\ \delta_{n,-2}$$

$$\langle n|\ \psi\rangle = \frac{1}{2} \qquad n=0 \tag{4.33}$$

$$\langle n|\ \psi\rangle = \frac{1}{2} \qquad n=-2. \tag{4.34}$$

According to equations (4.31), (4.32), (4.33) and (4.34) probabilities can be found as:

$$|\langle n|\ \psi\rangle|^2 = \frac{1}{4} \tag{4.35}$$

$$|\langle n|\ \psi\rangle|^2 = \frac{1}{2} \tag{4.36}$$

$$|\langle n|\ \psi\rangle|^2 = \frac{1}{4} \qquad n = -2. \tag{4.37}$$

It is clear that for the step t=3 $C(p)^3$ must be calculated:

$$\frac{1}{\sqrt{2}}\begin{pmatrix} e^{ip/\hbar} & e^{ip/\hbar} \\ e^{-ip/\hbar} & -e^{-ip/\hbar} \end{pmatrix}\frac{1}{2}\begin{pmatrix} e^{2ip/\hbar}+1 & e^{2ip/\hbar}-1 \\ 1-e^{-2ip/\hbar} & 1+e^{-2ip/\hbar} \end{pmatrix}$$

$$= \frac{1}{2\sqrt{2}}\begin{pmatrix} e^{3ip/\hbar}+2e^{ip/\hbar}-e^{-ip/\hbar} & e^{3ip/\hbar}+e^{-ip/\hbar} \\ e^{ip/\hbar}+e^{-3ip/\hbar} & e^{ip/\hbar}-2e^{-ip/\hbar}+e^{-3ip/\hbar} \end{pmatrix}.$$

After applying it to spin up of starting state:

$$\frac{1}{2\sqrt{2}}\begin{pmatrix} e^{3ip/\hbar}+2e^{ip/\hbar}-e^{-ip/\hbar} \\ e^{ip/\hbar}+e^{-3ip/\hbar} \end{pmatrix}. \tag{4.38}$$

There are 5 terms in equation (4.38) and by the same way in before steps 5 coefficients are found as follows:

$$\langle n|\ \psi\rangle = \frac{1}{2\sqrt{2}} \qquad n = 3 \tag{4.39}$$

$$\langle n|\ \psi\rangle = \frac{1}{\sqrt{2}} \qquad n = 1 \tag{4.40}$$

$$\langle n|\ \psi\rangle = -\frac{1}{2\sqrt{2}} \qquad n = -1 \tag{4.41}$$

$$\langle n|\ \psi\rangle = \frac{1}{2\sqrt{2}} \qquad n = 1 \tag{4.42}$$

$$\langle n|\ \psi\rangle = \frac{1}{2\sqrt{2}} \qquad n = -3. \tag{4.43}$$

By square power of above equations the probabilities can be found as:

$$|\langle 3|\ \psi\rangle|^2 = \frac{1}{8} \tag{4.44}$$

$$|\langle 1|\ \psi\rangle|^2 = \frac{5}{8} \tag{4.45}$$

$$|\langle -1|\ \psi\rangle|^2 = \frac{1}{8} \tag{4.46}$$

$$|\langle -3|\ \psi\rangle|^2 = \frac{1}{8}. \tag{4.47}$$

The probabilities of being at points +3, +1, -1, -3 are respectively equal to $\frac{1}{8}$, $\frac{5}{8}$, $\frac{1}{8}$ and $\frac{1}{8}$.

These results are the same as they had been generated in previous chapter using spatial expansion method. In table (3.1) the probabilities of ,there is 4 steps of Quantum Random Walk on a line have been presented. The values are exactly obtained in momentum space.

It is shown that the momentum space methods lead to the same results that was found by using the position space methods. In the next section a general form will be presented for the momentum space methods which lead us to finding a general formalism for t step quantum walk.

Finding general form of the wave function for t'th step by Hadamard coin

As it is discussed in the previous section, the general form of a t step of quantum walk can be obtained by calculating, t'th power of C(p). In order to calculate the t'th step of a quantum walk, one need to calculate the t'th power of the unitary time evolution matrix

$$C(p) = \begin{pmatrix} \frac{e^{ip/\hbar}}{\sqrt{2}} & \frac{e^{ip/\hbar}}{\sqrt{2}} \\ \frac{e^{-ip/\hbar}}{\sqrt{2}} & \frac{-e^{-ip/\hbar}}{\sqrt{2}} \end{pmatrix}^t.$$

Finding the t'th power is is not straightforward but if C(p) matrix can be diagonalized, it will be possible to find its powers in terms of its eigenvalues. To simplify writing process it is suitable to replace $\frac{P}{\hbar}$ with k. Hence the above matrix changes to:

$$C(K) = \begin{pmatrix} \frac{e^{ik}}{\sqrt{2}} & \frac{e^{ik}}{\sqrt{2}} \\ \frac{e^{-ik}}{\sqrt{2}} & -\frac{e^{-ik}}{\sqrt{2}} \end{pmatrix}^t. \tag{4.48}$$

To diagonalize the matrix in equation (4.48), determinant of the matrix should be calculated as:

$$det \begin{pmatrix} \frac{e^{ik}}{\sqrt{2}} - \lambda & \frac{e^{ik}}{\sqrt{2}} \\ \frac{e^{-ik}}{\sqrt{2}} & -\frac{e^{-ik}}{\sqrt{2}} - \lambda \end{pmatrix} = 0$$

$$\lambda^2 - \frac{2i\sin(k)}{\sqrt{2}}\lambda - 1 = 0.$$

From the determinant, the eigenvalues are obtained as:

$$\lambda_1 = \frac{i}{\sqrt{2}}\sin(k) + \sqrt{-\frac{\sin^2(k)}{2} + 1}$$

$$\lambda_2 = \frac{i}{\sqrt{2}}\sin(k) - \sqrt{-\frac{\sin^2(k)}{2} + 1}. \tag{4.49}$$

By changing variable,

$$-\frac{\sin(k)}{\sqrt{2}} = \sin(\omega) \tag{4.50}$$

Eigenvalues take a simpler form:

$$\lambda_1 = e^{-i\omega}$$

$$\lambda_2 = e^{i(\omega+\pi)}. \tag{4.51}$$

Normalized eigenvectors are given by solving the following matrix equation.

$$\begin{pmatrix} \frac{e^{ik}}{\sqrt{2}} & \frac{e^{ik}}{\sqrt{2}} \\ \frac{e^{-ik}}{\sqrt{2}} & -\frac{e^{-ik}}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = e^{-i\omega} \begin{pmatrix} x \\ y \end{pmatrix}$$

The first term is:

$$\frac{e^{ik}}{\sqrt{2}}(x+y) = e^{-i\omega}x$$

This form can be simplified to,

$$e^{ik}y = (\sqrt{2}e^{-i\omega} - e^{ik})x.$$

Hence the first eigenvector is:

$$\begin{pmatrix} e^{ik} \\ \sqrt{2}e^{-i\omega} - e^{ik} \end{pmatrix}.$$

Normalization of this eigenvector as:

$$\alpha^2 \begin{pmatrix} e^{-ik} & \sqrt{2}e^{+i\omega} - e^{-ik} \end{pmatrix} \begin{pmatrix} e^{ik} \\ \sqrt{2}e^{-i\omega} - e^{ik} \end{pmatrix} = 1$$

given,

$$\alpha = \frac{1}{\sqrt{2}}\left(1 + \cos^2(k) - \cos(k)\sqrt{1 + \cos^2(k)}\right)^{-\frac{1}{2}}. \tag{4.52}$$

Finally the first normalized eigenvector corresponding to the normalized eigenvalue λ is ob-

tained as:

$$|\phi_1\rangle = \frac{1}{\sqrt{2}}\left(1+\cos^2(k)-\cos(k)\sqrt{1+\cos^2(k)}\right)^{-\frac{1}{2}}\begin{pmatrix} e^{ik} \\ \sqrt{2}e^{-i\omega}-e^{ik} \end{pmatrix}. \tag{4.53}$$

Second normalized eigenvector which correspond to the second eigenvalue λ_2 is found in the same way as the first one.

$$|\phi_2\rangle = \frac{1}{\sqrt{2}}\left(1+\cos^2(k)+\cos(k)\sqrt{1+\cos^2(k)}\right)^{-\frac{1}{2}}\begin{pmatrix} -e^{ik} \\ +\sqrt{2}e^{i\omega}+e^{ik} \end{pmatrix}. \tag{4.54}$$

Now by deriving eigenvalues and eigenvectors of the C(p) matrix, the diagonalization process is finished.Therefore it is possible to find any power of C(p) matrix. C(p) can be expanded in the given vector space,

$$C(p) = \lambda_1 |\phi_1\rangle \langle\phi_1| + \lambda_2 |\phi_2\rangle \langle\phi_2| \tag{4.55}$$

Since $|\phi_1\rangle$ and $|\phi_2\rangle$ are normalized base vectors, the power of C(p) can be written simply as:

$$C(p)^t = \lambda_1^t |\phi_1\rangle \langle\phi_1| + \lambda_2^t |\phi_2\rangle \langle\phi_2| . \tag{4.56}$$

Above equation gives us an easy way to get the power of C. We must Find $|\phi_1\rangle \langle\phi_1| \, and \, |\phi_2\rangle \langle\phi_2|$ operators. First one is equal to:

$$\begin{aligned} |\phi_1\rangle \langle\phi_1| = & \\ & \frac{1}{2\left(1+\cos^2(k)-\cos(k)\sqrt{1+\cos^2(k)}\right)} \\ & \begin{pmatrix} e^{ik} \\ \sqrt{2}e^{-i\omega}-e^{ik} \end{pmatrix}\begin{pmatrix} e^{-ik} & \sqrt{2}e^{i\omega}-e^{-ik} \end{pmatrix} \\ & = \frac{1}{2\left(1+\cos^2(k)-\cos(k)\sqrt{1+\cos^2(k)}\right)} \\ & \begin{pmatrix} 1 & \sqrt{2}e^{i(k-\omega)}-1 \\ \sqrt{2}e^{-i(k-\omega)}-1 & 2+\sqrt{2}e^{-i(k-\omega)}-\sqrt{2}e^{i(k-\omega)}+1 \end{pmatrix} \end{aligned} \tag{4.57}$$

and the second one is:

$$
\begin{aligned}
&|\phi_2\rangle \langle\phi_2| = \\
&\frac{1}{2\left(1+\cos^2(k)+\cos(k)\sqrt{1+\cos^2(k)}\right)} \\
&\begin{pmatrix} -e^{ik} \\ \sqrt{2}e^{-i\omega}+e^{ik} \end{pmatrix}\begin{pmatrix} -e^{ik} & \sqrt{2}e^{i\omega}+e^{-ik} \end{pmatrix} \\
&= \frac{1}{2\left(1+\cos^2(k)+\cos(k)\sqrt{1+\cos^2(k)}\right)} \\
&\begin{pmatrix} 1 & -\sqrt{2}e^{i(k-\omega)}-1 \\ -\sqrt{2}e^{-i(k-\omega)}-1 & 2+\sqrt{2}e^{-i(k-\omega)}+\sqrt{2}e^{i(k-\omega)}+1 \end{pmatrix}
\end{aligned}
\quad . \tag{4.58}
$$

Similar to the second step in previous section in equation (4.28) by multipication of matrix C(p) to the up state,only 2 terms of the first column of matrix $C(p)^2$ are the answers that is needed here. because first wave function had spin up state, the other terms are vanished.

$$
\begin{pmatrix} C_{11} & C12 \\ C_{21} & C_{22} \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} C_{11} \\ C_{21} \end{pmatrix}. \tag{4.59}
$$

Hence, only the first column of the matrix $C(p)^t$ must be worked out. From equations (4.57) and (4.58) the first term of first column is:

$$
C_{11} = \frac{1}{2\left(1+\cos^2(k)-\cos(k)\sqrt{1+\cos^2(k)}\right)}e^{-i\omega t} - \frac{1}{2\left(1+\cos^2(k)+\cos(k)\sqrt{1+\cos^2(k)}\right)}e^{i\omega t}
$$

$$
= \frac{e^{-i\omega t}2\left(1+\cos^2(k)-\cos(k)\sqrt{1+\cos^2(k)}\right) - e^{i\omega t}2\left(1+\cos^2(k)+\cos(k)\sqrt{1+\cos^2(k)}\right)}{4\left(\left(1+\cos^2(k)\right)^2-\cos^2(k)\left(1+\cos^2(k)\right)\right)}.
$$

The denominator of the last fraction is equal to $4(1+\cos^2(k))$ so C_{11} is equal to:

$$
C_{11} = \frac{1}{2}\left(1+\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{-i\omega t} + \frac{(-1)^t}{2}e^{i\omega t}\left(1-\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{i\omega t}. \tag{4.60}
$$

Just like as the way of figuring out equation (4.21) it can be represented that:

$$\langle p|\ \psi(t)\rangle_{\uparrow} = \frac{1}{\sqrt{2\pi}}\frac{1}{2}\left(1+\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{-i\omega t}+\frac{(-1)^t}{2}e^{i\omega t}\left(1-\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{i\omega t}. \tag{4.61}$$

Using the equation (4.16) $\langle n|\ \psi\rangle_{\uparrow}$is found as follows:

$$\langle n|\ \psi\rangle_{\uparrow} = \frac{1}{2\pi}\int dk e^{ikn}\frac{1}{2}\left(1+\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{-i\omega t}+$$

$$\frac{(-1)^t}{2}e^{i\omega t}\left(1-\frac{\cos(k)}{\sqrt{1+\cos^2(k)}}\right)e^{i\omega t}. \tag{4.62}$$

Second coefficient C_{21} can be found by the same way as C_{11}.

So it is shown that by using momentum space representation of time evolution operator of quantum walk can be diagonalized and it is easy to find its t'th power analytically. On the other hand finding t'th power of random walk operator enables us to find t'th step of walk without finding $t-1$ previous steps.

In this section, as an specific example, Hadamard coin operator is used to calculate momentum space time evolution operator. In fact it is straightforward to generalized the results for the most general coin operator. This generalization will open the doors to find results for every coin that we need.

General form of the wave function for general coin

In previous section the general form of the wave function for Hadamard coin was calculated. Now the same process will follow again to find results for general form of coin operator. The general coin matrix for 2 dimensional spin Hilbert space is equation (3.16).

$$C = \begin{pmatrix} \cos(\gamma) & \sin(\gamma) \\ \sin(\gamma) & -\cos(\gamma) \end{pmatrix}.$$

By multiplying C(p) matrix with general coin above:

$$C(p) = \begin{pmatrix} e^{ip/\hbar}\cos(\gamma) & e^{ip/\hbar}\sin(\gamma) \\ e^{-ip/\hbar}\sin(\gamma) & -e^{-ip/\hbar}\cos(\gamma) \end{pmatrix}.$$

Again, as it is done in the previous section, it is suitable to use $k = p/\hbar$ to simplify writing. Power t of following matrix must be worked out:

$$C(k) = \begin{pmatrix} e^{ik}\cos(\gamma) & e^{ik}\sin(\gamma) \\ e^{-ik}\sin(\gamma) & -e^{-ik}\cos(\gamma) \end{pmatrix}^t. \tag{4.63}$$

In order to diagonalize the matrix in equation (4.63), eigenvalues and eigenvectors need to be calculated as follows:

$$det \begin{pmatrix} e^{ik}\cos(\gamma) - \lambda & e^{ik}\sin(\gamma) \\ e^{-ik}\sin(\gamma) & -e^{-ik}\cos(\gamma) - \lambda \end{pmatrix} = 0. \tag{4.64}$$

The eigenvalues are:

$$\lambda_1 = i\cos(\gamma)\sin(k) + \sqrt{-\cos^2(\gamma)\sin^2(k) + 1}$$

$$\lambda_1 = i\cos(\gamma)\sin(k) - \sqrt{-\cos^2(\gamma)\sin^2(k) + 1} \tag{4.65}$$

Changing the variables as follows,

$$\cos(\gamma)\sin(k) = \sin(\omega). \tag{4.66}$$

Simplify the form of the eigenvalues, two eigenvalues are:

$$\lambda_1 = e^{i\omega} \tag{4.67}$$

and

$$\lambda_2 = e^{-i\omega}. \tag{4.68}$$

The corresponding eigenvectors are:

$$\begin{pmatrix} e^{ik}\cos(\gamma) & e^{ik}\sin(\gamma) \\ e^{-ik}\sin(\gamma) & -e^{-ik}\cos(\gamma) \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = e^{i\omega} \begin{pmatrix} x \\ y \end{pmatrix}.$$

Two equation bellow is taken from the above matrix equation.

$$\cos(\gamma)e^{ik}x + \sin(\gamma)e^{ik}y = e^{i\omega}x$$

$$y = \frac{e^{i\omega} - \cos(\gamma)e^{ik}}{\sin(\gamma)e^{ik}}x.$$

By solving these two equations the first eigenvector is found as follows:

$$\begin{pmatrix} \sin(\gamma)e^{ik} \\ e^{i\omega} - \cos(\gamma)e^{ik} \end{pmatrix}.$$

The normalized eigenvectors are obtained,

$$\alpha^2 \begin{pmatrix} \sin(\gamma)e^{-ik} & e^{i\omega} - \cos(\gamma)e^{-ik} \end{pmatrix} \begin{pmatrix} \sin(\gamma)e^{ik} \\ e^{i\omega} - \cos(\gamma)e^{ik} \end{pmatrix} = 1$$

by calculating α where,

$$\alpha = \frac{1}{\sqrt{2}} \left(1 - \cos(\gamma) \left(\cos(k)\sqrt{1 - \cos^2(\gamma)\sin^2(k)} - \sin^2(k)\right)\right)^{-\frac{1}{2}}.$$

Finally the first normalized eigenvector is found as follows:

$$|\phi_1\rangle = \frac{1}{\sqrt{2}} \left(1 - \cos(\gamma) \left(\cos(k)\sqrt{1 - \cos^2(\gamma)\sin^2(k)} - \sin^2(k)\right)\right)^{-\frac{1}{2}} \begin{pmatrix} \sin(\gamma)e^{ik} \\ e^{i\omega} - \cos(\gamma)e^{ik} \end{pmatrix}. \tag{4.69}$$

The second eigenvector is also can be found in the same way. As the eigenvalues and eigenvectors of the matrix C(p) one obtained, C(p) can be expanded in terms of eigenvalues and their corresponding eigenvectors.

By finding eigenvectors matrix C(p) can be diagonalized as:

$$C(p) = \lambda_1 |\phi_1\rangle \langle\phi_1| + \lambda_2 |\phi_2\rangle \langle\phi_2|. \tag{4.70}$$

To find t'th step of walk it's t'th power can be derived to as:

$$C(p)^t = \lambda_1^n |\phi_1\rangle \langle\phi_1| + \lambda_2^n |\phi_2\rangle \langle\phi_2|. \tag{4.71}$$

Hence, it is not necessary to calculate the probability distribution step by step, but it is fully obtained by applying the t'th power of the time evolution operator on the initial state vector. The momentum space representation of the walk simplifies the calculations and envelope the possibilities of application of quantum random walk to various complicated problems. One of the most realistic class of systems to be studied are the quantum systems with external influence. When the system interacts with its environment, the quantum correlations are lost. The time duration and the amount of quantum correlation can be obtained by using the momentum space technique. In the next chapter the decoherence while result in the loss of quantum correlation will be discussed by using both spatial and momentum space wave functions. Before proceeding to the next chapter, in next section notation for fairly general

quantum walk will be prepared. This general notation is necessary to formulate decoherence in an appropriate way in next chapter.

General quantum walk on a line description

After detailed calculations for Hadamard walk on a line in position and momentum space and finding general form of wave function for general coin, now it is time to discuss and formulate fairly general quantum walk on a line without details. This symbolization method will give us a general point of view and it will summarize all it is done up to now. Moreover, this section and its notation is necessary to understand general discussions of the next chapter.

Position space

In previous chapters, because of its simplicity, the position of particle in discrete space represented by n and in quantum walk with eigenstates $|n\rangle$ with eigenvalues n. Here in the present subsection the position degree of freedom of quantum mechanical particle will be describe by position eigenstates $\{|x\rangle\}$ with eigenvalues x which x is an integer. Suppose position operator is **x** which $\mathbf{x}\,|x\rangle = x\,|x\rangle$. Spin degree of freedom is described by D-dimensional vector space spanned by the base vectors $|\phi\rangle$ whose initial state is $|\phi_0\rangle$. Orthogonal projection operators for Hilbert state of the coin described generally by operators S_+ and S_- and they are defined in a way that $S_+ + S_- = I$. I is Identity operator. These operators represent two possible outcomes of coin. Coin operator C is an unitary transformation in spin Hilbert state defined in such a way that when it acts on spin state, a superposition of eigenvalues on d-dimensional is obtained. Special example of such operator is Hadamard operator which is already discussed. Steps of quantum walk is given by the unitary operator:

$$U = (T_+ \otimes S_+ + T_- \otimes S_-)\,(I \otimes C)\,. \tag{4.72}$$

Special case for this operator is equation (3.17). Here T_+ and T_- are shift operators discussed in chapter 2. They have the property that can shift the particle to the right or left when they act on wave function of particle.

$$T_+\,|x\rangle = |x+1\rangle \tag{4.73}$$

$$T_-\,|x\rangle = |x-1\rangle\,. \tag{4.74}$$

Suppose initial state of walker is:

$$|\psi_0\rangle = |0\rangle \otimes |\phi_0\rangle\,. \tag{4.75}$$

Momentum space

Definition of momentum space is given by equation (4.3). on the other hand momentum space eigenvectors, $|k\rangle$, are defined as:

$$|k\rangle = \sum_x e^{-ikx} |x\rangle . \tag{4.76}$$

In equations (4.9) and (4.10) momentum space representation of shift operators are derived. By considering eigenvectors $|k\rangle$ for momentum Hilbert space of T_+ and T_- we have,

$$T_+ |k\rangle = e^{ik} |k\rangle \tag{4.77}$$

$$T_- |k\rangle = e^{-ik} |k\rangle . \tag{4.78}$$

Finally the time evolution operator in momentum space becomes:

$$U(|k\rangle \otimes |\phi\rangle) = |k\rangle \otimes \left(e^{ik} S_+ + e^{-ik} S_-\right) C |\phi\rangle \equiv |k\rangle \otimes C(k) |\phi\rangle \tag{4.79}$$

which C(k) is a unitary operator that acts only on coin degree of freedom. In next chapter this general notation for quantum walk will be used to explain decoherence effects analytically.

5. DECOHERENCE

Introduction

Quantum correlations are the key element for quantum computation and quantum information. Despite its importance, quantum correlations are very fragile since the interaction with the environment create decoherence and dephasing. For this reason quantitative understanding of decoherence plays an important role in order to advance the quantum technology. Prevention dephasing of states which exhibits quantum correlations is the major experimental task for advancing quantum technology. One class of technologically promising quantum systems is the discrete time quantum walk systems. The control over the discrete time quantum systems require coherent manipulation of a large quantum system[14]. The Hilbert space of an n-step quantum random walk is $2n$ -dimensional and hence it requires extremely sophisticated engineering and experimental techniques. In such large quantum systems there exist various decoherence mechanisms such as coin decoherence and spatial decoherence. The effect of different types of decoherence on probability distribution has been subjected to both numerically[15] and analytically[16], [17]. Analytical calculations have shown that the controlled decoherence may lead to distributions which are similar to those of obtained in classical random walk. This change on the probability distribution give an account of the quantum-to-classical transition[18], [17]. In the following sections the decoherence in the quantum random walk will be reviewed and particularly coin space decoherence effects on the quantum walk will be discussed using numerical techniques.

Decoherence in quantum walks

The decoherence in the quantum walk appears when a quantum system is under the influence of a non-unitary translation. The relationship between unitary and non-unitary operators on a system first shown in 1992 by Aharonov. [4].

In order to study decoherence the density matrix formalism is more convenient. Density operator can be used to classify the quantum systems. The density operator is defined as the outer product of state kets of the system:

$$\rho = |\psi\rangle \langle\psi| . \tag{5.1}$$

In general form, if the state of the system is classically mixed as follows:

$$|\psi\rangle = \sum a_i |\psi_i\rangle . \tag{5.2}$$

Here, classically mixed means that the state kets, $|\psi_i\rangle$, are not necessarily orthogonal base vectors of the Hilbert space. Therefore the density operator is:

$$\rho = \sum_i {a_i}^2 |\psi_i\rangle \langle\psi_i| \tag{5.3}$$

${a_i}^2$ is the probability of being in state i.

In quantum random walks, the state space is the direct product space of position and spin spaces. Hence, it is useful to label the state ket as $|n, s\rangle$ where n refers to position and s refers to spin degrees of freedoms of the particle respectively. Hence the density operator in this notation takes the form [35]

$$\rho = \sum_{n,s,n',s'} P_{n,s,n',s'} |n, s\rangle \langle n', s'| . \tag{5.4}$$

The important property of density operator is that it is a positive semi-definite Hermitian operator. For a pure state, $\rho^2 = \rho$ and also for a density operator $\mathrm{Tr}(\rho) = 1$. From Matrices theorems, for every density operator there exist a unitary operator that can diagonalize it.

The time evolution operator, $U = SC$, is applied to the state of the system to generate one time step of the quantum random walk. Here in the density operator formalism, the time evolution operator $U = SC$ will be applied to the density operator ρ. In each step after applying $U = SC$ the density matrix represents the system moved one step in time,

$$\rho' = U\rho U^\dagger. \tag{5.5}$$

Repeating the same operation t times, between the system at time t and the initial state have the relation,

$$\rho(t) = U^t \rho(0) {U^\dagger}^t. \tag{5.6}$$

This is the representation of an isolated system evolving through discrete time quantum walk process. If this system is not isolated, then various effects must be taken under consideration. System may be under the random influence of the environment or one may apply a measurement on the system. All such external influences are the sources of decoherence or dephasing in the system with quantum correlations. At each step of the walk application of the non-unitary operator corresponds to a measurement done on the system. The measurement, represented by a non-unitary operator N, results decoherence in the system. This means that at each time step an appropriate non-unitary operator is applied on the system together with the time evolution operator, $U = SC$. The resulting transformation on the density operator can be given in the form,

$$\rho' = N\left(SC\rho C^{\dagger}S^{\dagger}\right) \tag{5.7}$$

where N represents non-unitary super-operator representing measurement done on the system.

The specific form of the non-unitary operator N depends on the source of the external intervene. In the next section the form of the non-unitary operator will be discussed for coin space decoherence.

Coin decoherence in quantum walk

There are two different sources of decoherence, one of them is, the decoherence in the coin space. In this section the explicit form of the non-unitary operator which corresponds to measurement done on the coin space will be discussed in this section and the results of the controlled decoherence will be presented.

For this purpose a measurement operator will be applied on coin space at every step of the walk. A set of operator $\{M_n\}$ on 2×2 space which satisfy completeness relation as,

$$\sum_n M_n^{\dagger} M_n = I \tag{5.8}$$

are used for measurement.

Assuming measurement is done by using a non-unitary operator, the density operator of system becomes

$$\rho = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle \langle k'| \otimes \chi_{kk'}, \tag{5.9}$$

here, $\chi_{kk'}$ is the density operator on a vector space of linear operators on H_2.

After the measurement, a density operator χ on H_2 is transformed by

$$\chi \to \chi' = \sum_n M_n \chi M_n^{\dagger}. \tag{5.10}$$

After the measurement, the first step of the of the evolution under coin space decoherence, the density operator becomes as follows:

$$\rho' = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle \langle k'| \otimes \sum_n C_k M_n \chi_{kk'} M_n^{\dagger} C_{k'}^{\dagger}. \tag{5.11}$$

Considering $|0\rangle \otimes |\phi_0\rangle$, ob the initial state is given by the density operator:

$$\rho_0 = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle \langle k'| \otimes | |\phi_0\rangle \langle \phi_0| \,. \tag{5.12}$$

t steps of the walk can be given as,

$$\rho_t = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle \langle k'| \otimes \sum_{n_1,\ldots,n_t} C_k M_{n_t} \cdots C_k M_{n_1} |\phi_0\rangle \langle \phi_0| M_{n_1}^\dagger C_{k'}^\dagger \cdots M_{n_t}^\dagger C_{k'}^\dagger. \tag{5.13}$$

Defining a super-operator $\mathcal{L}_{kk'}$ to be an operator which maps $L(H_1)$ to $L(H_2)$:

$$\mathcal{L}_{kk'} B \equiv \sum_n C_k M_n B M_n^\dagger C_{k'}^\dagger, \ \forall B \in L(H_2), \tag{5.14}$$

then

$$\rho_t = \int \frac{dk}{2\pi} \int \frac{dk'}{2\pi} |k\rangle \langle k'| \otimes \mathcal{L}_{kk'}^t |\phi_0\rangle \langle \phi_0| \,. \tag{5.15}$$

The probability of reaching a point x at time t is given by,

$$\begin{aligned} p(x,t) &= \mathrm{Tr}\{(|x\rangle \langle x| \otimes I)\rho_t\} \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' \langle x|\ k\rangle \langle k'|\ x\rangle \,\mathrm{Tr}\{\mathcal{L}_{kk'}^t |\phi_0\rangle \langle \phi_0|\} \\ &= \frac{1}{(2\pi)^2} \int dk \int dk' e^{ix(k-k')} \,\mathrm{Tr}\{\mathcal{L}_{kk'}^t |\phi_0\rangle \langle \phi_0|\}. \end{aligned} \tag{5.16}$$

Calculating this probability have some difficulties, nevertheless, calculating the expectation value of the moments of the position operator is direct and essential for discussions of the decoherence by using this probability are useful. by definition,

$$\langle x^n \rangle_t = \sum_x x^n P(x,t) \tag{5.17}$$

putting equation (5.16) in this equation:

$$\langle x^n \rangle_t = \frac{1}{(2\pi)^2} \sum_x x^n \int dk \int dk' e^{ix(k-k')} \,\mathrm{Tr}\{\mathcal{L}_{kk'}^t |\phi_0\rangle \langle \phi_0|\}. \tag{5.18}$$

Using equation (4.7) from chapter 3 and summing over x by using the expansion,

$$\sum_x x^n e^{-ix(k-k')} = 2\pi(-i^n)\delta^n(k-k'). \tag{5.19}$$

The expectation values of the moments of x can be calculated.

$$\langle x^n \rangle_t = \frac{(-i^n)}{2\pi} \sum_x x^n \int dk \int dk' \delta^n(k-k') \, \mathrm{Tr}\{\mathcal{L}^t_{kk'} \left|\phi_0\right\rangle \left\langle\phi_0\right|\}. \tag{5.20}$$

The resulting expression can be integrated by parts. Under the assumptions below it will be done.

$$\frac{d}{dk} \mathrm{Tr}\{\mathcal{L}_{kk'}\Lambda\} = \mathrm{Tr}\{\frac{d\mathcal{L}_{kk'}}{dk}\Lambda\}. \tag{5.21}$$

Referring to the definition of super-operator $\mathcal{L}_{kk'}$ in equation (5.14) Inside the super-operator $\mathcal{L}_{kk'}$ only $C(k)$ is a function of k. In chapter 3 $C(k)$ was calculated for special case of Hadamard walk in equation (4.15) as:

$$C(k) = \begin{pmatrix} e^{ik} & e^{ik} \\ e^{-ik} & -e^{-ik} \end{pmatrix}. \tag{5.22}$$

The general form of time evolution operator, referring to equation (4.79) is:

$$C(k) = (e^{ik}S_+ + e^{-ik}S_-)C. \tag{5.23}$$

Hence for integration by parts we have:

$$\mathrm{Tr}\{\frac{d\mathcal{L}_{kk'}}{dk}\Lambda\} = \sum_n \mathrm{Tr}\{\frac{dC(k)}{dk} M_n \Lambda M_n^\dagger C^\dagger(k')\} \tag{5.24}$$

and

$$\frac{dC(k)}{dk} = i(S_+ - S_-)C(k) = iS'C(k) \tag{5.25}$$

$$\frac{dC^\dagger(k)}{dk} = -iC^\dagger(k)(S_+ - S_-) = iC^\dagger(k)S'. \tag{5.26}$$

Finally

$$\frac{d}{dk} \mathrm{Tr}\{\mathcal{L}_{kk'}\Lambda\} = i \, \mathrm{Tr}\{S' \left(\mathcal{L}_{kk'}\Lambda\right)\} = \tag{5.27}$$

where $(S_+ - S_-) = S'$.

super operator $\mathcal{L}_{kk'}$ for $k = k'$ conserves the trace :

$$\mathrm{Tr}\{\mathcal{L}_{kk}\Lambda\} = \mathrm{Tr}\{\Lambda\}. \tag{5.28}$$

Making use of equations (5.27) , (5.28) and equation (5.20) for the expectation value of x or position of particle we get:

$$\langle x\rangle_t = \frac{-1}{2\pi}\sum_t \int dk\, \mathrm{Tr}\{S'\mathcal{L}^t_{kk}\,|phi_0\rangle\,\langle\phi_0|\}. \tag{5.29}$$

Expectation value of square of the position can be found by the same integration method as follows:

$$\langle x^2\rangle_t = \frac{-1}{2\pi}\int dk \left(\sum_{i=1}^{t}\sum_{i'=1}^{i}\mathrm{Tr}\{S'\mathcal{L}^{i'}_{kk}\,|\phi_0\rangle\,\langle\phi_0|\} + \sum_{i=1}^{t}\sum_{i'=1}^{i-1}\mathrm{Tr}\{\mathcal{L}^{i'}_{kk}\,|\phi_0\rangle\,\langle\phi_0|\,S'\}\right). \tag{5.30}$$

Decoherence and non-unitary measurement process

In previous sections mentioned that the decoherence effect is described by a non-unitary measurement operator denoted by M. A special case for this kind of operators is called Kraus operators.$M_n, n = 0, 1, 2$

$$M_0 = \sqrt{p}\,|\uparrow\rangle\,\langle\uparrow| \tag{5.31a}$$

$$M_1 = \sqrt{p}\,|\downarrow\rangle\,\langle\downarrow| \tag{5.31b}$$

$$M_2 = \sqrt{1-p}(|\uparrow\rangle\,\langle\uparrow| + |\downarrow\rangle\,\langle\downarrow|). \tag{5.31c}$$

In this particular case, decoherence is produced by 3 operators in equation (5.31a). These operators represent a coin that is measured at each step with the probability p. This immediately implies that, by increasing p decoherence effects increases. Apart from the operators given by the equation (5.31a b,c), there are two other kind of operator sets which represent measurement on the coin space, and hence implies decoherence. One of them is pure dephasing method:

$$M'_0 = \frac{1}{\sqrt{2}}(e^{-i\phi}\,|\uparrow\rangle\,\langle\uparrow| + e^{i\phi}\,|\downarrow\rangle\,\langle\downarrow|) \tag{5.32}$$

$$M'_1 = \frac{1}{\sqrt{2}}(e^{i\phi}\,|\uparrow\rangle\,\langle\uparrow| + e^{-i\phi}\,|\downarrow\rangle\,\langle\downarrow|). \tag{5.33}$$

The second kind of decoherence is called weak measurement:

$$M''_0 = \frac{1}{\sqrt{2}}(\sqrt{q}\,|\uparrow\rangle\,\langle\uparrow| + \sqrt{1-q}\,|\downarrow\rangle\,\langle\downarrow|) \tag{5.34}$$

$$M''_1 = \frac{1}{\sqrt{2}}(\sqrt{1-q}\,|\uparrow\rangle\,\langle\uparrow| + \sqrt{q}\,|\downarrow\rangle\,\langle\downarrow|). \tag{5.35}$$

All sets of operators in equation (5.31a,b,c) have the same effect on density matrix. Hence

one can obtain a relation between different types of decoherence given by,

$$p = 1 - \cos(2\phi) = 1 - 2\sqrt{q - q^2}. \tag{5.36}$$

Here, in this thesis the first one is used for numerical calculations. In next result section, simulation results for this kind of decoherence has been derived for different values of p.

Entanglement and its measures

Consider a composite quantum system with n subsystems A,B,C,..., Hilbert space of this system is defined as $H_A \otimes H_B \otimes H_C, \ldots$. If the wave function can be written on the product of wave function of the subsystems,$|\psi\rangle_{ABC\ldots} = |\psi\rangle_A \otimes |\psi\rangle_B \otimes |\psi\rangle_c \otimes \ldots$, then the state is separable otherwise it is entangled.

Qualifying the degree of the entanglement is done by different methods. One of the most useful methods is to measure the reduced Von-Neumann entropy of the quantum system. Von-Neumann entropy defines as:

$$S(\rho) = -\operatorname{Tr}(\rho \log_2 \rho). \tag{5.37}$$

Suppose density matrix of a mixed state as:

$$|\rho\rangle = \sum_n \lambda_n |n\rangle \langle n| \tag{5.38}$$

which $|n\rangle$'s are the states of mixed system and λ_n's are eigenvalues of reduced density matrix ρ.

Then equation (5.37) can be written as:

$$S(\lambda) = -\sum_n \lambda_n \log_2 \lambda_n. \tag{5.39}$$

Equation (5.39)is used to determine the measure of the entanglement in this thesis.

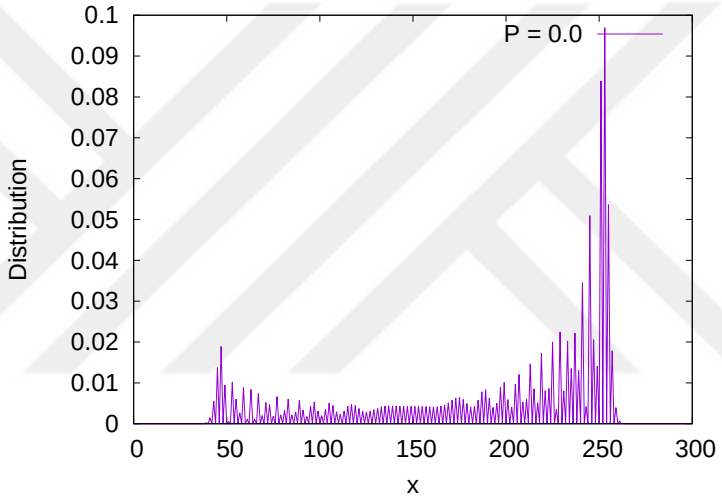
Since the Dynamics of a Quantum walk without decoherence is unitary and it is a reversible process, its Von-Neumann entropy doesn't change with respect to time. So if quantum walk starts with a pure state, it will continue in a pure state, Hence entropy of reduced density operator on the coin state can be used as a measure of its entanglement amount relative to the state of walker.

Decoherence effects on quantum walks is a non-unitary process, So maps quantum walk to a mixed state. Then the Von-Neumann entropy of total density matrix, isn't conserve and Von-Neumann entropy increases in time.[36].

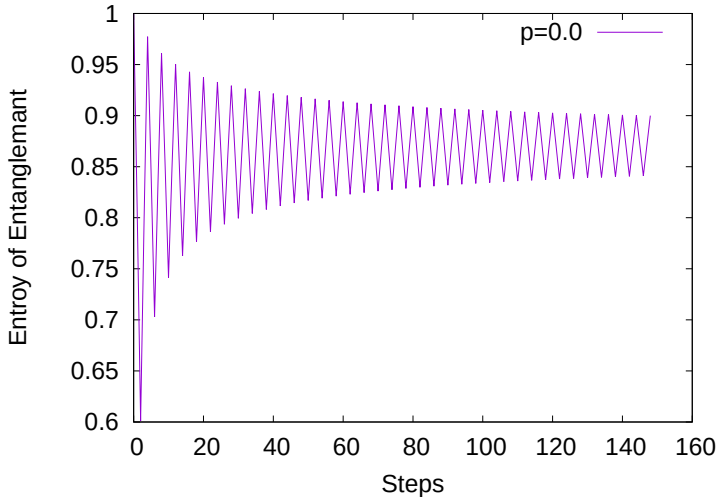
Results and discussions

As it is derived in chapter 2 and chapter 3 probability distribution of quantum walk with Hadamard coin for the case with no decoherence is fully quantum mechanical and non-classical. In figure (5.1) and (5.2) probability distribution, entanglement, position average, variance and standard deviation of pure quantum walk simulation results are presented for the case that p=0, the case without decoherence effects for comparison. Initial state of walker in the simulations fallen as $|\psi(t=0)\rangle = |0\rangle \otimes |\uparrow\rangle$.

In Hadamard walk without decoherence variance of position of walker, $\langle x^2 \rangle$, exhibits quadratic growth in time (figure (5.2b)). Hence, expectation value of position of walker or standard deviation, $\sqrt{\langle x^2 \rangle - \langle x \rangle^2}$, exhibits a linear increase with the number of steps of walk as it is expected figure (5.2c).

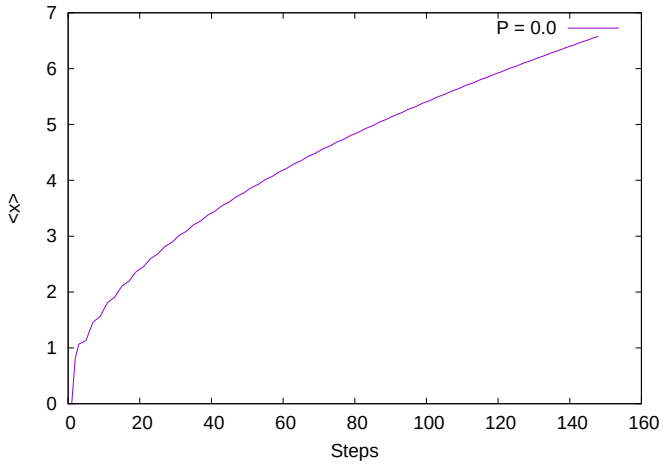


(a) Probability distribution

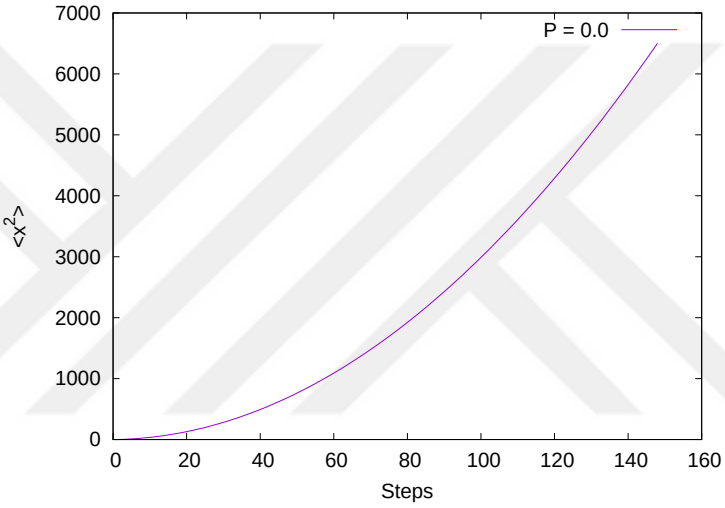


(b) Entanglement

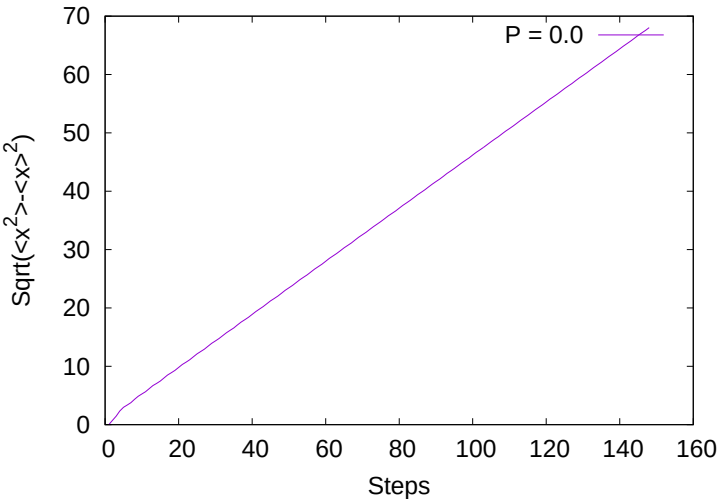
Figure 5.1: Simulation results for distribution(a) and Entanglement(b) of quantum random walk without decoherence for the case that p=0. Initial state of walker is $|\psi(t=0)\rangle = |0\rangle \otimes |\uparrow\rangle$.



(a) Position average



(b) Variance



(c) Standard deviation

Figure 5.2: Simulation results for position average, variance and standard deviation of quantum random walk without decoherence for the case that p=0.

Probability distribution of walker for Hadamard walk after 150 iterations with coin decoherence for 3 different amounts of decoherence are given in figure (5.3) p=0 represents the case with zero decoherence for comparison. As it is seen in figure by increasing p, probability distribution goes to classical Gaussian distribution. At p=0.1 it is completely classical. This means that in the case of coin decoherence, quantum correlations are lost very fast.

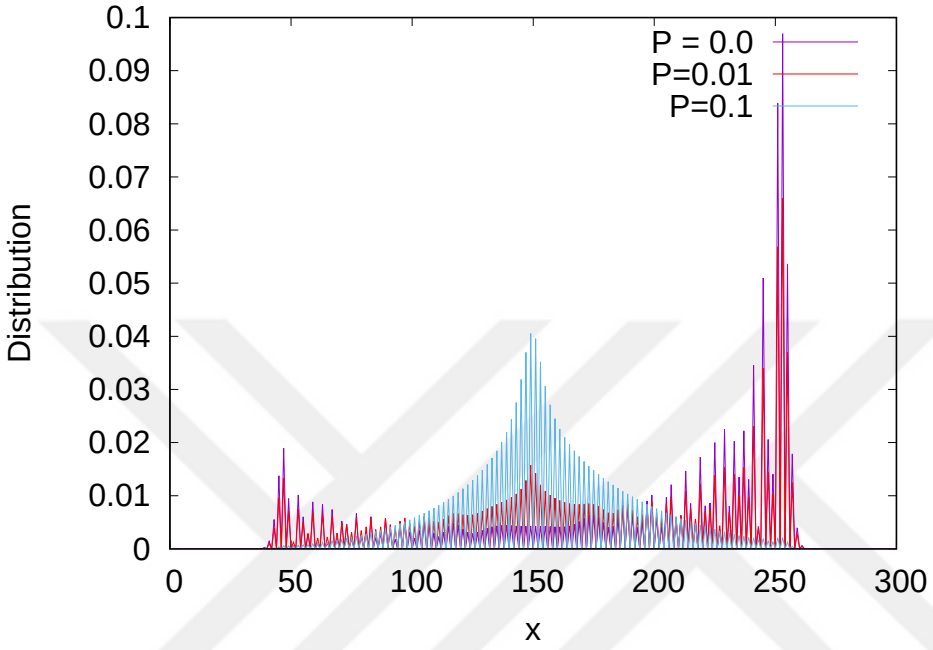


Figure 5.3: Probability distribution of walker by increasing decoherence effect for 150 iteration for p=0, p=0.01 and p=0.1. By increasing the decoherence, probability distribution goes fast to classical Gaussian distribution.

Average position of walker in classical case is equal to zero. Instead, in quantum random walks with asymmetric initial states this average grows as the square root of iterations. In figure (5.4) Average position of the walker for Hadamard walk is derived for 3 different cases. for p=0 this average has maximum value for each step. by increasing the decoherence this value decreases.

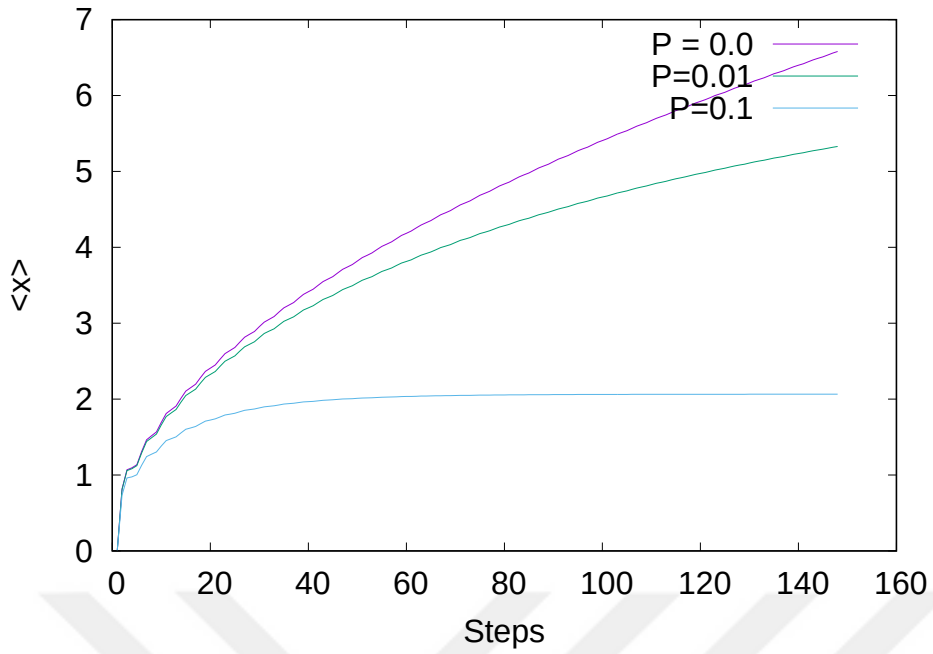


Figure 5.4: Average position of walker for Hadamard by increasing decoherence effect. it is seen that for p=0.1 average value decreases.

Expectation value of square of the position of walker in the case of Hadamard walk including decoherence is compared with the case of no decoherence in figure (5.5). As in previous cases , by increasing the decoherence it tends to exhibit classical generated random walk behavior. Even For p=0.1 the graphic (5.5) is almost linear with time.

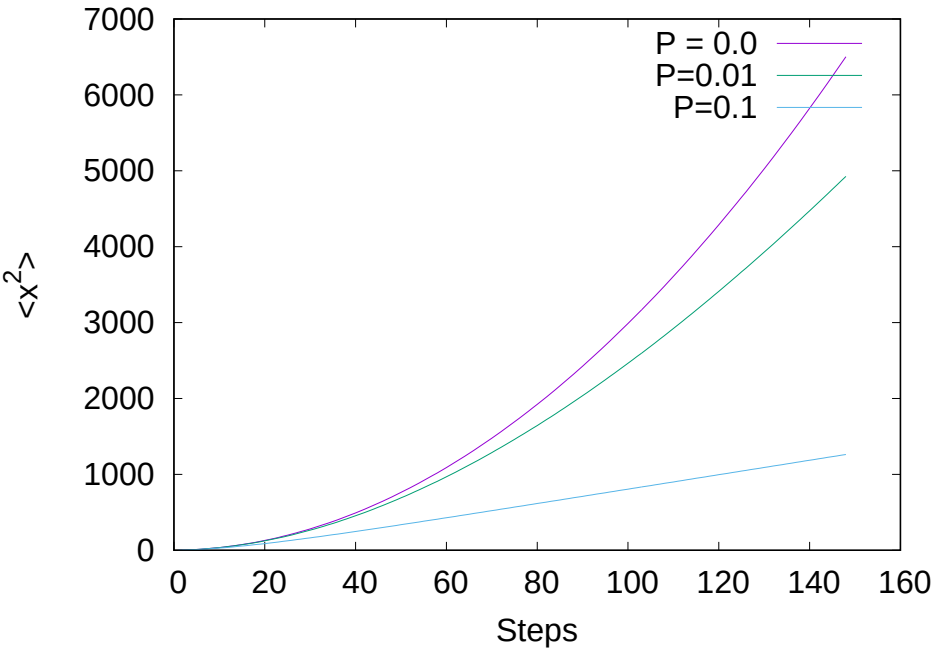


Figure 5.5: Average or expectation value of square of the position of walker or variance for Hadamard walk for p=0, p=0.01 and p=0.1. By increasing the decoherence variance tends to be linear with time.

As we maintained in previous section, entanglement measurement is done here by using reduced Von-Neumann entropy, equation (5.39). In case of pure quantum walk with p=0 (no decoherence case), entropy is measured and exhibited in figure (5.1b). In figure: (5.6) results of entropy measurements of the systems with decoherence are presented with Hadamard coin and asymmetric initial state, comparison with for p=0, p=0.01 and p=0.1 for decoherent systems. It can be seen that by increasing the decoherence and non unitary measurement, Von-Neumann entropy increases.

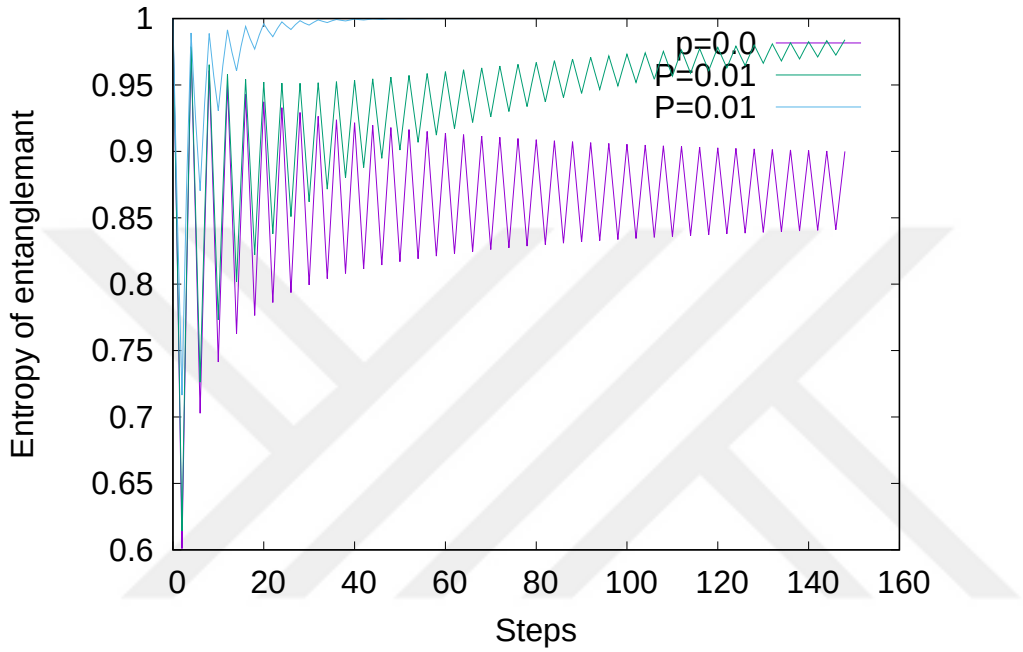


Figure 5.6: Entanglement between coin and position of walker for Hadamard walk by increasing the decoherence effect: It is shown that reduced Von-Neumann entropy increases with respect to time. for p=0.1 it shows very fast increase than the case with p=0.01

Standard deviation indicates propagation speed of the particle after t steps or speed of propagation of information in a quantum walk based algorithm. Quantum walks exhibits, linear increase in standard deviation with time. In classical random walks, expected position of particle increase with the square root of time steps, $\sqrt{n}$. Since classical random walk is one of the main techniques of simulation algorithms, quantum walk is expected simulator role in numerical comparison. Hence, it means that propagation of information in quantum algorithms is quadratically faster than its classical counterpart. In figure (5.7) by increasing the value of p it exhibits classically very fast. Hence, even small amount of decoherence in coin, gives classical properties to quantum walk.

As a result, coin decoherence in quantum walks, destroys quantum correlations and quantum entanglement, and makes quantum walk to exhibit classical.

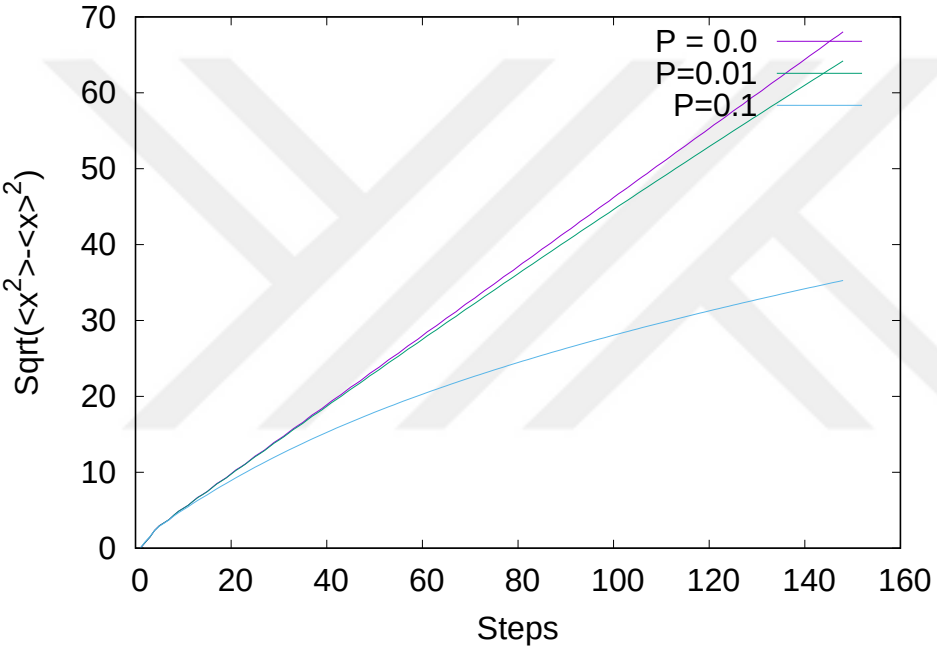


Figure 5.7: Standard deviation of position of walker for Hadamard walk by increasing decoherence effect. at p=0 the standard deviation is linearly with time. By increasing the value of p it exhibits by square root of position, $\sqrt{n}$. for p=0 it exhibits completely classical.

6. DISCUSSION

Quantum computation is expected to bring very important improvements on the computation algorithms and times on the most of the complicated quantum as well as classical problems. The main motivation of expectations of such huge advantage is that the quantum computation is inherently parallel. So far main advances are obtained in the lines of quantum algorithms, Grover's algorithm [19] and Shor's algorithm [20] are the most widely known and successful of all quantum algorithms. These algorithms provide quadratic and exponential improvements respectively comparing with their classical counterparts.

The classical random walk is a very useful tool for designing new algorithms. Quantum counterpart of the classical random walk has been shown to possesses various advantages comparing its classical counterpart. First of all, the quantum random walk can provide an increase in speed [22], [23], [24]. For this reason research on the quantum random walk has been an ever increasing interest among both the scientists studying physical systems and also persons using computation and information systems.

Algorithms based on the quantum walk appear to be compatible with the existing quantum algorithms. A quantum random-walk search algorithm proposed by Shenvi [25] and its improved version proposed by Potocek [26] appear to be the first successful algorithms. These two search algorithms are compatible in computational complexity to Grover's algorithm. Their advantages are in physical implementation and resistance to errors [27]. In recent years, many new quantum walk based algorithms are proposed and they are shown to be better than Grover's algorithm [28], [29].

In the practical side of the quantum algorithms, one knows that errors in quantum algorithms are inevitable. Usually, the errors are small but the scale of the problems are so large that these small errors accumulate to destroy the existing quantum correlations.

A particularly important source of error appears due to decoherence. Decoherence is created by interaction with environment which disturbs the quantum system. Many different types of random events can be mentioned here. One and particularly important random event type is random measurements. Random measurements will destroy superposition properties of the quantum system which in turn weakens the coherence.

In the quantum random walk based algorithms, the decoherence may have positive effects [30]. Controlled decoherence can create desired distribution as well as provid the required quantum speed up [31]. The effects of decoherence on quantum random walks have been studied [32], [33], [34] and it is found that a small amount of decoherence in a walk is beneficial, producing more uniform distributions.[30]. This is one of the major reasons that the studies of decoherence play an important role in understanding quantum random walk.

In this thesis work classical and quantum random walks are summarized, the basic analytical and numerical techniques presented in detail. Decoherence effects on the quantum walk have been the subject of the chapter 5 of the thesis. In this chapter, only the coin space decoherence have been the subject to investigations. Among many other types of decoherence which affect the quantum walk the coin space decoherence have a special importance since the control of decoherence is through technologically more feasible.

In chapter one, classical random walks, Markov-chains and its applications are introduced. To represent the importance of classical random walks in numerical solutions of differential equations, Laplace equation is solved by using Markov-chains. At the beginning of chapter two, general nature of quantum random walks on a line and continuous time and discrete time quantum walks as two components of general random walks are introduced. Then dynamics of discrete time quantum walks for Hadamard coin are formulated in detail and the main difference in results of classical random walks and quantum walks are obtained analytically for four steps of the walk. In order to derive a general formalism of quantum walk on a line in t steps, it is formulated in momentum space, this approach is presented in chapter three. At the end of this chapter, Fairly general formalism of quantum walk. Finally, the decoherence in quantum random walks are formulated and discussed as applying a non unitary operator to the state of the system. Then coin decoherence is calculated in detail analytically and numerically. Then the results are compared with purely quantum walk case and classical random walks.

It is concluded that, even a small amount of decoherence in coin, gives classical properties to the quantum walk. As a result, coin decoherence in quantum walks destroys quantum correlations and quantum entanglement, and makes quantum walk exhibit classical behavior.

It must be emphasized that the decoherence simulated and calculated in details was decoherene only in the coin degree of freedom. Effects of the decoherence in the position degree of freedom are indirect.

The subject is open to scientific and technological investigation since its immense possibilities of application.

A.1D QUANTUM RANDOM WALKS WITH COIN DECOHERENCE SIMULATION CODES IN C LANGUAGE

```
#include <stdio.h>
#include <math.h>
#include <complex.h>
#define NSteps 150
int main(){
  int i,j,k,l;
  double  d0[2*NSteps+1][2*NSteps+1][2][2];
  double  f0[2*NSteps+1][2*NSteps+1][2][2];
  double rho,theta,sum0,sum1,sum2,prb,av1,av2,susc;
  double  a,b,c,d,Sum[2][2];
  double  d00,d01,d10,d11,f00,f01,f10,f11;
  double  c00,c01,c10,c11;
  double  a000,a001,a010,a011;
  double  a100,a101,a110,a111;
  double  a200,a201,a210,a211;
  double di00,di01,di10,di11;
  double dj00,dj01,dj10,dj11;
  double sum00, sum01, sum10, sum11;
  double sum200, sum201, sum210, sum211;
  double lambda1,lambda2,Ent,p,ttt;
  FILE *ent,*dist,*aver;
  ent=fopen("Entanglement_0,01.dat","w");
  dist=fopen("Distribution_0,01.dat","w");
  aver=fopen("Averages_0,01.dat","w");

  p=0.01;

  a000 = 0.0;
  a001 = 0.0;
  a010 = 0.0;
  a011 = sqrt(p);

  a100 = sqrt(p);
  a101 = 0.0;
  a110 = 0.0;
```

```
a111 = 0.0;

a200 = sqrt(1-p);
a201 = 0.0;
a210 = 0.0;
a211 = sqrt(1-p);


for(j=0;j<=2*NSteps;j++){
  for(i=0;i<=2*NSteps;i++){
    d0[j][i][0][0] = 0.0;
    d0[j][i][0][1] = 0.0;
    d0[j][i][1][0] = 0.0;
    d0[j][i][1][1] = 0.0;
    f0[j][i][0][0] = 0.0;
    f0[j][i][0][1] = 0.0;
    f0[j][i][1][0] = 0.0;
    f0[j][i][1][1] = 0.0;
  }
}

d0[NSteps][NSteps][0][0] = 1.0;
d0[NSteps][NSteps][0][1] = 0.0;
d0[NSteps][NSteps][1][0] = 0.0;
d0[NSteps][NSteps][1][1] = 0.0;



for( k = 0;k<NSteps-1;k++){

  for(j=NSteps-k;j<=NSteps+k;j++){
    for(i=NSteps-k;i<=NSteps+k;i++){

      d00 = d0[j][i][0][0];
      d01 = d0[j][i][0][1];
      d10 = d0[j][i][1][0];
      d11 = d0[j][i][1][1];

      c00 = d00*a000 + d01*a010;
```

```
c01 = d00*a001 + d01*a011;
c10 = d10*a000 + d11*a010;
c11 = d10*a001 + d11*a011;

f00 = a000*c00 + a001*c10;
f01 = a000*c01 + a001*c11;
f10 = a010*c00 + a011*c10;
f11 = a010*c01 + a011*c11;

c00 = d00*a100 + d01*a110;
c01 = d00*a101 + d01*a111;
c10 = d10*a100 + d11*a110;
c11 = d10*a101 + d11*a111;

f00 = f00 + a100*c00 + a101*c10;
f01 = f01 + a100*c01 + a101*c11;
f10 = f10 + a110*c00 + a111*c10;
f11 = f11 + a110*c01 + a111*c11;

c00 = d00*a200 + d01*a210;
c01 = d00*a201 + d01*a211;
c10 = d10*a200 + d11*a210;
c11 = d10*a201 + d11*a211;

d00 = f00 + a200*c00 + a201*c10;
d01 = f01 + a200*c01 + a201*c11;
d10 = f10 + a210*c00 + a211*c10;
d11 = f11 + a210*c01 + a211*c11;


a = d00+d01;
b = d00-d01;
c = d10+d11;
d = d10-d11;

f0[j+1][i+1][0][0] = 0.5*(a+c);
f0[j+1][i-1][0][1] = 0.5*(b+d);
f0[j-1][i+1][1][0] = 0.5*(a-c);
f0[j-1][i-1][1][1] = 0.5*(b-d);
```

```
  }
}

for(j=NSteps-k-1;j<=NSteps+k+1;j++){
  for(i=NSteps-k-1;i<=NSteps+k+1;i++){

    d0[j+1][i+1][0][0] = f0[j+1][i+1][0][0];
    d0[j+1][i-1][0][1] = f0[j+1][i-1][0][1];
    d0[j-1][i+1][1][0] = f0[j-1][i+1][1][0];
    d0[j-1][i-1][1][1] = f0[j-1][i-1][1][1];

    f0[j+1][i+1][0][0] = (0.0+0.0*I);
    f0[j+1][i-1][0][1] = (0.0+0.0*I);
    f0[j-1][i+1][1][0] = (0.0+0.0*I);
    f0[j-1][i-1][1][1] = (0.0+0.0*I);

  }
}


for(i=NSteps-k-1;i<=NSteps+k+1;i++){
for(j=NSteps-k-1;j<=NSteps+k+1;j++){
  Sum[0][0]=0.0;
 Sum[0][1]=0.0;
 Sum[1][0]=0.0;
 Sum[1][1]=0.0;
for(l=NSteps-k-1;l<=NSteps+k+1;l++){

    di00 = d0[i][l][0][0];
    di01 = d0[i][l][0][1];
    di10 = d0[i][l][1][0];
    di11 = d0[i][l][1][1];

    dj00 = d0[l][j][0][0];
    dj01 = d0[l][j][0][1];
    dj10 = d0[l][j][1][0];
    dj11 = d0[l][j][1][1];

  Sum[0][0] += di00*dj00+di01*dj10;
```

```
    Sum[0][1] += di00*dj01+di01*dj11 ;
   Sum[1][0] += di10*dj00+di11*dj10 ;
   Sum[1][1] += di10*dj01+di11*dj11 ;
}
     f0[i][j][0][0] = Sum[0][0];
     f0[i][j][0][1] = Sum[0][1];
     f0[i][j][1][0] = Sum[1][0];
     f0[i][j][1][1] = Sum[1][1];
}}

sum00 = 0.0;
sum01 = 0.0;
sum10 = 0.0;
sum11 = 0.0;

sum200 = 0.0;
sum201 = 0.0;
sum210 = 0.0;
sum211 = 0.0;

for(i=NSteps-k-1;i<=NSteps+k+1;i++){

   sum00 = sum00 + d0[i][i][0][0];;
   sum01 = sum01 + d0[i][i][0][1];;
   sum10 = sum10 + d0[i][i][1][0];;
   sum11 = sum11 + d0[i][i][1][1];;

   sum200 = sum200 + f0[i][i][0][0];
   sum201 = sum201 + f0[i][i][0][1];
   sum210 = sum210 + f0[i][i][1][0];
   sum211 = sum211 + f0[i][i][1][1];

}

ttt = sum200 + sum211;

a = sum00;
b = sum01;
c = sum10;
```

```
    d = sum11;



    lambda1 =  (a + d – sqrt(a*a + 4*b*c – 2*a*d + d*d))/2.0;
    lambda2 =  (a + d + sqrt(a*a + 4*b*c – 2*a*d + d*d))/2.0;

    Ent=0 ;
    if(lambda1 != 0) Ent = –lambda1*log(lambda1)/log(2.0);
    if(lambda2 != 0) Ent = Ent – lambda2*log(lambda2)/log(2.0);


    fprintf(ent,” %d %f %f \n”,k,Ent, ttt);

    sum0 = 0;
    sum1 = 0;
    sum2 = 0;
    for(i=NSteps–k;i<NSteps+k;i++){
      prb = (d0[i][i][0][0]+d0[i][i][1][1]);
      sum0 = sum0 + prb ;
      sum1 = sum1 + prb * (i–NSteps);
      sum2 = sum2 + prb * (i–NSteps)*(i–NSteps);
    }
    av1 = sum1/sum0;
    av2 = sum2/sum0;
    susc = av2 – av1*av1;
    fprintf(aver,” %d %f %f %f %f \n”,k,prb,av1,av2,susc);

}


sum0 = 0;
sum1 = 0;
sum2 = 0;
for(i=0;i<2*NSteps;i++){
    prb = creal(d0[i][i][0][0]+d0[i][i][1][1]);
    sum0 = sum0 + prb ;
    sum1 = sum1 + prb * i;
    sum2 = sum2 + prb * i*i;
```

```
        av1 = sum1/sum0;
        av2 = sum2/sum0;
        susc = av2 - av1*av1;
        fprintf(dist," %d %f %f %f %f \n",i,prb,av1,av2,susc);
    }

}
```

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CURRICULUM VITAE

Credentials

Name/ Surname	:	Arash SALIMI KIA
Place of Birth	:	IRAN/URMIA more words.
E-Mail	:	arash.slm.kia@gmail.com
Address	:	Hacettepe University, Physics Engineering Department, ANKARA

Education

BSc. : Urmia Azad University, Applied Physics Department (2005 - 2009)

MSc. : Hacettepe University, Physics Engineering Department (2012-)

PhD. :

Foreign Language

English (Advanced) Persian (Fluent) Turkish (Fluent)

Work experience

International Baccalaureate Physics Teacher, Nesibe-Aydin College, IB college (2014 -)

Areas of Experience

Ankara-Turkey

Projects and Budgets

Publications

Oral and Poster Presentations

HACETTEPE UNIVERSITY
GRADUATE SCHOOL OF SCIENCE AND ENGINEERING
THESIS/DISSERTATION ORIGINALITY REPORT

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Department: Physics Engineering
Program: Physics Engineering
Status: ☒ Masters ☐ Ph.D. ☐ Integrated Ph.D.

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Prof. Dr. Yiğit GÜNDÜÇ
(Title, Name Surname, Signature)