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Spin Diffusion associated with a quantum random walk on a one-dimensional lattice

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Abstract

Classical random walks have found applications ranging from Brownian motion, diffusion of particles, designing computer algorithms, and even in the study of biological systems. Random walks can be used to explain the process of diffusion in the drift-diffusion model charge carrier motion in semiconductors. In the classical treatment of transport phenomena, the charge carrier transport can be characterized by a well defined diffusion coefficient $D$. Recently, there have been numerous proposals to make electronic and logic devices based on the spin property of electron like the Datta-Das Spin Field Effect Transistor. In such devices, the transport is non-classical (ballistic). This document examines the possibility of defining a spin diffusion coefficient for non-classical transport, using the study of quantum random walks as a starting point. In addition, this document also analyzes the effect of uniform noise on the behavior of quantum random walks and driving the quantum walk into classical regime.
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Chapter 1

Introduction

The theory of random walk has been of interest in several fields like physics, computer science, biology and economics. In a random walk, a ‘walker’ (or a particle) starts from a given point (the origin), and with a non-zero finite probability, takes a step in an arbitrary direction at each time step. The ‘steps’ and ‘time instants’ can be continuous variables (continuous-time random walk) or discrete (discrete-time random walk). Classically, random walk models have been used to describe a wide range of phenomena such as diffusion of particles (Brownian motion), motion of vacancies in a crystal, atoms on a crystalline surface, polymer chains and also biological systems.

The random walk phenomenon can occur in one dimension (line), two dimensions (plane) or three dimensions (space). The following discussion focuses exclusively on the random walk in one dimension, which is termed ‘discrete quantum walk on the line’. In this kind of discrete random walk, the line (space) and time are divided into discrete units. During each time step, the walker/particle takes one step in a random direction. This idea of walker taking discrete steps can naturally be extended to a random walk on a graph, giving rise to graph theoretic and computer science applications. Indeed, there are applications of Monte-Carlo Markov Chain (MCMC) algorithms, search algorithms and various other schemes based on random walk models in computer science.

There exist classical random walk models useful in several algorithmic applications and
it is natural to seek a quantum version of the random walk that is useful in building quantum algorithms. A good quantum algorithm should be faster/more efficient than a currently existing classical algorithm and should be robust to noise (the problem of decoherence). Although quantum computing has been thought of a very promising field, building good quantum algorithms had proved to be quite difficult. One proposed candidate to build good quantum algorithms is the **Quantum random walk**.

Quantum random walk was first proposed by Y. Aharanov, L. Davidovich and N. Zagury [1] as a quantum mechanical analog of the classical random walk, with applications in quantum optics. As with classical random walk, quantum (random) walks belong to one of the two cases: continuous-time and discrete-time. Various applications of quantum random walks have been proposed in quantum optics [1], quantum information and quantum computing, especially in quantum search algorithms [2]. Similar to classical random walks, quantum walks can occur in one (quantum walk on the line), two and three dimensions or on graphs (important for algorithmic applications). The information theoretic and computational properties and applications have been explored by several people; one such early exploration is by A. Vishwanath, A. Nayak, and A. Ambainis [3]. Simultaneously, various proposals have been made for the practical implementation of quantum walks in ion traps [4, 5], optical lattices [6], NMR [7] and Bose-Einstein condensates (BEC) [8].

Historically, before the advent of graph algorithms, an important use of classical random walks was to explain Brownian motion [9] which is used to explain the process of diffusion. Diffusion occurs in a wide variety of systems, including the movement of charge carriers in semiconductors. The movement of charge carriers in semiconductors is explained by the drift-diffusion model. The drift-diffusion model is based on the semi-classical Boltzmann Transport Equation, which is a semi-classical description of carrier transport. Modern semiconductor device sizes have become so small that the drift-diffusion model itself can no longer accurately predict the transport properties in such devices.

Now with the advent of proposals to make spin-based logic devices and transistors (such as the Datta-Das spinFET [10]), there have been attempts to use a diffusion coefficient for spin in such devices. This necessitates the need to examine if the ideas used in charge trans-
port can be applied to spin transport equally well. There are questions regarding the validity of assuming the same diffusion coefficient “$D$” to describe spin and charge transport \[11\]. The current work examines the characterization of spin transport in different regimes, and proceeds to check if a unique spin diffusion coefficient can be defined, which can be used to characterize spin transport in different conditions.

To understand the concept of a “diffusion coefficient” ($D$), consider a walker performing classical random walk, discrete or continuous. In the discussion in Sec. 2.1, the discrete classical random walk in one dimension is considered. Upon taking the continuum limit, one arrives at a coefficient which characterizes the diffusion phenomenon. This model does not take into account the kind of fields (or potentials) a charge carrier particle might experience, but the resulting parameter from this idealized model (diffusion coefficient) can be extended to describe the concept of diffusion in matter with external forces and fields, such as semiconductors.

Similarly, to understand spin transport and examine if a ‘spin diffusion coefficient’ can be analogously defined, consider an idealized model with no external interactions. In this model introduced shortly in Sec. 2.2, the walker performs discrete time quantum random walk in one dimension (on the line). The problem of mapping discrete time quantum walks (DTQW) to continuous time quantum walks (CTQW) has already been dealt with by several authors \[12\], and will not be discussed here. Among the possible types of discrete-time quantum random walks (DTQW) on the line, one variant of discrete-time quantum random walk known as the “Hadamard walk” is of special interest. It can be observed that quantum random walk has remarkably different properties compared to the classical random walk, such as a characteristic variance $\sigma^2 \propto t^2$ or $\sigma \propto t$ where $\sigma(t)$ is the standard deviation of the probability distribution $P_t(n)$ of the particle. Compared to this, the classical random walk has a standard deviation $\sigma \propto \sqrt{t}$. Later, noise is added to model non-ideal behavior and decoherence; and the noise was modelled by a uniform random number generator.

In the simulations shown in later chapters, it will be shown that the observable asymptotic trend is $\sigma^2 \propto t^\gamma$, where $\gamma = 2$ for the ideal, noiseless case (ballistic transport) and, as
the noise increases, $\gamma$ tends to 1 (diffusive transport). In Chapter 2, Sec. 2.1 describes the classical random walk on the line. It shows how, in the continuous limit, a diffusion coefficient can be defined. Next, Sec. 2.2 describes Hadamard walk and derives the equations of the discrete quantum random walk. It attempts to define a parameter analogous to the diffusion coefficient which was defined for the classical random walk. Later uniform random noise is added to the quantum random walk to model non-ideal behavior. It is shown that, in the presence of sufficiently large noise, the quantum random walk exhibits classical-like characteristics.

Chapter 3 shows the numerical simulation of the quantum random walk, starting with the ideal Hadamard walk (no noise) and goes on to show the effect of noise on the quantum random walk. It is shown that, in the case of very low noise, the noisy quantum random walk behaves like the ideal quantum random walk, and in the case of very high noise, the quantum random walk behaves like a random system. Further, it is shown that, in the case of low noise, the quantum random walk is highly sensitive to the initial spin state, and less so, with increasing noise. Chapter 4 discusses the possible implementation of noisy quantum random walk in various systems to verify the validity of the results presented, and extending the quantum random walk to two and three dimensions. Finally the appendix lists the core matlab code used to simulate the quantum random walk numerically.
Chapter 2

Background

2.1 Classical Random walks

In a classical random walk, a particle (or ‘walker’) is located on the origin, and at each time step, the walker hops from the current site to one of the nearest neighbors with a certain probability. In the unbiased random walk, if a site has \( c \) nearest neighboring sites, the probability of hopping to any of those sites is \( 1/c \). In one dimension, \( i.e. \), for the classical random walk on the line, the nearest neighbors are the lattice sites one step to the left or right of the walker. If the probability of moving to the left is, say, \( p \), then the probability of moving to the right would be \( 1-p \). In the case of unbiased random walk on the line, the probability of moving to the left (or right) is one-half, \( i.e. \) \( p = (1-p) = \frac{1}{2} \). The terms biased or unbiased are used analogous to coin-flipping experiments since the walker, like the coin, has two possibilities at each step.

Consider a walker on a one dimensional lattice (line) in which a unit step length is \( l \), and time for a single step is \( \tau \). Let the probability to find it at a site labelled by number \( n \) at time \( t \) be \( P_t(n) \). The time evolution at time \( t+1 \), by conservation of probability, requires that:

\[
P_{t+1}(n) = \frac{1}{2}[P_t(n-1) + P_t(n+1)], \quad \text{where } n = 0, \pm 1, \pm 2, \ldots
\]  

(2.1)
which, on subtracting \( P_t(n) \) on both sides becomes:

\[
P_{t+1}(n) - P_t(n) = \frac{1}{2}[P_t(n - 1) + P_t(n + 1) - 2P_t(n)]
\] (2.2)

Now the term on the left hand side of Eq. (2.2) varies only with time \( t \), and it can be written as:

\[
P_{t+1}(n) - P_t(n) = \tau \frac{\Delta P}{\Delta t}
\]

where \( \Delta t = (t + 1) - t = \tau \)

Also, the term of the right hand side of Eq. (2.2) varies with \( n \), and can be seen as the second derivative of \( P \) with respect to the spatial variable \( n \), which can be written as:

\[
\frac{1}{2}(P_t(n - 1) + P_t(n + 1) - 2P_t(n) = \ell^2 \frac{\Delta^2 P}{\Delta n^2}
\]

A continuous time description of the above random walk can be obtained by setting the lattice spacing \( \Delta n \to 0 \) and time step \( \Delta t \to 0 \). Under these limit conditions, the parameter \( D \) defined by

\[
D = \lim_{\ell \to 0} \lim_{\tau \to 0} \frac{\ell^2}{2\tau}
\]

is called the “diffusion coefficient”, which characterizes the rate at which the walker moves. In this continuous limit, the walk can be approximated to the diffusion equation:

\[
\frac{\partial P_t(n)}{\partial t} - D \frac{\partial^2 P_t(n)}{\partial n^2} = 0
\] (2.3)

where \( n \) and \( t \) are now continuous variables. The solution of this differential equation is the well-known Gaussian probability distribution

\[
P_t(n) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{n^2}{4Dt}}
\] (2.4)

Comparing this to the standard form of Gaussian distribution, the standard deviation is seen to be \( \sigma(t) = \sqrt{2Dt} \) i.e. \( \sigma(t) \propto \sqrt{t} \). This equation in the continuous limit describes the well known diffusion phenomena in one dimension.

2.2 Quantum Random walks

The basis states of the walker for the quantum random walk on the line are position states, denoted by \( |n\rangle \) for \( n = 0, \pm 1, \pm 2, \ldots \). In classical random walk, specifying the position of the walker is sufficient to complete the description of the state of walker. However,
the quantum random walk needs one more degree of freedom, called the “chirality” or “internal coin” which together with the position state, completes the description of the quantum walker. The term “coin” comes from classical random walk, where the movement of the walker at each step is decided by a ‘coin flip’. For an unbiased coin, the probabilities of the walker moving a step to the left or right are equal. In quantum random walk, the ‘coin’ (or chirality) is usually some (discrete) property of the system, like the spin of a particle or the polarization of a photon.

The basis states of chirality (internal coin) are \( |L\rangle \) and \( |R\rangle \), which usually represent a two level system. After each time-step, the walker moves one site to the left or right depending on whether the internal coin state is \( |L\rangle \) or \( |R\rangle \), respectively. In systems where the spin of the particle plays the role of internal coin, the basis states are also represented by \( |\downarrow\rangle \) and \( |\uparrow\rangle \), respectively. In this discussion, the coin states \( |R\rangle \) and \( |\uparrow\rangle \) are used interchangeably, and so are the symbols \( |L\rangle \) and \( |\downarrow\rangle \). The complete description of the walker is specified by the direct product of position and coin states as shown in Eq. (2.5)

\[
|\psi\rangle = |n\rangle |s\rangle \tag{2.5}
\]

where \( n = 0, \pm 1, \pm 2, \ldots \) and \( s \) can be \( R(\equiv \uparrow) \) or \( L(\equiv \downarrow) \).

In this representation, the walker moves to the right when the internal coin (spin) state is \( R(\uparrow) \) and to the left for \( L(\downarrow) \). An important property of quantum mechanical systems is the superposition of states. In the most general state, a quantum walker can be a superposition of the basis position and coin states. To see how the walker moves, let the walker start at origin \( (n = 0) \) and an arbitrary coin (spin) state \( (R \text{ or } L \text{ or any superposition of } R \text{ and } L) \) and then let the state of the walker evolve with time, as shown in Sec. 2.2.1.1.

2.2.1 Time evolution

2.2.1.1 Ideal Hadamard Walk

To describe time evolution, consider a walker/particle performing a discrete-time quantum random walk on a one-dimensional lattice (line). The mathematical description used in
this section closely follows that of Shapira et. al. [13], with a few changes. To see the time evolution of the walker, let the state of the walker at time $t$ be:

$$ |\psi(t)\rangle = \sum_{n=\infty}^{\infty} \sum_{s=L,R} a_{n,s}(t) |n\rangle |s\rangle $$  \hfill (2.6)

The state vector $|n\rangle$ ($n = 0, \pm 1, \pm 2, \ldots$) represents the spatial part of wavefunction at site $n$, and $|s\rangle$ ($s$ can be $L(\downarrow)$ or $R(\uparrow)$) is the spin (coin) part. The complex coefficients $a_{n,s}$ are probability amplitudes of the basis states $|n\rangle |s\rangle$. The complex numbers $a_{n,s}(t)$ are probability amplitudes, and hence obey the relation $\sum_{n,s} |a_{n,s}(t)|^2 = 1$. The coefficients $a_{n,s}(t+1)$ at the next time step depends on the spin/chirality state at time $t$. The time evolution of the quantum random walk is given by:

$$ |\psi(t+1)\rangle = \hat{Q} |\psi(t)\rangle $$ \hfill (2.7)

The time evolution operator $\hat{Q}$ is a product of two components $\hat{Q} = \hat{T}\hat{U}_0$. The order of operation is from right to left, so the operator $\hat{U}_0$ acts first, followed by $\hat{T}$. Now, $\hat{U}_0 = \hat{I} \otimes \hat{w}_0$ is an operator which acts only on the chiral (spin) state space (by $\hat{w}_0$) and leaves the position state unchanged (by acting with $\hat{I}$, the identity operator). In the next step, the $\hat{T}$ operator acts on the position space (moving the particle one step), leaving the coin state unchanged. This sequence of operations corresponds to the idea of flipping a coin, and then allowing the walker to take a step left or right depending on the outcome of coin-flip.

The requirement on $\hat{w}_0$ is that it should be a unitary operator, to conserve probability. So out of several possible choices, consider the standard “Hadamard” walk, in which a ‘Hadamard operator’ acts on the chiral (coin) state. The choice of the Hadamard matrix as the coin operator is not unique. There are other possible coin operators, such as the Grover coin operator. Several other possible approaches to control the quantum random walks by choices of initial states and different coin operators are described the works of Tregenna [14], and Brun [15, 16] etc.
Physically, the Hadamard operator takes a spin-up or spin-down state and produces an equal superposition state and the identity acting on the position ket leaves it unchanged. The action of the Hadamard operator can be represented as:

\[
\hat{w}_0 |\uparrow\rangle = \frac{|\uparrow\rangle + |\downarrow\rangle}{\sqrt{2}}
\]
\[
\hat{w}_0 |\downarrow\rangle = \frac{|\uparrow\rangle - |\downarrow\rangle}{\sqrt{2}}
\]  

(2.8)

i.e., the Hadamard operator (matrix) acting on a pure spin state sends them into one of two mutually orthogonal states (new-basis) in which the probabilities of |\uparrow\rangle and |\downarrow\rangle are equal.

For the quantum walk on the line, the coin state can take one of two possible values, physically implemented by two level systems like a spin-\(\frac{1}{2}\) system or plane-polarized photons. The basis states of the 2-level coin state can be represented as a 2-level spin system in which

\[
|R\rangle = |\uparrow\rangle \equiv \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad |L\rangle = |\downarrow\rangle \equiv \begin{bmatrix} 0 \\ 1 \end{bmatrix}
\]  

(2.9)

The Hadamard operator which converts these basis states into two (orthogonal) equal-superposition new basis states, in the above representation, is given by:

\[
\hat{w}_0 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}
\]  

(2.10)

After acting with \(U_0\), the position shift operator on the left i.e. \(\hat{T}\) acts on the position part of the state. The \(\hat{T}\) operator is a translation operator which shifts the position of the particle one step to the left or right depending on whether the chirality is \(\downarrow\) or \(\uparrow\), respectively.

\[
\hat{T} |n\rangle |\uparrow\rangle = |n+1\rangle |\uparrow\rangle
\]
\[
\hat{T} |n\rangle |\downarrow\rangle = |n-1\rangle |\downarrow\rangle
\]  

(2.11)

To see the time-evolution operator in action, start with the initial state specified in Eq. (2.6) and the time evolution as considered in Eq. (2.7).

\[
|\Psi(t+1)\rangle = \hat{T}\hat{U}_0 |\Psi(t)\rangle = \sum_{n=-\infty}^{\infty} \hat{T}\hat{U}_0 a_{n,\uparrow}(t) |n\rangle |\uparrow\rangle + \sum_{n=-\infty}^{\infty} \hat{T}\hat{U}_0 a_{n,\downarrow}(t) |n\rangle |\downarrow\rangle
\]
which, according to the action of Hadamard and time evolutions operators described in equations Eq. (2.8) and Eq. (2.11) respectively, becomes:

$$
\hat{Q} |\Psi(t)\rangle = \sum_{n=-\infty}^{\infty} \frac{a_{n,\uparrow}(t)}{\sqrt{2}} (|n+1\rangle |\uparrow\rangle + |n-1\rangle |\downarrow\rangle)
$$

$$
+ \sum_{n=-\infty}^{\infty} \frac{a_{n,\downarrow}(t)}{\sqrt{2}} (|n+1\rangle |\uparrow\rangle - |n-1\rangle |\downarrow\rangle) \quad (2.12)
$$

Collect the terms with identical kets:

$$
|\Psi(t+1)\rangle = \sum_{n=-\infty}^{\infty} \left\{ \left( \frac{a_{n,\uparrow}(t) + a_{n,\downarrow}(t)}{\sqrt{2}} \right) |n+1\rangle |\uparrow\rangle 
+ \left( \frac{a_{n,\uparrow}(t) - a_{n,\downarrow}(t)}{\sqrt{2}} \right) |n-1\rangle |\uparrow\rangle \right\} \quad (2.13)
$$

Comparing it to the standard form the state vector at time $t+1$ as described in Eq. (2.6), the relation between the coefficients $a_{n,s}$ at different time instants can be summarized as:

$$
a_{n,\uparrow}(t+1) = \frac{1}{\sqrt{2}} [a_{n-1,\uparrow}(t) + a_{n-1,\downarrow}(t)] \quad (2.14a)
$$

$$
a_{n,\downarrow}(t+1) = \frac{1}{\sqrt{2}} [a_{n+1,\uparrow}(t) - a_{n+1,\downarrow}(t)] \quad (2.14b)
$$

To solve these recursive relations, assume the walker starts at the origin ($n = 0$), and fix the chirality of the walker in a known state, say, $|\uparrow\rangle$ or $|\downarrow\rangle$ or any known superposition of $|\uparrow\rangle$ and $|\downarrow\rangle$. This way, once the initial state is known, the coefficients $a_{n,s}(t)$ at any finite time $t$ can be calculated and the state of the walker at any time is known.

The probability of finding the walker at position $n$ at time $t$ is $P_{t}(n)$. The quantity of interest is the standard deviation $\sigma(t)$ of the position of the walker performing the Hadamard walk, given by:

$$
\sigma^2(t) \equiv \langle n^2(t) \rangle - \langle n(t) \rangle^2
$$

where $\langle n \rangle$ and $\langle n^2 \rangle$ are first and second moments of the position, and are defined by:
\( \langle n^2(t) \rangle = \sum_{n=-t}^{t} n^2 \langle P_t(n) \rangle \)  
(2.15)

\( \langle n(t) \rangle = \sum_{n=-t}^{t} n \langle P_t(n) \rangle \)  
(2.16)

These relations, derived in the work of Shapira et. al. [13] and various other works, are valid for the ideal Hadamard walk (without noise, scattering or reflections).

### 2.2.1.2 Noisy Hadamard Walk

In the formalism described above, one way to introduce noise is to ‘bias’ the ideal coin, that is, change the Hadamard operator (matrix). Physically, instead of sending a pure spin into one of the two orthogonal equal-superposition states, this biased coin operator sends a spin into a superposition in which the probabilities of \( |\uparrow\rangle \) and \( |\downarrow\rangle \) are not equal; and hence the ‘bias’.

There were several works which study the effect of noise on quantum random walks. One work is the paper by Shapira et. al. [13] already discussed here. Further investigations which deal with the effect of noise/decoherence on quantum random walks are by Chandrashekar [17, 18], Olivera [19] among various others.

This current work tries to model the effect of uniform random noise on the walk using a generalized version of the Hadamard operator, which is required to be unitary. For this, a random variable ‘\( r \)’ is introduced, and can take any values in the range \([0, 1]\) (both inclusive). For the modified Hadamard operator to give the bias, the new, more general “coin” operator is defined to be:

\[
\hat{w} = \begin{bmatrix}
  r & \sqrt{1-r^2} \\
  \sqrt{1-r^2} & -r
\end{bmatrix}
\]  
(2.17)

It can be seen that the Hadamard matrix \( \hat{w}_0 \) is special case of \( \hat{w} \) shown above, when \( r = \frac{1}{\sqrt{2}} \). Also, the matrix \( \hat{w} \) can give rise to other important matrices for various values of \( r \):
\[ \hat{w}(r = 0) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \equiv \sigma_x, \quad \text{and} \quad \hat{w}(r = 1) = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \equiv \sigma_z \quad (2.18) \]

The action of the noisy Hadamard operator on the basis states in Eq. (2.9) is given by:

\[ \hat{w} \left| \uparrow \right\rangle = r \left| \uparrow \right\rangle + \sqrt{1 - r^2} \left| \downarrow \right\rangle \equiv \begin{bmatrix} r \\ \sqrt{1 - r^2} \end{bmatrix} \quad (2.19a) \]

\[ \hat{w} \left| \downarrow \right\rangle = \sqrt{1 - r^2} \left| \uparrow \right\rangle - r \left| \downarrow \right\rangle \equiv \begin{bmatrix} \sqrt{1 - r^2} \\ -r \end{bmatrix} \quad (2.19b) \]

Substitute these relations in the time evolution Eq. (2.7), where \( Q = \hat{T}\hat{U}_0 \). The operator \( \hat{U}_0 \) acts first, and its action is given by:

\[ \hat{U}_0 \left| n \right\rangle \left| \uparrow \right\rangle = (\hat{I} \otimes \hat{w}(r)) \left| n \right\rangle \otimes \left| \uparrow \right\rangle \]

\[ \hat{U}_0 \left| n \right\rangle \left| \uparrow \right\rangle = [\hat{I} \left| n \right\rangle] \otimes [\hat{w}(r) \left| \uparrow \right\rangle] \quad (2.20) \]

The action of the Hadamard operator \( \hat{w}(r) \) is given by Eq. (2.19), so that the above equation becomes

\[ \hat{U}_0 \left| n \right\rangle \left| \uparrow \right\rangle = \left| n \right\rangle \otimes \{ r \left| \uparrow \right\rangle + \sqrt{1 - r^2} \left| \downarrow \right\rangle \} \quad (2.21) \]

Instead, if the initial state of the walker is \( \left| n \right\rangle \left| \downarrow \right\rangle \), the resulting state after the operator \( U_0 \) acts becomes:

\[ \hat{U}_0 \left| n \right\rangle \left| \downarrow \right\rangle = \left| n \right\rangle \otimes \{ \sqrt{1 - r^2} \left| \uparrow \right\rangle - r \left| \downarrow \right\rangle \} \quad (2.22) \]

Now the translation operator \( \hat{T} \) acts on the resulting state \( \hat{U}_0 \left| n \right\rangle \left| s \right\rangle \) (where \( s = \uparrow \) or \( \downarrow \)) to complete the time evolution described in Eq. (2.7). The state of the walker at the next time step would be:

\[ \left| \psi(t + 1) \right\rangle = \hat{T} \left[ \sum_{n=-\infty}^{\infty} a_{n,\uparrow}(t) \left| n \right\rangle \left( r \left| \uparrow \right\rangle + \sqrt{1 - r^2} \left| \downarrow \right\rangle \right) \right. \]

\[ \left. + \sum_{n=-\infty}^{\infty} a_{n,\downarrow}(t) \left| n \right\rangle \left( \sqrt{1 - r^2} \left| \uparrow \right\rangle - r \left| \downarrow \right\rangle \right) \right] \quad (2.23) \]
Now using the properties of time-evolution operator $\hat{T}$ described in Eq. (2.11), the above equation becomes:

$$|\psi(t+1)\rangle = \sum_{n=-\infty}^{\infty} a_{n,\uparrow}(t) \left( r |n+1\rangle \uparrow + \sqrt{1-r^2} |n-1\rangle \downarrow \right)$$

$$+ \sum_{n=-\infty}^{\infty} a_{n,\downarrow}(t) \left( \sqrt{1-r^2} |n+1\rangle \uparrow - r |n-1\rangle \downarrow \right)$$

(2.24)

and rearranging the terms in a summation of single infinite series in terms of the corresponding state vectors:

$$|\psi(t+1)\rangle = \sum_{n=-\infty}^{\infty} \left[ (a_{n,\uparrow}(t) r + a_{n,\downarrow}(t) \sqrt{1-r^2}) |n+1\rangle \uparrow \right]$$

$$+ \left( a_{n,\uparrow}(t) \sqrt{1-r^2} - a_{n,\downarrow}(t) r \right) |n-1\rangle \downarrow \right]$$

(2.25)

To find out the relations between various coefficients $a_{n,\uparrow}$ and $a_{n,\downarrow}$, the above equation needs to be rewritten. Since the state vector is the sum of an infinite series, $|n+1\rangle$ can be replaced with $|n\rangle$ and replace $a_x$ with $a_{x-1}$ in the corresponding coefficient term. This amounts to "adjusting the window" to look at the term one step to the left. Similarly, replace the coefficients $a_n$ with $a_{n+1}$ and $|n-1\rangle$ with $|n\rangle$ in the second set of brackets, looking at one term to the right in the infinite sum. The resulting equation can be rewritten as:

$$|\psi(t+1)\rangle = \sum_{n=-\infty}^{\infty} \left[ (a_{n-1,\uparrow}(t) r + a_{n-1,\downarrow}(t) \sqrt{1-r^2}) |n\rangle \uparrow \right]$$

$$+ \left( a_{n+1,\uparrow}(t) \sqrt{1-r^2} - a_{n+1,\downarrow}(t) r \right) |n\rangle \downarrow \right]$$

(2.26)

These terms in parentheses are the coefficients of state vectors at time $t+1$ i.e. $a_{n,\uparrow}(t+1)$ and $a_{n,\downarrow}(t+1)$. Comparing the coefficients of basis vectors in the above equation to those in the time evolution equation Eq. (2.7), the following recursive relations are obtained:

$$a_{n,\uparrow}(t+1) = a_{n-1,\uparrow}(t) r + a_{n-1,\downarrow}(t) \sqrt{1-r^2}$$

(2.27a)

$$a_{n,\downarrow}(t+1) = a_{n+1,\uparrow}(t) \sqrt{1-r^2} - a_{n+1,\downarrow}(t) r$$

(2.27b)

However, unlike the ideal Hadamard walk described in Sec. 2.2.1.1 in our work, the standard deviations of spin-up (related $a_{n,\uparrow}$) and spin-down (related to $a_{n,\downarrow}$) are considered
separately. This is in line with our goal, outlined in the introduction, of finding difference in diffusion coefficients for different spin orientations. In the following chapters, it is shown that under ideal conditions (very low noise/decoherence), the values of $\sigma_{\uparrow}^2(t)$ and $\sigma_{\downarrow}^2(t)$ are significantly different for different initial spin injection conditions. To examine the effect of noise, $r$ is allowed to vary as a uniformly distributed random variable. In order to calculate values of $\sigma^2$, the first and second moments of spatial distributions of particle/walker and the corresponding probability amplitudes.

The probability of finding a spin-up particle at time $t$ at position $n$ is given by:

$$P_{\uparrow}^t(n) = |a_{n,\uparrow}(t)|^2$$

and similarly, the corresponding probability for a spin-down particle is:

$$P_{\downarrow}^t(n) = |a_{n,\downarrow}(t)|^2$$

With these definitions, the first and second moments of spatial distribution of a particle starting in spin-up state ($\uparrow$) are:

$$\langle n_{\uparrow}(t) \rangle = \sum_{n=-t}^{t} n \langle P_{\uparrow}^t(n) \rangle$$

$$\langle n^2_{\uparrow}(t) \rangle = \sum_{n=-t}^{t} n^2 \langle P_{\uparrow}^t(n) \rangle$$

Similarly, for a particle starting in the spin-down state ($\downarrow$), the first and second moments of spatial distribution are:

$$\langle n_{\downarrow}(t) \rangle = \sum_{n=-t}^{t} n \langle P_{\downarrow}^t(n) \rangle$$

$$\langle n^2_{\downarrow}(t) \rangle = \sum_{n=-t}^{t} n^2 \langle P_{\downarrow}^t(n) \rangle$$

Using these definitions of first and second moments, the standard deviation of spatial distribution for spin-up and spin-down is written as:

$$\sigma_{\uparrow}(t) = \sqrt{\langle n_{\uparrow}(t) \rangle - \langle n_{\uparrow}(t) \rangle^2}$$

$$\sigma_{\downarrow}(t) = \sqrt{\langle n_{\downarrow}(t) \rangle - \langle n_{\downarrow}(t) \rangle^2}$$
Chapter 3

Simulations

3.1 Design of Simulations

The ideal quantum walk described in section 2.2.1.1 has been subject to several investigations by several authors, both analytically [20, 21] and numerically [13, 17]. It has been already observed in section 2.1 that classical random walk gives rise to a Gaussian probability distribution. Numerical simulations of quantum random walk show a different behavior, with a probability distribution which is symmetric about the origin. For a given number of time-steps, quantum random walk spreads much further on the lattice than its classical counterpart, with two peaks at each end of the line and is rather flat at the center (origin) as show in Fig. 3.1.

For the ideal quantum walk whose spatial probability distribution is given in Fig. 3.1, the variance of the walk $\sigma^2$ varies as $t^2$ (or for the standard deviation, $\sigma \propto t$), which is shown in Fig. 3.2. However, the quantity of interest is the ratio $\left(\frac{\sigma^2}{t}\right)$, which in the classical scenario is related to the diffusion coefficient (upto some constant). Hence the plot of ratio $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for the ideal quantum random walk is show in Fig. 3.3.

This is the standard behavior of quantum random walk which is explained in several works. However, most works do not explore the sensitivity of $\sigma$ to the initial injection condition; even if it is, it is explored only in the ideal (noiseless Hadamard) case. If the initial
Figure 3.1: Spatial probability distribution of quantum random walk with the Hadamard coin, in the ideal case starting with equal superposition

condition of the walker is right chirality (R) or spin-up (↑), the probability distribution is skewed to the right as shown in Fig. 3.4. Similarly, if the walker starts with left chirality (L) or spin-down (↓), the probability distribution is skewed to the left as shown in Fig. 3.5.
Figure 3.2: Variance of quantum random walk with the Hadamard coin, in the ideal case

Figure 3.3: Plot of \( (\sigma^2 t) \) as a function of \( t \) for ideal quantum random walk with the Hadamard coin, with the walker starting in an equal superposition of spin-up and spin-down
Figure 3.4: Spatial probability distribution of quantum random walk with the Hadamard coin, in the ideal case starting with spin-up

Figure 3.5: Spatial probability distribution of quantum random walk with the Hadamard coin, in the ideal case starting with spin-down
The corresponding plots of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ are shown in Fig. 3.4 (for the walker starting in spin-up state) and Fig. 3.5 (for the walker starting in spin-down state) respectively. It can be clearly seen that the value of the quantity $\left(\frac{\sigma^2}{t}\right)$ exhibits a strong dependence on the initial configuration of the walker. For a walker starting with a spin-up configuration (Fig. 3.4), the ratio $\left(\frac{\sigma^2}{t}\right)_{↑}$, which is proportional to the classical diffusion coefficient for spin-up configuration is clearly significantly greater than $\left(\frac{\sigma^2}{t}\right)_{↓}$ for spin-down. Similarly, if the walker starts with spin-down, the value of $\left(\frac{\sigma^2}{t}\right)_{↓}$ is significantly greater than $\left(\frac{\sigma^2}{t}\right)_{↑}$ as shown in Fig. 3.5.

Figure 3.6: Plot of $\left(\frac{\sigma^2}{t}\right)$ as a function of $t$ for ideal quantum random walk with the Hadamard coin, with the walker starting in spin-up state.
Figure 3.7: Plot of $\left(\sigma^2/t\right)$ as a function of $t$ for an ideal quantum random walk with the Hadamard coin, with the walker starting in spin-down state.

It can be seen in Fig. 3.3, the quantity $\left(\sigma^2/t\right)$ is exactly linear in $t$, as expected in the case of quantum random walk with no noise. To find the variation of the quantities $\sigma^2$ and $\left(\sigma^2/t\right)$ as a function of time $t$, numerical simulations were done in MATLAB. Each simulation was averaged over 1,000 iterations, with each iteration having 1,000 simulation steps.

In the simulations described in this work, uniform random noise is used to modify the Hadamard coin operator. The noise is modelled by a random number $r$ generated by the random number generating function “rand” in MATLAB. This modified Hadamard operator sends each spin state into a superposition of spin-up and spin-down basis states such that total overall probability is 1 (so the coin operator is unitary). This modified Hadamard operator $\hat{w}$ is unitary with the property $\hat{w} = \hat{w}^\dagger$, such that the probability is conserved after each step. The unitarity is also verified in the simulations as well, the sum of probabilities being equal to 1 after each step.

In the work of Shapira et. al. [13], the noise is modeled as an unitary operator of the
form $e^{i\hat{a}(t)}$, where $\hat{a}(t) = \alpha_1(t)\sigma_x + \alpha_2(t)\sigma_y + \alpha_3(t)\sigma_z$, where $\sigma_x$, $\sigma_y$ and $\sigma_z$ are Pauli matrices. The noise is characterized by $\alpha$ which is the standard deviation of $\alpha_1$, $\alpha_2$, $\alpha_3$. The paper [13] also specifies that the classical behavior overtakes the quantum behavior in case of strong noise i.e. $\alpha \geq 0.07$. There are two ways to induce noise/decoherence in the quantum walk: decoherence in the position space or noise in the coin (chiral/spin)space (also called ‘de-phasing the coin’). In the model described above, the coin is ‘de-phased’ while retaining the position space noise-free. There have been several other works which deal with the problem of quantum random walks with de phased coins [15] and the quantum to classical transition in quantum random walks [16].

The decoherence is modelled by a single parameter $r$ which modifies the Hadamard operator as seen from Eq. (2.27) in Sec. 2.2.1.1 while maintaining unitarity. In Sec. 2.2.1.2 the generalized coin operator was represented by $\hat{w}(r)$. It reduces to the standard Hadamard operator $\hat{w}_0$ when $r = \frac{1}{\sqrt{2}}$ (represented by $a_0$ in this discussion). The simulations were done with different ‘coin’ operators by varying the parameter $r$ of the generalized Hadamard coin operator. The plots described in Fig. 3.3, 3.6 and 3.7 correspond to the ideal case when $r = a_0 = \frac{1}{\sqrt{2}}$. The parameter $r$ is varied as a uniform random number, and at each time step, $r$ is allowed to lie in a certain range of values. Starting with $r = a_0$ for the ideal case, the range of $r$ is increased in steps, $a_0 - 0.01 \leq r \leq a_0 + 0.01$, $a_0 - 0.02 \leq r \leq a_0 + 0.02$, $a_0 - 0.05 \leq r \leq a_0 + 0.05$, $a_0 - 0.07 \leq r \leq a_0 + 0.07$, and so on, expanding the range to $0 \leq r \leq 1$ which corresponds to maximum decoherence.

This chapter shows the plots of $\left(\frac{\sigma^2}{T}\right)$ vs $t$ and the corresponding spatial probability distribution $P(n)$ of the walker vs the spatial variable $n$. For each value of the parameter $r$, three initial conditions were considered; the walker performing quantum walk starting in (a) equal superposition of spin-up ($\uparrow$) and spin-down ($\downarrow$), (b) spin up ($\uparrow$), and (c) spin down ($\downarrow$).

As it can be seen in Fig. 3.8 adding a very small amount of noise does not alter the nature of quantum walk significantly. The following pages show further simulations for various allowed ranges of the parameter $r$. In the work of Shapira [13], a significant change in the probability distribution happens when $\alpha = 0.07$. Hence the curves are plotted for low noise.
in small increments, and once the quantum to classical transition is apparent, the increments can be made large.

It is clearly observed that classical behavior becomes significant when allowed deviation is $\pm 0.07$ from the value of $a_0$, i.e. the value of $r$ lies in the range $a_0 - 0.07 \leq r \leq a_0 + 0.07$. It can be conjectured that the classical nature becomes stronger as the range of $r$ is allowed to increase. The next few pages show the transition of the walk from quantum to classical like regime.
Figure 3.8: Plot of \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.01 \leq r \leq a_0 + 0.01 \), with the walker starting in (a)equal superposition of spin-up and spin-down, (c)spin-up state, and (e)spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.9: Plot of $\left( \frac{\sigma^2}{t} \right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.02 \leq r \leq a_0 + 0.02$, with the walker starting in (a)equal superposition of spin-up and spin-down, (c)spin-up state, and (e)spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.10: Plot of $\frac{\sigma^2}{t}$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.05 \leq r \leq a_0 + 0.05$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.11: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.07 \leq r \leq a_0 + 0.07$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.12: Plot of \( \frac{\langle \sigma^2 \rangle}{t} \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.1 \leq r \leq a_0 + 0.1 \), with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.13: Plot of $\left( \frac{\sigma^2}{t} \right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.125 \leq r \leq a_0 + 0.125$; with the walker starting in (a)equal superposition of spin-up and spin-down, (c)spin-up state, and (e)spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.14: Plot of $\langle \sigma^2 \rangle$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.15 \leq r \leq a_0 + 0.15$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.15: Plot of $\left( \frac{\sigma^2}{t} \right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.2 \leq r \leq a_0 + 0.2$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.16: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.25 \leq r \leq a_0 + 0.25$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.17: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $0 \leq r \leq 1$, with the walker starting in (a)equal superposition of spin-up and spin-down, (c)spin-up state, and (e)spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
3.2 Classical limit

Also, although the walk does not become exactly classical, it is asymptotically classical with increasing time-steps, as seen in figures Fig. 3.18, 3.19, and 3.20. In this classical limit, the expected behavior is \( \left( \frac{\sigma^2}{t} \right) \propto t^0 \) or constant and similarly, \( \left( \frac{\sigma'^2}{t} \right) \propto t^0 \).

In the work of Brun et. al. [15], the authors observe that “The usual classical solution is recovered in the limit where the coin decoheres completely every step”. The MATLAB code used for the simulations is characterized by a parameter \( r \), a random number generated at every instant of time and before taking each step. It can be observed that the random walk behaves in a classical manner when the allowed range of \( r \) becomes maximum, \( i.e. \) \( 0 \leq r \leq 1 \). However, the ratios \( \left( \frac{\sigma^2}{t} \right) \) and \( \left( \frac{\sigma'^2}{t} \right) \) tends to a constant in the asymptotic limit; however, it is not exactly a constant for 1,000 steps. Hence the a sampling of the simulations were repeated with 2,000 steps averaged over a 1,000 iterations and the plots are presented in Fig. 3.18, 3.19, and 3.20.
Figure 3.18: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 2000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.07 \leq r \leq a - 0 + 0.07$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.19: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 2000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.20 \leq r \leq a - 0 + 0.20$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
Figure 3.20: Plot of $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 2000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $0 \leq r \leq 1$, with the walker starting in (a) equal superposition of spin-up and spin-down, (c) spin-up state, and (e) spin-down state. The plots (b), (d), and (f) show the probability distribution of the walker for the corresponding initial conditions.
3.3 Curve Fitting

3.3.1 Power law

For the ideal quantum random walk discussed in Sec. 2.2.1.1 and verified by numerical simulations in Fig. 3.3, 3.6, and 3.7, 
\( \left( \frac{\sigma^2}{t} \right) \propto t \) or \( t^1 \) and \( \left( \frac{\sigma^2}{t} \right) \propto t \); and in general, 
\( \left( \frac{\sigma^2}{t} \right) \neq \left( \frac{\sigma^2}{t} \right) \) except in the case when the walker starts in an equal superposition of spin basis states 
\( \left( \frac{\sigma^2}{t} \right) \) such as the case highlighted in Fig. 3.3. In the limit of large noise (classical limit), the expected behavior is 
\( \left( \frac{\sigma^2}{t} \right) \propto t^0 \) or constant and similarly, \( \left( \frac{\sigma^2}{t} \right) \propto t^0 \). This naturally brings forth the question if there exists a simple relation between the quantities 
\( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) and \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) which can be characterized by a power law of the form

\[ y = at^\gamma \]  

(3.1)

where \( y \) is one of the quantities \( \left( \frac{\sigma^2}{t} \right) \) or \( \left( \frac{\sigma^2}{t} \right) \); \( t \) is the time (discrete) and \( \gamma \) is an exponent whose value is 1 for the ideal quantum walk and 0 for the classical random walk.

To check if a power law of the form shown in Eq. (3.1) exists, a sample from the simulations shown in Sec. 3.1 were considered, and attempted to fit the \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) (where \( s = \uparrow \) or \( \downarrow \)) curves against the power law equation \( y = at^\gamma \). The following Figures show the fitted curve plotted against the results obtained by numerical simulations. For each fit, the values of coefficients \( a \), \( \gamma \), and the goodness of the fit (measured by the value of \( R^2 \)) are given.
Figure 3.21: Fitted curves of (a) $\left( \frac{\sigma^2}{t} \right)$ vs $t$ and (b) $\left( \frac{\sigma^2}{t} \right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r = a_0$ with the walker starting in equal superposition of spin-up and spin-down. The coefficients and $R^2$ values are: (a) $a = 0.1226$, $\gamma = 1.003$ and $R^2 = 1$ (b) $a = 0.1226$, $\gamma = 1.003$ and $R^2 = 1$

Figure 3.22: Fitted curves of (a) $\left( \frac{\sigma^2}{t} \right)$ vs $t$ and (b) $\left( \frac{\sigma^2}{t} \right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r = a_0$ with the walker starting in spin-up state. The coefficients and $R^2$ values are: (a) $a = 0.1183$, $\gamma = 1.001$ and $R^2 = 1$ (b) $a = 0.08556$, $\gamma = 1.004$ and $R^2 = 1
Figure 3.23: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r = a_0$ with the walker starting in spin-down state. The coefficients and $R^2$ values are: (a) $a = 0.08567$, $\gamma = 1.004$ and $R^2 = 1$ (b) $a = 0.1117$, $\gamma = 1.008$ and $R^2 = 1$

Figure 3.24: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.07 \leq r \leq a_0 + 0.07$ with the walker starting in equal superposition of spin-up and spin-down. The coefficients and $R^2$ values are: (a) $a = 1.004$, $\gamma = 0.5668$ and $R^2 = 0.9845$ (b) $a = 0.9672$, $\gamma = 0.5722$ and $R^2 = 0.9839$
Figure 3.25: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.07 \leq r \leq a_0 + 0.07$ with the walker starting in spin-up state. The coefficients and $R^2$ values are: (a) $a = 1.073$, $\gamma = 0.5619$ and $R^2 = 0.9811$ (b) $a = 0.5168$, $\gamma = 0.6526$ and $R^2 = 0.9894$

Figure 3.26: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.07 \leq r \leq a_0 + 0.07$ with the walker starting in spin-down state. The coefficients and $R^2$ values are: (a) $a = 0.5186$, $\gamma = 0.6518$ and $R^2 = 0.9896$ (b) $a = 1.019$, $\gamma = 0.5692$ and $R^2 = 0.9799
Figure 3.27: Fitted curves of (a)\(\frac{\sigma^2}{t}\) vs \(t\) and (b)\(\frac{\sigma^2}{t}\) vs \(t\) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \(r\) in the range \(a_0 - 0.125 \leq r \leq a_0 + 0.125\) with the walker starting in equal superposition of spin-up and spin-down. The coefficients and \(R^2\) values are: (a) \(a = 2.015, \gamma = 0.3337\) and \(R^2 = 0.9408\) (b) \(a = 1.933, \gamma = 0.3397\) and \(R^2 = 0.9385\)

Figure 3.28: Fitted curves of (a)\(\frac{\sigma^2}{t}\) vs \(t\) and (b)\(\frac{\sigma^2}{t}\) vs \(t\) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \(r\) in the range \(a_0 - 0.125 \leq r \leq a_0 + 0.125\) with the walker starting in spin-up state. The coefficients and \(R^2\) values are: (a) \(a = 2.232, \gamma = 0.3198\) and \(R^2 = 0.9329\) (b) \(a = 1.396, \gamma = 0.3843\) and \(R^2 = 0.9843\)
Figure 3.29: Fitted curves of (a) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) and (b) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.125 \leq r \leq a_0 + 0.125 \) with the walker starting in spin-down state. The coefficients and \( R^2 \) values are: (a) \( a = 0.1409, \gamma = 0.3829 \) and \( R^2 = 0.9483 \) (b) \( a = 2.086, \gamma = 0.3296 \) and \( R^2 = 0.9301 \)

Figure 3.30: Fitted curves of (a) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) and (b) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.2 \leq r \leq a_0 + 0.2 \) with the walker starting in equal superposition of spin-up and spin-down. The coefficients and \( R^2 \) values are: (a) \( a = 1.986, \gamma = 0.2065 \) and \( R^2 = 0.8842 \) (b) \( a = 1.887, \gamma = 0.2141 \) and \( R^2 = 0.8777 \)
Figure 3.31: Fitted curves of (a) \( \frac{\sigma^2}{t} \) vs \( t \) and (b) \( \frac{\sigma^2}{t} \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.2 \leq r \leq a_0 + 0.2 \) with the walker starting in spin-up state. The coefficients and \( R^2 \) values are: (a) \( a = 2.169, \gamma = 0.1935 \) and \( R^2 = 0.8712 \) (b) \( a = 1.641, \gamma = 0.2337 \) and \( R^2 = 0.8843 \)

Figure 3.32: Fitted curves of (a) \( \frac{\sigma^2}{t} \) vs \( t \) and (b) \( \frac{\sigma^2}{t} \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.2 \leq r \leq a_0 + 0.2 \) with the walker starting in spin-down state. The coefficients and \( R^2 \) values are: (a) \( a = 1.634, \gamma = 0.2345 \) and \( R^2 = 0.8951 \) (b) \( a = 1.96, \gamma = 0.2089 \) and \( R^2 = 0.8739 \)
Figure 3.33: Fitted curves of (a) \(\frac{\sigma^2}{\tau} \) vs \( t \) and (b) \(\frac{\sigma^2}{\tau} \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( 0 \leq r \leq 1 \) with the walker starting in equal superposition of spin-up and spin-down. The coefficients and \( R^2 \) values are: (a) \( a = 0.523, \gamma = 0.09166 \) and \( R^2 = 0.8367 \) (b) \( a = 0.4655, \gamma = 0.1096 \) and \( R^2 = 0.788 \)

Figure 3.34: Fitted curves of (a) \(\frac{\sigma^2}{\tau} \) vs \( t \) and (b) \(\frac{\sigma^2}{\tau} \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( 0 \leq r \leq 1 \) with the walker starting in spin-up state. The coefficients and \( R^2 \) values are: (a) \( a = 0.5553, \gamma = 0.08116 \) and \( R^2 = 0.7767 \) (b) \( a = 0.4846, \gamma = 0.1019 \) and \( R^2 = 0.7475 \)
Figure 3.35: Fitted curves of (a) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) and (b) \( \left( \frac{\sigma^2}{t} \right) \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( 0 \leq r \leq 1 \) with the walker starting in spin-down state. The coefficients and \( R^2 \) values are: (a) \( a = 0.5236, \gamma = 0.090311 \) and \( R^2 = 0.818 \) (b) \( a = 0.4805, \gamma = 0.1038 \) and \( R^2 = 0.7475 \)

### 3.3.2 Stretched exponential

As seen in figures from Fig. 3.30 to Fig. 3.35, the plots deviate significantly from power law behavior with increasing noise. The functional dependence of \( \left( \frac{\sigma^2}{t} \right) \) on \( t \) no longer follows a simple power law, \( i.e. \), the general law \( \left( \frac{\sigma^2}{t} \right) \propto t^\gamma \) no longer holds which can be inferred from the decreasing \( R^2 \) values shown in Sec. 3.3.1. Sec. 3.2 shows the plots when the lattice size and the number of time steps were increased to 2000. It is shown that even in the case of maximum noise, the quantity \( \left( \frac{\sigma^2}{t} \right) \) approaches a constant value only asymptotically (after a very large time).

This behavior is reminiscent of the charging of a capacitor which, in principle, takes infinitely long time to complete. The discharge of a capacitor, a similar process, was first described by Kohlrausch [22] using a function of the form \( f_\beta(t) = e^{-t^\beta} \), which is called the "stretched exponential" function, where \( \beta < 1 \) usually. The exponential function is recovered when \( \beta \) is set to 1. This stretched exponential is the modified to the form \( f_\beta(t) = e^{-\left( \frac{t}{\tau} \right)^\beta} \) which has been used phenomenologically in disordered systems [23, 24] and various types of glasses [25, 26] and networks [27].
The stretched exponential has been modified to a form

\[ y_\beta(t) = y_0 \left[ 1 - \exp\left(\frac{-t}{\tau}\right)^\beta \right] \]  

(3.2)

which takes a very long time to reach the final value \( y_0 \). The plots of \( \left(\frac{\sigma^2}{t}\right) \) vs \( t \) have been fit to Eq. (3.2), with fitting parameters \( y_0, \tau \) and the exponent \( \beta \). There have been a few “magic numbers” observed for the value of the exponent \( \beta \) \cite{25,27}, \( \beta = \frac{3}{5} (= 0.6) \) and \( \beta = \frac{3}{7} (= 0.42857) \). In the fits shown in this section, it is observed that the values of \( \beta \) obtained in the fits are most likely to be close to one of the two “magic numbers”.

![Graphs](image)

Figure 3.36: Fitted curves of (a) \( \left(\frac{\sigma^2}{t}\right) \) vs \( t \) and (b) \( \left(\frac{\sigma^2}{t}\right) \) vs \( t \) for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter \( r \) in the range \( a_0 - 0.2 \leq r \leq a_0 + 0.2 \) with the walker starting in equal superposition of spin-up and spin-down. The coefficients and \( R^2 \) values are: (a) \( y_0 = 4.827, \tau = 57.0998, \beta = 0.6233 \) and \( R^2 = 0.9906 \) (b) \( y_0 = 4.8054, \tau = 62.004, \beta = 0.6677 \) and \( R^2 = 0.9873 \)
Figure 3.37: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.2 \leq r \leq a_0 + 0.2$ with the walker starting in spin-up state. The coefficients and $R^2$ values are: (a) $y_0 = 4.8904$, $\tau = 53.375$, $\beta = 0.6019$ and $R^2 = 0.9904$ (b) $y_0 = 4.838$, $\tau = 73.6463$, $\beta = 0.697$ and $R^2 = 0.9915$

Figure 3.38: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $a_0 - 0.2 \leq r \leq a_0 + 0.2$ with the walker starting in spin-down state. The coefficients and $R^2$ values are: (a) $y_0 = 4.793$, $\tau = 70.671$, $\beta = 0.661$ and $R^2 = 0.9902$ (b) $y_0 = 4.8$, $\tau = 60.121$, $\beta = 0.6514$ and $R^2 = 0.9842$
Figure 3.39: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $0 \leq r \leq 1$ with the walker starting in equal superposition of spin-up and spin-down. The coefficients and $R^2$ values are: (a) $y_0 = 0.9558$, $\tau = 19.563$, $\beta = 0.411664$ and $R^2 = 0.9834$ (b) $y_0 = 0.9437$, $\tau = 29.485$, $\beta = 0.532$ and $R^2 = 0.9822$

Figure 3.40: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $0 \leq r \leq 1$ with the walker starting in spin-up state. The coefficients and $R^2$ values are: (a) $y_0 = 0.9367$, $\tau = 16.0708$, $\beta = 0.4468$ and $R^2 = 0.9744$ (b) $y_0 = 0.9284$, $\tau = 26.359$, $\beta = 0.5724$ and $R^2 = 0.9746$
Figure 3.41: Fitted curves of (a) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ and (b) $\left(\frac{\sigma^2}{t}\right)$ vs $t$ for quantum random walk for 1000 steps averaged over 1000 iterations with the Hadamard parameter $r$ in the range $0 \leq r \leq 1$ with the walker starting in spin-down state. The coefficients and $R^2$ values are: (a) $y_0 = 0.9442$, $\tau = 19.543$, $\beta = 0.4313$ and $R^2 = 0.9819$ (b) $y_0 = 0.9331$, $\tau = 27.352$, $\beta = 0.563$ and $R^2 = 0.9790$

3.4 Observations

3.4.1 Sensitivity to initial state

As the range of allowed values of $r$ (and hence the noise) increases, the quantum to classical transition of the random walk on the lattice is apparent. The spatial probability distribution of the walker $P(n)$ is predominantly Gaussian-like, and the spread of $P(n)$ decreases. Also, as the range of noise increases, the values of $\left(\frac{\sigma^2}{t}\right)$ and $\left(\frac{\sigma^2}{t}\right)$ converge asymptotically regardless of the initial state of the walker.

For the ideal quantum walk shown in Fig. 3.3, 3.6 and 3.7 the ratios $\left(\frac{\sigma^2}{t}\right)$ and $\left(\frac{\sigma^2}{t}\right)$ depend on the initial state (bias) of the walker and are generally quite different except when the walker starts in an equal superposition of the two states. It is also clear that $\left(\frac{\sigma^2}{t}\right)$ and $\left(\frac{\sigma^2}{t}\right)$ are linear in $t$, i.e. $\left(\frac{\sigma^2}{t}\right) \propto t$ for both possible spin orientations ($\uparrow$ or $\downarrow$), which is characteristic of ballistic transport.

The value of $\left(\frac{\sigma^2}{t}\right) > \left(\frac{\sigma^2}{t}\right)$ when the walker starts in an up($\uparrow$) spin state initially. Sim-
ilarly, \((\sigma^2_t)^{\uparrow} < (\sigma^2_t)^{\downarrow}\) when the walker starts in a down(\(\downarrow\)) spin state initially. These trends continue as the noise increases, although the difference between \((\sigma^2_t)^{\uparrow}\) and \((\sigma^2_t)^{\downarrow}\) sharply decreases, and both the values become nearly equal when the noise is maximum.

3.4.2 Quantum to classical transition

The random walk with noisy Hadamard coin shows a gradual transition from purely quantum to (almost) classical behavior. In the work dealing with quantum walk with unitary noise [13], the classical behavior overtakes the quantum nature of the walk when the parameter characterizing the noise \(\alpha\), has a standard deviation \(\alpha = 0.07\). It can observed that the classical behavior becomes more prominent in the simulations in Sec. 3.1 when the noisy Hadamard parameter \(r\) grows to \(r = 0.07\) and beyond.

The quantum walk with the modified Hadamard coin shown in Fig. 3.8 to Fig. 3.17 shows a gradual transition from a fully quantum behavior to almost classical-like behavior. For very low deviations of \(r\) from the ideal value \(a_0(= 1/\sqrt{2} = 0.7071)\), especially in the range \(|r - a_0| < 0.07\) (i.e. \(0.7001 < r < 0.7141\)), the walk mostly resembles the quantum walk, with the peaks on either ends bigger than the Gaussian envelope in the center. When the range of allowed values of \(r\) is increased to \(0 \leq r \leq 1\) as shown in Fig. 3.11 to Fig. 3.17, the random walk transitions from quantum walk to strongly classical-like, but resembling a disordered system, as shown in Sec. 3.3.2.

3.4.3 Separation of \(\left(\sigma^2_t\right)^{\uparrow}\) and \(\left(\sigma^2_t\right)^{\downarrow}\)

It is very evident that the values of \(\left(\sigma^2_t\right)^{\uparrow}\) and \(\left(\sigma^2_t\right)^{\downarrow}\) are very different for the ideal quantum walk as shown in Fig. 3.3, 3.6 and 3.7. The separation of \(\left(\sigma^2_t\right)^{\uparrow}\) and \(\left(\sigma^2_t\right)^{\downarrow}\) becomes less distinct with increasing noise, as evidenced in plots from Fig. 3.8 to Fig. 3.17 (maximum noise) when both the quantities are nearly equal as the random walk shows classical-like
behavior.

Asymptotically, the ratios \( \left( \frac{\sigma^2}{t} \right) \) \((s = \uparrow \text{ and } \downarrow)\) both converge, it is clear that \( \left( \frac{\sigma^2}{t} \right) \) approaches a constant value asymptotically, as observed in Sec. 3.3. However, allowing the Hadamard parameter \( r \) to take all possible allowed values \((0 \leq r \leq 1)\) does not result in a perfectly classical behavior which can be described a power-law of the form described by Eq. (3.1). Instead, the dependence of \( \left( \frac{\sigma^2}{t} \right) \) on \( t \) assumes the form of Eq. (3.2), a stretched exponential which takes infinitely long time to become a constant, which is the typical behavior of a disordered system.
Chapter 4

Future work

4.1 Classical limit

It can be observed that the walk becomes more classical-like with increasing noise when
the walker is allowed to take a large number of steps. Other properties of the quantum
walk as observed in Sec. 3.4 hold equally good for the walk with higher number of time
steps. However, instead of the expected behavior of \( \left( \frac{s^2}{t} \right) \) (being independent of time \( t \)), the
ratio \( \left( \frac{s^2}{t} \right) \) shows a stretched exponential dependence like a disordered system, as shown in
Sec. 3.3.2.

This leads to the problem of deciding when a quantum random walk can be seen “classical enough”, which is not well-defined and the problem remains open. The ideal dis-
crete time quantum walks (DTQW) have been mapped to continuous time quantum walks
(CTQW) \[12\], but the problem of mapping the noisy discrete time quantum walks, such as
the one presented in this work, to a continuous time quantum walk is yet to be solved.

4.2 Choice of coin operators

The quantum random walk presented here depends on the presence of a property called
‘chirality’, and the action of a “coin operator” on the chiral state. The ideal quantum random
walk presented in Sec. 2.2.1.1 uses what is called a “Hadamard coin”. Similarly, the noisy
quantum random walk presented in Sec. 2.2.1.2 used a generalized Hadamard coin. However, this choice of the coin operators is not unique. Several other choices of the coin operators have been explored, most notably the Grover coin [28, 29]. Prediction of the behavior of quantum walk when other coins are allowed to be noisy is has not been done yet. Further, it is not clear if the noisy Hadamard walk behaves in the same way as noisy Grover walk or any other coined quantum walk subjected to noise.

4.3 Generalization to higher dimensions

The simulations shown in Chap. 3 were done for quantum random walk on the line (one dimension). However, in all semiconductor devices, the charge/spin carriers move in higher (two or three) dimensions. The quantum random walk discussed has been generalized to two dimensions [29, 30], but for different methods of decoherence. The noisy quantum random walk described in Sec. 2.2.1.2 needs to be generalized to two and three dimensions. There is only one “coin” in the one-dimensional quantum random walk. Generalizing the quantum walk to higher dimensions requires using extra coins or coin states with more than two levels [18].

4.4 Implementation

One important problem is the verification of results presented in Sec. 2.2.1.2 by suitable experimental systems. Ideal quantum walks, such as those presented in Sec. 2.2.1.1 have been implemented or proposed to be implemented in several candidate systems such as ion traps [4, 5], Nuclear Magnetic Resonance(NMR) systems [7], optical lattices [6] and Bose-Einstein Condensates [8].

However, there are very few proposals to implement the generalized noisy quantum walk such as the one presented in Sec. 2.2.1.2. The results presented there and the numerical simulations presented in Chap. 3 need to be verified against experiment. Although the spintronics applications have been emphasized in this work, working with other systems such as ion traps, NMR or optical lattices has proven to be easier to implement ideal quantum
walks. The choice of a suitable system to implement the noisy quantum walk is yet to be made, and it is to be seen if it could likely be one of the several existing candidates.
Appendix A

MATLAB Code

This appendix contains the core MATLAB code used to generate the plots shown in Chapter 3. The “basic recurrence relations” pointed out in the code refer to Equations (2.27). The curve-fitting was mostly done with the “Curve Fitting Toolbox” (cftool) in MATLAB. The code for curve fitting and rendering the plots into ‘pdf’ format is not included here.

```matlab
%--- The ideal Hadamard parameter
a0 = 1/sqrt(2);

j = 1000;         %--- Number of time steps
iter = 1000;      % --- Number of iterations

%--- astart and bstar are the lower and upper limits of Hadamard parameter r ---
astar = 0;         %a0-0.07;
bstar = 1;         %a0+0.07;
%--------------------------------------------------------------------------------

%-------------- Location of astart and bstar on the bloch sphere----------------
theta1 = asind(astar);
theta2 = asind(bstar);
%--------------------------------------------------------------------------------

pup = zeros(j,1,'double');
pdown = zeros(j,1,'double');
pupsq = zeros(j,1,'double');
pdownsq = zeros(j,1, 'double');
```

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%------- Check and p are arrays, the sum of which is the total probability (should be 1)
p = zeros((2*j)+1,iter,'double');
check = zeros(j,1,'double');

%-------- The ratios sigma^2/t for spin up and spin down-------------------------
ratio_up = zeros(j,1, 'double');
ratio_down = zeros(j,1,'double');
%----------------------------------------------------------------------------------

for k = 1:1:iter
    aup = zeros((2*j)+1, j, 'double');
adown = zeros((2*j)+1, j, 'double');

    %--------initial conditions (corresponding to equal superpositions)--------
    aup(j+1, 1) = 1/sqrt(2);
adown(j+1, 1) = 1i/sqrt(2);
    %--------------------------------------------------------------------------

    for t = 1:1:j-1 %timesteps
        r = astar + ((bstar - astar) * rand(1,1));
        for x = 1:1:(2*j) % steps in space, -j to j i.e. 2j+1 steps
            if x == 1
                %-------------Starting point, doesn't depend on lower values of x-----------------
            else
                %basic recurrence relations from Chapter 2---------------------

                aup(x,t+1) = double((aup(x-1,t) * r) + (sqrt(1 - (r^2)) * adown(x-1,t)));
adown(x,t+1) = double((aup(x+1,t) * (sqrt(1 - (r^2)))) - (r * adown(x+1,t)));
            end
        end
    end

    %matlab starts indexing from 1(no negative x). So for us, the origin is at 'j' (=500); we vary x
    %from 1 to 2*j+1 instead of -j to +j and hence we multiply with (x-j)
    %rather than x.

    for t = 1:1:j
        for x = 1:1:(2*j)
            if t == 1
                %%%%%%%%%%%%%%%%%-Starting point, doesn't depend on lower values of x----------------
            else
                %basic recurrence relations from Chapter 2---------------------

                aup(x,t+1) = double((aup(x-1,t) * r) + (sqrt(1 - (r^2)) * adown(x-1,t)));
adown(x,t+1) = double((aup(x+1,t) * (sqrt(1 - (r^2)))) - (r * adown(x+1,t)));
            end
        end
    end

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else
    pup(t) = pup(t) + ((x-j).*\(\text{abs}(a_{\text{up}}(x,t)) \cdot 2)));
    pupsq(t) = pupsq(t) + ((x-j)^2).*\(\text{abs}(a_{\text{up}}(x,t)) \cdot 2));
    pdown(t) = pdown(t) + ((x-j).*\(\text{abs}(a_{\text{down}}(x,t)) \cdot 2));
    pdownsq(t) = pdownsq(t) + ((x-j)^2).*\(\text{abs}(a_{\text{down}}(x,t)) \cdot 2));
end
end
end

%----- This loop is just to check the sum of probabilities "p" remains 1 ----------------------
for t = 1:1:j
    for x = 1:1:2*j
        if x == 1
            else
                p(x,k) = ((\text{abs}(a_{\text{up}}(x,t)) \cdot 2) + (\text{abs}(a_{\text{down}}(x,t)) \cdot 2));
        end
    end
end
end

end

%------ Calculate the values of \sigma^2 for spin up and spin down
sigmasq_up = abs((pupsq./iter) - ((pup./iter)).^2));
sigmasq_down = abs((pdownsq./iter) - ((pdown./iter)).^2));

for t = 1:j
    ratio_up(t) = sigmasq_up(t) ./t;
    ratio_down(t) = sigmasq_down(t) ./t;
end

%------------------Code for the plots--------------------------
figure
plot(1:j, sigmasq_up , 'g', 1:j, sigmasq_down , 'r');
legend('spin-up', 'spin-down')
title(strcat('{\sigma^2} vs t for a_{1} =', num2str(astar), '\(\theta_{1}=', num2str(theta1), ') and a_{2} = ', num2str(bstar), '\(\theta_{2}=', num2str(theta2), ')' )
ylabel('{\sigma^2}')
xlabel('{t}')
figure
plot(1:j, ratio_up , 'g', 1:j, ratio_down, 'r' );
legend('spin-up', 'spin-down' )
ylabel('\sigma^2 / t')
xlabel('t')

figure
plot(-j:j, sum(p.')./iter );
title(strcat('P(n) vs n for n = ', num2str(j)))
ylabel('P(n)')
xlabel('n')
Bibliography


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