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QUANTUM RANDOM WALKS UNDER DECOHERENCE

A Dissertation
Submitted to
the Temple University Graduate Board

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in Partial Fulfillment
of the Requirements for the Degree of
DOCTOR OF PHILOSOPHY

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by
Zhongzhi Liu
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ABSTRACT

QUANTUM RANDOM WALKS UNDER DECOHERENCE

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DOCTOR OF PHILOSOPHY

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Wei-Shih Yang, Chair

In this thesis, we consider quantum random walks on finite dimensional Hilbert spaces when decoherence is introduced. From the pure mathematics definition of history, we assign probabilities to histories according to R. Feynman's integral principle, and give out master equations and Green functions. We prove that decoherent quantum processes are ergodic. On finite lattices, we show that they have the same limiting distributions as classical random walks. This is an extension of the results on classical random walks, and it verifies that classical physical properties can be induced from the quantum theory under the decoherence theory frame.

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To my family

my mother, wife and son

with all my love.

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CHAPTER 1

Introduction

Random walks form one of the algorithmic tools in physics, computation science and financial mathematics. They have been applied to a variety of problems, such as estimating the volume of a convex body and solving certain differential equations. Since R.Feynman gave his idea of a quantum computer [1], quantum algorithms have been developed, such as Shor's factoring algorithm [2] and Grover's search algorithm [23]. Quantum random walks are expected to play the same roles as classical random walks in future computation science. From a quantum mechanics point of view, quantum random walks are quantum system evolutions and connected with the fundamental theory of quantum dynamic. Quantum random walks are of mathematical interest in their own right.

The basic idea of quantum walks can be traced back to the dynamics of quantum diffusion. Using a discrete time step to study quantum dynamics is described as quantum random walk. The discrete time quantum random walks were first used by R.Feynman for discretizing the Dirac equation [4]. The term " quantum random walks" appeared in the late 1980s from Gudder (1988) [5], Grossing and Zeilinger (1988) and Aharonov, Davidovich and Zagury in (1993) [6] . Motivated by quantum information and quantum computation, quantum random walks were studied again by Meyer in [7]. Recently, Aharonov, Ambainis, Kempe and Vazirani studied quantum random walks on general graphs with rigorous proofs. As a result, several rigorous results for quantum random walks were obtained.

This research has uncovered many effects that are different from the classical random walks, both from the physical point of view as well as from computer or information theory perspective. Kempe gave review on the differences in [8]. For example, in classical random walk, the probability of being absorbed by a wall at the original point 0 is 1 for a particle starting at position 1. But in quantum random Hadamard walk, the probability of being absorbed is $\frac{2}{\pi}$.

Interference phenomena are a well-known feature of quantum mechanics. The theory of decoherence is the study of interactions between a system and its environment. Decoherence occurs when a system loses phase coherence between different portions of its quantum states. Decoherence is caused by interactions with the second system, which may be considered as either the environments or a measuring device. As a result of the interaction, the wave functions of the system and the measuring device become entangled with each other. Since the measuring device has many degrees of freedom, the system behaves as a classical statistical ensemble of the different portions of the system states. In each member of the ensemble, the system appears to have collapsed onto a state with precise values. Some classical physical properties can be induced from the quantum theory under the decoherence theory frame. Decoherence plays a fundamental role in transforming from the quantum to the classical regime.

In quantum mechanics, the decoherent histories approach was initiated in 1984 by Robert Griffiths [9], and independently proposed by Roland Omns [10] shortly after. It was subsequently rediscovered by Murray Gell-Mann and James Hartle [11].

In mathematics, decoherence can be regarded as describing a stochastic process with intrinsic randomness. The histories for which decoherence is concerned are random histories of interactions with the environments. It is a useful idea to assign probabilities to histories, but it is not so easy to achieve.

In physics, decoherence assigns probabilities only to histories belonging to special families which satisfy a certain decoherence condition guaranteeing that $P(x)$ is additive, and hence provide a consistent assignment of probabilities to elements.

A pure mathematical decoherent process can be described as follows. Let H be a Hilbert space spanned by particle states $\phi_1, \phi_2, \dots \phi_n \dots$, which is an orthonormal basis of H. Let U be a unitary operator. If we choose an initial state ϕ_0, a pure quantum random walk with some discrete time t is $\psi_t = U^t(\phi_0)$.

We also choose $A_0 = \sqrt{1-p}I$, and $A_i = \sqrt{p}\Pi_i$, where I is the unit , Π_i is the projection from H to the subspace $C\phi_i$ spanned by ϕ_i, and p is a real number in the interval $[0,1]$. These operators can be considered as the interferences or measurements.

A decoherent quantum random walk (process) with an initial state ϕ_i with some discrete time t is

$$\Omega_t \phi_i \equiv (A_{j_t} \circ U)(A_{j_{t-1}} \circ U) \dots (A_{j_2} \circ U)(A_{j_1} \circ U)\phi_i$$

for a sequence $\Omega_t = (A_{j_t} \circ U) \circ (A_{j_{t-1}} \circ U) \dots (A_{j_1} \circ U)$, $j_l \in \{0, 1, 2, \dots, n, \dots\}$. We call this decoherent quantum random walk an Ω_t process, since it is determined by the order sequence Ω_t.

Under an Ω_t process and an initial state ϕ_i, the probability of the particle being measured at state ϕ_j is $|< \phi_j, \Omega_t \phi_i >|^2$. According to R.Feynman's famous path integral principle, we define the following as the probability that a quantum particle is found at ϕ_j at time t.

$$P_t^i(j) = \sum_{\Omega_t \in \Xi_t} |< \phi_j, \Omega_t \phi_i >|^2$$

where Ξ_t is the set of all order Ω_t.

If $p = 0, A_{j_t}$ are zero, and A_0 is the unit operator, then the decoherent quantum walk is a pure quantum walk $\psi_t = U^t(\phi_0)$.. On the other hand, if $p = 1$, then A_0 is zero, and A_{j_t} is a projector for all j_t, then the decoherent quantum random walk is a classical Markov chain.

We know that a classical Markov chain is ergodic , but not a pure quantum random walk. In this thesis, we prove that a decoherent quantum random walk is ergodic for $p \neq 0$ when H is finite Hilbert space. There are many ways to approach this problem. We will apply the generating function technique to work on the problem.

The structure of this thesis is as follows: First, in Chapter 2, we present some basic concepts and facts of quantum mechanics, such as state of quantum system, density matrix and Schrödinger equation. In Chapter 3, the pure mathematics definition of history is introduced. We associate a kind of probability with the histories, and give out the master equation (3.9)

$$P^i_{t+1}(j) = \sum_{s=1}^{t+1} p(1-p)^{s-1} \sum_{l=1}^{N} \left| W^{(s)}_{jl} \right|^2 P^i_{t+1-s}(l),$$

for $t \geq 0$. By the generating function technique, we prove that the limiting distribution exists. For finite case, under a family of Grover diffusion matrices, we show that the limiting distribution is $\frac{1}{N}$ on N points lattice. This is the same result as classical random walks. In this chapter, we also show that in a infinite dimensional space the probabilities still satisfy the above master equation. In Chapter 4. we deal with some hitting time questions of pure quantum walks in a half plane.

CHAPTER 2

Quantum Mechanics Preliminaries

2.1 States, Observables and Density Operators of Quantum Systems

In quantum mechanics, one of the major differences from classical mechanics is the superposition principle: Physical states are represented as vectors of a complex Hilbert space H. Two vectors α and β represent the same state of a quantum system if and only if they differ by a non-zero multiplication constant. In other word, α and β represent the same quantum state if there is a non-zero complex number $c \in C$ such that

$$\alpha = c\beta.$$

So if H is an n dimensional space, quantum states are just the elements of the projective space CP^{n-1}. In general, under an orthonormal basis $\{e_i\}$ of H, a state of a system ψ is

$$\psi = \sum x_i e_i,$$

where

$$\sum |x_i|^2 = 1.$$

The quantity $|< e_i, \psi >|^2 = |x_i|^2$ is the probability to find the system in the state e_i in a measure. With this explanation, a state of a system is a distribution function on all the unit vectors of H. If we identify the dual space of H with itself, a physical state in quantum system can be treated as a linear functional on H.

Another special concept for quantum mechanics is observable. An observable is simply a Hermitian operator on a Hilbert space. This means that A is an observable if and only if for any α, β of H,

$$< A\alpha, \beta >=< \alpha, A\beta > .$$

Two observables A and B are simultaneously measurable if

$$[A, B] = AB - BA = 0.$$

A family of observables $\{A_1, A_2, \dots A_n\}$ are simultaneously measurable if the corresponding operators commute with each other. If e is the common eigenvector, and

$$A_i(e) = \lambda_i e,$$

then the joint probability of simultaneously observables in a state ψ is

$$|< e, \psi >|^2 .$$

A linear operator P is a projector on H if and only if P is a Hermitian operator such that

$$P^2 = P.$$

A projector is an observable. Actually, projector operators play a fundamental role in quantum measurements.

A family of projectors $\{P_1, P_2, \dots P_n\}$, is said to be mutually orthogonal if and only if when $i \neq j$, $P_i P_j = 0$. It is said to be complete if and only if $\sum P_i = I$, where I is the identity of H.

A mutually orthogonal family of projectors are simultaneously measurable. An Hermitian operator is diagonalizable. It has real eigenvalues and orthogonal eigenvectors. If its spectrum is discrete and we denote by e_i its eigenvectors and λ_i the corresponding eigenvalues. Then

$$A = \sum \lambda_i e_i \otimes \bar{e_i},$$

where $\bar{e_j}$ are elements in the dual space of H, and satisfy $\bar{e_j}(e_i) = \delta_i^j$.
For a state of system ψ, the quantity $|< e_i, \psi >|^2$ is interpreted as the probability to find the value λ_i in a measure of the physical observable associated to A. For a Hermitian A and a state ψ, the quantity

$$< \psi|A|\psi >=< \psi, A(\psi) >= \sum \lambda_i |< e_i, \psi >|^2$$

is interpreted as the expected value of a measurement with respect to an observable A of a quantum system in a state ψ.
The quantity

$$|A(\psi)|^2 =< A(\psi), A(\psi) >$$

is the second moment of the measures of the observable associated with A. Since A is Hermitian, the expectation value is real.

The second quantity has different versions in physics. We would like to explain that by using notations from physics. Dirac has introduced the kets $|e_i >$ to denote vectors of Hilbert space H, and the bras $< e_j|$ for the elements of the dual space of H. Using $|e_i >< e_j|$. to denote the tensor product $e_i \otimes \bar{e_j}$.
For a state ψ,

$$\psi = \sum x_i e_i,$$

the dual is

$$\bar{\psi} = \sum \bar{x_i} \bar{e_i},$$

where $\bar{x_i}$ is the complex conjugate x_i.
From

$$|e_i >< e_j| = e_i \otimes \bar{e_j},$$

we have

$$|\psi >< \psi| = \psi \otimes \bar{\psi} = \sum x_i \bar{x}_j e_i \otimes \bar{e_j}.$$

$$= \begin{pmatrix} |x_1|^2 & x_1\bar{x_2} & \dots & x_1\bar{x_n} & \dots \\ x_2\bar{x_1} & |x_2|^2 & \dots & x_2\bar{x_n} & \dots \\ x_n\bar{x_1} & x_n\bar{x_2} & \dots & |x_n| & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix} \tag{2.1}$$

Thus

$$|\psi|^2 = trac(|\psi >< \psi|).$$

Now if A is represented by a matrix

$$A(e_i) = \sum a_{ij}e_j,$$

we have

$$\bar{A}(\bar{e_i}) = \sum \bar{a_{li}}\bar{e_l}.$$

Then

$$|A(\psi)|^2 = trac(|A(\psi) >< A(\psi)|).$$

For density operators, we have a pure mathematics definition. A linear operator on a Hilbert space is a density operator if it is a semi-definite Hermitian operators of trace 1. It is clear that for a state ψ of system, $\rho = \psi \otimes \bar{\psi}$ is a density operator. In physics, it is called a pure ensemble. It can be shown that a density operator represents a pure ensemble if and only if the operator is a projector. From $A(\psi) = \sum x_i a_{ij} e_j$, it is easy to see that

$$< \psi, A(\psi) >= trace(\rho A).$$

2.2 Quantum Evolution and Schrödinger Equation

In a closed quantum system, evolution is determined by the action of an unitary operator U. Let the initial state be $\psi(t_0)$, and $U(t, t_0)$ be the unitary operator, then at moment t, the state of the system is described by the vector

$$\psi(t) = U(t, t_0)\psi(t_0). \tag{2.2}$$

$U(t, t_0)$ is called the evolution operator. If two times translation are performed successively, the corresponding evolution operators are assumed to satisfy the following composition law:

$$U(t, t_0) = U(t, t_1)U(t_1, t_0)$$

This composition law is the analog of the Markov property for transition probabilities in the theory of stochastics. However, $U(t, t_0)$ forms a one parameter transform subgroup of the unitary group. The transition of probabilities in stochastic theory define only semigroup.

If $U(t, t_0)$ is differentiable as a function of t, $\psi(t)$ satisfies

$$ih\frac{\partial\psi}{\partial t} = H\psi(t) \tag{2.3}$$

where h is the Planck constant, H is the Hamiltonian. This equation is the basic equation of quantum mechanics. It is called Schrödinger equation. From mathematical perspective, Schrödinger equation is

$$\frac{\partial U(t)}{\partial t} = -\frac{i}{h}H(t)U(t), \tag{2.4}$$

where $-\frac{i}{h}H(t)$ is a skew-Hermitian operator.

If the Hamiltonian $H(t)$ is independent of time t, in other word, $H(t) = H$, then all matrices commute and the above equation has a simple solution

$$U(t) = e^{-\frac{i}{h}Ht}.$$

Generally, the solution is given by the path integral.

As a function of time, the expectation value of an operator A can be written as

$$< \psi(t), A\psi(t) >=< U(t,t_0)\psi(t_0), AU(t,t_0)\psi(t_0) >$$

$$=< \psi(t_0), U(t,t_0)^* AU(t,t_0)\psi(t_0) >$$

Then we have the Heisenberg representation of operator A,

$$A(t) = U(t,t_0)^* AU(t,t_0).$$

The operators $A(t)$ satisfies the evolution equation:

$$ih\frac{\partial A(t)}{\partial t} = [H, A(t)]. \tag{2.5}$$

Since a state ψ associated with a density operator $\rho = |\psi><\psi|$, the evolution of state induces the evolution of density operators.

$$\rho(t) = U(t,t_0)\rho(t_0)U^*(t.t_0).$$

The equation (2.1) appears in another form

$$ih\frac{\partial \rho}{\partial t} = [H, \rho(t)]. \tag{2.6}$$

2.3 Quantum Random Walks

In the classical discrete random walks, a particle is located at one of a finite or countable set of definite positions, such as the set of integers on the line or a graph of finite vertices. In response to a random event, the particle moves either right or left. The iterated process represents the basic example of a Markov chain. Generally, A Markov chain be characterized by a pair$(W(t_n), p(0))$, where $W(t_n) = W_{ij}(t_n)$ is a transition probability matrix or a stochastic matrix. Let $p(0) = (p_1(0), p_2(0), \dots p_n(0))^T$ be the initial probability distribution vector. At time t_n, the probability distribution $p(t_n)$ is determined by $W(t_n)$ as

$$p(t_n) = W(t_n)p(t_0). \tag{2.7}$$

Since $p(t_n)$ is a probability distribution, $W(t_n)$ is a stochastic matrix, so we have

$$\sum_i p_i(t_n) = 1, \; 0 \leq p_i(t_n) \leq 1,$$

and

$$\sum_i W_{ij}(t_n) = 1, \; 0 \leq W_{ij}(t_n) \leq 1.$$

For a classical random walk on the real line, the matrix is

$$W(t_n) = (W(t_0))^n,$$

where $W_{ij}(t_0) = \frac{1}{2}$, when $|i - j| = 1$, otherwise $W_{ij}(t_0) = 0$. By comparing 2.7 with 2.2, we define quantum random walks as quantum evolutions.

According to the evolution operators, quantum random walks are classified as discrete quantum walks and continuous quantum walks. For time parameter t, if the evolution operators $U(t)$ form a discrete subgroup of some unitary group, then the quantum walk is discrete. Similarly, if $U(t)$ form a continuous subgroup of a unitary group, the quantum walk is continuous. Generally, we use integer n as the time parameter of a discrete quantum walk, and notation

$$U(t_n) = (U)^n,$$

for some unitary operator U on the states space H.

At continuous cases, $U(t)$ is determined by its Hamiltonian $\mathcal{H}$, in other word,

$$U(t) = e^{-t\frac{i}{\hbar}\mathcal{H}}.$$

In direct analogy to classical random walks on the line, we have the following example. Let Z denote the integers on the real line and let $D = \{R, L\}$, where we make identification $R = right$ and $L = left$. The quantum systems will have the state set $Z \otimes D$. The quantum states of the system are unit vectors in the Hilbert space $H \equiv l^2(Z) \otimes l^2(D)$ with an orthonormal basis $\{n \otimes d,\ n \in Z, d \in D\}$. For Hadamard operator A on $l^2(D)$, and identity I on $l^2(Z)$, we have a unitary operator $I \otimes A$ on whole space H. Next, define another unitary operator, shift operator on H as follows

$$S(n \otimes R) = (n+1) \otimes R,$$

$$S(n \otimes L) = (n-1) \otimes L.$$

Finally, the composition $S \circ (I \otimes A)$ is the unitary operator for Hadamard walk.

2.4 Quantum Decoherence

In quantum mechanics. for a closed system, decoherent histories approach is to find sets of histories and to assign probabilities to histories. Such sets of histories are called consistent or decoherent. The approach provides a framework from which we can discuss classical properties from quantum mechanics.

The histories of a closed system are sequences of alternative at a succession of time. For example, in a typical experiment, a particle is emitted from a decaying nucleus at time t_1, then it passes through a magnetic field at time t_2, then it is absorbed by a detector at time t_3.

In quantum mechanics, properties of a system at a fixed time are represented by a set of projection operators $\{A_i, A_j \ldots\}$. At each time t, if the system appears at i, the projection operator A_i effect a partition of the possible alternative i. The set of operators satisfy exhaustive and exclusive conditions

$$\sum_j A_j A_j^* = 1, \; A_i A_j = \delta_i^j A_i.$$

A quantum mechanical history is characterized by a sequence of time dependent projections

$$\Omega_{t_n} \equiv A_{j_1}(t_1) A_{j_2}(t_2) \ldots A_{j_n}(t_n)$$

and an initial state ψ_0. The candidate probability for such histories is

$$< \psi, \Omega_{t_n} \psi >= trace(\Omega_{t_n}^* \rho \Omega_{t_n}).$$

It is easy to show that this number is non-negative. However it does not satisfy all the axioms of probability theory. It does not satisfy the axiom of additivity. The standard example is the double slit experiment. In this experiment, the histories consist of projections at two moments of time. At time t_1, the first projection determines which slit the particle went through. the second projection determines the point at which the particle hit the screen at time t_2. It is well known that the probability distribution for the interference pattern on the screen can not be written as a sum of the probabilities for going through each slit.

There are certain types of histories for which this candidate probability satisfies the sum rules. We have the following necessary and sufficient condition for that types histories: for any two histories Ω_t and Ω_s,

$$D(\Omega_t, \Omega_s) = trace(\Omega_t^* \rho \Omega_s) = 0.$$

We call this decoherence functional. Intuitively, it measures the amount of interference between pairs of histories.

CHAPTER 3

Decoherent Quantum Walks on Finite Lattices

3.1 Definitions and Generating Functions

Let H be an n dimensional Hilbert space over C spanned by particle states $\phi_1, \phi_2, \dots \phi_n$, which is an orthonormal basis of H. Let U be a unitary matrix. We also choose $A_0 = \sqrt{1-p}I$, and $A_i = \sqrt{p}\Pi_i$, where I is the unit matrix, Π_i is the projection from H to the subspace $\mathcal{C}\phi_i$ spanned by ϕ_i, and p is a real number in interval $[0, 1]$.

For an order sequence of operators $\Omega_t = (A_{j_t} \circ U) \circ (A_{j_{t-1}} \circ U) \dots (A_{j_1} \circ U)$, $j_l \in \{0, 1, 2, \dots n\}$, if we choose some ϕ_i as an initial state , a decoherent quantum random walk (process) start at ϕ_i with some discrete time $t = \{1, 2, \dots\}$ is

$$\Omega_t \phi_i \equiv (A_{j_t} \circ U)(A_{j_{t-1}} \circ U) \dots (A_{j_2} \circ U)(A_{j_1} \circ U)\phi_i.$$

We call this decoherent quantum random walk an Ω_t process, since it is determined by the order sequence Ω_t, and call $\Omega_t\phi_i$ a history.

Each unit vector in H represents a state of the particle. Let ϕ be a unit vector. Under an Ω_t process, the probability of the particle being measured at state ϕ is $|< \phi, \Omega_t\phi_i >|^2$.

According to the Feynman's famous paths integral principle, we define the probability that a quantum particle is found at ϕ at time t as follows,

$$P_t^i(\phi) = \sum_{\Omega_t \in \Xi_t} |< \phi, \Omega_t \phi_i >|^2 ,$$

where Ξ_t is the set of all operator sequences Ω_t, and we postulate that $P_0^i(\phi) = |< \phi, \phi_i >|^2$. We will prove that $P_t^i(\phi) \leq 1$ for all $t \geq 0$.

Remark : If $p = 0$, A_{j_t}'s are zero, and A_0 is the unit matrix, then the decoherent quantum walk is a pure quantum walk. On the other side, if $p = 1$, then A_0 is zero, and A_{j_t} is a projector for all j_t, the decoherent quantum random walk is a classical Markov chain.

We know that a classical Markov chain is ergodic , but not a pure quantum random walk. We hope that a decoherent quantum random walk is ergodic for $p \neq 0$. There are many ways to approach this problem. We consider generating functions.

$$g_j^i(z) = \delta_j^i + \sum_{t=1}^{\infty} P_t^i(j) z^t,$$

where $P_t^i(j) = P_t^i(\phi_j)$.

Before describing this function, we need to estimate some quantities. First we prove that $P_t^i(\phi) \leq 1$ for every t, and any unit vector $\phi \in H$, when $i, = 1, 2, \ldots N$.

We prove that by induction on t. At $t = 0$, by the definition and Schwarz inequality, we have $P_0^i(\phi) = |< \phi, \phi_i >|^2 \leq 1$.

Let $\phi = \sum_{l=1}^{N} a_l \phi_l$ be a unit vector, then a_l satisfy $\sum_{l=1}^{N} |a_l|^2 = 1$.

We assume that the claim is true for $t = k$ and any unit vector ϕ in H. We will prove that for $t = k + 1$.

Let $\Omega_k = (A_{j_k} \circ U) \ldots (A_{j_2} \circ U)(A_{j_1} \circ U)$ be a general element of Ξ_k. We introduce an operation

$$A_{j_{k+1}} \circ U \circ \Xi_k = \{A_{j_{k+1}} \circ U \circ \Omega_k = (A_{j_{k+1}} \circ U) \circ (A_{j_k} \circ U) \ldots (A_{j_2} \circ U)(A_{j_1} \circ U) | \forall \Omega_k \in \Xi_k\},$$

then we have a partition of Ξ_{k+1}

$$\Xi_{k+1} = \bigcup_{l=0}^{N} A_l \circ U \circ \Xi_k.$$

Thus

$$P^i_{k+1}(\phi) = \sum_{\Omega_{k+1}\in\Xi_{k+1}} |< \phi, \Omega_{k+1}\phi_i >|^2$$
$$= \sum_{l=0}^{N} \sum_{A_l\circ U\circ\Xi_k} |< \phi, A_l \circ U \circ \Omega_k\phi_i >|^2$$
$$= \sum_{\Xi_k}(|< \phi, A_0 \circ U \circ \Omega_k\phi_i >|^2 + \sum_{\Xi_k}\sum_{l=1}^{N} |< \phi, A_l \circ U \circ \Omega_k\phi_i >|^2) \tag{3.1}$$

Note that $A_l \circ U \circ \Omega_k = A_l \circ U \circ \Omega_k$, then

$$|< \phi, A_0 \circ U \circ \Omega_k\phi_i >|^2 = |< (U^* \circ A_0^*)\phi, \Omega_k\phi_i >|^2$$
$$= (1-p)\,|< U^*\phi, \Omega_k\phi_i >|^2 . \tag{3.2}$$

Similarly

$$|< \phi, A_l \circ U \circ \Omega_k\phi_i >|^2 = |< (U^* \circ A_l^*)\phi, \Omega_k\phi_i >|^2$$
$$= p\,|a_l|^2\,|< U^*\phi_l, \Omega_k\phi_i >|^2 . \tag{3.3}$$

Equation(3.1) becomes

$$P^i_{k+1}(\phi) = (1-p)\sum_{\Xi_k} |< U^*\phi, \Omega_k\phi_i >|^2 + p\sum_{l=1}^{N} |a_l|^2 \sum_{\Xi_k} |< U^*\phi_l, \Omega_k\phi_i >|^2 . \tag{3.4}$$

So that, for $k \geq 0$, we have

$$P^i_{k+1}(\phi) = (1-p)P^i_k(U^*\phi) + p\sum_{l=1}^{N} |a_l|^2\, P^i_k(U^*\phi_l). \tag{3.5}$$

By the assumption,

$$P^i_k(U^*\phi) \leq 1$$

and

$$P^i_k(U^*\phi_l) \leq 1,$$

We have proved that

$$P^i_{k+1}(\phi) \leq 1.$$

As a result of the inequality. we have the follow proposition.

Proposition 3.1 *The generating functions* $g_j^i(z) = \delta_j^i + \sum_{t=1} P_k^i(j)z^t$ *is analytic on* $\{z, |z| < 1\}$.

From (3.5), we see that if $\phi = \phi_j$, then

$$P_{k+1}^i(j) = P_k^i(U^*\phi_j). \tag{3.6}$$

Moreover if we choose $\phi_j, j = 1, 2, \dots N$ as the eigenvectors of U^*, and the respective eigenvalues are λ_j, $|\lambda_j|^2 = 1$.
In this case,

$$\begin{aligned} P_{t+1}^i(j) &= P_t^i(U^*\phi_j) \\ &= |\lambda_j|^2 P_t^i(j) \\ &= P_t^i(j). \end{aligned} \tag{3.7}$$

Since $P_0^i(j) = \delta_j^i$, so that

$$g_j^i(z) = \delta_j^i + \sum_{t=1}^{\infty} P_t^i(j)z^t$$

$$g_j^i(z) = \frac{\delta_j^i}{1-z}.$$

This is the trivial case for solving function $g_j^i(z)$.
Now we want to find a recursion formula for solving $g_j^i(z)$ in general case.
If $U^*\phi_j = \sum_{l=1}^N W_{jl}^{(1)}\phi_l$, by the general equation (3.5), for $t \geq 1$, we get

$$P_t^i(U^*\phi_j) = (1-p)P_{t-1}^i((U^*)^2\phi_j) + p\sum_{l=1}^N \left|W_{jl}^{(1)}\right|^2 P_{t-1}^i(U^*\phi_l)$$

Using equation 3.6, we have

$$P_{t+1}^i(j) = (1-p)P_{t-1}^i((U^*)^2\phi_j) + p\sum_{l=1}^N \left|W_{jl}^{(1)}\right|^2 P_t^i(\phi_l).$$

Let

$$(U^*)^2\phi_j = \sum_{l=1}^N W_{jl}^{(2)}\phi_l,$$

and repeating the process on

$$P_{t-1}((U^*)^2\phi_j) = (1-p)P^i_{t-2}((U^*)^3\phi_j) + p\sum_{l=1}^{N}\left|W^{(2)}_{jl}\right|^2 P^i_{t-1}(l).$$

For $t \geq 0$, we obtain that

$$P^i_{t+1}(j) = \sum_{s=0}^{t-1} p(1-p)^s \sum_{l=1}^{n} |W^{(s+1)}_{jl}|^2 P^i_{t-s}(l) + (1-p)^t P^i_0((U^*)^{t+1}\phi_j). \quad (3.8)$$

If $p = 0$, decoherence quantum walks become pure quantum walks, we have only the last term in the above equation

$$P^i_{t+1}(j) = P^i_0((U^*)^{t+1}\phi_j).$$

Now we suppose $p \neq 0$, and

$$(U^*)^s\phi_j = \sum_{l=1}^{N} W^{(s)}_{jl}\phi_l,$$

by the definition,

$$P^i_0((U^*)^{t+1}\phi_j) = |W^{(t+1)}_{ji}|^2,$$

we can rewrite the last term as

$$(1-p)^t P^i_0((U^*)^{t+1}\phi_j) = p(1-p)^t \frac{1}{p}|W^{(t+1)}_{ji}|^2$$

$$= \sum_{l=1}^{n} p(1-p)^t |W^{(t+1)}_{jl}|^2 \frac{1}{p}\delta^l_i.$$

Now, for $t \geq 0$, replacing s for $s+1$, equation 3.8 becomes,

$$P^i_{t+1}(j) = \sum_{s=1}^{t+1} p(1-p)^{s-1} \sum_{l=1}^{N}\left|W^{(s)}_{jl}\right|^2 P^i_{t+1-s}(l), \quad (3.9)$$

where we reset $P^i_0(l) = \frac{1}{p}\delta^i_l$. This is our recursion formula of $P^i_{t+1}(j)$.

Remark: In this recursion formula, we reset that $P^i_0(l) = \frac{1}{p}\delta^i_l$. This number can not be induced from the definition of $P^i_t(j)$ for $t \geq 1$. Since it is not a probability, it lives only in this recursion formula. At time $t = 0$, we have supposed the δ_j^i to be the initial probability.

Now we can write out the generating function $g_j^i(z)$ as follows:

$$\begin{aligned} g_j^i(z) &= \delta_j^i(z) + \sum_{t=0}^{\infty} P_{t+1}^i(j) z^{t+1} \\ &= \delta_j^i(z) + \sum_{t=0}^{\infty}\sum_{s=1}^{t+1} p(1-p)^{s-1} \sum_{l=1}^{N} \left|W_{jl}^{(s)}\right|^2 P_{t+1-s}^i(l) z^{t+1} \\ &= \delta_j^i(z) + \sum_{s=1}^{\infty}\sum_{t=s-1}^{\infty} p(1-p)^{s-1} \sum_{l=1}^{N} \left|W_{jl}^{(s)}\right|^2 P_{t+1-s}^i(l) z^{t+1} \\ &= \delta_j^i(z) + \sum_{s=1}^{\infty} pz((1-p)z)^{s-1} \sum_{l=1}^{N} \left|W_{jl}^{(s)}\right|^2 \sum_{t=s-1}^{\infty} P_{t-s+1}^i(l) z^{t-s+1}, \end{aligned} \tag{3.10}$$

but

$$\sum_{t=s-1}^{\infty} P_{t-s+1}^i(l) z^{t-s+1} = g_l^i(z) + \frac{1}{p}\delta_l^i - \delta_l^i.$$

Let

$$Q_{jl} = \sum_{s=1}^{\infty} pz((1-p)z)^{s-1} \left|W_{jl}^{(s)}\right|^2,$$

from the above equation, we have

$$G = I + QG + \frac{1}{p}Q - Q. \tag{3.11}$$

Since the norm of Q is less than 1 on $\{z, |z| \leq 1\}$, then $(I-Q)^{-1}$ exists on the disk.

Thus

$$G = I + \frac{1}{p}(I-Q)^{-1}Q. \tag{3.12}$$

on $\{z, |z| \leq 1\}$.

Note that $Q = -(I-Q) + I$, so that

$$G = -\frac{q}{p}I + \frac{1}{p}(I-Q)^{-1}. \tag{3.13}$$

We write this as our first theorem.

Theorem 3.1 *For any decoherent quantum random walk in a finite dimensional Hilbert space H, the generating function of the walk is*

$$G = -\frac{q}{p}I + \frac{1}{p}(I - Q)^{-1}$$

which is meromorphic on $\{z, |z| < \frac{1}{q}\}$*, and the poles are on or outside the unit circle.*

Since G is analytic on $|z| < 1$, and $det(I - Q)$ is analytic on $|z| < \frac{1}{q}$, by the equation 3.13, then the theorem holds.

Before we prove that the decoherence quantum walks are ergodic, we introduce some notations. Let

$$|(U^*)^s|^2 = \begin{pmatrix} \left|W_{11}^{(s)}\right|^2 & \left|W_{12}^{(s)}\right|^2 & \cdots & \left|W_{1N}^{(s)}\right|^2 \\ \left|W_{21}^{(s)}\right|^2 & \left|W_{22}^{(s)}\right|^2 & \cdots & \left|W_{2N}^{(s)}\right|^2 \\ \cdots & \cdots & \cdots & \cdots \\ \left|W_{N1}^{(s)}\right|^2 & \left|W_{12}^{(s)}\right|^2 & \cdots & \left|W_{NN}^{(s)}\right|^2 \end{pmatrix}$$

Then $Q(z)$ is a generating matrix by the sequence of matrices

$$|U^*|^2, \left|(U^*)^2\right|^2, \ldots, |(U^*)^n|^2, \ldots.$$

From $det(I - Q(z)) = 0$, we know that 1 is a eigenvalue of $Q(z)$. By analyzing the eigenvalues of $Q(z)$, for some decoherent quantum walk, we will show that $G(z)$ has only one pole $z = 1$ on the unit circle. Instead of directly proving this claim, we prove a more general theorem on the properties of a sequence of double stochastic matrices. The reason is that $Q(z)$ is a generating matrix of the sequence

$$|U^*|^2, \left|(U^*)^2\right|^2, \ldots, |(U^*)^n|^2, \ldots.$$

Since $(U^*)^n$ is unitary for any n, then $|(U^*)^n|^2$ are double stochastic matrices for $n = 1, 2, \ldots$.

We say a stochastic matrix W has gap property if and only if W has an eigenvalue $\lambda_1 = 1$ with multiplicity 1, and all other eigenvalues λ_i satisfy $|\lambda_i| < 1$ for $i = 2, \ldots, N$.

Theorem 3.2 *Let $0 < p < 1$, and $W_n, n = 1, 2, \ldots$, be a sequence of stochastic matrices, and $Q(z) = \frac{p}{q}\sum_{n=1}^{\infty}(qz)^n W_n$. Suppose for some W_{n_0} has the gap property. Then eigenvalues $\lambda(z)$ of $Q(z)$ satisfy $|\lambda(z)| < 1$, for any $|z| \leq 1, z \neq 1$. At $z = 1$, $Q(1)$ has the gap property.*

let $V_0 = (1, 1, \ldots, 1)^T$. Since W_n is stochastic for any n, V_0 is a common eigenvector of all W_n. Then

$$Q(z)V_0 = \lambda_0(z)V_0,$$

where

$$\lambda_0(z) = \frac{pz}{1 - qz}.$$

Thus $|\lambda_0(z)| < 1$ when $|z| \leq 1$ except $z = 1$. Suppose $\lambda(z)$ is another eigenvalue of $Q(z)$ for some fixed z. The corresponding eigenvector is $V(z)$. It is clear that $< V(z), V_0 >= 0$, otherwise $\lambda(z) = \lambda_0(z)$. We assume that $|V(z)| = 1$. For any $n \neq n_0$, we have

$$|< V(z), W_n V(z) >| \leq 1$$

for W_n are stochastic matrices. From assumption, we know that

$$|< V(z), W_{n_0} V(z) >| < 1.$$

otherwise, it will contradict with that W_{n_0} has gap property. Then

$$|\lambda(z)| = |< V(z), Q(z)V(z) >| = \left|\frac{p}{q}\sum_{n=1}^{\infty}(qz)^n < V(z), W_n V(z) >\right|$$

$$\leq \frac{p}{q}\sum_{n=1}^{\infty} q^n \, |< V(z), W_n V(z) >| < 1$$

Corollary 3.1 *In finite dimensional space H, if $|U^*|$ has gap property, then for the decoherent quantum walks, the generating matrix of functions is analytic on the unit disk $|z| \leq 1$ except $z = 1$.*

Suppose $z_0, |z_0| \geq 1$, makes $det(I - Q(z)) = 0$, then z_0 is a pole of $G(z)$. But $det(I - Q(z))$ is analytic on the disk $\{z, |z| < \frac{1}{q}\}$, so that for some small positive number $0 < \delta < \frac{p}{q}$, $det(I - Q(z))$ has finite zero points on the circle $\{z, |z| = 1\}$, but does not have zero points on the disk $|z| \leq 1 + \delta$. This means that $G(z)$ is meromorphic on disk $\{z, |z| < 1 + \delta\}$, and $G(z)$ is analytic on the circle $|z| = 1 + \delta$. So that by the Residue theorem, for some positive ξ, we have

$$\frac{1}{2\pi i} \oint_{|z|=\xi} \frac{G(z)}{z^{t+1}} dz = \frac{1}{2\pi i} \oint_{|z|=1+\delta} \frac{G(z)}{z^{t+1}} dz + \sum_i Res(\frac{G(z)}{z^{t+1}})|_{z_i}. \tag{3.14}$$

From the definition of $G(z)$, we know that

$$P_t^i(j) = \frac{1}{2\pi i} \oint_{|z|=\xi} \frac{G(z)}{z^{t+1}} dz. \tag{3.15}$$

On the other hand,

$$\lim_{t\to\infty} \oint_{|z|=1+\delta} \frac{G(z)}{z^{t+1}} dz = 0.$$

So that

$$\lim_{t\to\infty} P_t^i(j) = \lim_t \sum_i Res(\frac{G(z)}{z^{t+1}})|_{z_i}.$$

If $G(z)$ has only one pole $z = 1$ on $|z| = 1$, or equivalently, by our corollary, $|U^*|$ with gap property, the above equation means that the decoherent quantum walk on H is ergodic. We have proved the following theorem.

Theorem 3.3 *In a finite Hilbert space, if $|U^*|$ has gap property, then the decoherent quantum walks are ergodic.*

3.2 Decoherent Grover Quantum Random Walks

In this section, we will apply the theorems of the above section to some examples. Grover diffusion matrix appears in quantum mechanics and computer sciences. Grover matrix D can be written as

$$\begin{pmatrix} a & b & b & \dots & b \\ b & a & b & \dots & b \\ \dots & \dots & \dots & \dots & \dots \\ b & b & \dots & \dots & a \end{pmatrix},$$

where $a = \frac{2}{N} - 1$, and $b = \frac{2}{N}$.
For a vector $k \in Z_2^N$, we use $S(k)$ to denote the matrix

$$\begin{pmatrix} I_{N-|k|} & 0 \\ 0 & -I_{|k|} \end{pmatrix},$$

where I_l is the $l \times l$ identity matrix, $|k|$ is the L^1 norm of k, i.e. the number of 1 in vector k.
We let U be a general Grover matrix.

$$S(k)D = \begin{pmatrix} \frac{2}{N} - 1 & \frac{2}{N} & \dots & \frac{2}{N} & \frac{2}{N} \\ \frac{2}{N} & \frac{2}{N} - 1 & \dots & \frac{2}{N} & \frac{2}{N} \\ \dots & \dots & \dots & \dots & \dots \\ -\frac{2}{N} & -\frac{2}{N} & \dots & -\frac{2}{N} + 1 & -\frac{2}{N} \\ -\frac{2}{N} & -\frac{2}{N} & \dots & -\frac{2}{N} & -\frac{2}{N} + 1 \end{pmatrix}.$$

In order to give the explicit expression of $Q(z)$, we have to calculate $\left|(S(k)D)^{\prime t}\right|$. First we diagonalize matrix $S(k)D$. The characteristic polynomial of $S(k)D$ is

$$|\lambda I - S(k)D| = 0.$$

That is

$$\begin{vmatrix} a-\lambda & b & b & \dots & b \\ b & a-\lambda & b & \dots & b \\ \dots & \dots & \dots & \dots & \dots \\ -b & -b & \dots & -a-\lambda & -b \\ -b & -b & \dots & -b & -a-\lambda \end{vmatrix} = 0.$$

By simplifying, the characteristic polynomial becomes

$$(1+\lambda)^{N-|k|-2}(1-\lambda)^{|k|-1}\begin{vmatrix} a-\lambda & b & 0 \\ (N-|k|-1)b & a-\lambda+(N-|k|-2)b & |k|(1+\lambda) \\ -b & -b & 1-\lambda. \end{vmatrix} = 0.$$

That is

$$(1+\lambda)^{N-|k|-2}(1-\lambda)^{|k|-1}\begin{vmatrix} a-b-\lambda & b & 0 \\ b-a+\lambda & a-\lambda+(N-|k|-2)b & |k|(1+\lambda) \\ 0 & -b & 1-\lambda \end{vmatrix} = 0.$$

Further simplifying yields

$$(1+\lambda)^{N-|k|-1}(1-\lambda)^{|k|-1}[\lambda^2 - 2(1-|k|\,b)\lambda + 1] = 0.$$

Then $S(k)D$ has eigenvalues 1 and -1 with multiplicity $|k|-1$ and $N-|k|-1$ respectively. The left two eigenvalues are $e^{i\theta_k}$, $e^{-i\theta_k}$, where $cos(\theta_k) = 1 - \frac{2|k|}{N}$ and $sin(\theta_k) = \frac{2}{N}\sqrt{|k|\,(N-|k|)}$.

Now we want to find all eigenvectors corresponding to these eigenvalues.

From

$$(I + S(k)D)X = 0$$

we get $N-|k|-1$ eigenvectors corresponding to $\lambda = -1$

$$X_1 = (1, -1, \ldots, 0),^T$$
$$X_2 = (1, 0, -1, \ldots, 0),^T$$
$$\ldots, \ldots, \ldots, \ldots,$$
$$X_{N-|k|-1} = (1, 0, 0, \ldots, -1, \underbrace{0 \ldots, 0}_{|k|})^T.$$

Similarly from

$$(I - S(k)D)X = 0,$$

we have $|k| - 1$ eigenvectors corresponding to $\lambda = 1$

$$Y_1 = (\underbrace{0, 0, \ldots, 0,}_{N-|k|} 1, -1, 0, \ldots 0)^T,$$
$$Y_2 = (0, 0, \ldots, 0, 1, 0, -1 \ldots, 0)^T,$$
$$\ldots, \ldots, \ldots, \ldots,$$
$$Y_{|k|-1} = (0, 0, \ldots, 0, 1, 0, \ldots, 0, -1)^T.$$

The last two eigenvectors come from the equation

$$(S(k)D - \lambda_{N-1}I)X = 0.$$

They are

$$Z_1 = (-\frac{i}{\sqrt{N-|k|}}, \ldots, -\frac{i}{\sqrt{N-|k|}}, \frac{1}{\sqrt{|k|}}, \ldots, \frac{1}{\sqrt{|k|}})^T,$$
$$Z_2 = (\frac{i}{\sqrt{N-|k|}}, \ldots, \frac{i}{\sqrt{N-|k|}}, \frac{1}{\sqrt{|k|}}, \ldots, \frac{1}{\sqrt{|k|}})^T,$$

where there are $|k|$ terms of $\frac{1}{\sqrt{|k|}}$ in each vector above.
Let S be

$$S = (X_{N-|k|-1}, \ldots X_2, X_1, Z_1, Z_2, Y_1, \ldots, Y_{|k|-1}),$$

and

$$M = \begin{pmatrix} -I_{N-|k|-1} & 0 & 0 \\ 0 & E & 0 \\ 0 & 0 & I_{|k|-1} \end{pmatrix},$$

where

$$E = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix}.$$

From

$$S(k)D = SMS^{-1},$$

for any integer t, we have

$$(S(k)D)'^{t} = (S')^{-1}M^{t}S'.$$

By calculating directly,

$$S' = \left(\begin{array}{ccccc|ccccc} 1 & 0 & 0 & \dots & -1 & 0 & 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots\dots & \dots & \dots & \dots & \\ 1 & 0 & -1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ 1 & -1 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ -\frac{i}{\sqrt{N-|k|}} & -\frac{i}{\sqrt{N-|k|}} & -\frac{i}{\sqrt{N-|k|}} & \dots & -\frac{i}{\sqrt{N-|k|}} & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \dots & \frac{1}{\sqrt{|k|}} \\ \hline \frac{i}{\sqrt{N-|k|}} & \frac{i}{\sqrt{N-|k|}} & \frac{i}{\sqrt{N-|k|}} & \dots & \frac{i}{\sqrt{N-|k|}} & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \dots & \frac{1}{\sqrt{|k|}} \\ 0 & 0 & 0 & \dots & 0 & 1 & -1 & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & -1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & & \\ 0 & 0 & 0 & \dots & 0 & 1 & 0 & 0 & \dots & -1 \end{array}\right).$$

By rewriting it as a block matrix

$$S' = \begin{pmatrix} A & B \\ C & E \end{pmatrix}.$$

From the formula

$$S'^{-1} = \begin{pmatrix} (A - BE^{-1}C)^{-1} & -A^{-1}B(E - CA^{-1}B)^{-1} \\ -E^{-1}C(A - BE^{-1}C)^{-1} & (E - CA^{-1}B)^{-1} \end{pmatrix},$$

and that

$$A^{-1} = \frac{1}{i\sqrt{(N-|k|)}} \begin{pmatrix} \frac{i}{\sqrt{N-|k|}} & \frac{i}{\sqrt{N-|k|}} & \cdots & \frac{i}{\sqrt{N-|k|}} & -1 \\ \frac{i}{\sqrt{N-|k|}} & \frac{i}{\sqrt{N-|k|}} & \cdots & \frac{-(N-|k|-1)i}{\sqrt{N-|k|}} & -1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{i}{\sqrt{N-|k|}} & \frac{-(N-|k|-1)i}{\sqrt{N-|k|}} & \cdots & \frac{i}{\sqrt{N-|k|}} & -1 \\ \frac{-(N-|k|-1)i}{\sqrt{N-|k|}} & \frac{i}{\sqrt{N-|k|}} & \cdots & \frac{i}{\sqrt{N-|k|}} & -1 \end{pmatrix},$$

$$E^{-1} = \frac{1}{\sqrt{|k|}} \begin{pmatrix} 1 & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \cdots & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} \\ 1 & -\frac{|k|-1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \cdots & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} \\ 1 & \frac{1}{\sqrt{|k|}} & -\frac{|k|-1}{\sqrt{|k|}} & \cdots & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & \frac{1}{\sqrt{|k|}} & \frac{1}{\sqrt{|k|}} & \cdots & \frac{1}{\sqrt{|k|}} & -\frac{|k|-1}{\sqrt{|k|}} \end{pmatrix},$$

we have

$$(A - BE^{-1}C)^{-1} = \frac{1}{2i\sqrt{(N-|k|)}}$$

$$\begin{pmatrix} \frac{2i}{\sqrt{N-|k|}} & \frac{2i}{\sqrt{N-|k|}} & \cdots & \frac{2i}{\sqrt{N-|k|}} & -1 \\ \frac{2i}{\sqrt{N-|k|}} & \frac{2i}{\sqrt{N-|k|}} & \cdots & \frac{-2(N-|k|-1)i}{\sqrt{N-|k|}} & -1 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \frac{2i}{\sqrt{N-|k|}} & \frac{-2(N-|k|-1)i}{\sqrt{N-|k|}} & \cdots & \frac{2i}{\sqrt{N-|k|}} & -1 \\ \frac{-2(N-|k|-1)i}{\sqrt{N-|k|}} & \frac{2i}{\sqrt{N-|k|}} & \cdots & \frac{2i}{\sqrt{N-|k|}} & -1 \end{pmatrix},$$

and

$$(E - CA^{-1}B)^{-1} = \frac{1}{2\sqrt{|k|}} \begin{pmatrix} 1 & \frac{2}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} & \cdots & \frac{2}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} \\ 1 & -\frac{2(|k|-1)}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} & \cdots & \frac{2}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} \\ 1 & \frac{2}{\sqrt{|k|}} & -\frac{2(|k|-1)}{\sqrt{|k|}} & \cdots & \frac{2}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & \frac{2}{\sqrt{|k|}} & \frac{2}{\sqrt{|k|}} & \cdots & \frac{2}{\sqrt{|k|}} & -\frac{2(|k|-1)}{\sqrt{|k|}} \end{pmatrix},$$

the other two matrices are

$$-A^{-1}B(E-CA^{-1}B)^{-1}=\frac{1}{i2\sqrt{(N-|k|)}}\begin{pmatrix}1&0&0&\dots&0\\1&0&0&\dots&0\\\dots&\dots&\dots&\dots&\dots\\1&0&0&\dots&0\end{pmatrix},$$

$$-E^{-1}C(A-BE^{-1}C)^{-1}=\frac{1}{2\sqrt{|k|}}\begin{pmatrix}0&0&0&\dots&1\\0&0&0&\dots&1\\\dots&\dots&\dots&\dots&\dots\\0&0&0&\dots&1\end{pmatrix}.$$

Then we have

$$(S(k)D)'^{t}=\begin{pmatrix}a_t&b_t&b_t&\dots&b_t&c_t&c_t&\dots&c_t\\b_t&a_t&b_t&\dots&b_t&c_t&c_t&\dots&c_t\\\dots&\dots&\dots&\dots&\dots&\dots&\dots&\dots&\dots\\b_t&b_t&b_t&\dots&a_t&c_t&c_t&\dots&c_t\\d_t&d_t&d_t&\dots&d_t&e_t&f_t&\dots&f_t\\d_t&d_t&d_t&\dots&d_t&f_t&e_t&\dots&f_t\\\dots&\dots&\dots&\dots&\dots&\dots&\dots&\dots&\dots\\d_t&d_t&d_t&\dots&d_t&f_t&f_t&\dots&e_t\end{pmatrix},$$

where

$$a_t=\frac{(-1)^t(N-|k|-1)+cos(t\theta)}{N-|k|},$$

$$b_t=\frac{cos(t\theta)-(-1)^t}{N-|k|},$$

$$c_t=\frac{-sin(t\theta)}{\sqrt{|k|\,(N-|k|)}},$$

$$d_t=\frac{sin(t\theta)}{\sqrt{|k|\,(N-|k|)}},$$

$$e_t=\frac{cos(t\theta)+|k|-1}{|k|},$$

$$f_t=\frac{cos(t\theta)-1}{|k|}.$$

Further

$$\left|(S(k)D)'^t\right|^2 = \begin{pmatrix} |a_t|^2 & |b_t|^2 & |b_t|^2 & \dots & |b_t|^2 & |c_t|^2 & |c_t|^2 & \dots & |c_t|^2 \\ |b_t|^2 & |a_t|^2 & |b_t|^2 & \dots & |b_t|^2 & |c_t|^2 & |c_t|^2 & \dots & |c_t|^2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ |b_t|^2 & |b_t|^2 & |b_t|^2 & \dots & |a_t|^2 & |c_t|^2 & |c_t|^2 & \dots & |c_t|^2 \\ |d_t|^2 & |d_t|^2 & |d_t|^2 & \dots & |d_t|^2 & |e_t|^2 & |f_t|^2 & \dots & |f_t|^2 \\ |d_t|^2 & |d_t|^2 & |d_t|^2 & \dots & |d_t|^2 & |f_t|^2 & |e_t|^2 & \dots & |f_t|^2 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ |d_t|^2 & |d_t|^2 & |d_t|^2 & \dots & |d_t|^2 & |f_t|^2 & |f_t|^2 & \dots & |e_t|^2 \end{pmatrix}.$$

Recall that

$$Q(z) = \frac{p}{q}\sum_{t=1}^{\infty}(qz)^t\left|(S(k)D)'^t\right|^2,$$

thus

$$Q(z) = \begin{pmatrix} Q_{11} & Q_{12} & Q_{12} & \dots & Q_{12} & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ Q_{12} & Q_{11} & Q_{12} & \dots & Q_{12} & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ Q_{12} & Q_{12} & Q_{12} & \dots & Q_{11} & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{NN} & Q_{|k|N} & \dots & Q_{|k|N} \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{|k|N} & Q_{NN} & \dots & Q_{|k|N} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{|k|N} & Q_{|k|N} & \dots & Q_{NN} \end{pmatrix}(z),$$

where

$$Q_{11}(z) = \frac{p}{q}\sum_t |a_t|^2 (qz)^t,$$

$$Q_{12}(z) = \frac{p}{q}\sum_t |b_t|^2 (qz)^t,$$

$$Q_{1N}(z) = \frac{p}{q}\sum_t |c_t|^2 (qz)^t,$$

$$Q_{N1}(z) = \frac{p}{q}\sum_t |d_t|^2 (qz)^t,$$

$$Q_{NN}(z) = \frac{p}{q}\sum_t |e_t|^2 (qz)^t,$$

$$Q_{|k|N}(z) = \frac{p}{q}\sum_t |f_t|^2 (qz)^t.$$

By Theorem 3.3, we know that $Q(z)$ has eigenvalues $\lambda(z)$ with norm strictly less than 1 for all $|z| = 1$ except $z = 1$. Therefore

$$G(z) = -\frac{p}{q}I + \frac{1}{p}(I - Q(z))^{-1}$$

has a unique pole on $|z| = 1$ at $z = 1$. But here we would like to verify that by directly calculating. First we calculate the eigenvalues of $Q(z)$. From

$$\begin{vmatrix} Q_{11}-\lambda & Q_{12} & Q_{12} & \dots & Q_{12} & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ Q_{12} & Q_{11}-\lambda & Q_{12} & \dots & Q_{12} & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ Q_{12} & Q_{12} & Q_{12} & \dots & Q_{11}-\lambda & Q_{1N} & Q_{1N} & \dots & Q_{1N} \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{NN}-\lambda & Q_{|k|N} & \dots & Q_{|k|N} \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{|k|N} & Q_{NN}-\lambda & \dots & Q_{|k|N} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ Q_{N1} & Q_{N1} & Q_{N1} & \dots & Q_{N1} & Q_{|k|N} & Q_{|k|N} & \dots & Q_{NN}-\lambda \end{vmatrix} = 0,$$

we get

$$(Q_{11} - \lambda - Q_{12})^{N-|k|-1}(Q_{NN} - \lambda - Q_{|k|N})^{|k|-1}$$
$$\begin{vmatrix} 1 & 0 & 0 & \dots & Q_{12} & Q_{1N} & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & Q_{12} & Q_{1N} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ -1 & -1 & -1 & \dots & Q_{11}-\lambda & Q_{1N} & 0 & \dots & 0 \\ 0 & 0 & 0 & \dots & Q_{N1} & Q_{NN}-\lambda & -1 & \dots & -1 \\ 0 & 0 & 0 & \dots & Q_{N1} & Q_{|k|N} & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & Q_{N1} & Q_{|k|N} & 0 & \dots & 1 \end{vmatrix} = 0. \quad (3.16)$$

So that the eigenvalues of $Q(z)$ are

$$\lambda = Q_{11} - Q_{12}$$

with multiplicity of $N-|k|-1$ and

$$\lambda = Q_{NN} - Q_{|k|N}$$

of multiplicity of $|k|-1$, and the roots of

$$\begin{vmatrix} Q_{11} - \lambda + (N-|k|-1)Q_{12} & (N-|k|)Q_{1N} \\ |k|\, Q_{N1} & Q_{NN} - \lambda + (|k|-1)Q_{|k|N} \end{vmatrix} = 0.$$

From $a_t = b_t + (-1)^t$ and $e_t = f_t + 1$, and expressions of $Q(11), Q_{12}, Q_{NN}$ and $Q_{|k|N}$, we have the following equations.

$$Q_{11}(z) - Q_{12}(z) = \frac{2p}{(N-|k|)q} \sum_t (-1)^t cos(t\theta)(qz)^t + \frac{N-|k|-2}{N-|k|} h(z),$$

where

$$h(z) = \frac{pz}{1-qz}.$$

For any $|z| = 1$, since

$$|Q_{11}(z) - Q_{12}(z)| < 1,$$

thus $Q_{11}(z) - Q_{12}(z) \neq 1$ on the unit circle.
Similarly, we have

$$Q_{NN}(z) - Q_{|k|N}(z) = \frac{2p}{|k|\, q} \sum_t cos(t\theta)(qz)^t + \frac{|k|-2}{|k|} h(z),$$

and

$$|Q_{NN}(z) - Q_{|k|N}(z)| < 1$$

on the unit circle.
From

$$Q_{11} - \lambda + (N-|k|-1)Q_{12} = \frac{N-|k|-1}{N-|k|} h(z) - \lambda + \frac{p}{(N-|k|)q} \sum_t cos^2(t\theta)(qz)^t,$$

and

$$Q_{NN} - \lambda + (|k|-1)Q_{|k|N} = \frac{|k|-1}{|k|} h(z) - \lambda + \frac{p}{|k|\, q} \sum_t cos^2(t\theta)(qz)^t,$$

we obtain the last two eigenvalues

$$\lambda_{N-1} = h(z) - \frac{pN}{|k|\,(N-|k|)q}\sum_t sin^2(t\theta)(qz)^t,$$

$$\lambda_N = h(z).$$

We know that $h(z) < 1$ on $|z| = 1$ except $z = 1$. Next we want to show that $\lambda_{N-1} \neq 1$ on the unit circle.

Rewrite λ_{N-1} as

$$\frac{|k|\,p}{|k|\,q}\sum_t [cos^2(t\theta)+sin^2(t\theta)](qz)^t - \frac{p}{|k|\,q}\sum_t sin^2(t\theta)(qz)^t - \frac{p}{(N-|k|)q}\sum_t sin^2(t\theta)(qz)^t$$

$$= \frac{p}{q}\sum_t cos^2(t\theta)(qz)^t + [\frac{(|k|-1)p}{|k|\,q} - \frac{p}{(N-|k|)q}]\sum_t sin^2(t\theta)(qz)^t$$

$$= \frac{p}{q}\sum_t cos^2(t\theta)(qz)^t + [\frac{(|k|\,(N-|k|)-N)p}{|k|\,(N-|k|)q}]\sum_t sin^2(t\theta)(qz)^t.$$

From this equation, we have $|\lambda_{N-1}| < 1$ when $|z| = 1$. Therefore, $G(z)$ has a unique pole on the unit circle $|z| = 1$ at $z = 1$. This means that, for some $\delta > 0$, the contour integral of $G(z)$ on the circle $|z| = 1 + \delta$ comes from the single residue of $G(z)$ at $z = 1$. Next we calculate the residue directly from the expression of $G(z)$.

From

$$\begin{aligned} det(Q(z)-I) =&(Q_{11} - Q_{12} - 1)^{N-|k|-1}(Q_{NN} - Q_{|k|N} - 1)^{|k|-1} \\ &(h(z)-1)(h(z) - \frac{pN}{|k|\,(N-|k|)q}\sum_t sin^2(t\theta)(qz)^t - 1), \end{aligned} \tag{3.17}$$

the cofactor of $Q_{11} - 1$ in $Q(z) - I$ is

$$A_{11} = (Q_{11} - Q_{12} - 1)^{N-|k|-2}(Q_{NN} - Q_{|k|N} - 1)^{|k|-1}$$

$$\begin{vmatrix} Q_{11} - 1 + (N-|k|-2)Q_{12} & (N-|k|-1)Q_{1N} \\ |k|\,Q_{N1} & Q_{NN} - 1 + (|k|-1)Q_{|k|N} \end{vmatrix}.$$

Thus

$$res(G(z)_{11})_{z=1} = -res\left(\frac{1}{p}\frac{A_{11}(z)}{det(Q(z)-1)}\right)_{z=1}$$

$$= -\left(\frac{1}{(Q_{11}-Q_{12}-1)(-\frac{pN}{|k|(N-|k|)q}\sum_t sin^2(t\theta)(qz)^t)}\right.$$

$$\left.\begin{vmatrix} Q_{11}-1+(N-|k|-2)Q_{12} & (N-|k|-1)Q_{1N} \\ |k|\,Q_{N1} & Q_{NN}-1+(|k|-1)Q_{|k|N}\end{vmatrix}\right)_{z=1},$$

but

$$(Q_{11}-Q_{12}-1)_{z=1} = \frac{2p}{(N-|k|)q}(\sum_t(-1)^t cos^2(t\theta)q^t - 2),$$

$$(Q_{NN}-1+(|k|-1)Q_{|k|N})_{z=1} = -\frac{p}{|k|\,q}\sum_t sin^2(t\theta)q^t,$$

and

$$|k|\,Q_{N1}Q_{1N} = \frac{p^2}{|k|\,(N-|k|)^2q^2}(\sum_t sin^2(t\theta)q^t)^2.$$

Then

$$\begin{vmatrix} Q_{11}-1+(N-|k|-2)Q_{12} & (N-|k|-1)Q_{1N} \\ |k|\,Q_{N1} & Q_{NN}-1+(|k|-1)Q_{|k|N}\end{vmatrix}_{z=1}$$

$$= \frac{p}{|k|\,q}(\sum_t sin^2(t\theta)q^t)^2\frac{1}{(N-|k|)}(Q_{11}-Q_{12}-1).$$

Thus the residue is $\frac{1}{N}$. By similarly calculation, we obtain

$$res(G(z)_{ij})_{z=1} = -res\left(\frac{1}{p}\frac{A_{ij}}{det(Q(z)-1)}\right)_{z=1} = \frac{1}{N}.$$

From the equation,

$$G(z) = -\frac{p}{q}I + \frac{1}{p}\frac{1}{det(I-Q(z))}(I-Q(z))^*,$$

we know that the order of the pole of $G(z)$ at $z=1$ is one. Finally we have

$$\lim_{t\to\infty} P_t^i(j) = \frac{1}{N}.$$

This prove the theorem.

Theorem 3.4 *In a finite Hilbert space H, the decoherent Grover quantum walk is ergodic. The limit distribution is*

$$\lim_{t\to\infty} P_t^i(j) = \frac{1}{N}.$$

The limit speed in $\lim_{t\to\infty} P_t^i(j) = \frac{1}{N}$ is controlled by the distance between the unit circle and set of the poles of $G(z)$ except $z = 1$. We would like to show that this gap will disappear when either p approaches 0 or N goes to infinity. We will prove that in two steps. First we claim that there is at least one pole of $G(z)$ in $\{z, 1 < |z| < \frac{1}{q}\}$. Second we prove that all the poles in the region approach 1 when either p goes to 0 or N goes to infinity. Since the poles are the points z_0 that make $Q(z_0)$ has eigenvalue 1, we will analyze the eigenvalues of $Q(z)$. Recall that the eigenvalues are

$$h(z) = \frac{pz}{1-qz},$$

$$h(z) - \frac{pN}{|k|\,(N-|k|)q} \sum_t sin^2(t\theta)(qz)^t,$$

$$Q_{11}(z) - Q_{12}(z),$$

$$Q_{NN}(z) - Q_{|k|N}(z).$$

Now we prove the first claim by considering the roots of

$$Q_{11}(z) - Q_{12}(z) = 1.$$

That is

$$\frac{N-|k|-2}{(N-|k|)}h + \frac{2p}{(N-|k|)q}\sum_{t=1}^{\infty}(-1)^t(qz)^t cos(t\theta) = 1.$$

Simplifying

$$\frac{1}{1+qze^{i\theta}} + \frac{1}{1+qze^{-i\theta}} = \frac{N-|k|}{p} - \frac{N-|k|-2}{1-qz}.$$

It is a third degree polynomial equation of z with real coefficients, so that there is at least one real root.

First we suppose that the root is $-r$, for some $r > \frac{1}{q}$. By rewriting the equation as

$$\frac{1}{1-qre^{i\theta}} + \frac{1}{1-qre^{-i\theta}} = \frac{N-|k|}{p} - \frac{N-|k|-2}{1+qr}.$$

In this equation, the right side is a positive number. The left side is 2 times a real part of $\frac{1}{1-qre^{i\theta}}$. But

$$Re(\frac{1}{1-qre^{i\theta)}}) = \frac{Re(1-qre^{-i\theta})}{1+(qr)^2 - 2qrcos(\theta)}.$$

From

$$1+(qr)^2 - 2qrcos(\theta) = (1-qr)^2 + 2qr(1-cos(\theta)) > \frac{4\,|k|}{N},$$

we obtain that

$$\frac{1}{1-qre^{i\theta}} + \frac{1}{1-qre^{-i\theta}} < 2\frac{N}{4\,|k|}(1-cos(\theta)) = 1.$$

So that

$$\frac{N-|k|}{p} - \frac{N-|k|-2}{1+qr} < 1.$$

On the other hand,

$$\frac{N-|k|}{p} - \frac{N-|k|-2}{1+qr} > \frac{2}{p} > 2.$$

This is a contradiction. So that the real root r is in the region $\{z, |z| < \frac{1}{q}\}$ or is positive.

Now suppose that r is positive. Since real part of $\frac{1}{1+qre^{i\theta}}$ is less 1, then we have

$$\frac{1}{1+qre^{i\theta}} + \frac{1}{1+qre^{-i\theta}} < 2.$$

So that

$$\frac{N-|k|}{p} - \frac{N-|k|-2}{1-qr} < 2.$$

From this we get

$$1-qr > 0.$$

Thus

$$r < \frac{1}{q}.$$

We have proved the first claim.

For the second claim, when p approach 0, then $\frac{1}{q}$ approach 1. Then the claim is clear. Now we only consider N goes to infinity.

Now suppose some complex number $z, 1 < |z| < \frac{1}{q}$ is a root of $Q_{11}-Q_{12} = 1$. Since $cos\theta = \frac{N-2|k|}{N}$, so we can think z as a function of p, $|k|$ and N. We rewrite the above equation as

$$\frac{2p}{(N-|k|)q}\sum_{t=1}^{\infty}(-1)^t(qz(p,N))^t cos(t\theta) = \frac{z(p,N)-1}{1-qz(p,N)} - \frac{2pz(p,N)}{(N-|k|)(1-qz(p,N))}.$$

From this we see that

$$\lim_{p\to 0} z(p,N) = \lim_{N\to\infty} z(p,N) = 1.$$

Similarly, if $z, 1 < |z| < \frac{1}{q}$, is a root of $Q_{NN}(z) - Q_{|k|N}(z) = 1$, then z is a root of

$$\frac{2p}{|k|\,q}\sum_{t=1}^{\infty}(qz)^t cos^2(t\theta) + \frac{|k|-2}{|k|}h(z) = 1.$$

Let $N \to \infty$, then $cos(\theta) = 1$, from this equation we have $z \to 1$. Finally if $z, 1 < |z| < \frac{1}{q}$, is a root of

$$h(z) - \frac{pN}{|k|\,(N-|k|)q}\sum_t sin^2(t\theta)(qz)^t = 1.$$

$N \to \infty$ implies that $sin(\theta) \to 0$, the above equation implies that z approaches 1. So that we prove the second claim. From two claims, we can say that the gap disappears when N goes to infinity or p approaches 0. Recall that equation (3.14)

$$\frac{1}{2\pi i}\oint_{|z|=\xi}\frac{G(z)}{z^{t+1}}dz = \frac{1}{2\pi i}\oint_{|z|=1+\delta}\frac{G(z)}{z^{t+1}}dz + \sum_i Res(\frac{G(z)}{z^{t+1}})|_{z_i}.$$

If we use $K(N,p)$ to denote some constant such that

$$\oint_{|z|=1+\delta}\frac{G(z)}{z^{t+1}}dz = K(N,p)\oint_{|z|=1+\delta}\frac{1}{z^{t+1}}dz,$$

we can rewrite the theorem (3.4) as

Theorem 3.5 *In a finite Hilbert space H, the decoherent Grover quantum walk is ergodic. The limit distribution is*

$$P_t^i(j) = \frac{1}{N} + K(N,p)\mathcal{O}(e^{-C(p,N)t}),$$

where

$$\lim_{p\to 0} C(p,N) = \lim_{N\to\infty} C(p,N) = 0.$$

3.3 Decoherent Quantum Walks on Hypercubes

Quantum random walks on the hypercube are related to many quantum algorithms, they have been studied recently by many people [32]. The geometric properties of the hypercube make the quantum random walks exhibit a numbers of features different from that of other graph such as cycles. For an example, a quantum walk on the n-cycle mixes in time $O(nlogn)$, however on the hypercube it mixes faster than $O(nlogn)$. when decoherence is introduced, under continuous cases, Alagic and Russell [12] give the exact mixing times. In this section, we will study the limit distribution function when the quantum walks are discrete and subjected to decoherence. First we introduce some notations and finite Fourier transform.

Let Z_2^N be the N-dimensional hypercube, i.e, Z_2^N is a N dimensional vector space on the field Z_2. It has a regular basis of vectors $B = \{\alpha_i = (0,\ldots,1,\ldots 0), i = 1,2,\ldots,N\}$. Under the classical inner product $<,>$, Z_2^N is an Euclidean space.

Let $L(Z_2^N)$ and $L(B)$ be the Hilbert spaces of complex functions on Z_2^N and B respectively. We consider $H = L(Z_2^N) \otimes L(B)$ as a Hilbert space with inner product

$$< f \otimes h, g \otimes l >=< f, g >< h, l >$$

An orthonormal basis in H is

$$\{\delta_x \otimes \delta_{\alpha_i} | x \in Z_2^N, \alpha \in B\}.$$

Under this basis, any element Ψ in H can be expressed as

$$\Psi = \sum_{(x,\alpha_i) \in Z_2^N \otimes B} \Psi_{(x,\alpha_i)} \delta_x \otimes \delta_{\alpha_i},$$

where $\Psi_{(x,\alpha_i)}$ is the coordinate. By arranging the order, for a fixed x, we have $n-$dimensional vector

$$\Psi(x) \equiv (\Psi_{(x,\alpha_1)}, \Psi_{(x,\alpha_2)}, \Psi_{(x,\alpha_N)}).$$

Then we can consider Ψ as a vector valued function on Z_2^N

$$\Psi : Z_2^N \to C^N.$$

For any two elements Ψ and Φ, the inner product is

$$\begin{aligned} < \Psi, \Phi > &= \sum_{(x,\alpha)} \Psi_{(x,\alpha_i)} \bar{\Phi}_{(x,\alpha_i)} \\ &= \sum_x < \Psi(x), \Phi(x) > \end{aligned} \tag{3.18}$$

where $< \Psi(x), \Phi(x) >$ is the inner product of $\Psi(x)$ and $\Phi(x)$ in C^N with the classical Hermitian.

The Fourier transform of Ψ is $\mathcal{F}(\Psi) = \hat{\Psi}$:

$$\hat{\Psi}(k) = \frac{1}{\sqrt{2^N}} \sum_x (-1)^{<x,k>} \Psi(x).$$

From

$$\begin{aligned} < \mathcal{F}(\Psi), \mathcal{F}(\Phi) > &= \sum_k < \mathcal{F}(\Psi)(k), \mathcal{F}(\Phi)(k) > \\ &= \frac{1}{2^N} \sum_k < \sum_x (-1)^{<x,k>} \Psi(x), \sum_y (-1)^{<y,k>} \Psi(y) > \\ &= \sum_x < \Psi(x), \Phi(x) > \\ &=< \Psi, \Phi >, \end{aligned} \tag{3.19}$$

we get a lemma.

Lemma 3.1

$$< \hat{\Psi}, \hat{\Phi} >=< \Psi, \Phi > .$$

The shift operator S is defined as

$$S(\Psi)(x) = (\Psi_1(x \oplus \alpha_1), \Psi_2(x \oplus \alpha_2), \ldots \Psi_n(x \oplus \alpha_n)).$$

By definition, we have

$$\begin{aligned} < S(\Psi), S(\Phi) > &= \sum_{(x,\alpha)} S(\Psi)_{(x,\alpha)} S(\bar{\Phi})_{(x,\alpha)} \\ &= \sum_{(x,\alpha)} \Psi_{(x+\alpha,\alpha)} \bar{\Phi}_{(x+\alpha,\alpha)} \\ &=< \Psi, \Phi > . \end{aligned} \tag{3.20}$$

Then we obtain a lemma.

Lemma 3.2

$$< S(\Psi), S(\Phi) >=< \Psi, \Phi > .$$

The property of exchanging the order of S and $\mathcal{F}$ is the following.

Lemma 3.3 *For any* $k = (k_1, k_2, \dots, k_N)$ *in* Z_2^N,

$$\mathcal{F} \circ S(\Psi)(k) = \begin{pmatrix} (-1)^{k_1} & 0 & 0 & \dots & 0 \\ 0 & (-1)^{k_2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & (-1)^{k_N} \end{pmatrix} \mathcal{F}(\Psi)(k)$$

By the definitions of S and $\mathcal{F}$, we have

$$\begin{aligned} \mathcal{F} \circ S(\Psi)(k) &= \sum_x (-1)^{<xk>} S(\Psi)(x) \\ &= \frac{1}{\sqrt{2^N}} \sum_x (-1)^{<xk>} (\Psi_1(x \oplus \alpha_1), \Psi_2(x \oplus \alpha_2), \dots \Psi_n(x \oplus \alpha_n)) \\ &= \begin{pmatrix} (-1)^{k_1} & 0 & 0 & \dots & 0 \\ 0 & (-1)^{k_2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & (-1)^{k_N} \end{pmatrix} \mathcal{F}(\Psi)(k). \end{aligned} \tag{3.21}$$

We use $\hat{S}(k)$ denote the matrix

$$\begin{pmatrix} (-1)^{k_1} & 0 & 0 & \dots & 0 \\ 0 & (-1)^{k_2} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & (-1)^{k_N} \end{pmatrix}$$

for $k = (k_1, k_2, \dots k_N)$ and $k_i \in \{0, 1\}$.

For any $N \times N$ matrix $D = (D_{ij})$, we define a linear operator on $L(Z_2^N) \otimes L(B)$ as

$$D\Psi(x) = D(\Psi_1(x), \Psi_2(x), \dots \Psi_N(x))^T.$$

Since

$$\begin{aligned}(D\circ\mathcal{F})(\Psi)(k) &= D\frac{1}{\sqrt{2^N}}\sum_x(-1)^{<x,k>}\Psi(x)\\ &= \frac{1}{\sqrt{2^N}}\sum_x(-1)^{<x,k>}D\Psi(x) \\ &= \mathcal{F}(D\Psi)(k),\end{aligned} \tag{3.22}$$

therefore, we have proved the following lemma.

Lemma 3.4

$$\mathcal{F}\circ D = D\circ\mathcal{F}.$$

For a fixed unitary D and initial state Ψ_0, the first step quantum walk is

$$\Psi_1(x) = (S\circ D)\Psi_0(x).$$

For discrete time t, the quantum walk is the process

$$\Psi_t(x) = (S\circ D)^t\Psi_0(x).$$

From Lemma 3.3 and Lemma 3.4, we get

$$\hat{\Psi}_t(k) = (\hat{S}(k)\circ D)^t\mathcal{F}(\Psi_0)(k).$$

Let $U_k = \hat{S}(k)\circ D$, the above equation is

$$\hat{\Psi}_t(k) = U_k^t\mathcal{F}(\Psi_0)(k).$$

Next, we introduce operators $A_j = I\otimes\sqrt{p}\Pi_j, j = 1,\ldots,N$, and $A_0 = I\otimes\sqrt{1-p}I$ on $L(Z_2^N)\otimes L(B)$. As Todd A.Brun and H, A. Carteret did in paper [13], we consider the decoherence only on the coin space.

For a history

$$\Omega_t = (A_{j_t}\circ S\circ D)(A_{j_{t-1}}\circ S\circ D)\ldots(A_{j_0}\circ S\circ D),$$

and two states $\delta_y\otimes\delta_\beta$ and $\delta_x\otimes\delta_\alpha$, we consider the quantity

$$P_t^{(x,\alpha)}(\delta_y\otimes\delta_\beta) = \sum_{\Omega_t\in\Xi_t}|<\delta_y\otimes\delta_\beta,\Omega_t(\delta_x\otimes\delta_\alpha)>|^2.$$

By the equation (3.18)

$$< \delta_y \otimes \delta_\beta, \Omega_t(\delta_x \otimes \delta_\alpha) >= \sum_k < \mathcal{F}(\delta_y \otimes \delta_\beta)(k), \mathcal{F}(\Omega_t \delta_x \otimes \delta_\alpha)(k) >,$$

and

$$\begin{aligned} \mathcal{F}(\delta_y \otimes \delta_\beta)(k) &= \frac{1}{\sqrt{2^N}} \sum_x (-1)^{<k,x>} (\delta_y \otimes \delta_\beta)(x) \\ &= \frac{1}{\sqrt{2^N}} (-1)^{<k,y>} \delta_\beta, \end{aligned} \tag{3.23}$$

$$\begin{aligned} \mathcal{F}(\Omega_t(\delta_x \otimes \delta_\alpha)(k) &= (A_{j_t} \circ U_k) \ldots (A_{j_0} \circ U_k)(\mathcal{F}(\delta_x \otimes \delta_\alpha)(k) \\ &= (A_{j_t} \circ U_k) \ldots (A_{j_0} \circ U_k) \frac{1}{\sqrt{2^N}} (-1)^{<k,x>} \delta_\alpha. \end{aligned} \tag{3.24}$$

Therefore

$$\begin{aligned} &< \delta_y \otimes \delta_\beta, \Omega_t(\delta_x \otimes \delta_\alpha) > \\ &= \frac{1}{2^N} \sum_k < (-1)^{<k,y>} \delta_\beta, (-1)^{<k,x>} \hat{\Omega}_t(k) \delta_\alpha > \\ &= \frac{1}{2^N} \sum_k (-1)^{<k,y+x>} < \delta_\beta, \hat{\Omega}_t(k)(\delta_\alpha) > \\ &= \frac{1}{2^N} < \delta_\beta, \sum_k (-1)^{<k,y+x>} \hat{\Omega}_t(k)(\delta_\alpha) > \end{aligned} \tag{3.25}$$

where, we use $\hat{\Omega}_t(k)$ denote $(A_{j_t} \circ U_k) \ldots (A_{j_0} \circ U_k)$.
Then

$$\begin{aligned} &\sum_{\Omega_t} |< \delta_y \otimes \delta_\beta, \Omega_t(\delta_x \otimes \delta_\alpha) >|^2 \\ &= \frac{1}{4^N} \sum_{\Omega_t} \left| < \delta_\beta, \sum_k (-1)^{<k,x+y>} \hat{\Omega}_t(k)(\delta_\alpha) > \right|^2 \end{aligned} \tag{3.26}$$

For an easy estimation of above quantities, we suppose that $|x + y|$ is an odd number. We divide Z_2^N into two parts. One is the set of k such that

$< k, x+y >$ is an odd number, denote by $\mathcal{A}$. The rest is $Z_2^N - \mathcal{A}$. The above equation becomes

$$\sum_k (-1)^{<k,x+y>} \hat{\Omega}_t(k)(\delta_\alpha) = \sum_{k \in Z_2^N - \mathcal{A}} \hat{\Omega}_t(k)(\delta_\alpha) - \sum_{k \in \mathcal{A}} \hat{\Omega}_t(k)(\delta_\alpha). \tag{3.27}$$

Since $< (1,1,\ldots,1), x+y >= |x+y|$ is an odd number, $(1,1,\ldots,1)$ is in $\mathcal{A}$ and

$$\mathcal{A} + (1,1,\ldots 1) = Z_2^N - \mathcal{A}.$$

From the definition of $\hat{S}(k)$, for each element k in $Z_2^N - \mathcal{A}$, we have a unique element $\bar{k}$ in $\mathcal{A}$ such that

$$\hat{S}(k) = \hat{S}(\bar{k})(-I),$$

equivalently,

$$U_{\bar{k}} = -U_k.$$

Therefore, for a fixed decoherent history $\Omega_t = (A_{jt} \circ U_k) \ldots (A_{j0} \circ U_k)$, we have a corresponding history $(A_{jt} \circ U_{\bar{k}}) \ldots (A_{j0} \circ U_{\bar{k}}) = (-1)^t \Omega_t$. Then for an even number t,

$$\sum_k (-1)^{<k,x+y>} \hat{\Omega}_t(k) = 0$$

That means when $|x+y|$ is odd and t is even,

$$P_y^x(t) = 0.$$

For a general case, by introducing row and column exchange matrix $E(i,j)$, for any pair of (i,j), we have

$$E(i,j)E(i,j) = I.$$

If D is Grover's matrix, $D_{ij} = \frac{2}{N} - \delta_i^j$, then

$$E(i,j)DE(i,j) = D.$$

For a fixed k, we have a product of a sequence of exchange matrices $E(k)$, such that

$$E(k)\hat{S}(k)E(k) = S(k).$$

Then we can rewrite $\hat{\Omega}_t(k)$ as $E(k)\left((A_{j_t} \circ S(k) \circ D) \ldots (A_{j_0} \circ S(k) \circ D)\right) E(k)$. We have

$$< \delta_\beta, \hat{\Omega}_t(k)(\delta_\alpha) >=< E(k)^*(\delta_\beta), \Omega_t(E(k)\delta_\alpha) >,$$

where the Ω_t is the same as that in Section 3.2. So that we can apply Theorem 3.5 to the last term in the inequality (3.25), we obtain

$$\lim_t \sum_{\Omega_t} |< \delta_y \otimes \delta_\beta, \Omega_t(\delta_x \otimes \delta_\alpha) >|^2 \leq \frac{1}{N}. \tag{3.28}$$

For fixed positions x, y and a start state $\delta_x \otimes \delta_\alpha$, the limiting distribution function of quantum walk with decoherence $P_x(y)$ satisfies:

$$\begin{aligned} P_x(y) = \lim_t \sum_{\beta} |< \delta_y \otimes \delta_\beta, \Omega_t(\delta_x \otimes \delta_\alpha) >|^2 \\ \leq \sum^{N} \frac{1}{N} = 1. \end{aligned} \tag{3.29}$$

We summarize what was done as follows.

Theorem 3.6 *In the hypercube Z_2^N, for the decoherence introduced only in the direction space, if $x + y$ has an odd first norm, and time t is even, $P_y^x(t) = 0$. In general, $\lim_t P_y^x \leq 1$.*

3.4 Decoherent Walks on Infinite Dimensional Spaces

In this section, we will show that in an infinite dimensional case Green functions $G(z)$ satisfies the equation

$$G = -\frac{q}{p}I + \frac{1}{p}(I - Q)^{-1}.$$

A general quantum random walk on the line provide us with a simple infinity case. One dimensional Hadamard walk defined as follows: Let H be the Hilbert space spanned by the particle states $\{\phi_{xi}, x \in Z, i = 1, 2\}$, which is an orthonormal basis of H.
$U : H \longrightarrow H$ is the unitary operator:

$$\begin{cases} U(\phi_{x1}) = \frac{1}{\sqrt{2}}(\phi_{(x+1)1} + \phi_{(x-1)2}). \\ U(\phi_{x2}) = \frac{1}{\sqrt{2}}(\phi_{(x+1)1} - \phi_{(x-1)2}). \end{cases}$$

Then for an initial state ψ_0, one dimensional quantum random walk is the process

$$\psi_t = U^t \psi_0.$$

Now we consider a general decoherent quantum random walk on the line. Let $A_{xi} = \sqrt{p}\Pi_{xi}$, where Π_{xi} is the projector operator from H to the subspace spanned by ϕ_{xi}, and $A_\nu = \sqrt{1-p}I$, I is the unit operator on H. If we choose the initial state of the particle ψ_0, where ψ_0 is a unit vector in H, a decoherent quantum random walk is the process

$$\Omega_t(\psi_0) = (A_{\mu_t} \circ U)(A_{\mu_{t-1}} \circ U) \ldots (A_{\mu_1} \circ U)\psi_0,$$

where $\mu_i \in \{\nu, xi\}$.

For a unit vector ψ of H, the probability of the particle be found at ψ in a Ω_t process is defined by

$$|< \psi, \Omega_t \psi_0 >|^2.$$

We still use the notation Ξ_t to denote the set of all Ω_t.

Let

$$P_t^{\psi_0}(\psi) = \sum_{\Omega_t \in \Xi_t} |< \psi, \Omega_t \psi_0 >|^2 .$$

We have to prove that $P_t^{\psi_0}(\psi) \le 1$ for any t and unit vector ψ of H. The proof is similar to that in section 1. But here $\psi = \sum_X \psi_{xi}\phi_{xi}$, where X is an infinity set $\{xi, z \in Z, i = 1, 2.\}$. Since ψ is a unit vector, all the coefficients ψ_{xi} satisfy

$$\sum_X |\psi_{xi}|^2 = 1.$$

When $t = 1$,

$$P_1^{\psi_0}(\psi) = \sum_{\Omega_1 \in \Xi_t} |< \psi, \Omega_1 \psi_0 >|^2$$

$$= (1-p)\,|< \psi, U\psi_0 >|^2 + \sum_X |\psi_{xi}|^2\, p\, |< \phi_{xi}, U\psi_0 >|^2 .$$

By Schwarz's inequality, $P_1^{\psi_0}(\psi) \le 1$.

For general t, we have

$$P_{t+1}^{\psi_0}(\psi) = (1-p)P_t^{\psi_0}(U^*\psi) + p\sum_X |\psi_{xi}|^2\, P_t^{\psi_0}(U^*\phi_{xi}). \tag{3.30}$$

By induction, we prove that the claim is true for each t. For the generating function

$$g_{yj}^{xi}(z) = \sum_{t=0}^{\infty} P_t^{xi}(\phi_{yj}) z^t,$$

we have the same proposition as **Proposion1.1**

Proposition 3.2 *For any decoherent quantum random walk in Hilbert space H, the generating function of the walk is analytic on $\{z, |z| < 1\}$.*

We consider the recursion formula of $P_t^{xi}(\phi_{yj})$. From (2.1), we obtain that

$$P_{t+1}^{xi}(\phi_{yj}) = P_t^{xi}(U^*\phi_{yj}).$$

As we did in section 1, we repeat using equation (2.1). If we suppose

$$(U^*)^s\phi_{yj} = \sum_X W_{yj,rk}^{(s)}\phi_{rk},$$

the recursion formula for $P_t^{xi}(\phi_{yj})$ is

$$P_{t+1}^{xi}(\phi_{yj}) = \sum_{s=1}^{t+1} p(1-p)^{s-1} \sum_{rk\in X} \left|W_{yj,rk}^{(s)}\right|^2 P_{t+1-s}^{xi}(\phi_{rk}). \tag{3.31}$$

As in Section 1, let

$$Q_{yj,rk} = \sum_{s=1}^{\infty} pz((1-p)z)^{s-1} \left|W_{yj,rk}^{(s)}\right|^2.$$

Using G denote the infinity matrix $g_{yj}^{xi}(z), xi, yj \in X$, we have equation

$$G = I + QG + \frac{1}{p}Q - Q \tag{3.32}$$

Since $(U^*)^s$ is unitary for any s, so that the norm $\|Q\| < 1$ on $\{z, |z| < 1\}$, then $(I-Q)^{-1}$ exists as an operator on H when $|z| < 1$. From the above equation, we get

$$G = I + \frac{1}{p}(I-Q)^{-1}Q \tag{3.33}$$

on $\{z, |z| < 1\}$.

note that $Q = -(I-Q) + I$, so that

$$G = -\frac{q}{p}I + \frac{1}{p}(I-Q)^{-1}.$$

We have shown that the gap between the eigenvalues disappears when the dimension goes to infinity. Even though $G(z)$ satisfies the above equation, we can not use Cauchy integral formula to find the limit distribution. However this equation provides us with a choice for further analysis.

CHAPTER 4

Quantum Random Walks on Half Spaces

As in classical random walks, some quantities are introduced in quantum random walks, such as hitting time, limit distribution. In order to deal with quantities, several mathematical methods have been used. The most commonly used techniques are diagonalization of the shift operator and Fourier transform. Diagonalization of the shift operator is limited to the situation where it can be diagonalized, e.g., quantum random walks on the whole space. When we restrict a quantum random walk in a subset such as a half plan, Fourier transform and diagonalization shift operator can not give good results. Under this situation, path integral is a useful method. In this chapter, we will use path integral to investigate some hitting time problems in a half space of Z^d.

4.1 Notations and Definitions

We shall start with the definition of quantum random walks in a d-dimensional space. Let Z^d be a d-dimensional integer lattice. For a d-dimensional quantum random walk, the position Hilbert space is the Hilbert space H_p spanned by an orthonormal basis $\{|x>, x \in Z^d\}$. For convenience, we use Dirac notation for vectors in this chapter. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j>, j = 1, 2, ..., 2d.\}$. The state space is defined by $H = H_p \otimes H_c$.

The evolution of the quantum random walk is defined as follows. Let $e_1 = (1, 0, ..., 0)$, $e_2 = (0, 1, 0, ..., 0)$, ..., $e_d = (0, 0, ..., 0, 1)$ be the standard orthonormal basis for Z^d, and $e_{d+j} = -e_j$, for $j = 1, 2, ..., d$. The shift operator $S : H \to H$ is defined by

$$S(|x> \otimes |j>) = |x + e_j> \otimes |j>,$$

for all j. The coin operator $A : H_c \to H_c$ is a unitary operator. Then the evolution operator for the quantum random walk is defined by $U = S(I \otimes A)$, where I denotes the identity operator on H_p.
Let $\psi_0 \in H$ and $\psi_t = U^t \psi_0$. The sequence $\{\psi_t\}_0^\infty$ is called a d-dimensional quantum random walk with initial state ψ_0. We will mainly consider Hadamard walks by the following Hadamard matrix.

The 1-dimensional Hadamard walk is the quantum random walk on Z^1 with $A = H_2$,

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

The 2-dimensional Hadamard walk is the quantum random walk on Z^2 with

$$A = H_2 \otimes H_2 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$

Grover's walk in 2 dimensions is the quantum random walk on Z^2 with

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

The measurements for a quantum random walk are defined as follows. Let Π_x^j be the orthogonal projection operator of H onto the linear span of $|x> \otimes |j>$ and Π_x the orthogonal projection of H onto the linear span of $\{|x> \otimes |j>; j = 1, 2, ..., 2d\}$. The position operators $X = (X_1, ..., X_d)$ are unbounded linear operators on H such that

$$X_i(|x> \otimes |j>) = x_i|x> \otimes |j>,$$

for all $x \in Z^d$, $j = 1, 2, ..., 2d$, and $i = 1, 2, ..., d$.

Let $\psi_t = \sum_{j=1}^{2d} \sum_{x \in Z^d} \psi_t(x, j)|x> \otimes |j>$ be the quantum random walk at time t, where $\psi_t(x, j)$ is the coefficient at $|x> \otimes |j>$. Let $|\psi_t(x, j)|^2$ be the probability that the particle is found at state $|x> \otimes |j>$ at time t, and $p_t(x) = p_t(x, 1) + p_t(x, 2) + ... + p_t(x, 2d)$ be the probability that the particle is found at state $|x>$ at time t.

4.2 The Path Integral

Our formulation of path integral is described as follows. A path w is defined by $w = (w_0, w_1, ..., w_n)$, where $w_i \in Z^d$, and $|w_i - w_{i-1}| = 1$. The length of w is defined by $|w| = n$. Let $e_{j_i} = w_i - w_{i-1}$ be the increment at i-th step of w. Then $w = (w_0, w_1, ..., w_n)$ can be 1-1 identified with $(w_0; e_{j_1}, ..., e_{j_n})$. We use Ω^n denote the set of path of length n, i.e. $\Omega_n = \{w; |w| = n\}$.

Definition 4.1 *(Amplitude function) For $1 \leq i, j \leq 2d$, $x \in Z^d$, the amplitude function is defined for $w \in \Omega^n$,*

$$\Psi_j^{i,x}(w) = \delta_j(j_n) a_{j_n j_{n-1}} a_{j_{n-1} j_{n-2}} ... a_{j_1 i}, \tag{4.1}$$

here $w_i - w_{i-1} = e_{j_i}$ and $w_0 = x$; otherwise $\Psi_j^{i,x}(w) = 0$. Here $\delta_j(k) = 0$ if $k \neq j$ and $\delta_j(k) = 1$ if $k = j$.

Let B be the transpose of A. Then we have

$$\Psi_j^{i,x}(w) = b_{ij_1} b_{j_1 j_2} ... b_{j_{n-1} j_n} \delta_j(j_n). \tag{4.2}$$

Definition 4.2 *Let $\Gamma \subseteq \Omega^n$. The amplitude of a Γ is defined by*

$$\Psi_j^{i,x}(\Gamma) = \sum_{w \in \Gamma} \Psi_j^{i,x}(w). \tag{4.3}$$

Let $\Omega = \cup_{n=0}^{\infty} \Omega^n$. For $\Gamma \subseteq \Omega$ with $\Gamma^n = \Gamma \cap \Omega^n$, we also define

$$\Psi_j^{i,x}(\Gamma) = \sum_{n=0}^{\infty} \Psi_j^{i,x}(\Gamma_n), \tag{4.4}$$

and

$$\Psi^{i,x}(\Gamma) = \sum_j \Psi_j^{i,x}(\Gamma).$$

For any $\psi \in H$, we shall write

$$\psi = \sum_{i=1}^{2d} \sum_{x \in Z^d} \psi(x, i) |x> \otimes |i> .$$

By definition of U,

$$U^t|x>\otimes|i>=U^{t-1}(\sum_j a_{ji}|x+e_j>\otimes|j>)$$

$$=U^{t-2}(\sum_{j_2}\sum_{j_1} a_{j_2j_1}a_{j_1i}|x+e_{j_1}+e_{j_2}>\otimes|j_2>).$$

By induction, the above

$$=\sum_{j_t,...,j_1} a_{j_tj_{t-1}}...a_{j_2j_1}a_{j_1i}|x+e_{j_1}+e_{j_2}+...+e_{j_t}>\otimes|j_t>$$

$$=\sum_{y,j}\Psi_j^{ix}(\omega_t=y)|y>\otimes|j>.$$

Therefore, we have the following proposition.

Proposition 4.1 *If $\psi_t=U^t|x>\otimes|i>$, then for all $y\in Z^d, j=1,...,2d$, we have*

$$\psi_t(y,j)=\Psi_j^{ix}(\omega_t=y),$$

The above proposition unifies the path integrals for quantum random walks and classical random walks, if a non-unitary A is allowed. Indeed, if we let $a_{ij}=1/2d$, for all i,j, then for the d-dimensional classical simple random walk, $(X_t)_{t=0}^{\infty}$, on Z^d, the conditional probability

$$P(X_t=y|X_0=x)=\Psi^{ix}(\omega_t=y),$$

for all $y\in Z^d$, and any $i=1,...,2d$.

The above proposition works for general quantum random walks on Cayley graph as well. Let G be a group. Let E be a set of generators of G such that the identity $x_0\notin E$. Let (G,E) be the Cayley graph associated with G and E. The position Hilbert space is H_p spanned by an orthonormal basis $\{|x>,x\in G\}$. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j>,e_j\in E\}$. The state space is $H=H_p\otimes H_c$.

The shift operator $S:H\to H$ is

$$S(|x>\otimes|j>)=|x\cdot e_j>\otimes|j>,$$

for all j, where $\cdot$ is the operation of the group. The coin operator $A : H_c \longrightarrow H_c$ is any unitary operator. The evolution operator for the quantum random walk on $(G, E)$is defined by $U = S(I \otimes A)$, where I denotes the identity operator on H_p. Let $\psi_0 \in H$ and $\psi_t = U^t\psi_0$. The sequence $\{\psi_t\}_0^\infty$ is called a quantum random walk on (G, E) with initial state ψ_0. Then Proposition 4.1 holds for quantum random walks on (G, E)

4.3 Quantum Random Walks on Half Plane

Now we apply the path integral to quantum random walks in half-spaces. The following method works for any d, but for convenience of presentation, we will consider $d = 2$ only.

Let $D = \{(x, y) \in Z^2, x \leq 0\}$ be the left half-space. Let $\tau = \tau(w) = \inf\{t > 0; w_t \in D\}$ be the first hitting time of D by w.

The amplitude Green function for the quantum random walk in the right half-space with zero boundary conditions is given by

$$f_j^{i,n}(y) = f_j^{i,n}(y, z) = \sum_{t=1}^{\infty} \Psi_j^{in}(w_t = (0, y), \tau = t) z^t.$$

Here i is the initial type, j is the ending type, n is the initial position in the x-axis, y is the ending position in the y-axis, and z is a complex number. We note that $\Psi_j^{in}(w_t = (0, y), \tau = t)$ is in $L^2(y, t)$ (see (4.17) and (4.18) below). Therefore the Green function is absolutely convergent for $|z| < 1$. It exists in the sense of $L^2(\theta)$, for $z = e^{i\theta}$ and satisfies

$$\|\Psi_j^{in}(w_t = (0, y), \tau = t)\|_{L^2(t)}^2 = \frac{1}{2\pi} \int_0^{2\pi} d\theta f_j^{i,n}(y, e^{i\theta}) f_j^{i,n}(y, e^{-i\theta}). \qquad (4.5)$$

Similarly, let

$$f_j^{i,n}(k, z) = \sum_y e^{iky} f_j^{i,n}(y, z), 0 \leq k \leq 2\pi$$

and

$$f_j^{i,n}(k, t) = \sum_y e^{iky} \Psi_j^{in}(w_t = (0, y), \tau = t), 0 \leq k \leq 2\pi$$

be the Fourier transforms. Note that we continue to use $f_j^{i,n}(k, z)$ instead of $\hat{f}_j^{i,n}(k, z)$ for the Fourier transform. The Fourier transform is understood by its variables. Then

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_0^{2\pi} |f_j^{i,n}(k, e^{i\theta})|^2 dk = \|\Psi_j^{in}(w_t = (0, y), \tau = t)\|_{L^2(y,t)}^2 < \infty.$$

Therefore, for a.e. k,

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta |f_j^{i,n}(k, e^{i\theta})|^2 < \infty.$$

This implies $\sum_t |f_j^{i,n}(k,t)|^2 < \infty$ and $f_j^{i,n}(k,z)$ is analytic in $|z| < 1$, for a.e. k, and $f_j^{i,n}(k, re^{i\theta}) \to f_j^{i,n}(k, e^{i\theta})$ in $L^2(\theta)$, as $r \uparrow 1$. In particular, we put $f_j^i = f_j^{i,0}$. Let F be a 4×4 matrix with entries $F_{ij} = f_j^i(k,z)$. We also let $\tilde{A}$ denote the matrix obtained from A by interchanging the first and the third columns.

Since $\Psi_j^{i0}(w_t = (0,y), \tau = t) = 0$ if $t < |y|$. So that

$$\sum_y |f_j^i(y,z)| = \sum_{y \neq 0} |\sum_{t=|y|}^{\infty} \Psi_j^{i0}(w_t = (0,y), \tau = t) z^t| + |\sum_{t=1}^{\infty} \Psi_j^{i0}(w_t = (0,0), \tau = t) z^t|.$$

Since $\Psi_j^{i0}(w_t = (0,y), \tau = t)$ is in $L^2(y,t)$, it is bounded by a constant M. Therefore, the above sum is bounded by

$$M \sum_{y \neq 0} \sum_{t=|y|}^{\infty} |z|^t + M \sum_{t=1}^{\infty} |z|^t$$

$$\leq [\frac{2M}{1-|z|} + M] \frac{|z|}{1-|z|},$$

which goes to 0 as $|z| \to 0$. We have shown that

$$\lim_{z \to 0} \sum_y |f_j^i(y,z)| = 0. \tag{4.6}$$

Now, by considering a sample path of cases $\tau = 1$, $\tau = 2$, and for $\tau \geq 3$, it visits the vertical line $x = 1$ exactly $l + 1$ times before hitting D. We obtain the following recursive relations:

$$f_j^i(y,z) = zb_{i2}\delta_2(j)\delta_1(y) + zb_{i4}\delta_4(j)\delta_{-1}(y) + zb_{i1}zb_{13}\delta_3(j)\delta_0(y)$$

$$+zb_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \cdots j_l} \sum_{y_1 y_2 \cdots y_{l-1}} f_{j_1}^1(y_1,z) f_{j_2}^{j_1}(y_2 - y_1, z) \ldots f_{j_l}^{j_{l-1}}(y - y_{l-1}, z) zb_{j_l 3}\delta_3(j).$$

The infinite series of the above sum is bounded by $\sum_l 4^l C^l$, where $C = \max_{i,j} \|f_j^i(y,z)\|_{L^1(y)}$ and $\|f_j^i(y,z)\|_{L^1(y)} = \sum_y |f_j^i(y,z)|$. By (4.6), $C < 1$ if $|z|$ is sufficiently small. Therefore the series is convergent for sufficiently small $|z|$. Applying the Fourier transform, we have

$$f_j^i(k,z) = zb_{i2}\delta_2(j)e^{ik} + zb_{i4}\delta_4(j)e^{-ik}$$

$$+[zb_{i1}zb_{13} + zb_{i1}\sum_{l=1}^{\infty}\sum_{j_1j_2\cdots j_l} f^1_{j_1}(k,z)f^{j_1}_{j_2}(k,z)\ldots f^{j_{l-1}}_{j_l}(k,z)zb_{j_l3}]\delta_3(j)$$

$$= zb_{i2}\delta_2(j)e^{ik} + zb_{i4}\delta_4(j)e^{-ik} + \{zb_{i1}(zB)_{13} + zb_{i1}[\sum_{l=1}^{\infty} F^l zB]_{13}\}\delta_3(j).$$

So that

$$f^i_j(k,z) = zb_{i2}e^{ik}\delta_2(j) + zb_{i4}e^{-ik}\delta_4(j) + zb_{i1}[\frac{I}{I-F}zB]_{13}\delta_3(j).$$

Note that by (4.6), the above series is convergent for sufficiently small $|z|$ and $I - F$ is invertible. This implies the following proposition.

Proposition 4.2 *For each fixed k, there exists $\delta > 0$ such that for all $|z| < \delta$, the Green functions satisfy*

$$F = z\tilde{A}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & e^{ik} & 0 & 0 \\ 0 & 0 & ([1-F]^{-1}zA)_{13} & 0 \\ 0 & 0 & 0 & e^{-ik} \end{pmatrix}. \quad (4.7)$$

To simplify the notation, we put

$$([1-F]^{-1}zA)_{13} = g(k,z), \text{ for } |z| < \delta. \quad (4.8)$$

For the related Green functions with other initial positions, we note that for $n \geq 1$, $f^{i,n}_j(y) = 0$, for all $j \neq 3$. For $j = 3$, we have

$$f^{i,1}_3(k,z) = ([1-F]^{-1}zA)_{i3}, \text{ for } |z| < \delta. \quad (4.9)$$

In particular,

$$f^{1,1}_3(k,z) = ([1-F]^{-1}zA)_{13} = g, \text{ for } |z| < \delta. \quad (4.10)$$

$$f^1_3(k,z) = za_{11}f^{1,1}_3(k,z) = za_{11}g, \text{ for } |z| < \delta. \quad (4.11)$$

and

Corollary 4.1 *For $n \geq 1$, $|z| < \delta$,*

(a) $f^{i,n}_3(k) = f^{i,1}_3(k)(f^{3,1}_3(k))^{n-1}$.

(b) $f^{3,n}_3(k) = (f^{3,1}_3(k))^n$, and $f^{3,1}_3(k) = ([1-F]^{-1}zA)_{33}$.

For some matrices A, the equation (4.7) has a solution $h_j^i(k,z)$ such that for every k, $h_j^i(k,z)$ is analytic in $|z|<1$, relatively continuous in $|z|\le 1$ and equal to $f_j^i(k,z)$ for $|z|<\delta$. For example, when $d=2$, we put

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

in (4.7). We solve (4.7) and get $g(z)=0$ for $z=0,e^{ik},e^{-ik}$. And for $0<|z|<\delta$, $z\neq 0,e^{ik},-e^{-ik}$,

$$g=\frac{-z^4+iz^3\sin k+iz\sin k+1-R(z)}{z(-z+e^{ik})(z+e^{-ik})}, \tag{4.12}$$

where

$$R(z)=\sqrt{(-1+z^2)(-1+z^6-2iz\sin k-2iz^5\sin k+z^2\sin^2 k-z^4\sin^2 k)}. \tag{4.13}$$

To show that the solution function is analytic inside of the unit disk and relatively continuous in the closed unit disk, by (4.7), it is sufficient to show that for every k, $g(k,z)$ is analytic in $|z|<1$ and continuous in $|z|\le 1$. Let $h(k,z)$ be the right hand side of (4.12). We shall first show that for every k, $h(k,z)$ is analytic in $|z|<1$ and continuous in $|z|\le 1$. Let

$$K=(-1+z^2)(-1+z^6-2iz\sin k-2iz^5\sin k+z^2\sin^2 k-z^4\sin^2 k).$$

Then $R^2(z)=K$. Considering K on the unit circle, we have

$$K(k,e^{i\theta})=4e^{4i\theta}\sin\theta(\sin\theta\sin^2 k+2\cos 2\theta\sin k-\sin 3\theta).$$

Also,

$$\sin\theta\sin^2 k+2\cos 2\theta\sin k-\sin 3\theta=2(\sin\frac{\theta}{2}\sin k+\cos\frac{3\theta}{2})(\cos\frac{\theta}{2}\sin k-\sin\frac{3\theta}{2}).$$

This is a quadratic equation of $\sin k$. For every θ, there is only one solution for $\sin k$ (the other solution has absolute value greater than one).

Note that $\sin\frac{\theta}{2}$ and $\sin\frac{3\theta}{2}$ are periodic. Hence for every k, there are six θ's corresponding to $\sin k$, which give the six roots on the unit circle for every k. Taking 1 and -1 into account, $K(k, z)$ has eight zeros on the unit circle. These are all the zeros for $K(k, z)$ on the complex plane since $K(k, z)$ is a polynomial of degree 8 in z, for every k. We can choose a branch cut for $R(z)$ such that it is analytic in the unit disk and $R(0) = 1$. This implies that h is meromorphic inside the unit disk. Let z_0 be the pole of h with smallest norm. Suppose $|z_0| = r < 1$. Then h is analytic for $|z| < r$. However, this implies that $f_3^{11} = h$ for $|z| < r$. Note that f_3^{11} is analytic for all $|z| < 1$, hence $\lim_{z\to z_0} h(z) = \lim_{z\to z_0} f_3^{11}(k, z)$ exists. This contradicts to the fact that z_0 is a pole for h. Therefore, h is analytic in the unit disk. We have thus proved that both h and g are analytic inside the unit disk and relatively continuous in the closed unit ball.

By solving equation (4.7), we have $f_3^{31}(k, 0) = 0$, and for $0 < |z| < \delta$,

$$f_3^{31}(k, z) = \frac{z(-1 + z^2 + z\cos k - iz\sin k)}{1 - z^2 + z^4 - iz(-1 + z^2)\sin k + R(z)}. \tag{4.14}$$

The above expression for $f_3^{31}(k, z)$ can be extended to $|z| < 1$. Since both denominator and numerator of $f_3^{31}(k, z)$ are relatively continuous in the closed unit ball, to show that $f_3^{31}(k, z)$ is relatively continuous in the closed unit ball, it is sufficient to show that the denominator is non-zero on $|z| = 1$. To this end, we write

$$f_3^{31}(k, z) = \frac{N}{T + R(z)},$$

where

$$N = z(-1 + z^2 + z\cos k - iz\sin k),$$

$$T = 1 - z^2 + z^4 - iz(-1 + z^2)\sin k,$$

$$R^2(z) = K,$$

$$K = (-1 + z^2)(-1 + z^6 - 2iz\sin k - 2iz^5\sin k + z^2\sin^2 k - z^4\sin^2 k).$$

By comparing the real part and the imaginary part of $(T^2 - K)(k, e^{i\theta}) = 0$, we have

$$T^2 - K = 0$$

if and only if

$$\sin k = \frac{3 - 2\cos 2\theta}{4\sin\theta}.$$

However,

$$|\frac{3 - 2\cos 2\theta}{4\sin\theta}| = |\frac{1}{4\sin\theta} + \sin\theta| \geq 1.$$

Hence, the only two solutions for $T + R(z) = 0$ are $\theta = \frac{\pi}{6}, k = \frac{\pi}{2}$ and $\theta = -\frac{\pi}{6}, k = -\frac{\pi}{2}$. By evaluating the function at these points, we see $T + R(z) \neq 0$. Therefore the denominators of $f_3^{31}(k, e^{i\theta})$ is never zero.

Since $P_3^{3n} \leq 1$, for all n, we have $0 \leq |f_3^{31}(-k, e^{i\theta})| \leq 1$, for a.e. $k, \theta \in [0, 2\pi]$. We are interested in the decay property of $|f_3^{31}(-k, e^{i\theta})|$. Let $L = \{(k,\theta) || f_3^{31}(k, e^{i\theta})| = 1\}$. We first show that

$$|f(k, e^{i\theta})| = 1 \iff \sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta) \leq 0. \quad (4.15)$$

By direct calculation, we have

$$|T^2 - K| = |N|^4,$$

$$|N|^2 = 1 + 4\sin\theta(\sin\theta - \sin k),$$

$$|R(z)|^2 = |4\sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta)|,$$

$$|T|^2 = (1 - 4\sin^2\theta + 2\sin\theta\sin k)^2.$$

Also, note that $|T + R(z)|^2 = \frac{|N^2|}{|f|^2}$ and $|T - R(z)|^2 = \frac{|T^2 - K||f|^2}{|N|^2}$. Then we have

$$|T^2 - K|^2|f|^4 - 2(|T|^2 + |R(z)|^2)|N|^2|f|^2 + |N|^4 = 0.$$

Hence, $|f| = 1$ if and only if

$$|T^2 - K|^2 - 2(|T|^2 + |R(z)|^2)|N|^2 + |N|^4 = 0,$$

i.e.,

$$-4\sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta) = |4\sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta)|,$$

which holds only when the left hand side is non-negative. This implies (4.15) and $L = \{\theta, k; \sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta) \leq 0\}$.

Let $k_1 = k_1(\theta) = \arcsin(\frac{\sin\frac{3\theta}{2}}{\sin\frac{\theta}{2}})$ and $k_2 = k_2(\theta) = \arcsin(-\frac{\cos\frac{3\theta}{2}}{\sin\frac{\theta}{2}})$. Then in the square $\{(\theta, k) \in [0, 2\pi] \times [0, 2\pi]\}$, L^c is the region

$$
\begin{aligned}
& \{\theta \in [0, \tfrac{\pi}{4}], k \in (k_1, \pi - k_1)\} \\
\cup\ & \{\theta \in [\tfrac{\pi}{4}, \tfrac{\pi}{3}], k \in (\pi - k_2, 2\pi + k_2))\} \\
\cup\ & \{\theta \in [\tfrac{\pi}{3}, \tfrac{\pi}{2}], k \in (0, k_2) \cup (\pi - k_2, 2\pi)\} \\
\cup\ & \{\theta \in [\tfrac{\pi}{2}, \tfrac{2\pi}{3}], k \in (0, k_1) \cup (\pi - k_1, 2\pi)\} \\
\cup\ & \{\theta \in [\tfrac{2\pi}{3}, \tfrac{3\pi}{4}], k \in (\pi - k_1, 2\pi + k_1)\} \\
\cup\ & \{\theta \in [\tfrac{3\pi}{4}, \pi], k \in (k_2, \pi - k_2)\} \\
\cup\ & \{\theta \in [\pi, \tfrac{5\pi}{4}], k \in (\pi - k_2, 2\pi + k_2)\} \\
\cup\ & \{\theta \in [\tfrac{5\pi}{4}, \tfrac{4\pi}{3}], k \in (k_1, \pi - k_1)\} \\
\cup\ & \{\theta \in [\tfrac{4\pi}{3}, \tfrac{3\pi}{2}], k \in (0, \pi - k_1) \cup (2\pi + k_1, 2\pi)\} \\
\cup\ & \{\theta \in [\tfrac{3\pi}{2}, \tfrac{5\pi}{3}], k \in (0, \pi - k_2) \cup (2\pi + k_2, 2\pi)\} \\
\cup\ & \{\theta \in [\tfrac{5\pi}{3}, \tfrac{7\pi}{4}], k \in (k_2, \pi - k_2)\} \\
\cup\ & \{\theta \in [\tfrac{7\pi}{4}, 2\pi], k \in (\pi - k_1, 2\pi + k_1)\},
\end{aligned}
$$

This implies that L has a positive Lebesgue measure. The numerical value of the Lebesgue measure of $L \approx 0.556$.

4.4 The First Hitting Probabilities on Half Plane

The first hitting probability of D by a quantum random walk starts with initial state $|(n,0)> \otimes|i>$ is related to the following Green function

$$f_j^{i,n}(y,z) = \sum_{t=1}^{\infty} \Psi_j^{in}(w_t = (0,y), \tau = t) z^t. \tag{4.16}$$

The probability that a 2-dimensional quantum random walk in the right half-space D^c exits from D^c at $(0,y)$ is given by

$$P_3^{i,n}(y) = \sum_{t=1}^{\infty} |\Psi_3^{in}(w_t = (0,y), \tau = t)|^2 = \|\Psi_3^{in}(w_t = (0,y), \tau = t)\|^2_{L^2(t)}. \tag{4.17}$$

By (4.17), $\Psi_3^{in}(w_t = (0,y), \tau = t)$ is in $L^2(t)$, therefore $f_3^{i,n}(y,z)$ is in $L^2(\theta)$, for $z = e^{i\theta}$. For $n \geq 1$, the probability that the quantum random walk ever exits from the right half-space is

$$P_3^{i,n} = \sum_{y} \sum_{t=1}^{\infty} |\Psi_3^{in}(w_t = (0,y), \tau = t)|^2 = \|\Psi_3^{in}(w_t = (0,y), \tau = t)\|^2_{L^2(y,t)}. \tag{4.18}$$

By Fourier transform, we have

$$P_j^{i,n}(k) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_0^{2\pi} f_j^{i,n}(k - k_1, e^{i\theta}) f_j^{i,n}(k_1, e^{-i\theta}) dk_1, \tag{4.19}$$

and

$$P_j^{i,n} = P_j^{i,n}(k)|_{k=0} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_0^{2\pi} f_j^{i,n}(-k_1, e^{i\theta}) f_j^{i,n}(k_1, e^{-i\theta}) dk_1. \tag{4.20}$$

Suppose that the quantum random walk starts with initial state $|(n,0)> \otimes|i>$. We have known that $\lim_{n\to\infty} P_3^{i,n}$ is exists and equal to the positive Lebesgue measure of $L = \{(k,\theta)||f_3^{31}(k,e^{i\theta})| = 1\}$ [38]. We will consider the asymptotic behavior of $P_3^{i,n}$ as n go to ∞.

For simplicity, we write f for f_3^{31}. Let $\xi_1 = 0$, $\xi_2 = \pi/4$, $\xi_3 = \pi/2$, $\xi_4 = 3\pi/4$, $\xi_5 = \pi$, $\xi_6 = 5\pi/4$, $\xi_7 = 3\pi/2$, $\xi_8 = 7\pi/4$, and $\xi_9 = 2\pi$. For a fixed $\theta \neq \xi_i$, L^c is an union of open intervals, $\cup_j I_j$. Let $p_1(\theta) < p_2(\theta) < ... < p_l(\theta)$

be the endpoints of the intervals. Let $k_1(\theta) = \arcsin \frac{\sin\frac{3\theta}{2}}{\sin\frac{\theta}{2}}$. Then k_1 is a root of the quadratic equation

$$\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta = 0.$$

For $\theta \in (0, \frac{\pi}{4})$, $p_1(\theta) = k_1(\theta)$ and $p_2(\theta) = \pi - k_1(\theta)$. Let $\Omega = \{\theta \in (0, \frac{\pi}{4}), k \in (k_1, \pi/2)\}$. We will consider the behavior of $|f|^2$ over Ω only, since the other regions can be treated similarly. In Ω, we have

$$\begin{aligned}|f|^2 &= \frac{1 - 4\sin\theta\sin k + 4\sin^2\theta}{\{1 - 4\sin^2\theta + 2\sin\theta\sin k + 2\sqrt{\sin\theta(\sin\theta\sin^2 k + 2\cos 2\theta\sin k - \sin 3\theta)}\}^2} \\ &= \frac{N_0}{(T_0 + 2\sqrt{K_0})^2}.\end{aligned}$$

Hence,

$$\begin{aligned}1 - |f|^2 &= \frac{8K_0 + 4T_0\sqrt{K_0}}{(T_0 + 2\sqrt{K_0})^2} \\ &= \frac{4\sqrt{K_0}}{T_0 + 2\sqrt{K_0}}.\end{aligned}$$

Fix θ, as $k \to k_1$ from Ω or equivalently, $\sin k \to \frac{\sin\frac{3\theta}{2}}{\sin\frac{\theta}{2}}$, we have

$$T_0 + 2\sqrt{K_0} \to -1 + 2\cos\theta \geq C > 0,$$

where C is independent of $\theta \in [0, \pi/4]$. This implies that

$$1 - |f|^2 \sim O(\sqrt{K_0}). \tag{4.21}$$

Now we show upper bound for $1 - |f|^2$. For a fixed θ, we have

$$\partial_k K_0 = \cos k(2\sin\theta\sin k + 2\cos 2\theta)\sin\theta. \tag{4.22}$$

Since the right side of (4.22) is less than a positive constant for all (θ, k) in Ω, by the Mean Value Theorem, we have

$$K_0(\theta, k) \leq C_1(k - k_1), \tag{4.23}$$

for all (θ, k) in Ω. By (4.21), we then have

$$1 - |f|^2 \leq C_1\sqrt{k - k_1}, \tag{4.24}$$

for all (θ, k) in Ω.

If we let $I_j = (a_j, b_j)$, and $c_j = \frac{a_j+b_j}{2}$, for all sufficiently small positive constant ϵ, $O_{ij} = \{\xi_i < \theta < \xi_{i+1}; a_j+\epsilon < c_j\}$ and $O'_{ij} = \{\xi_i < \theta < \xi_{i+1}; b_j - \epsilon > c_j\}$ have positive Lebesgue measures. On these set,

$$1 - |f(k, e^{i\theta})|^2 \leq C\sqrt{|k - a_j|},$$

for all $\xi_i < \theta < \xi_{i+1}$, and $a_j < k < c_j$, here C is a universal positive constant. The same asymptotic behavior also holds for the other end of the interval, i.e.,

$$1 - |f(k, e^{i\theta})|^2 \leq C\sqrt{|k - b_j|},$$

for all $\xi_i < \theta < \xi_{i+1}$, and $b_j > k > c_j$.

We shall consider $\Omega = \{\theta \in (0, \frac{\pi}{4}), k \in (k_1, \pi/2)\}$ only for lower bound of $1 - |f(k, e^{i\theta})|^2$, since the rest can be treated similarly. Let $\Omega_1 = \{\theta \in (0, \frac{\pi}{4} - \eta), k \in (k_1, \pi/2)\}$ and $\Omega_2 = \{\theta \in (\frac{\pi}{4} - 2\eta, \frac{\pi}{4}), k \in (k_1, \pi/2)\}$. For fixed k, let θ_1 be such that $k_1(\theta_1) = k$. We shall show

$$1 - |f|^2 \geq C_2\sqrt{\theta - \theta_1}, \tag{4.25}$$

for all (θ, k) in Ω_2, and

$$1 - |f|^2 \geq C_2\sqrt{\theta}\sqrt{k - k_1}, \tag{4.26}$$

for all (θ, k) in Ω_1.

By

$$\partial_\theta K_0 = \cos\theta(\sin\theta + 2\cos 2\theta - \sin 3\theta) + \sin\theta(\cos\theta - 4\sin 2\theta - 3\cos 3\theta), \tag{4.27}$$

we have

$$-\partial_\theta K_0(\frac{\pi}{4}, \frac{\pi}{2}) > 0,$$

and since $\partial_\theta K_0$ is continuous everywhere, there exists $\alpha > 0$, such that

$$-\partial_\theta K_0 \geq C_2 > 0, \tag{4.28}$$

for all (θ, k) in Ω_2. By the Mean Value Theorem,

$$K_0 \geq C_2(\theta - \theta_1), \tag{4.29}$$

for all (θ, k) in Ω_2. By (4.21), we have thus proved (4.25).

To prove (4.26), we take partial derivative in k. By (4.22),

$$\partial_k K_0 = \cos k(2\sin\theta\sin k + 2\cos 2\theta)\sin\theta.$$

Let

$$Z(\theta, k) = \cos k(2\sin\theta\sin k + 2\cos 2\theta).$$

Then Z is continuous everywhere. Note that $Z(\theta, k_1)$ is positive and bounded away from zero uniformly in $0 \le \theta \le \pi/4 - \eta$, and $C_2\theta < \sin\theta$, for some $C_2 > 0$, there exists a sufficiently small γ such that

$$\partial_k K_0 \ge C_2\theta, \tag{4.30}$$

for all $0 < \theta < \pi/4 - \eta$, $k_1 < k < k_1 + \gamma$. By the Mean Value Theorem and (4.21), we have

$$1 - |f|^2 \ge C_2\sqrt{\theta}\sqrt{k - k_1}, \tag{4.31}$$

for all $0 < \theta < \pi/4 - \eta$, $k_1 < k < k_1 + \gamma$. Since $1 - |f|^2$ is positive and uniformly bounded away from zero on $0 < \theta < \pi/4 - \eta$, $k_1 + \gamma \le k \le \pi/2$, we have proved (4.26) by choosing a sufficiently small $C_2 > 0$.

Now we consider the equation

$$P_3^{3n} - P_3^{3\infty} = \frac{1}{(2\pi)^2}\int_{L^c} |f|^{2n} d\theta dk = \frac{1}{(2\pi)^2}\sum_{i=1}^{t-1}\sum_j \int_{\xi_i}^{\xi_{i+1}}\int_{I_j} |f|^{2n} dk d\theta. \tag{4.32}$$

We shall show that each term has the same asymptotic behavior as $n \to \infty$. First we introduce a lemma.

Lemma 4.1 *Let g and h be functions on interval (α, β) such that the integral $f(n) = \int_\alpha^\beta g(u)e^{nh(u)}du$ exists for all sufficiently large positive n. Suppose h is a real-valued function, continuous at $u = \alpha$, continuously differentiable for $\alpha < u \le \alpha + \eta$, with $\eta > 0$. Suppose further that $h' < 0$, for $\alpha < u \le \alpha + \eta$, and $h(u) \le h(\alpha) - \epsilon$, with $\epsilon > 0$, for $\alpha + \eta \le u \le \beta$. If $h'(u) \sim -A(u-\alpha)^{\nu-1}$ and $g(u) \sim B(u-\alpha)^{\lambda-1}$ as $u \to \alpha$, $\lambda > 0$, $\nu > 0$, then*

$$f(n) = \int_\alpha^\beta g(u)e^{nh(u)}du \sim \frac{B}{\nu}\Gamma(\frac{\lambda}{\nu})(\frac{\nu}{An})^{\frac{\lambda}{\nu}}e^{nh(\alpha)}$$

as $n \to \infty$.

Let

$$Q = \frac{1}{(2\pi)^2} \int_{\xi_i}^{\xi_{i+1}} \int_{a_j}^{c_j} |f|^{2n} dk d\theta. \tag{4.33}$$

be one of the terms in the above sum. We will consider Q only since the rest can be treated in the same way.

First f is continuous in (a_j, c_j), $|f(a_j)| = 1$, $|f(c_j)| < 1$ and $|f|$ is strictly less than 1 in (a_j, c_j). Moreover, by what we have proved before Lemma 4.1 , there is a sufficiently small positive constant ϵ, independent of θ such that

$$O_{ij} = \{\xi_i < \theta < \xi_{i+1}; a_j + \epsilon < k < c_j\}$$

has a positive Lebesgue measure, and on this set

$$1 - |f(k, e^{i\theta})|^2 \leq C\sqrt{|k - a_j|}. \tag{4.34}$$

For all $\xi_i < \theta < \xi_{i+1}$, $a_i < k \leq a_i + \epsilon$,

$$C\sqrt{|k - a_j|} \leq \frac{1}{2},$$

and for all $\xi_i < \theta < \xi_{i+1}$, $a_i + \epsilon < k < c_i$,

$$|f|^2 \leq \alpha < 1. \tag{4.35}$$

For the lower bound of Q, we have

$$Q \geq \frac{1}{(2\pi)^2} \int_{O_{ij}} \int_{a_j}^{(a_j+\epsilon)} |1 - C(k - a_j)^{\frac{1}{2}}|^n dk d\theta.$$

Applying Lemma 4.1, with

$$h(k) = \ln[1 - C(k - a_j)^{\frac{1}{2}}],$$

$$g(k) = 1, \lambda = 1, \nu = \frac{1}{2},$$

we have

$$\frac{1}{(2\pi)^2} \int_{O_{ij}} \int_{a_j}^{(a_j+\epsilon)} |1 - C(k - a_j)^{\frac{1}{2}}|^n dk d\theta \sim \int_{O_{ij}} C n^{-2} d\theta \sim O(n^{-2}),$$

as $n \to \infty$, since O_{ij} has a positive Lebesgue measure.

For the upper bound, let $Q_1 = \frac{1}{(2\pi)^2}\int_{\Omega_1}|f|^{2n}dkd\theta$, and $Q_2 = \frac{1}{(2\pi)^2}\int_{\Omega\setminus\Omega_1}|f|^{2n}dkd\theta$. Then

$$Q = Q_1 + Q_2.$$

Let $\Omega_{11} = \{\xi_i < \theta < \xi_{i+1} - \eta, a_j < k < a_j + \gamma\}$, $\Omega_{12} = \{\xi_i < \theta < \xi_i + \gamma, a_j < k < c_j\}$, and $\Omega_{13} = \Omega_1 \setminus (\Omega_{11} \cup \Omega_{12})$. if γ is sufficiently small, then

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \le 1 - |f(k, e^{i\theta})|^2, \text{ in } \Omega_{11}, \tag{4.36}$$

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \le 1 - |f(k, e^{i\theta})|^2, \text{ in } \Omega_{12}, \tag{4.37}$$

$$|f(k, e^{i\theta})|^2 \le \alpha < 1, \text{ in } \Omega_{13}, \tag{4.38}$$

and

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \le \frac{1}{2}.$$

We have

$$Q_1 \le Q_{11} + Q_{12} + Q_{13},$$

where

$$Q_{11} = \frac{1}{(2\pi)^2}\int_{\xi_i}^{\xi_{i+1}-\eta}\int_{a_j}^{(a_j+\gamma)}|f|^{2n}dkd\theta,$$

$$Q_{12} = \frac{1}{(2\pi)^2}\int_{\xi_i}^{\xi_i+\gamma}\int_{a_j}^{c_j}|f|^{2n}dkd\theta,$$

$$Q_{13} = \frac{1}{(2\pi)^2}\int_{\Omega_{13}}|f|^{2n}dkd\theta.$$

By (4.38), $Q_{13} = O(e^{-cn})$, as $n \to \infty$, for some $c > 0$. For the upper bound of Q_{11}, by (4.36), for any $\delta > 0$,

$$Q_{11} \le \frac{1}{(2\pi)^2}\int_{\xi_i}^{\xi_{i+1}-\eta}\int_{a_j}^{(a_j+\gamma)}|1 - C(\theta - \xi_i)^{\frac{1}{2}}(k - a_j)^{\frac{1}{2}+\delta}|^n dkd\theta.$$

Applying Lemma 4.1, with

$$h(k) = \ln[1 - C|\theta - \xi_i|^{\frac{1}{2}}(k - a_j)^{\frac{1}{2}+\delta}],$$

$$g(k) = 1, \lambda = 1, \nu = \frac{1}{2} + \delta, A = C|\theta - \xi_i|^{\frac{1}{2}}, B = 1,$$

we have

$$\frac{1}{(2\pi)^2}\int_{\xi_i}^{\xi_{i+1}-\eta}\int_{a_j}^{(a_j+\gamma)}|1-C(\theta-\xi_i)^{\frac{1}{2}}(k-a_j)^{\frac{1}{2}+\delta}|^n dkd\theta$$

$$\sim \int_{\xi_i}^{\xi_{i+1}-\eta}(\frac{1}{C(\theta-\xi_i)^{\frac{1}{2}}n})^{(\frac{1}{2}+\delta)^{-1}}d\theta.$$

As $n \to \infty$, the last term is at the same order $n^{-2+\epsilon}$, where ϵ can be chosen arbitrary small if δ is chosen small enough. Similarly, $Q_{12} \leq O(n^{-2+\epsilon})$, as $n \to \infty$. For Q_2, let $\Omega_{21} = \{k_1(\xi_{i+1}-\eta) < k < c_j, \theta_1 - \gamma < \theta < \theta_1\}$, $\Omega_{22} = (\Omega \setminus \Omega_1) \setminus \Omega_{21}$. By (4.31), if γ is sufficiently small, then

$$C\sqrt{|\theta-\theta_1|} \leq 1 - |f(k,e^{i\theta})|^2, \text{ in } \Omega_{21}, \tag{4.39}$$

$$|f(k,e^{i\theta})|^2 \leq \alpha < 1, \text{ in } \Omega_{22}, \tag{4.40}$$

and

$$C\sqrt{|\theta-\theta_1|} \leq \frac{1}{2}.$$

Let

$$Q_{21} = \frac{1}{(2\pi)^2}\int_{\Omega_{21}}|f|^{2n}dkd\theta,$$

$$Q_{22} = \frac{1}{(2\pi)^2}\int_{\Omega_{22}}|f|^{2n}dkd\theta.$$

Then $Q_2 = Q_{21} + Q_{22}$. By (4.40), $Q_{22} = O(e^{-cn})$, as $n \to \infty$, for some $c > 0$. By a similar argument as that in the lower bound, $Q_{21} \leq O(n^{-2})$, as $n \to \infty$. We have thus obtained

Theorem 4.1 *For Hadamard walks on Z^2, for any $\epsilon > 0$,*

$$c_1 n^{-2} \leq P_3^{3n} - P_3^{3\infty} \leq c_2(\epsilon) n^{-2+\epsilon}, \tag{4.41}$$

as $n \to \infty$, where c_1, $c_2(\epsilon)$ are positive constants.

For the first hitting time τ at the left half-space. It is well-known that the expectation of τ is infinite for classical random walks. We will show that for a quantum random walk, if it hits, then the conditional expectation of τ

is finite. To this end, we need some properties of function f. Recall that for Hadamard walks,

$$f(k, e^{i\theta}) = \frac{N}{T + R(z)},$$

where

$$N = z(-1 + z^2 + z\cos k - iz\sin k),$$

$$T = 1 - z^2 + z^4 - iz(-1 + z^2)\sin k,$$

$$R^2(z) = K,$$

$$K = (-1 + z^2)(-1 + z^6 - 2iz\sin k - 2iz^5\sin k + z^2\sin^2 k - z^4\sin^2 k).$$

For every k, $K(k, z)$ is a polynomial in z of order 8. By factoring $K(k, z)$, we get

$$K(k, z) = (z + 1)^2(z - 1)^2(z - e^{i\theta_1})(z - e^{-i\theta_1})(z - e^{i\theta_2})(z - e^{-i\theta_2})$$

where $\theta_1 = \arccos\frac{1-\cos k}{2}$, $\theta_2 = \arccos\frac{-1-\cos k}{2}$. Therefore all the zeros of $K(k, z)$ are on the unit circle, for every k. Now, for $K(k, z)$, we write the roots of K as $\{e^{i\theta_j}\}$, $\theta_j = \theta_j(k)$ such that $\sum_{j=1}^{8}\theta_j = 0$. For each j, set $h_{\theta_j}(z) = R_{\pi+\theta_j}(e^{i\theta_j} - z)$. We then have the following properties: 1. $h_{\theta_j}(z)$ is analytic except $\{z; |z| \geq 1, \arg z = \theta_j\}$; 2. $h_{\theta_j}(z)$ is analytic in $\{z; |z| < 1\}$ and relatively continuous in $|z| \leq 1$; 3. $h_{\theta_j}(0) = e^{\frac{i\theta_j}{2}}$. If we define $R(z) = \prod_{j=1}^{8} h_{\theta_j}$, then $R^2(z) = K$ and $R(0) = 1$. Therefore $R(z)$ can be defined as analytic in $|z| < 1$, relatively continuous in $|z| \leq 1$ and $R(0) = 1$.

Let $r = e^{-s}$. Then

$$\begin{aligned} |\frac{\partial f}{\partial s}| &= |\partial_z f \partial_s z| \\ &= |\frac{\partial_z N(T + R(z)) - N(\partial_z T + \partial_z R(z))}{(T + R(z))^2}(-e^{-s}e^{i\theta})|. \end{aligned}$$

Note that $T + R(z)$ is never zero on the unit circle, N and T are polynomials in z. Therefore to estimate $\partial_z R(z)$ it is sufficient to obtain an upper bound of $|\frac{\partial f}{\partial s}|$.

From $R(z) = \prod_{j=1}^{8} h_{\theta_j}$, we have

$$|h'_{\theta_j}(z)| = |R'_{\pi+\theta_j}(e^{i\theta_j} - z)(-1)| = |\frac{1}{2R_{\pi+\theta_j}(e^{i\theta_j} - z)}|$$

$$= \frac{1}{2\sqrt{|e^{i\theta_j} - z|}} \leq \frac{C}{\sqrt{|\theta_j - \theta|}},$$

if $z = re^{i\theta}$, $0 < r_0 < r < 1$.

$$|h_{\theta_j}(z)| = |R_{\pi+\theta_j}(e^{i\theta_j} - z)|$$

$$= \sqrt{|e^{i\theta_j} - z|} \leq C,$$

for all $|z| \leq 1$. By the Product Rule, we have obtained the following lemma.

Lemma 4.2 *For every k, there exists a set $D_k = [0, 2\pi] \backslash \{\theta_1(k), \theta_2(k), ..., \theta_m(k)\}$ such that the partial derivative $\partial_r f(k, re^{-i\theta})$ exists and is continuous in $0 < r < 1$, $\theta \in D_k$. Moreover there exists a constant C, independent of k, θ, r such that*

$$|\partial_r f(k, re^{i\theta})| \leq C \sum_{i=1}^{m} \frac{1}{\sqrt{|\theta - \theta_i|}},$$

for all $k \in [0, 2\pi]$, $r_0 < r < 1$, for some $0 < r_0 < 1$, and all $\theta \in D_k$.

For a probability measure and its Laplace transform, we have the following lemma.

Lemma 4.3 *Let μ be a probability measure supported in $[0, \infty)$. Let $\rho(s) = \int_0^\infty e^{-st} d\mu(t)$ be the Laplace transform of μ. For all $n = 1, 2, ...,$ the following statements hold.*

(a) If $\int_0^\infty t^n d\mu(t) < \infty$, then $(-1)^n \frac{d^n \rho(s)}{ds^n} = \int_0^\infty t^n e^{-st} d\mu(t) < \infty$.

(b) If $(-1)^n \frac{d^n \rho(s)}{ds^n}|_0$ exists, then $\int_0^\infty t^n d\mu(t) < \infty$.

Let

$$\rho(s) = \sum_{t=1}^{\infty} e^{-st} P_j^{i,n}(t)$$

be the Laplace transform. By the same argument as that in (4.20), we have

$$\rho(s) = \frac{1}{2\pi} \int_0^{2\pi} d\theta \frac{1}{2\pi} \int_0^{2\pi} f_j^{i,n}(-k, e^{-s+i\theta}) f_j^{i,n}(k, e^{-i\theta}) dk \tag{4.42}$$

$$= \frac{1}{2\pi}\int_0^{2\pi} d\theta \frac{1}{2\pi}\int_0^{2\pi} [f_j^{i,1}(-k, e^{-s+i\theta}) f_j^{i,1}(k, e^{-i\theta})]^n dk.$$

We will consider the case $i = j = 3$ only, since other cases can be treated the same. The derivative of the above integrand is

$$\partial_s[f(-k, e^{-s+i\theta}) f(k, e^{-i\theta})]^n = n[f(-k, e^{-s+i\theta})]^{n-1} \partial_s f(-k, e^{-s+i\theta})[f(k, e^{-i\theta})]^n.$$

By Lemma 4.2, $|f| \leq 1$ and for every k, there exists a set $D_k = [0, 2\pi] \setminus \{\theta_1(k), \theta_2(k), ..., \theta_m(k)\}$ such that the partial derivative $\partial_r f(k, re^{-i\theta})$ exists and is continuous in $0 < r < 1$, $\theta \in D_k$. Moreover there exists a constant, independent of k, θ, r such that

$$|\partial_r f(k, re^{i\theta})| \leq C \sum_{i=1}^{m} \frac{1}{\sqrt{|\theta - \theta_i|}},$$

for all $k \in [0, 2\pi]$, $\frac{1}{2} < r < 1$ and $\theta \in D_k$. Therefore, the derivative of the integrand in (4.42) is bounded by

$$C \sum_{i=1}^{m} \frac{1}{\sqrt{|\theta - \theta_i|}},$$

which is independent of s and integrable. By the Dominated Convergence Theorem, $\rho(s)$ is differentiable. Then Lemmas 4.2 and 4.3 imply the following theorem.

Theorem 4.2 *For Hadamard walks on Z^2, when τ is finite, then conditional expectation of τ, with respect to P^{3n}, is finite.*

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