

**QUANTUM RANDOM WALKS ON ONE AND TWO
DIMENSIONAL LATTICES**

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DOCTOR OF PHILOSOPHY

by
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ABSTRACTQUANTUM RANDOM WALKS ON ONE AND TWO DIMENSIONAL
LATTICES

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In this thesis, we study quantum random walks on one and two dimensional lattices. We derive an asymptotic formula for characteristic function $E(e^{i\zeta \frac{X_t}{t}})$ and a formula for the variance $\sigma^2(X_t)$ in term of t with a different and simplified description for the result obtained by Konno [10], using the method introduced by Grimmett et al. [6]. Here $X_t = U^{+t} X U^t$ be the process at time t , U is an evolution, and X is the position operator. We find the asymptotic fomulas for hitting probabilities of one dimensional Hadamard quantum walk and corresponding classical random walk with a hitting point, using the method of asymptotic expansions of Fourier integrals. By using a sample path analysis, we also obtain several exact analytical expressions of the hitting probabilities, limiting distributions for two dimensional Hadamard and Grover random walks with a hitting vertical half space. The sample path integral also works for two dimensional classical random walk hitting 45° half space. We obtain the hitting probabilities and the asymptotic formula for the conditional expectation of $\frac{Y_n(w)}{n}$, where $Y_n(w)$ denotes the random variable defined by $w_\tau = (Y_n(w), Y_n(w))$ for a path w with initial position $w_0 = (0, n)$. We partially justify a conjecture pointed out by Ambainis et al. [1].

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CHAPTER 1

INTRODUCTION

Classical random walks are very well-studied processes. In the simplest variation, a simple particle moves on a two-way infinite, one-dimensional lattice. At each step, the particle moves one position left or right, depending on the flip of a fair coin. Such random walks may be generalized to more complicated lattices and to finite or infinite graphs. Kemeny and Snell [7] gave many basic facts regarding random walks. In this thesis we consider quantum variations of random walks on one and two dimensional lattices—we refer to such processes as *quantum random walks*.

Consider a quantum particle that moves freely on the integer points on the line, and has an additional degree of freedom, its *chirality*, that takes values RIGHT and LEFT. A walk on the line by such a particle may be described as follows: at every time step, its chirality undergoes a unitary transformation and then the particle moves according to its (new) chirality state. We call this kind of walk the *one dimensional quantum random walk*. Similarly a quantum particle doing two dimensional quantum random walk may be described as follows: it moves freely on the sites on two dimensional lattices, at every time step, its chirality which takes values RIGHT, UP, LEFT and DOWN undergoes a unitary transformation and then the particle moves according to its (new) chirality state.

The study of quantum walks was begun by Meyer [13]. Then it has been investigated by a number of groups. The recent concentrated studies make clear mathematical properties of the one and two dimensional quantum walks. In particular [1, 2, 6, 10] have presented the properties of quantum walks in detail. The behavior of quantum walks differs from that of classical random walks in several striking ways (for instance, hitting probabilities and the variance). The reason for this is quantum interference. Whereas there can not be destructive interference in a classical random walk, in a quantum walk two separate paths leading to the same point may be out of phase and cancel one another.

In this thesis we investigate the properties of quantum walks on one and two dimensional lattices. Our results may be summarized as follows. In chapter 2, we derive an asymptotic formula for characteristic function $E(e^{i\zeta \frac{X_t}{t}})$ and a formula for the variance $\sigma^2(X_t)$ in term of t with a different and simplified description for the result obtained by Konno [10], using method introduced by Grimmett et al. [6]. Here $X_t = U^{\dagger t} X U^t$ be the process at time t , U is an evolution, and X is the position operator. We find the asymptotic formulas for hitting probabilities of one dimensional Hadamard quantum walk and corresponding classical random walk with a hitting point, using the method of asymptotic expansions of Fourier integrals. Then we partially justify a conjecture pointed out by Ambainis et al. [1]. In chapter 3, by using a sample path analysis, we obtain several exact analytical expressions of the hitting probabilities, limiting distributions for two dimensional Hadamard and Grover random walks with a hitting vertical half space. The sample path integral also works for two dimensional classical random walk hitting 45° half space. We obtain the hitting probabilities and the asymptotic formula for the conditional expectation of $\frac{Y_n(w)}{n}$, where $Y_n(w)$ denotes the random variable defined by $w_\tau = (Y_n(w), Y_n(w))$ for a path w with initial position $w_0 = (0, n)$.

The thesis is organized as follows. Chapter 2 deals with three types of

one dimensional quantum walks, in addition, we discuss properties of classical random walks hitting a fixed point. In Chapter 3, we study the properties of two dimensional quantum walks hitting vertical half-space. We also study two dimensional classical random walk hitting 45° half space.

CHAPTER 2

ONE DIMENSIONAL QUANTUM RANDOM WALK

2.1 Definitions and known results

We begin this chapter with formally defining our notion of quantum walks and giving descriptions of main known results regarding quantum walks on one dimensional lattices.

Definition 2.1 The Space. *For a 1-dimensional quantum random walk, the position Hilbert space H_p is spanned by an orthonormal basis $\{|x \rangle; x \in Z\}$. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j \rangle; j = 1, 2\}$. The state space is $H = H_p \otimes H_c$.*

Definition 2.2 The Evolution. *The shift operator $S : H \rightarrow H$ is defined by*

$$S(|x \rangle \otimes |j \rangle) = |x + 1 \rangle \otimes |j \rangle, \text{ if } j = 1,$$

$$S(|x \rangle \otimes |j \rangle) = |x - 1 \rangle \otimes |j \rangle, \text{ if } j = 2.$$

So $j = 1$ means "right" and $j = 2$ means "left".

The coin operator $A : H_c \rightarrow H_c$ is a unitary operator.

The evolution operator is defined by $U = S(I \otimes A)$.

Let $\psi_0 \in H$ with $\|\psi_0\| = 1$ and $\psi_t = U^t\psi_0$. The sequence $\{\psi_t\}_0^\infty$ is called a 1-dimensional quantum random walk (or two-way infinite timed quantum walk) with initial state ψ_0 .

Example 2.1 Hadamard Walk. Let $A = \text{Hadamard gate} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}$.

The quantum random walk is called a Hadamard walk if A is a Hadamard gate.

Definition 2.3 Measurements.

Position operator X is defined by

$$X(|x \rangle \otimes |j \rangle) = x|x \rangle \otimes |j \rangle .$$

Projection operator $\Pi_x^j =$ orthogonal projection onto linear span of $|x \rangle \otimes |j \rangle$.

Projection operator $\Pi_x =$ orthogonal projection onto linear span of $\{|x \rangle \otimes |j \rangle; j = 1, 2\}$.

Definition 2.4 Quantum Probability.

Let $\psi_t = \sum_{j=1,2} \sum_{x \in Z} \psi_t(x, j)|x \rangle \otimes |j \rangle$ be the quantum random walk at time t .

Let $p_t(x, j) = \langle \psi_t, \Pi_x^j \psi_t \rangle = |\psi_t(x, j)|^2$ be the probability that the particle is found at state $|x \rangle \otimes |j \rangle$ at time t , and $p_t(x) = p_t(x, 1) + p_t(x, 2)$ be the probability that the particle is found at state $|x \rangle$ at time t .

Known results 1.

In [1], Ambainis, Bach, Nayak, Vishwanath and Watrous (2001) obtained the following results.

Suppose that the initial state is $\psi_0 = |0 \rangle \otimes |1 \rangle$.

1. Let $x = \alpha t \rightarrow \infty$ with α fixed. Suppose $-1 < \alpha < \frac{-1}{\sqrt{2}}$ or $\frac{1}{\sqrt{2}} < \alpha < 1$. Then there is a $c > 1$ for which $p_t(x, j) = O(c^{-x})$, for all j .

2. Let $\epsilon > 0$ be any constant. Suppose α is in the interval $(\frac{-1}{\sqrt{2}} + \epsilon, \frac{1}{\sqrt{2}} - \epsilon)$. Then as $t \rightarrow \infty$, we have (uniformly in x)

$$p_t(x, 1) \sim \frac{2(1 + \alpha)}{\pi(1 - \alpha)\sqrt{1 - 2\alpha^2t}} \cos^2(-\omega t + \frac{\pi}{4}),$$

$$p_t(x, 2) \sim \frac{2}{\pi\sqrt{1 - 2\alpha^2t}} \cos^2(-\omega t + \frac{\pi}{4} - \rho),$$

where $\omega = \alpha\rho + \theta$, $\rho = \arg(-B + \sqrt{\Delta})$, $\theta = \arg(-B + 2 + \sqrt{\Delta})$, $B = \frac{2\alpha}{1-\alpha}$, and $\Delta = B^2 - 4(B + 1)$.

For a Markov chain, the mixing time is defined by

$$\tau_\epsilon = \max_u \min_t \{t; \|p_u(\cdot, t') - \pi\| \leq \epsilon, \forall t' \geq t\},$$

where $p_u(\cdot, t')$ is the distribution of the Markov chain at time t' with initial condition u , and π is the limiting distribution.

For a quantum random walk, due to periodic character, the limiting distribution does not exist. So the mixing time is defined as

$$\tau_\epsilon = \max_u \min_t \{t; \|p_u(\cdot, t) - \pi\| \leq \epsilon\},$$

where $p_u(\cdot, t)$ is the distribution of the quantum random walk at time t with initial condition u , and π is a target distribution.

The results 1 and 2 suggest that $\tau_\epsilon = \Omega(\frac{1}{\epsilon})$, for a 1-dimensional quantum random walk where π is the uniform distribution. For a 1-dimensional classical random walk, $\tau_\epsilon = \Omega(\frac{1}{\epsilon^2})$.

Definition 2.5 The Semi-infinite Walk.

The quantum random walk on $[0, \infty)$ is defined as follows.

Step 1. Let the initial state be $|1\rangle \otimes |1\rangle$.

Step 2. Apply U , and then apply the measurement $\{\Pi_0, 1 - \Pi_0\}$.

Step 3. If the result of the measurement is 0, then terminate the process, otherwise repeat step 2.

Notation 2.1 Let p_∞ be the probability that the process is eventually terminated.

Then we have $p_\infty = \frac{2}{\pi} = .6366$.

Remark 2.1 $p_\infty = 1$, for 1-dimensional classical random walk.

Definition 2.6 The Finite Walk.

The quantum random walk on $[0, n]$, $n > 1$ is defined as follows.

Step 1. Let the initial state be $|1\rangle \otimes |1\rangle$.

Step 2. Apply U , apply the measurement $\{\Pi_0, 1 - \Pi_0\}$, and then apply the measurement $\{\Pi_n, 1 - \Pi_n\}$.

Step 3. If the result of either measurement is either 0 or n , then terminate the process, otherwise repeat step 2.

Notation 2.2 Let p_n be the probability that quantum random walk on $[0, n]$ is eventually terminated at 0.

Then we have $\lim_{n \rightarrow \infty} p_n = \frac{1}{\sqrt{2}} = .7071$.

It is interesting that $\frac{1}{\sqrt{2}} > \frac{2}{\pi}$, and $\lim_{n \rightarrow \infty} p_n > p_\infty$. This is not the case for classical random walks, where $p_n \leq p_\infty$, for all $n > 0$.

Known results 2: Scaling limit of quantum random walks on Z .

In [6], Grimmett, Janson, and Scudo (2003) obtained the scaling limit of a quantum random walk on Z^d .

In [10], Konno (2003), also obtained scaling limit but with a different description of the distribution.

S can be diagonalized in k -space (i.e. $L^2([0, 2\pi))$) as follows.

Notation 2.3 Let $\psi = \sum_{j=1,2} \sum_{x \in Z} \psi(x, j) |x\rangle \otimes |j\rangle \in H$.

$$\text{Let } \psi(x) = \begin{pmatrix} \psi(x, 1) \\ \psi(x, 2) \end{pmatrix}.$$

Let $\psi(k) = \sum_{x \in Z} \psi(x) e^{ikx}$ be the Fourier transform of $\psi(x)$.

Then we have

$$\psi(x) = \int_0^{2\pi} e^{-ikx} \psi(k) \frac{dk}{2\pi},$$

and

$$\langle \psi, \phi \rangle = \sum_{x,j} \bar{\psi}(x,j) \phi(x,j) = \sum_j \int_0^{2\pi} \bar{\psi}(k,j) \phi(k,j) \frac{dk}{2\pi}.$$

By definition,

$$S \begin{pmatrix} \psi(x,1) \\ \psi(x,2) \end{pmatrix} = \begin{pmatrix} \psi(x-1,1) \\ \psi(x+1,2) \end{pmatrix}.$$

Then in k -space,

$$S \begin{pmatrix} \psi(k,1) \\ \psi(k,2) \end{pmatrix} = \begin{pmatrix} e^{ik} \psi(k,1) \\ e^{-ik} \psi(k,2) \end{pmatrix}.$$

Therefore,

$$U\psi = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} A \begin{pmatrix} \psi(k,1) \\ \psi(k,2) \end{pmatrix} = U(k)\psi(k).$$

The evolution in terms of k -space is then

$$\psi_t(k) = U(k)^t \psi_0(k).$$

Notation 2.4 $U(k)$ has two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ with $|\lambda_j(k)| = 1$, and the corresponding orthonormal eigenvectors are denoted by $v_1(k)$ and $v_2(k)$. If $\lambda_1(k) = \lambda_2(k)$, then $U(k)$ is diagonal and A is also diagonal and the state evolves trivially either to the right or to the left. Therefore, we assume that $\lambda_1(k) \neq \lambda_2(k)$ from now on.

By eigenvector expansion, we have

$$\begin{aligned} \psi_t(k) &= U(k)^t \psi_0(k) \\ &= \lambda_1(k)^t \langle v_1(k), \psi_0(k) \rangle v_1(k) + \lambda_2(k)^t \langle v_2(k), \psi_0(k) \rangle v_2(k). \end{aligned}$$

The r -th moment of position operator is

$$E(X_t^r) = \langle \psi_t, X^r \psi_t \rangle = \int_0^{2\pi} \langle \psi_t(k), D^r \psi_t(k) \rangle \frac{dk}{2\pi},$$

where $D = -id/dk$ is the position operator in k -space. We assume that the initial state ψ_0 has all finite moments $E(X_0^r)$.

By Leibniz' rule, we have

$$D^r \psi_t(k) = \sum_j P(t, r) \lambda_j(k)^{t-r} (D\lambda_j(k))^r \langle v_j(k), \psi_0(k) \rangle v_j(k) + O(t^{r-1}),$$

where $P(t, r) = t(t-1)\dots(t-r+1)$. Therefore, as $t \rightarrow \infty$, we have

$$\begin{aligned} & E[(X_t/t)^r] \\ &= \int_0^{2\pi} \sum_j \lambda_j(k)^{t-r} (D\lambda_j(k))^r \langle v_j(k), \psi_0(k) \rangle \langle \psi_t(k), v_j(k) \rangle \frac{dk}{2\pi} + O(t^{-1}) \\ &= \int_0^{2\pi} \sum_j \left(\frac{D\lambda_j(k)}{\lambda_j(k)} \right)^r |\langle v_j(k), \psi_0(k) \rangle|^2 \frac{dk}{2\pi} + O(t^{-1}). \end{aligned}$$

Notation 2.5 Let $\Omega = [0, 2\pi] \times \{1, 2\}$ and μ a probability measure on Ω such that

$$\mu = |\langle v_j(k), \psi_0(k) \rangle|^2 \frac{dk}{2\pi}$$

on $[0, 2\pi] \times \{j\}$. Let h be a function defined on Ω such that $h(k, j) = \lambda_j(k)^{-1} D\lambda_j(k)$.

Then we have

$$\lim_{t \rightarrow \infty} E[(X_t/t)^r] = \int_{\Omega} h^r d\mu.$$

In [6], Grimmett, Janson, and Scudo (2003) obtained the following result. Let $X_t = U^{\dagger t} X U^t$ be the position operator at time t . If all the r -th moments are finite at time 0, then $\lim_{t \rightarrow \infty} \frac{1}{t} X_t = Y = h(Z)$, weakly, where Z is a random element of Ω with distribution μ .

Remark 2.2 Similar argument also works for d -dimensional case.

Remark 2.3 To obtain the above result, we need to assume that $\int_0^{2\pi} O(t^{-1}) \frac{dk}{2\pi} = O(t^{-1})$, for the quantum random walk considered.

Example 2.2 Hadamard Walk. For Hadamard walk,

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

The eigenvalues are

$$\lambda_j(k) = \frac{i}{\sqrt{2}} \sin k \pm \sqrt{1 - \frac{1}{2} \sin^2 k},$$

and the corresponding eigenvectors are

$$v_1(k) = \frac{1}{\sqrt{2N(\pi - k)}} \begin{pmatrix} e^{-ik} \\ -\sqrt{2}e^{-i\omega_k} + e^{-ik} \end{pmatrix},$$

and

$$v_2(k) = \frac{1}{\sqrt{2N(k)}} \begin{pmatrix} e^{-ik} \\ \sqrt{2}e^{i\omega_k} + e^{-ik} \end{pmatrix},$$

where $\omega_k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ satisfies $\sin(\omega_k) = \frac{\sin k}{2}$, and

$$N(k) = (1 + \cos^2 k) + \cos k \sqrt{1 + \cos^2 k}.$$

Therefore,

$$h(k, j) = \frac{-i\lambda'_j(k)}{\lambda_j(k)} = \pm \frac{\cos k}{\sqrt{2 - \sin^2 k}}.$$

The limiting distribution is concentrated on the interval $[\min h, \max h] = [-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]$.

If the initial state is $|0\rangle > |i\rangle$, where $i = 1$ or 2 , then $\psi_0(k) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ or $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$, respectively, and $\mu = |v_{ji}(k)|^2 \frac{dk}{2\pi}$ on $[0, 2\pi] \times \{j\}$. If the random walk starts at a mixed initial state $|0\rangle > |1\rangle$ with probability $\frac{1}{2}$ and $|0\rangle > |2\rangle$ with probability $\frac{1}{2}$, then $\mu = \frac{1}{2} \sum_{i=1}^2 |v_{ji}(k)|^2 \frac{dk}{2\pi} = \frac{dk}{4\pi}$ on $[0, 2\pi] \times \{j\}$. This means that μ is the uniform distribution on Ω . In this case, the density of Y is given by

$$f(y) = \frac{1}{\pi(1 - y^2)\sqrt{1 - 2y^2}},$$

for $y \in [-\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}]$.

2.2 Two-way infinite timed quantum walk

In this section, we let ψ_0 be the initial state in $H = H_p \otimes H_c$ with finite moments $E(X_0)$ and $E(X_0^2)$. Let

$$U(k) = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix} A.$$

Here A is a unitary operator from H_c to H_c . Let $X_t = U^{\dagger t} X U^t$ be the position operator at time t .

$U(k)$ has two eigenvalues $\lambda_1(k)$ and $\lambda_2(k)$ with $|\lambda_j(k)| = 1$, and the corresponding orthonormal eigenvectors are denoted by $v_1(k)$ and $v_2(k)$. If $\lambda_1(k) = \lambda_2(k)$, then $U(k)$ is diagonal and A is also diagonal and the state evolves trivially either to the right or to the left. Therefore, we assume that $\lambda_1(k) \neq \lambda_2(k)$ from now on.

By using the technique introduced in [6], we obtain the asymptotics of characteristic function $E(e^{i\xi \frac{X_t}{t}})$, result in this direction has been obtained by Konno [10]. We obtain it with a different description of distribution and simplify that result.

Theorem 2.1 $\lim_{t \rightarrow \infty} E(e^{i\xi \frac{X_t}{t}}) =$

$$\int_0^{2\pi} [e^{\xi \overline{\lambda_1(k)} \frac{d\lambda_1(k)}{dk}} | \langle v_1(k), \psi_0(k) \rangle |^2 + e^{\xi \overline{\lambda_2(k)} \frac{d\lambda_2(k)}{dk}} | \langle v_2(k), \psi_0(k) \rangle |^2] \frac{dk}{2\pi}.$$

Proof. The expectation of the random variable function $e^{i\xi \frac{X_t}{t}}$ is given in term of the operator X according to the standard formula as follows,

$$E(e^{i\xi \frac{X_t}{t}}) = \langle \psi_t, e^{i\xi \frac{X}{t}} \psi_t \rangle$$

Using the isometry between $l^2(Z)$ and $L^2([0, 2\pi))$, the above expectation may be written as

$$\begin{aligned}
E(e^{i\xi\frac{X_t}{t}}) &= \int_0^{2\pi} \langle \psi_t(k), \psi_t(k + \frac{\xi}{t}) \rangle \frac{dk}{2\pi} \\
&= \int_0^{2\pi} [T_1(k, t, \xi) + T_2(k, t, \xi) + T_3(k, t, \xi) + T_4(k, t, \xi)] \frac{dk}{2\pi}.
\end{aligned}$$

Here $\psi_t(k) = \lambda_1(k)^t \langle v_1(k), \psi_0(k) \rangle v_1(k) + \lambda_2(k)^t \langle v_2(k), \psi_0(k) \rangle v_2(k)$, and $T_i, i = 1, 2, 3, 4$, denote the following expression respectively.

$$\begin{aligned}
&[\overline{\lambda_1(k)} \lambda_1(k + \frac{\xi}{t})]^t \overline{\langle v_1(k), \psi_0(k) \rangle} \langle v_1(k + \frac{\xi}{t}), \psi_0(k + \frac{\xi}{t}) \rangle \langle v_1(k), v_1(k + \frac{\xi}{t}) \rangle \\
&[\overline{\lambda_1(k)} \lambda_2(k + \frac{\xi}{t})]^t \overline{\langle v_1(k), \psi_0(k) \rangle} \langle v_2(k + \frac{\xi}{t}), \psi_0(k + \frac{\xi}{t}) \rangle \langle v_1(k), v_2(k + \frac{\xi}{t}) \rangle \\
&[\overline{\lambda_2(k)} \lambda_1(k + \frac{\xi}{t})]^t \overline{\langle v_2(k), \psi_0(k) \rangle} \langle v_1(k + \frac{\xi}{t}), \psi_0(k + \frac{\xi}{t}) \rangle \langle v_2(k), v_1(k + \frac{\xi}{t}) \rangle \\
&[\overline{\lambda_2(k)} \lambda_2(k + \frac{\xi}{t})]^t \overline{\langle v_2(k), \psi_0(k) \rangle} \langle v_2(k + \frac{\xi}{t}), \psi_0(k + \frac{\xi}{t}) \rangle \langle v_2(k), v_2(k + \frac{\xi}{t}) \rangle
\end{aligned}$$

Noting that $v_1(k)$ and $v_2(k)$ are orthonormal, and applying to Mean Value Theorem, then we have the following facts:

$$\begin{aligned}
(1) \quad &[\overline{\lambda_1(k)} \lambda_1(k + \frac{\xi}{t})]^t = [\overline{\lambda_1(k)} \lambda_1(k) + \overline{\lambda_1(k)} \frac{d\lambda_1(k_{\frac{\xi}{t}})}{dk} \frac{\xi}{t}]^t \\
&= \{ [1 + \overline{\lambda_1(k)} \frac{d\lambda_1(k_{\frac{\xi}{t}})}{dk} \frac{\xi}{t}]^{\frac{t}{\xi \overline{\lambda_1(k)} \frac{d\lambda_1(k_{\frac{\xi}{t}})}{dk} \frac{\xi}{t}}} \}^{\xi \overline{\lambda_1(k)} \frac{d\lambda_1(k_{\frac{\xi}{t}})}{dk} \frac{\xi}{t}}
\end{aligned}$$

goes to $e^{\xi \overline{\lambda_1(k)} \frac{d\lambda_1}{dk}}$, as t goes to ∞ .

Here $k_{\frac{\xi}{t}}$ is some number between k and $k + \frac{\xi}{t}$.

Similarly,

$$(2) \quad [\overline{\lambda_2(k)} \lambda_2(k + \frac{\xi}{t})]^t \text{ goes to } e^{\xi \overline{\lambda_2(k)} \frac{d\lambda_2}{dk}}, \text{ as } t \text{ goes to } \infty.$$

The above arguments implies

$$\begin{aligned}
&\lim_{t \rightarrow \infty} E(e^{i\xi\frac{X_t}{t}}) \\
&= \int_0^{2\pi} [e^{\xi \overline{\lambda_1(k)} \frac{d\lambda_1}{dk}} |\langle v_1(k), \psi_0(k) \rangle|^2 + e^{\xi \overline{\lambda_2(k)} \frac{d\lambda_2}{dk}} |\langle v_2(k), \psi_0(k) \rangle|^2] \frac{dk}{2\pi}.
\end{aligned}$$

*Computer simulation shows the probability distribution of the Hadamard walk at time $t = 100$ with initial state $\psi_0 = |0\rangle \otimes |2\rangle$. Note that it has a drift toward left. So the quantum random walk is asymmetric with respect to $j = 1$ (right) and 2 (left). Unlike the classical random walk with Gaussian character, it is bimodal and spread out through the whole interval. It is spread out faster than the classical random walk. The variance for classical random walk is $\sigma^2(t) = t$ while $\sigma^2(t) = ct^2$ is expected for quantum random walk, where c is a constant and depends on the initial state and the evolution. Next we give a formula for the variance for quantum random walk. It follows from some technique in [6].

Theorem 2.2 *The variance $\sigma^2(X_t) = ct^2 + O(t)$, where*

$$c = \sum_j |\overline{[\lambda_j(k)]^2} \langle v_j(k), \psi_0(k) \rangle|^2 [D\lambda_j(k)]^2,$$

and $D = -id/dk$ is the position operator in k -space.

Proof. By eigenvector expansion, we have

$$\begin{aligned} \psi_t(k) &= U(k)^t \psi_0(k) \\ &= \lambda_1(k)^t \langle v_1(k), \psi_0(k) \rangle v_1(k) + \lambda_2(k)^t \langle v_2(k), \psi_0(k) \rangle v_2(k). \end{aligned}$$

The r -th moment of position operator is

$$E(X_t^r) = \langle \psi_t, X^r \psi_t \rangle = \int_0^{2\pi} \langle \psi_t(k), D^r \psi_t(k) \rangle \frac{dk}{2\pi},$$

where $D = -id/dk$ is the position operator in k -space. We assume that the initial state ψ_0 has all finite moments $E(X_0^r)$.

By Leibniz' rule, we have

$$D^r \psi_t(k) = \sum_j P(t, r) \lambda_j(k)^{t-r} (D\lambda_j(k))^r \langle v_j(k), \psi_0(k) \rangle v_j(k) + O(t^{r-1}),$$

where $P(t, r) = t(t-1)\dots(t-r+1)$.

$$\begin{aligned}
E(X_t^2) &= \langle \psi_t, X^2 \psi_t \rangle = \int_0^{2\pi} \langle \psi_t(k), D^2 \psi_t(k) \rangle \frac{dk}{2\pi} \\
&= \int_0^{2\pi} B_1(k, t) \frac{dk}{2\pi} = t(t-1) \int_0^{2\pi} B_2(k) \frac{dk}{2\pi} + O(t).
\end{aligned}$$

Here $B_1(k, t)$ and $B_2(k)$ denote the following expression respectively,

$$\begin{aligned}
\langle \psi_t(k), \sum_{j=1}^2 t(t-1) \lambda_j(k)^{t-2} (D\lambda_j(k))^2 \langle v_j(k), \psi_0(k) \rangle v_j(k) + O(t) \rangle, \\
\sum_{j=1}^2 \overline{\lambda_j(k)^2} |\langle v_j(k), \psi_0(k) \rangle|^2 (D\lambda_j(k))^2.
\end{aligned}$$

And also notice that

$$\begin{aligned}
E(X_t) &= \langle \psi_t, X \psi_t \rangle = \int_0^{2\pi} \langle \psi_t(k), D \psi_t(k) \rangle \frac{dk}{2\pi} \\
&= \int_0^{2\pi} B_3(k, t) \frac{dk}{2\pi} = t \int_0^{2\pi} B_4(k) \frac{dk}{2\pi} + O(1).
\end{aligned}$$

Here $B_1(k, t)$ and $B_2(k)$ denote the following expression respectively,

$$\begin{aligned}
\langle \psi_t(k), \sum_{j=1}^2 t \lambda_j(k)^{t-1} D\lambda_j(k) \langle v_j(k), \psi_0(k) \rangle v_j(k) + O(1) \rangle, \\
\sum_{j=1}^2 \overline{\lambda_j(k)} |\langle v_j(k), \psi_0(k) \rangle|^2 D\lambda_j(k).
\end{aligned}$$

So we have $\sigma(X_t) = E(X_t^2) - [E(X_t)]^2 = ct^2 + O(t)$, where

$$c = \sum_j \overline{[\lambda_j(k)]^2} |\langle v_j(k), \psi_0(k) \rangle|^2 [D\lambda_j(k)]^2.$$

2.3 Semi-infinite Hadamard walk

In this section we will study the asymptotic behavior of hitting probabilities of one-dimensional Hadamard quantum walk and corresponding classical random walk with starting state $|1\rangle$ and the hitting point right to the left of starting position.

2.3.1 Path integral for 1-d quantum random walk

A path $w = (w_0, w_1, \dots, w_n)$, where $w_l \in Z$. The length of w is $|w| = n$. Let $e_{j_l} = w_l - w_{l-1}$ be the increment at l -th step, where $e_1 = 1$, $e_2 = -1$. Note that $w = (w_0, w_1, \dots, w_n)$ can be 1-1 identified with $(w_0, e_{j_1}, \dots, e_{j_n})$ or (w_0, j_1, \dots, j_n) .

Notation 2.6 Let $\Omega^n = \{w; |w| = n\}$. Let $A = (a_{ij})_{2 \times 2}$.

Definition 2.7 Amplitude function

The amplitude function is defined by

$$\Psi_j^{i,x}(w) = a_{ij_1} a_{j_1 j_2} \dots a_{j_{n-1} j_n} \delta_j(j_n),$$

here $w_l - w_{l-1} = e_{j_l}$ and $w_0 = x$; otherwise $\Psi_j^{i,x}(w) = 0$.

Definition 2.8 Let $\Gamma \subseteq \Omega^n$. The amplitude of a set is

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

We also let

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

Note that $\Psi^{i,x}$ does not satisfy the "consistency condition" needed to define a measure on the space of all sample paths as in the theory of random processes. This is seen from the following

Example 2.3 Consider Hadamard walk in 1 dimension. $\Psi^{i,0}(w_1 = 1) = a_{i1}$. $\Psi^{i,0}(w_1 = 1, w_2 = 2 \text{ or } 0) = a_{i1}a_{11} + a_{i1}a_{12} \neq a_{i1}$.

Notation 2.7 Let $\Omega = \sum_{n=0}^{\infty} \Omega^n$. Let $\Gamma \subseteq \Omega$ and $\Gamma^n = \Gamma \cap \Omega^n$.

Definition 2.9

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

and

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

For $\psi \in H$, we write $\psi = \sum_{i=1}^2 \sum_{x \in Z} \psi(x, i) |x \rangle |i \rangle$.

We have the following theorem.

Theorem 2.3 (a) Suppose $\psi_t = U^t |x \rangle |i \rangle$, then

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

for all $y \in Z, j = 1, 2$.

(b) Suppose $\psi_t = U^t \psi_0$. Then for any $\psi_0 \in H$, we have

$$\psi_t(y, j) = \sum_i \sum_x \psi_0(x, i) \Psi_j^{ix}(w_t = y).$$

Remark 2.4 The above theorem unifies the path integrals for quantum random walks and classical random walks. In fact, if we let

$$A = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad (2.1)$$

then for the classical simple random walk, $(X_t)_{t=0}^{\infty}$, on Z , we have

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

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

Proof (a). By definition of U ,

$$U^t |x \rangle |i \rangle = U^{t-1} \left(\sum_j a_{ij} |x + e_j \rangle |j \rangle \right)$$

$$= U^{t-2} \left(\sum_{j_2} \sum_{j_1} a_{j_1 j_2} a_{i j_1} |x + e_{j_1} + e_{j_2} > |j_2 \rangle \right).$$

By induction, the above

$$\begin{aligned} &= \sum_{j_t, \dots, j_1} a_{j_t - 1 j_t} \dots a_{j_1 j_2} a_{i j_1} |x + e_{j_1} + e_{j_2} + \dots + e_{j_t} > |j_t \rangle \\ &= \sum_{y, j} \Psi_j^{ix}(w_t = y) |y > |j \rangle, \end{aligned}$$

by definition.

(b) follows from (a) and the linearity.

2.3.2 1-dimensional quantum random walk hitting a fixed point

Definition 2.10 Green function for amplitudes. Let $D = 0$ be the hitting point. Let $\tau(w) = \inf\{t > 0; w_t = 0\}$ be the first hitting time by w .

Let

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

Here i is the initial type, and j is the ending type, n is the initial position in the line.

In particular, we put $f_j^i = f_j^{i,0}$.

Notation 2.8 Let F be a 2×2 matrix with entries $f_{ij} = f_j^i$.

In the following theorem we let \tilde{A} be the matrix obtained from A by interchanging the first and the second columns.

Using sample path analysis, we obtain the following theorem.

Theorem 2.4

$$F = z\tilde{A} \begin{pmatrix} 0 & 0 \\ 0 & ([1 - F]^{-1}zA)_{12} \end{pmatrix}.$$

Proof. By considering a sample path of case $\tau = 2$, and for $\tau \geq 4$, it visits the point $x = 1$ exactly $l + 1$ times before it hits D , we obtained the following recursive relations:

$$\begin{aligned} f_j^i(z) &= [za_{i1}za_{12} + za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^1(z) f_{j_2}^{j_1}(z) \dots f_{j_l}^{j_{l-1}}(z) za_{j_l 2}] \delta_2(j) \\ &= [za_{i1}(zA)_{12} + za_{i1} (\sum_{l=1}^{\infty} F^l zA)_{12}] \delta_2(j) \end{aligned}$$

So we have

$$f_j^i(z) = za_{i1} \left[\frac{I}{I - F} zA \right]_{12} \delta_2(j)$$

This implies the theorem.

For a short notation, we put

Notation 2.9

$$([1 - F]^{-1} zA)_{12} = g(z)$$

Related Functions.

Note that $f_1^{i,n}(z) = 0$, for both $i=1$ and 2 , and for all n . By a similar argument as that in the proof of Theorem 1.4, we have

$$f_2^{i,1}(z) = ([1 - F]^{-1} zA)_{i2}.$$

In particular,

$$f_2^{1,1}(z) = ([1 - F]^{-1} zA)_{12} = g(z),$$

and

$$f_2^1(z) = za_{11} f_2^{1,1}(z) = za_{11} g.$$

Using sample path analysis, we also obtain

Theorem 2.5 (a) $f_2^{i,n}(z) = f_2^{i,1}(z) (f_2^{2,1}(z))^{n-1}$, for $n \geq 1$.
 (b) $f_2^{2,n}(z) = (f_2^{2,1}(z))^n$, and $f_2^{2,1}(z) = ([1 - F]^{-1} zA)_{22}$.

Quantities to be considered.

Notation 2.10 Let $p(t)$ denotes the probability that the Hadamard walk with initial state $|1\rangle|1\rangle$ is observed for the first time at location 0 exactly after t steps.

By the definition of $p(t)$, $p(t) = |\Psi_2^{11}(w_t = 0, \tau = t)|^2$.

We are interested in the following problems.

Problem 1. Find $\lim_{t \rightarrow \infty} p(t)$, if it exists.

Problem 2. Find the expectation of τ given that $\tau < \infty$, if it exists.

For Hadamard walk, we put

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

in the equation of Theorem 1.4 and solve. We have

$$f_2^{1,1}(z) = g(z) = \frac{1 + z^2 - \sqrt{1 + z^4}}{\sqrt{2}z},$$

Remark 2.5 The above function is already obtained by Ambainis, Bach, Nayak, Vishwanath and Watrous (2001).

Notation 2.11 Let $A(t) = \frac{1}{2\pi} \int_0^{2\pi} f_2^{1,1}(e^{-i\theta}) e^{it\theta} d\theta$.

Note that

$$\begin{aligned} A(t) &= \frac{1}{2\pi} \int_0^{2\pi} f_2^{1,1}(e^{-i\theta}) e^{it\theta} d\theta \\ &= \frac{1}{2\pi} \int_0^{2\pi} \sqrt{2} \cos\theta e^{it\theta} d\theta - \frac{\sqrt{2}}{4\pi} \int_0^{2\pi} \sqrt{1 + e^{-4i\theta}} e^{i(t+1)\theta} d\theta \end{aligned}$$

Problem Find $\lim_{t \rightarrow \infty} A(t)$, if it exists.

We need the following lemma and propositions.

Proposition 2.1 1) For $0 < \theta < \pi$, $\sqrt{-e^{2i\theta}} = -ie^{i\theta}$.

2) For $0 < \theta < \pi$, $\sqrt{-e^{-2i\theta}} = ie^{-i\theta}$.

3) For $0 < \theta < \pi/2$, $\sqrt{e^{2i\theta}} = e^{i\theta}$.

4) For $\pi/2 < \theta < \pi$, $\sqrt{e^{2i\theta}} = -e^{i\theta}$.

5) For $0 < \theta < \pi/2$, $\sqrt{e^{-2i\theta}} = e^{-i\theta}$.

6) For $\pi/2 < \theta < \pi$, $\sqrt{e^{-2i\theta}} = -e^{-i\theta}$.

By the theorem on page 49 in [4], we have the following lemma.

Lemma 2.1 If $\phi(\theta)$ is N times continuously differentiable for $\alpha \leq \theta \leq \beta$, and $0 < \lambda \leq 1$, $0 < \mu \leq 1$, then

$$\int_{\alpha}^{\beta} e^{it\theta} (\theta - \alpha)^{\lambda-1} (\beta - \theta)^{\mu-1} \phi(\theta) d\theta = B_N(t) - A_N(t) + O(t^{-N}) \text{ as } t \rightarrow \infty,$$

where

$$A_N(t) = \sum_{n=0}^{N-1} \frac{\Gamma(n+\lambda)}{n \downarrow} e^{\pi i(n+\lambda-2)/2} t^{-n-\lambda} e^{it\alpha} \frac{d^n [(\beta - \alpha)^{\mu-1} \phi(\alpha)]}{d\alpha^n}$$

$$B_N(t) = \sum_{n=0}^{N-1} \frac{\Gamma(n+\mu)}{n \downarrow} e^{\pi i(n-\mu)/2} t^{-n-\mu} e^{it\beta} \frac{d^n [(\beta - \alpha)^{\lambda-1} \phi(\beta)]}{d\beta^n},$$

and $O(t^{-N})$ may be replaced by $o(t^{-N})$ if $\lambda = \mu = 1$.

By the Proposition 3.1.14 on page 165 in [5], we have the following proposition.

Proposition 2.2 Suppose that $g \in L^1([0, 2\pi])$ and that

$$\sum_{t \in \mathbb{Z}} |\widehat{g}(t)| < \infty,$$

$$\text{where } \widehat{g}(t) = \frac{1}{2\pi} \int_{[0, 2\pi]} g(\theta) e^{-it\theta} d\theta.$$

$$\text{Then } g(\theta) = \sum_{t \in \mathbb{Z}} \widehat{g}(t) e^{it\theta} \text{ a.e.,}$$

and therefore g is almost everywhere equal to a continuous function.

Proposition 2.3 $\frac{1}{2\pi} \int_0^{2\pi} \sqrt{2} \cos \theta e^{it\theta} d\theta$

$$= \begin{cases} 0 & \text{if } t \geq 2 \\ \sqrt{2}/2 & \text{if } t = 1 \end{cases}$$

Proof $\frac{1}{2\pi} \int_0^{2\pi} \sqrt{2} \cos \theta e^{it\theta} d\theta = \frac{\sqrt{2}}{\pi} \int_0^\pi \cos(\theta) \cos(t\theta) d\theta$

$$= \begin{cases} 0 & \text{if } t \geq 2 \\ \sqrt{2}/2 & \text{if } t = 1 \end{cases}$$

Proposition 2.4 $\int_0^{2\pi} \sqrt{1 + e^{-4i\theta}} e^{i(t+1)\theta} d\theta$

$$= \begin{cases} 8 \int_0^{\pi/4} \cos(t\theta) \sqrt{2\cos(2\theta)} d\theta & \text{if } t = 4k + 3, \text{ where } k \text{ is a nonnegative integer} \\ 0 & \text{otherwise} \end{cases}$$

Proof By Proposition 2.1, we have $\int_0^{2\pi} \sqrt{1 + e^{-4i\theta}} e^{i(t+1)\theta} d\theta$

$$= \int_0^\pi \sqrt{1 + e^{-4i\theta}} e^{i(t+1)\theta} d\theta + \int_0^\pi \sqrt{1 + e^{4i\theta}} e^{-i(t+1)\theta} d\theta$$

$$= \int_0^{\pi/4} \sqrt{2\cos(2\theta)} e^{it\theta} d\theta + \int_{\pi/4}^{\pi/2} i\sqrt{-2\cos(2\theta)} e^{it\theta} d\theta +$$

$$\int_{\pi/2}^{3\pi/4} i\sqrt{-2\cos(2\theta)} e^{it\theta} d\theta + \int_{3\pi/4}^\pi -\sqrt{2\cos(2\theta)} e^{it\theta} d\theta +$$

$$\int_0^{\pi/4} \sqrt{2\cos(2\theta)} e^{-it\theta} d\theta + \int_{\pi/4}^{\pi/2} -i\sqrt{-2\cos(2\theta)} e^{-it\theta} d\theta +$$

$$\int_{\pi/2}^{3\pi/4} -i\sqrt{-2\cos(2\theta)} e^{-it\theta} d\theta + \int_{3\pi/4}^\pi -\sqrt{2\cos(2\theta)} e^{-it\theta} d\theta$$

$$= \int_0^{\pi/4} 2\cos(t\theta) \sqrt{2\cos(2\theta)} d\theta + \int_{\pi/4}^{\pi/2} -2\sin(t\theta) \sqrt{-2\cos(2\theta)} d\theta$$

$$\begin{aligned}
& + \int_{\pi/2}^{3\pi/4} -2\sin(t\theta)\sqrt{-2\cos(2\theta)}d\theta + \int_{3\pi/4}^{\pi} -2\cos(t\theta)\sqrt{2\cos(2\theta)}d\theta \\
& = \begin{cases} 8 \int_0^{\pi/4} \cos(t\theta)\sqrt{2\cos(2\theta)}d\theta & \text{if } t = 4k + 3, k \text{ is a nonegitive integer.} \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}$$

Proposition 2.5 $\int_0^{\pi/4} \cos(t\theta)\sqrt{2\cos(2\theta)}d\theta = -2\Gamma(3/2)e^{i\pi(t+1)/4}t^{-3/2}+O(t^{-2})$,
as $t \rightarrow \infty$.

Proof Note that

$$\int_0^{\pi/4} e^{(it\theta)}\sqrt{2\cos(2\theta)}d\theta = \int_0^{\pi/4} (\pi/4 - t)^{-1/2}(\pi/4 - t)^{1/2}\sqrt{2\cos(2\theta)}e^{(it\theta)}d\theta$$

We apply Lemma 2.1 to the above integral, where $\lambda = 1$, $\mu = \frac{1}{2}$,
and $\phi(\theta) = (\frac{\pi}{4} - \theta)^{\frac{1}{2}}\sqrt{2\cos(2\theta)}$.

Proposition 2.6

$$A(t) = \begin{cases} \frac{2\sqrt{2}}{\sqrt{\pi}}t^{-\frac{3}{2}} + O(t^{-2}) & \text{if } t = 4k + 3 \rightarrow \infty, \text{ where } k \text{ is an integer} \\ \frac{\sqrt{2}}{2} & \text{if } t=1 \\ 0 & \text{otherwise} \end{cases}$$

Proof It follows the definition of $A(t)$, Proposition 2.3, Proposition 2.4 and Proposition 2.5.

Theorem 2.6 $p(t)$

$$= \begin{cases} \frac{8}{\pi}t^{-3} + O(t^{-4}) & \text{if } t = 4k + 3 \rightarrow \infty, \text{ where } k \text{ is an integer} \\ \frac{1}{2} & \text{if } t=1 \\ 0 & \text{otherwise} \end{cases}$$

Proof. By Proposition 2.6 and Proposition 2.2,

$$g(e^{-i\theta}) = \sum_{t=1}^{\infty} A(t)e^{-it\theta}.$$

On the other hand, by the definition of $g(z)$,

$$g(e^{-i\theta}) = \sum_{t=1}^{\infty} \Psi_2^{11}(w_t = 0, \tau = t)e^{-it\theta}.$$

Since $\{e^{-it\theta}\}_{t \in \mathbb{Z}}$ is a complete orthonormal system of Hilbert space $L^2([0, 2\pi])$, we have

$$A(t) = \Psi_2^{11}(w_t = 0, \tau = t).$$

So $p(t) = (|\Psi_2^{11}(w_t = 0, \tau = t)|)^2 = [A(t)]^2$, the theorem follows.

Corollary 2.1 *Let $E(\tau)$ denote the expectation of τ . Then $E(\tau|\tau < \infty) = \sum_{t=1}^{t=\infty} tp(t) < \infty$.*

2.3.3 1-dimensional classical symmetric random walk hitting a fixed point

Notation 2.12 *Let $p_c(t)$ denotes the probability that the classical random walk (symmetric) with initial state $|1\rangle$ is observed for the first time at location 0 exactly after t steps.*

For this classical random walk, we put

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

in the equation of Theorem 2.4 and solve. We have

$$f_c(z) = \frac{1 - \sqrt{1 - z^2}}{z},$$

where $f_c(z)$ is the green function for the corresponding classical random walks.

Theorem 2.7 $p_c(t)$

$$= \begin{cases} \sqrt{\frac{2}{\pi}} t^{-\frac{3}{2}} + O(t^{-2}) & \text{if } t = 2k + 1 \rightarrow \infty, \text{ where } k \text{ is an integer} \\ 0 & \text{otherwise} \end{cases}$$

Proof Since $f_c(z) = \sum_{t=1}^{\infty} \Psi_2^{11}(w_t = 0, \tau = t) z^t = \frac{1 - \sqrt{1 - z^2}}{z}$,

$$f_c(1) = \sum_{t=1}^{\infty} \Psi_2^{11}(w_t = 0, \tau = t) = 1$$

By Proposition 2.2, $\Psi_2^{11}(w_t = 0, \tau = t) = \frac{1}{2\pi} \int_0^{2\pi} f_c(e^{-i\theta}) e^{it\theta} d\theta$.

By the definition of $p_c(t)$, $p_c(t) = \Psi_2^{11}(w_t = 0, \tau = t)$.

$$\begin{aligned} \text{So } p_c(t) &= \frac{1}{2\pi} \int_0^{2\pi} f_c(e^{-i\theta}) e^{it\theta} d\theta = \frac{1}{2\pi} \int_0^{2\pi} (e^{i\theta} - e^{i\theta} \sqrt{1 - e^{-2i\theta}}) e^{it\theta} d\theta \\ &= -\frac{1}{2\pi} \int_0^{\pi} (\pi - \theta)^{-\frac{1}{2}} \theta^{-\frac{1}{2}} \psi_1(\theta) e^{i(t+1)\theta} d\theta \\ &\quad - \frac{1}{2\pi} \int_{\pi}^{2\pi} (2\pi - \theta)^{-\frac{1}{2}} (\theta - \pi)^{-\frac{1}{2}} \psi_2(\theta) e^{i(t+1)\theta} d\theta, \end{aligned}$$

where $\psi_1(\theta) = (\pi - \theta)^{\frac{1}{2}} \theta^{\frac{1}{2}} \sqrt{1 - e^{-2i\theta}}$, $\psi_2(\theta) = (2\pi - \theta)^{\frac{1}{2}} (\theta - \pi)^{\frac{1}{2}} \sqrt{1 - e^{-2i\theta}}$.

By applying the Lemma 2.1 to the above integrals, after doing a lot of calculations, we obtain this theorem.

Remark 2.6 *By investigating their long time behaviors, it is easy to see their time expectations which are $\sum_{t=0}^{\infty} tp(t)$ and $\sum_{t=0}^{\infty} tp_c(t)$ respectively are different. One is finite, the other is infinite.*

2.4 The quantum events and finite Hadamard walk

2.4.1 The quantum events.

Let H be the physical Hilbert space.

Definition 2.11 *Let $\{M_m; m = 0, 1, \dots, N\}$ be operators on H . $\{M_m; m = 0, 1, \dots, n\}$ is called a measurement if $\sum_m M_m^\dagger M_m = 1$, where M_m^\dagger is the Hermitian conjugate of M_m .*

Definition 2.12 *Let $\{M_m; m = 0, 1, \dots, N\}$ be a measurement. Then $M_m^\dagger M_m$ is called an event. It is the event that m occurs when the measurement $\{M_m; m = 0, 1, \dots, N\}$ is performed.*

Note that an event is an observable, i.e., a self-adjoint operator.

Example 2.4 *Let $\{\psi_0, \psi_1\}$ be an orthonormal basis of H . Let $M_i = M_{\psi_i}$ be the orthogonal projection onto ψ_i . Then $\{M_0, M_1\}$ is a measurement. Since $M_0^\dagger = M_0$ and $M_0^\dagger M_0 = M_0 M_0 = M_0$, M_0 is an event.*

Notation 2.13 *Let U_t , $t=0, 1, 2, \dots$ be a quantum dynamics on H . For any operator B on H , let $B_t = U_t^\dagger B U_t$.*

Proposition 2.7 *Suppose $\{M_m; m = 0, 1, \dots, n\}$ is a measurement. Then $\{(M_m)_t; m = 0, 1, \dots, n\}$ is also a measurement.*

Proposition 2.8 *Let $\{M_m; m = 0, 1, \dots, n\}$ and $\{M'_m; m = 0, 1, \dots, n'\}$ be measurement. Then $\{M'_m M_m; m = 0, 1, \dots, n, m' = 0, 1, \dots, n'\}$ is also a measurement.*

Proposition 2.9 *Let $\{M_m; m = 0, 1, \dots, n\}$ is a measurement. Then*

$$\{(M_{m_l})_{t_l} \dots (M_{m_1})_{t_1} M_{m_0}; m_0, \dots, m_l = 0, 1, \dots, n\}$$

is also a measurement, for all $0 < t_1 < \dots < t_l$.

Corollary 2.2 *Let $B = (M_{m_l})_{t_l} \dots (M_{m_1})_{t_1} M_{m_0}$. Then $B^\dagger B$ is an event.*

Proposition 2.10 *Given that the initial state is ϕ_0 , the probability that the event $B^\dagger B$ occurs is $P_{\phi_0}(B^\dagger B) = \langle \phi_0, B^\dagger B \phi_0 \rangle = \|B\phi_0\|^2$.*

Example 2.5 *Consider 1-d quantum random walk on $[0, \infty)$ with initial state $\phi_0 = \psi_{1,R}$. Let Π_x be the orthogonal projection onto the linear span of $\{\psi_{x,j}, j = R, L\}$. Let $\Pi'_x = 1 - \Pi_x$.*

Notation 2.14 *Let τ be the first hitting time of quantum random walk at 0. Let $B = (U^\dagger)^3 \Pi_0 U \Pi'_0 U \Pi'_0 U \Pi'_0$.*

Then

$$P_{\phi_0}(\tau = 3) = P_{\phi_0}(B^\dagger B) = \|B\phi_0\|^2.$$

Note that $B^\dagger \neq B$, therefore B is not an orthogonal projection.

Example 2.6 *Let $I \subseteq Z^1$. Let Π_I be the orthogonal projection onto the linear span of $\{\psi_{x,j}; x \in I, j = R, L\}$. Let $\Pi'_I = 1 - \Pi_I$. Let $B = \Pi_I U \dots \Pi_{I_1} U$. Then $B^\dagger B$ is the event $\{w; w_1 \in I_1, \dots, w_l \in I_l\}$.*

$$P_{\phi_0}(\{w; w_1 \in I_1, \dots, w_l \in I_l\}) = P_{\phi_0}(B^\dagger B) = \|B\phi_0\|^2.$$

If $\phi_0 = \psi_{0,i}$. Then the above

$$= \sum_{x \in I_l, j=R,L} |\Psi_j^{i,0}(\{w; w_1 \in I_1, \dots, w_{l-1} \in I_{l-1}, w_l = x\})|^2.$$

Theorem 2.8 *Let $B_l = \Pi_{I_l} U \dots \Pi_{I_1} U$, for $l = 1, 2, \dots$, and $B = (B_l)_{l=1}^\infty$ be a sequence of operators on H . Then there exists an operator E_B on H , $0 \leq E \leq 1$ such that*

$$\lim_{l \rightarrow \infty} B_l^\dagger B_l = E_B,$$

in weak operator topology.

Proof

$$\begin{aligned} P_\phi(B_l^\dagger B_l) &= \langle \phi, B_l^\dagger B_l \phi \rangle = \|B_l \phi\|^2 = \|\Pi_{I_l} U \dots \Pi_{I_1} U \phi\|^2 \\ &\leq \|U \Pi_{I_{l-1}} U \dots \Pi_{I_1} U \phi\|^2 = \|\Pi_{I_{l-1}} U \dots \Pi_{I_1} U \phi\|^2 = P_\phi(B_{l-1}^\dagger B_{l-1}). \end{aligned}$$

Since the above sequence is nonnegative and decreasing,

$$\lim_{l \rightarrow \infty} \langle \phi, B_l^\dagger B_l \phi \rangle$$

exists. By Polarization Identity on Page 63 in [17].

$$\lim_{l \rightarrow \infty} \langle \phi, B_l^\dagger B_l \psi \rangle$$

also exists,

$$\begin{aligned} \langle \phi, B_l^\dagger B_l \psi \rangle &= \frac{1}{4} \{ \langle (\phi + \psi), B_l^\dagger B_l (\phi + \psi) \rangle - \langle (\phi - \psi), B_l^\dagger B_l (\phi - \psi) \rangle \\ &\quad - i [\langle (\phi + i\psi), B_l^\dagger B_l (\phi + i\psi) \rangle - \langle (\phi - i\psi), B_l^\dagger B_l (\phi - i\psi) \rangle] \}. \end{aligned}$$

It follows from Theorem VI.1 (Page 184, in [17]) that there exists a bounded operator E_B such that $\lim_{l \rightarrow \infty} B_l^\dagger B_l = E_B$. Since $0 \leq B_l^\dagger B_l \leq 1$, we have $0 \leq E_B \leq 1$.

2.4.2 The finite Hadamard walk .

Now we consider the finite Hadamard walk.

Notation 2.15 *For each $n > 1$, Let p_n and q_n be the probability that a 1-dimensional Hadamard walk in $[0, n]$ with initial condition $\psi_{1,R}$ that exists from 0 and n , respectively.*

In [1], Ambainis, Bach, Nayak, Vishwanath and Watrous (2001) pointed out that $p_n + q_n = 1$, for all $n > 1$, but they did not give any proof. We think that is only their conjecture. We shall give proof only in case $n=3$, and 4.

Notation 2.16 Let Ω^n be the set of all paths with length n . Let Ω_x^n be the set of all path w with $w_n = x$. Let $\Gamma \subseteq \Omega^n$ and $\Gamma_x = \Gamma \cap \Omega_x^n$. Let $\phi_0 = \psi_{y,i}$. Then

$$P_{\phi_0}(\Gamma) = \sum_x P_{\phi_0}(\Gamma_x) = \sum_x |\Psi^{i,y}(\Gamma_x)|^2.$$

Lemma 2.2

$$P_{\phi_0}(\Gamma) \leq \sup_x |\Gamma_x| P_c^y(\Gamma) = \sup_x P_c^y(\Gamma_x) 2^n P_c^y(\Gamma).$$

Proof

$$\begin{aligned} P_{\phi_0}(\Gamma) &= \sum_x P_{\phi_0}(\Gamma_x) = \sum_x |\Psi^{i,y}(\Gamma_x)|^2 \\ &= \sum_x \left| \sum_{w \in \Gamma_x} \Psi^{i,y}(w) \right|^2. \end{aligned}$$

By the Cauchy-Schwarz Inequality, the above

$$\begin{aligned} &\leq \sum_x \sum_{w \in \Gamma_x} |\Psi^{i,y}(w)|^2 |\Gamma_x| \\ &= \sum_x P_c^y(\Gamma_x) |\Gamma_x| \leq \sum_x |\Gamma_x| P_c^y(\Gamma) = \sup_x P_c^y(\Gamma_x) 2^n P_c^y(\Gamma). \end{aligned}$$

Proposition 2.11 We have $p_3 + q_3 = 1$.

Proof Let τ be the first hitting time of the walk at either 0 or 3. We shall apply Lemma 2.2 by letting $\Gamma = \{w; |w| = n, \tau > n\}$. Since the initial position is 1, $\Gamma = \Gamma_2$ if n is odd, and $\Gamma = \Gamma_1$ if n is even. Since $P_c^1(\Gamma) = (\frac{1}{2})^n$, the proposition follows from Lemma 2.2.

Proposition 2.12 We have $p_4 + q_4 = 1$.

Proof Let τ be the first hitting time of the walk at either 0 or 4. Let $\Gamma = \{w; |w| = n, \tau > n\}$. By observation and induction on n , we have $P_{\phi_0}(\Gamma) = P_c^1(\Gamma) = \frac{2^{\frac{n-1}{2}}}{2^n}$ if n is odd, and $P_{\phi_0}(\Gamma) = P_c^1(\Gamma) = \frac{2^{\frac{n}{2}}}{2^n}$ if n is even. The Proposition follows from that fact $\lim_{n \rightarrow \infty} P_{\phi_0}(\Gamma) = 0$.

CHAPTER 3

TWO DIMENSIONAL QUANTUM RANDOM WALKS HITTING HALF-SPACE

3.1 Path integral for 2-d quantum random walk.

In this chapter, we develop a sample path analysis for quantum random walks in a vertical half space. We obtain a formula for the first exit time. Based on this formula, we analyze the resulting Fourier integrals, and obtain hitting probabilities, asymptotic properties for quantum random walks in 2-dimensional vertical half space. The sample path integral also works for two dimensional classical random walk hitting 45° half space. We obtain the hitting probabilities and the asymptotic formula for the conditional expectation of $\frac{Y_n(w)}{n}$, where $Y_n(w)$ denotes the random variable defined by $w_\tau = (Y_n(w), Y_n(w))$ for a path w with initial position $w_0 = (0, n)$. We begin this chapter with the following definition.

Definition 3.1 The spaces. For a 2-dimensional quantum random walk, the position Hilbert space H_p is spanned by an orthonormal basis $\{|x \rangle; x \in \mathbb{Z}^2\}$. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j \rangle; j = 1, 2, 3, 4.\}$. The state space is $H = H_p \otimes H_c$.

Notation 3.1 Let $e_1 = (1, 0)$, $e_2 = (0, 1)$ be the standard orthonormal basis for \mathbb{Z}^2 , and $e_3 = -e_1$, $e_4 = -e_2$.

Definition 3.2 The evolution. The shift operator $S : H \rightarrow H$ is defined by

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

for all $j=1, 2, 3, 4$.

The coin operator $A : H_c \rightarrow H_c$ is a unitary operator.

The evolution operator is defined by $U = S(I \otimes A)$.

Let $\psi_0 \in H$ with $\|\psi_0\| = 1$ and $\psi_t = U^t \psi_0$. The sequence $\{\psi_t\}_0^\infty$ is called a 2-dimensional quantum random walk with initial state ψ_0 .

Example 3.1 (2-dimensional Hadamard walk.) Let

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

Example 3.2 (2-dimensional Grover walk.) Let

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

Notation 3.2 A path $w = (w_0, w_1, \dots, w_n)$, where $w_i \in Z^2$. The length of w is $|w| = n$. Let $e_{j_i} = w_i - w_{i-1}$ be the increment at i -th step. Note that $w = (w_0, w_1, \dots, w_n)$ can be 1-1 identified with $(w_0, e_{j_1}, \dots, e_{j_n})$ or (w_0, j_1, \dots, j_n) .

Notation 3.3 Let $\Omega^n = \{w; |w| = n\}$. Let $A = (a_{ij})_{4 \times 4}$.

Definition 3.3 Amplitude function. The amplitude function is defined by

$$\Psi_j^{i,x}(w) = a_{ij_1} a_{j_1 j_2} \dots a_{j_{n-1} j_n} \delta_j(j_n),$$

here $w_l - w_{l-1} = e_{j_l}$ and $w_0 = x$; otherwise $\Psi_j^{i,x}(w) = 0$.

Definition 3.4 Let $\Gamma \subseteq \Omega^n$. The amplitude of a set is

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

We also let

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

Note that $\Psi^{i,x}$ does not satisfy the "consistency condition" needed to define a measure on the space of all sample paths as in the theory of random processes. This is seen from the following

Example 3.3 Consider Hadamard walk in 1 dimension. $\Psi^{i,0}(w_1 = 1) = a_{i1}$. $\Psi^{i,0}(w_1 = 1, w_2 = 2 \text{ or } 0) = a_{i1}a_{11} + a_{i1}a_{12} \neq a_{i1}$.

Definition 3.5 Let $\Omega = \sum_{n=0}^{\infty} \Omega^n$. Let $\Gamma \subseteq \Omega$ and $\Gamma^n = \Gamma \cap \Omega^n$. We define

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

and

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

For $\psi \in H$, we write $\psi = \sum_{i=1}^4 \sum_{x \in Z^2} \psi(x, i) |x \rangle |i \rangle$. We have the following theorem.

Theorem 3.1 (a) Suppose $\psi_t = U^t |x \rangle |i \rangle$, then

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

for all $y \in Z^2, j = 1, 2, 3, 4$. (b) Suppose $\psi_t = U^t \psi_0$. Then for any $\psi_0 \in H$, we have

$$\psi_t(y, j) = \sum_i \sum_x \psi_0(x, i) \Psi_j^{ix}(w_t = y).$$

Remark 3.1 The above theorem unifies the path integrals for quantum random walks and classical random walks in 2-dim. lattices. In fact, if we let

$$A = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},$$

then for the classical simple random walk, $(X_t)_{t=0}^{\infty}$, on Z^2 , we have

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

for all $y \in Z^2$, and any $i=1, 2, 3, 4$.

Proof. (a). By definition of U ,

$$\begin{aligned} U^t |x \rangle |i \rangle &= U^{t-1} \left(\sum_j a_{ij} |x + e_j \rangle |j \rangle \right) \\ &= U^{t-2} \left(\sum_{j_2} \sum_{j_1} a_{j_1 j_2} a_{i j_1} |x + e_{j_1} + e_{j_2} \rangle |j_2 \rangle \right). \end{aligned}$$

By induction, the above

$$= \sum_{j_t, \dots, j_1} a_{j_t - 1 j_t} \dots a_{j_1 j_2} a_{i j_1} |x + e_{j_1} + e_{j_2} + \dots + e_{j_t} \rangle |j_t \rangle$$

$$= \sum_{y,j} \Psi_j^{ix}(w_t = y) |y \rangle |j \rangle,$$

by definition.

(b) follows from (a) and the linearity.

3.2 Application I. 2-dimensional quantum random walk hitting half-space

3.2.1 Green function for amplitudes

Definition 3.6 **Green function for amplitudes.** *Let $D = \{(x, y) \in \mathbb{Z}^2, x \geq 0\}$ be the left half-space. Let $\tau(w) = \inf\{t > 0; w_t \in D\}$ be the first hitting time of D by w .*

Let

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

Here i is the initial type, and j is the ending type, n is the initial position in x -axis, y is the ending position in y -axis.

Let $f_j^{i,n}(k, z) = \sum_y e^{iky} f_j^{i,n}(y)$, $0 \leq k \leq 2\pi$ be the Fourier transform. Then $f_j^{i,n}(k, z)$ is called Green function for amplitudes.

In particular, we put $f_j^i = f_j^{i,0}$.

Notation 3.4 *Let F be a 4×4 matrix with entries $F_{ij} = f_j^i(k, z)$.*

In the following theorem we let \tilde{A} be the matrix obtained from A by interchanging the first and the third columns.

Using sample path analysis, we obtain the following theorem.

Theorem 3.2

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

proof. 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 hits D , we obtained the following recursive relations:

$$\begin{aligned} f_j^i(y, z) &= za_{i2}\delta_2(j)\delta_1(y) + za_{i4}\delta_4(j)\delta_{-1}(y) + za_{i1}za_{13}\delta_3(j)\delta_0(y) \\ &+ za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} \sum_{y_1 y_2 \dots y_{l-1}} f_{j_1}^1(y_1, z) f_{j_2}^{j_1}(y_2 - y_1, z) \dots f_{j_l}^{j_{l-1}}(y - y_{l-1}, z) za_{j_l 3} \delta_3(j). \end{aligned}$$

Applying the Fourier transform, we have

$$\begin{aligned} f_j^i(k, z) &= za_{i2}\delta_2(j)e^{ik} + za_{i4}\delta_4(j)e^{-ik} \\ &+ [za_{i1}za_{13} + za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^1(k, z) f_{j_2}^{j_1}(k, z) \dots f_{j_l}^{j_{l-1}}(k, z) za_{j_l 3}] \delta_3(j) \\ &= za_{i2}\delta_2(j)e^{ik} + za_{i4}\delta_4(j)e^{-ik} + \{za_{i1}(zA)_{13} + za_{i1}[\sum_{l=1}^{\infty} F^l zA]_{13}\} \delta_3(j). \end{aligned}$$

So we have

$$f_j^i(k, z) = za_{i2}e^{ik}\delta_2(j) + za_{i4}e^{-ik}\delta_4(j) + za_{i1}[\frac{I}{I - F}zA]_{13}\delta_3(j).$$

This implies the theorem.

Notation 3.5 For a short notation, we put

$$([I - F]^{-1}zA)_{13} = g(k, z).$$

Proposition 3.1 Note that for $n \geq 1$, $f_j^{i,n}(k, z) = 0$, for all $j \neq 3$. By a similar argument as that in the proof of Theorem 3.2, we have

$$f_3^{i,1}(k, z) = ([I - F]^{-1}zA)_{i3}.$$

In particular,

$$f_3^{1,1}(k, z) = ([I - F]^{-1}zA)_{13} = g,$$

and

$$f_3^1(k, z) = za_{11}f_3^{1,1}(k, z) = za_{11}g.$$

Using sample path analysis, we also obtain

Theorem 3.3 We have

- (a) $f_3^{i,n}(k, z) = f_3^{i,1}(k, z)(f_3^{3,1}(k, z))^{n-1}$, for $n \geq 1$.
- (b) $f_3^{3,n}(k, z) = (f_3^{3,1}(k, z))^n$, and $f_3^{3,1}(k, z) = ([I - F]^{-1}zA)_{33}$.

The hitting probability of half-space is related to the green function for amplitudes in half-space:

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

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

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

For $n \geq 1$, the probability that the quantum random walk ever exists from the right half-space is

$$P_j^{i,n} = \sum_y \sum_{t=1}^{\infty} |\Psi_j^{in}(w_t = (0, y), \tau = t)|^2 = \|\Psi_j^{in}(w_t = (0, y), \tau = t)\|_{L^2(y,t)}^2.$$

By Plancherel Theorem, we have

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

We are interested in the following problems.

Problem 1. Find $\lim_{n \rightarrow \infty} P_j^{i,n}$, if it exists.

Problem 2. Find α such that the scaling limit $\lim_{n \rightarrow \infty} \frac{1}{P_j^{i,n}} P_j^{i,n}(\frac{k}{n^\alpha})$ exists and find its limit.

3.2.2 Applications to Hadamard Walk

For Hadamard walk in 2 dimensions, 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 the equation of Theorem 3.2 and solve. We have

$$g = \frac{2}{z} \frac{1 - z^4 + iz \sin k + iz^3 \sin k - S}{2 - 2z^2 + 4iz \sin k},$$

where

$$S = [(-1 + z^2)(-1 + z^6 - 2iz \sin k - 2iz^5 \sin k + z^2(\sin k)^2 - z^4(\sin k)^2)]^{\frac{1}{2}}.$$

We also have

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

Proposition 3.2 P_3^{3n} decreases as n increase, and $\lim_{n \rightarrow \infty} P_3^{3n} < 1$.

Proof. $p_3^{3n} = P_3^{3n}(k)|_{k=0}$

$$\begin{aligned} &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} f_3^{3n}(-k_1, e^{i\theta}) f_3^{3n}(k_1, e^{-i\theta}) dk_1 d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} (f_3^{31}(-k_1, e^{i\theta}))^n (f_3^{31}(k_1, e^{-i\theta}))^n dk_1 d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} [f_3^{31}(-k_1, e^{i\theta}) \overline{f_3^{31}(-k_1, e^{i\theta})}]^n dk_1 d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} |f_3^{31}(-k_1, e^{i\theta})|^{2n} dk_1 d\theta, \end{aligned}$$

for all $n=1, 2, \dots$

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. $k, \theta \in [0, 2\pi]$.

Therefore, P_3^{3n} decreases as n increase. The limit exists as n goes to ∞ . Moreover, by the Dominated Convergence Theorem, we have

$$\begin{aligned} \lim_{n \rightarrow \infty} P_3^{3n} &= \lim_{n \rightarrow \infty} \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} |f_3^{31}(-k_1, e^{i\theta})|^{2n} dk_1 d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} \lim_{n \rightarrow \infty} |f_3^{31}(-k_1, e^{i\theta})|^{2n} dk_1 d\theta \\ &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} L(k, \theta) dk_1 d\theta, \end{aligned}$$

where L is the indicator function of $\{k, \theta \in [0, 2\pi]; |f_3^{31}(-k_1, e^{i\theta})| = 1\}$.

The limit is less than 1 because $P_3^{31} < 1$.

By Proposition 3.2, $\lim_{n \rightarrow \infty} P_3^{3n}$ exists and we put

Notation 3.6

$$\lim_{n \rightarrow \infty} P_3^{3n} = P_3^{3\infty}.$$

Remark 3.2 By calculating the integral $\frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} L(k, \theta) dk_1 d\theta$ numerically, we have

$$P_3^{3\infty} \approx 0.556.$$

It is proved in [2] that $P_3^{3\infty} = \frac{1}{2}$, for $d = 1$.

Notation 3.7 Let $Y_n = Y_n(w)$ be a random variable defined by $w_\tau = (0, Y_n(w))$, for a path w with initial position $w_0 = (0, n)$. Let E^{in} denote the expectation with respect to the distribution P^{in} .

Theorem 3.4 Given that $\tau < \infty$, the conditional expectation of $\frac{Y_n}{n}$, with respect to P^{3n} , has the following limit.

$$\begin{aligned} & \lim_{n \rightarrow \infty} E^{3n} [e^{it \frac{Y_n}{n}} | \tau < \infty] \\ &= \frac{1}{P_3^{3\infty} (2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} L(k, \theta) e^{t\partial_k f_3^{31}(k, e^{-i\theta}) [f_3^{31}(k, e^{-i\theta})]^{-1}} dk_1 d\theta \end{aligned}$$

Proof.

$$\begin{aligned} E^{3n} [e^{it \frac{Y_n}{n}} | \tau < \infty] &= \frac{1}{P_3^{3n}} \sum_{y \in Z} e^{i \frac{y}{n} t} P_3^{3n}(y) \\ &= \frac{1}{P_3^{3n} (2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k + \frac{t}{n}, e^{-i\theta}) dk d\theta. \end{aligned}$$

By Theorem 3.3 (b) and the Mean Value Theorem, the above

$$= \frac{1}{P_3^{3n} (2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} [f_3^{31}(-k, e^{i\theta})]^n [f_3^{31}(k, e^{-i\theta}) + \frac{t}{n} \frac{\partial f_3^{31}(\eta_{k\theta}, e^{-i\theta})}{\partial k}]^n dk d\theta,$$

where $k < \eta_{k\theta} < k + \frac{t}{n}$. The integrand of the above goes to

$$L(k, \theta) e^{t\partial_k f_3^{31}(k, e^{-i\theta}) [f_3^{31}(k, e^{-i\theta})]^{-1}},$$

as n goes to ∞ . Since $0 \leq |f_3^{31}(-k, e^{i\theta})| \leq 1$, for a.e. $k, \theta \in [0, 2\pi]$, and by the Dominated Convergence Theorem, we have proved the theorem.

Remark 3.3 For a classical random walk on Z^2 , Y_n/n converges to a Cauchy distribution with parameter 1 (characteristic function $e^{-|t|}$), as n goes to infinity.

3.2.3 Applications to Grover's Walk

For Grover's walk in 2 dimensions, 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 the equation of Theorem 3.2 and solve. We have

$$f_3^{31}(k, z) = \frac{z - z^3}{-1 + z^4 + z(-1 + z^2) \cos k - S},$$

where

$$S = [(-1 + z^2)^2(1 + z^2 + z^4 + 2(z + z^3) \cos k + z^2 \cos^2 k)]^{\frac{1}{2}}.$$

Proposition 3.3 We have

$$\lim_{n \rightarrow \infty} [f_3^{31}(-k, e^{i\theta}) f_3^{31}(k, e^{-i\theta})]^n = L(k, \theta),$$

where $L(k, \theta)$ is the indicator function of $\{(k, \theta); (2 \cos \theta + \cos k)^2 < 1\}$.

Proof. By the definitions of $f_3^{31}(k, z)$ and S ,

$$\begin{aligned} f_3^{31}(k, e^{-i\theta}) &= -2 \cos \theta - \cos k \\ &+ \frac{2ie^{-2i\theta} \sin \theta \sqrt{-4 \sin^2 \theta e^{-4i\theta} [(2 \cos \theta + \cos k)^2 - 1]}}{-4 \sin^2 \theta e^{-4i\theta}}. \end{aligned}$$

It follows that for $0 < \theta < \pi$,

$$f_3^{31}(k, e^{-i\theta}) = -2 \cos \theta - \cos k - \frac{i}{2} e^{2i\theta} \sqrt{-4e^{-4i\theta}[(2 \cos \theta + \cos k)^2 - 1]},$$

and for $\pi < \theta < 2\pi$,

$$f_3^{31}(k, e^{-i\theta}) = -2 \cos \theta - \cos k + \frac{i}{2} e^{2i\theta} \sqrt{-4e^{-4i\theta}[(2 \cos \theta + \cos k)^2 - 1]}.$$

Since $|f_3^{31}(k, e^{-i\theta})| \leq 1$, $L(k, \theta)$ is the indicator function of the set $\{(k, \theta); |f_3^{31}(k, e^{-i\theta})| = 1\}$. By using the following properties of the square roots, we see that it is equivalent to the indicator function of $\{(k, \theta); (2 \cos \theta + \cos k)^2 < 1\}$.

- 1) For $0 < \theta < \frac{\pi}{2}$, $\sqrt{-e^{4i\theta}} = -ie^{2i\theta}$.
- 2) For $0 < \theta < \frac{\pi}{2}$, $\sqrt{-e^{-4i\theta}} = ie^{-2i\theta}$.
- 3) For $\frac{\pi}{2} < \theta < \pi$, $\sqrt{-e^{4i\theta}} = ie^{2i\theta}$.
- 4) For $\frac{\pi}{2} < \theta < \pi$, $\sqrt{-e^{-4i\theta}} = -ie^{-2i\theta}$.
- 5) For $\frac{\pi}{4} < \theta < \frac{3\pi}{4}$, $\sqrt{e^{4i\theta}} = -e^{2i\theta}$.
- 6) For $0 < \theta < \frac{\pi}{4}$, $\sqrt{e^{-4i\theta}} = e^{-2i\theta}$.
- 7) For $\frac{\pi}{4} < \theta < \frac{3\pi}{4}$, $\sqrt{e^{-4i\theta}} = -e^{-2i\theta}$.
- 8) For $\frac{3\pi}{4} < \theta < \frac{5\pi}{4}$, $\sqrt{e^{4i\theta}} = e^{2i\theta}$.
- 9) For $\frac{3\pi}{4} < \theta < \frac{5\pi}{4}$, $\sqrt{e^{-4i\theta}} = e^{-2i\theta}$.
- 10) For $\frac{5\pi}{4} < \theta < \frac{7\pi}{4}$, $\sqrt{e^{-4i\theta}} = -e^{-2i\theta}$.
- 11) For $\frac{7\pi}{4} < \theta < 2\pi$, $\sqrt{e^{-4i\theta}} = e^{-2i\theta}$.

Theorem 3.5 We have $\lim_{n \rightarrow \infty} P_3^{3n}$

$$= \frac{4}{(2\pi)^2} \int_0^\pi \left[\arccos\left(\frac{-1 - \cos k}{2}\right) - \arccos\left(\frac{1 - \cos k}{2}\right) \right] dk \approx 0.387. \quad (3.1)$$

$$c_1 n^{-2} \leq P_3^{3n} - P_3^{3\infty} \leq c_2 n^{-\frac{3}{2}}, \quad (3.2)$$

as $n \rightarrow \infty$, where c_1, c_2 are positive constants and $P_3^{3\infty}$ is the limit in (2.1).

Remark 3.4 *It is proved in [2] that*

$$P_3^{3n} - P_3^{3\infty} \sim cn^{-2},$$

for a Hadamard walk in $d=1$.

Proof of (2.1). The first equation (3.1) follows from Proposition 3.3, the Dominated Convergence Theorem and the symmetries of k and θ in $f_3^{31}(k, e^{-i\theta})$.

Proof of (3.2).

$$\begin{aligned} P_3^{3n} &= \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{2\pi} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) dk d\theta \\ &= \frac{4}{(2\pi)^2} \int_0^\pi \int_0^\pi f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) dk d\theta \end{aligned}$$

$$\begin{aligned} &= \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_0^{\arccos \frac{1-\cos k}{2}} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right] \\ &+ \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_{\arccos \frac{1-\cos k}{2}}^{\arccos \frac{-1-\cos k}{2}} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right] \quad (3.3) \\ &+ \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_{\arccos \frac{-1-\cos k}{2}}^\pi f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right] \end{aligned}$$

$$\begin{aligned} &= P_3^{3\infty} \\ &+ \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_0^{\arccos \frac{1-\cos k}{2}} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right] \quad (3.4) \end{aligned}$$

$$+ \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_{\arccos \frac{-1-\cos k}{2}}^\pi f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right], \quad (3.5)$$

since the integrand in (3.3) is equal to 1.

Let I_1 and I_2 be the integral terms in (3.4) and (3.5), respectively. To prove (3.1) and (3.2), it is sufficient to prove that $c_1 n^{-2} \leq I_1, I_2 \leq c_2 n^{-\frac{3}{2}}$.

To this end, we shall use the following lemma on Laplace's method (see the Theorem on page 37 in [4]).

Lemma 3.1 *Let g and h be functions on the interval $[\alpha, \beta]$ for which the integral $f(n) = \int_{\alpha}^{\beta} g(u)e^{nh(u)}du$ exists for each sufficiently large positive n . Suppose h is real, continuous at $u = \alpha$, continuously differentiable for $\alpha < u \leq \alpha + \eta$, with $\eta > 0$. Suppose further that $h' < 0$ for $\alpha < u \leq \alpha + \eta$, and $h(u) \leq h(\alpha) - \epsilon$, with $\epsilon > 0$, for $\alpha + \eta \leq u \leq \beta$. If $h'(u) \sim -a(u - \alpha)^{\nu-1}$ and $g(u) \sim b(u - \alpha)^{\lambda-1}$ as $u \rightarrow \alpha$, $\lambda > 0$, $\nu > 0$, then*

$$f(n) = \int_{\alpha}^{\beta} g(u)e^{nh(u)}du \sim \frac{b}{\nu} \Gamma\left(\frac{\lambda}{\nu}\right) \left(\frac{\nu}{an}\right)^{\frac{\lambda}{\nu}} e^{nh(\alpha)}$$

as $n \rightarrow \infty$

By (3.4),

$$\begin{aligned} I_1 &= \frac{4}{(2\pi)^2} \int_0^{\pi} dk \left[\int_0^{\arccos \frac{(1-\cos k)}{2}} f_3^{3n}(-k, e^{i\theta}) f_3^{3n}(k, e^{-i\theta}) d\theta \right] \\ &= \frac{4}{(2\pi)^2} \int_0^{\pi} dk \int_0^{\arccos \frac{(1-\cos k)}{2}} [f_3^{31}(-k, e^{i\theta}) f_3^{31}(k, e^{-i\theta})]^n d\theta \\ &= \frac{4}{(2\pi)^2} \int_0^{\pi} dk \int_0^{\arccos \frac{(1-\cos k)}{2}} [-2 \cos \theta - \cos k + \sqrt{(2 \cos \theta + \cos k)^2 - 1}]^{2n} d\theta. \end{aligned}$$

Let $e^{-u} = (-2 \cos \theta - \cos k + \sqrt{(2 \cos \theta + \cos k)^2 - 1})^2$. Then we have

$$\theta = \arccos \left(\frac{\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - \cos k}{2} \right).$$

Therefore,

$$\frac{d\theta}{du} = - \frac{\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}}{\sqrt{1 - \left(\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2} \cos k\right)^2}}.$$

Note that

$$u = -2 \ln (2 \cos \theta + \cos k - \sqrt{(2 \cos \theta + \cos k)^2 - 1}).$$

If θ goes from 0 to $\arccos \frac{1-\cos k}{2}$, then u goes from

$$-2 \ln (2 + \cos k - \sqrt{(2 + \cos k)^2 - 1})$$

to 0. Integration by substitution gives

$$\begin{aligned}
I_1 &= \frac{4}{(2\pi)^2} \int_0^\pi dk \left[\int_0^{-2 \ln(2+\cos k - \sqrt{(2+\cos k)^2 - 1})} \frac{\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k)^2}} e^{-nu} du \right] \\
&= \frac{4}{(2\pi)^2} \int_0^{-2 \ln(3-\sqrt{8})} \left(\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}} \right) e^{-nu} du \\
&\quad \times \int_0^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \frac{1}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k)^2}} dk. \tag{3.6}
\end{aligned}$$

Proposition 3.4 *We have*

$$c_1 \ln(u^{-1}) \leq \int_0^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \frac{1}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k)^2}} dk \leq c_2 u^{-\frac{1}{2}},$$

as $u \rightarrow 0$, where c_1 and c_2 are positive numbers.

Proof of Proposition 3.4. Let

$$I_3 = \int_0^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \frac{1}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k)^2}} dk.$$

Since

$$\begin{aligned}
&\frac{1}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k)^2}} \\
&= \frac{1}{\sqrt{1 - \frac{1}{4}e^{\frac{u}{2}} - \frac{1}{4}e^{-\frac{u}{2}} + \frac{1}{2}\cos k}} \frac{1}{\sqrt{1 + \frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k}} \\
&\geq \frac{M}{\sqrt{\frac{1}{2} + \frac{1}{2}\cos k}},
\end{aligned}$$

for $u \rightarrow 0$, we have

$$I_3 \geq \int_0^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \frac{M}{\sqrt{\frac{1}{2} + \frac{1}{2}\cos k}} dk$$

$$= M_1 \ln \left(\frac{1 + \sin \frac{k}{2}}{1 - \sin \frac{k}{2}} \right) \Big|_0^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} = c_1 \ln(u^{-1}) + o(u).$$

On the other hand, let

$$M_u = \int_0^{\frac{\pi}{2}} \frac{1}{\sqrt{1 - (\frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2} \cos k)^2}} dk.$$

Then M_u is bounded as $u \rightarrow 0$, and

$$I_3 = M_u + \int_{\frac{\pi}{2}}^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)}$$

$$\frac{1}{\sqrt{1 - \frac{1}{4}e^{\frac{u}{2}} - \frac{1}{4}e^{-\frac{u}{2}} + \frac{1}{2} \cos k}} \frac{1}{\sqrt{1 + \frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2} \cos k}} dk.$$

Let $s = \frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2$. Then $s \rightarrow -1$, and $\arccos s \rightarrow \pi$, as $u \rightarrow 0$. We write

$$1 - \frac{1}{4}e^{\frac{u}{2}} - \frac{1}{4}e^{-\frac{u}{2}} + \frac{1}{2} \cos k = \frac{1}{2}(\cos k - \cos(\arccos s)),$$

and by the Mean Value Theorem,

$$= \frac{1}{2}[-\sin(\arccos s)(k - \arccos s) - \frac{1}{2}(\cos \xi)(k - \arccos s)^2],$$

where $k < \xi < \arccos s$. For k , $\arccos s$ near π , $\cos \xi < 0$. Therefore,

$$1 - \frac{1}{4}e^{\frac{u}{2}} - \frac{1}{4}e^{-\frac{u}{2}} + \frac{1}{2} \cos k \geq \frac{1}{2}(\sin \arccos s)(\arccos s - k),$$

for k , $\arccos s$ near π .

Therefore

$$I_3 \leq M_u + \int_{\frac{\pi}{2}}^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \frac{\sqrt{2}}{\sqrt{\sin(\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2))(\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2) - k)}} \times \frac{1}{\sqrt{1 + \frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2} \cos k}} dk.$$

$$\begin{aligned}
&= M_u + \frac{\sqrt{2}}{\sqrt{\sin(\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2))}} \int_{\frac{\pi}{2}}^{\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2)} \\
&\frac{1}{\sqrt{(\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2) - k)}} \frac{1}{\sqrt{1 + \frac{1}{4}e^{\frac{u}{2}} + \frac{1}{4}e^{-\frac{u}{2}} - \frac{1}{2}\cos k}} dk.
\end{aligned}$$

Since the above integral is finite and

$$\frac{\sqrt{2}}{\sqrt{\sin(\arccos(\frac{1}{2}e^{\frac{u}{2}} + \frac{1}{2}e^{-\frac{u}{2}} - 2))}} = c_2 u^{-\frac{1}{2}},$$

as $u \rightarrow 0$, the proposition is proved.

Now, by Proposition 3.4 and (3.6), we have

$$I_1 \leq c_2 \int_0^{-2\ln 3 - \sqrt{8}} (\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}) u^{-\frac{1}{2}} e^{-nu} du.$$

By Lemma 3.1, with $g(u) = (\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}})u^{-\frac{1}{2}} \sim \frac{1}{8}u^{\frac{1}{2}} = \frac{1}{8}u^{\frac{3}{2}-1}$ as $u \rightarrow 0$, we have $I_1 \leq c_4 n^{-\frac{3}{2}}$, for some constant c_4 , as $n \rightarrow \infty$.

For the lower bound for I_1 , by Proposition 3.4 and (3.6),

$$\begin{aligned}
I_1 &\geq c_1 \int_0^{-2\ln 3 - \sqrt{8}} (\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}) \ln u^{-1} e^{-nu} du \\
&\geq c_1 \int_0^{-2\ln 3 - \sqrt{8}} (\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}) e^{-nu} du.
\end{aligned}$$

By Lemma 3.1, we have $\int_0^{-2\ln 3 - \sqrt{8}} (\frac{1}{8}e^{\frac{u}{2}} - \frac{1}{8}e^{-\frac{u}{2}}) e^{-nu} du \sim c_3 n^{-2}$, for some constant c_3 , as $n \rightarrow 0$.

3.3 Application II. 2-dimensional classical random walk hitting 45° half-space

3.3.1 Green function for amplitudes

Definition 3.7 Green function for amplitudes Let $D = \{(x, y) \in \mathbb{Z}^2, y \geq x\}$ be the left half-space. Let $\tau(w) = \inf\{t > 0; w_t \in D\}$ be the first hitting time of D by w .

Let

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

Here i is the initial type, and j is the ending type, n is the initial position in x -axis, y is the ending position in the line $y = x$.

Let $f_j^{i,n}(k, z) = \sum_y e^{iky} f_j^{i,n}(y)$, $0 \leq k \leq 2\pi$ be the Fourier transform. Then $f_j^{i,n}(k, z)$ is called Green function for amplitudes.

In particular, we put $f_j^i = f_j^{i,0}$.

Notation 3.8 Let F be a 4×4 matrix with entries $F_{ij} = f_j^i(k, z)$.

Using sample path analysis, we obtain the following theorem.

Theorem 3.6

$$F = zA \begin{pmatrix} 0 & ([I - F]^{-1}zA)_{12}e^{ik} & ([I - F]^{-1}zA)_{13} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & ([I - F]^{-1}zA)_{42} & ([I - F]^{-1}zA)_{43}e^{-ik} & 0 \end{pmatrix}.$$

proof. By considering a sample path of cases $\tau = 1$, $\tau = 2$, and for $\tau \geq 3$, it visits the line $y = x - 1$ exactly $l + 1$ times before hits D , we obtained the following recursive relations:

$$\begin{aligned} f_j^i(y, z) &= za_{i1}za_{13}\delta_3(j)\delta_0(y) \\ &+ za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} \sum_{y_1 y_2 \dots y_{l-1}} f_{j_1}^1(y_1, z) f_{j_2}^{j_1}(y_2 - y_1, z) \dots f_{j_l}^{j_{l-1}}(y - y_{l-1}, z) za_{j_l 3} \delta_3(j) \\ &\quad + za_{i1}za_{12}\delta_2(j)\delta_1(y) \end{aligned}$$

$$\begin{aligned}
& +za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} \sum_{y_1 \dots y_{l-1}} f_{j_1}^1(y_1, z) f_{j_2}^{j_1}(y_2 - y_1, z) \dots f_{j_l}^{j_{l-1}}(y - 1 - y_{l-1}, z) za_{j_l 2} \delta_2(j) \\
& \quad + za_{i4} za_{42} \delta_2(j) \delta_0(y) \\
& +za_{i4} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} \sum_{y_1 y_2 \dots y_{l-1}} f_{j_1}^4(y_1, z) f_{j_2}^{j_1}(y_2 - y_1, z) \dots f_{j_l}^{j_{l-1}}(y - y_{l-1}, z) za_{j_l 2} \delta_2(j) \\
& \quad + za_{i4} za_{43} \delta_3(j) \delta_{-1}(y) \\
& +za_{i4} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} \sum_{y_1 \dots y_{l-1}} f_{j_1}^4(y_1, z) f_{j_2}^{j_1}(y_2 - y_1, z) \dots f_{j_l}^{j_{l-1}}(y + 1 - y_{l-1}, z) za_{j_l 3} \delta_3(j).
\end{aligned}$$

Applying the Fourier transform, we have

$$\begin{aligned}
& f_j^i(k, z) \\
& = [za_{i1} za_{13} + za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^1(k, z) f_{j_2}^{j_1}(k, z) \dots f_{j_l}^{j_{l-1}}(k, z) za_{j_l 3}] \delta_3(j) \\
& + [za_{i1} za_{12} + za_{i1} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^1(k, z) f_{j_2}^{j_1}(k, z) \dots f_{j_l}^{j_{l-1}}(k, z) za_{j_l 2}] \delta_2(j) e^{ik} \\
& + [za_{i4} za_{42} + za_{i4} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^4(k, z) f_{j_2}^{j_1}(k, z) \dots f_{j_l}^{j_{l-1}}(k, z) za_{j_l 2}] \delta_2(j) \\
& + [za_{i4} za_{43} + za_{i4} \sum_{l=1}^{\infty} \sum_{j_1 j_2 \dots j_l} f_{j_1}^4(k, z) f_{j_2}^{j_1}(k, z) \dots f_{j_l}^{j_{l-1}}(k, z) za_{j_l 3}] \delta_3(j) e^{-ik} \\
& = \{za_{i1}(zA)_{13} + za_{i1} [\sum_{l=1}^{\infty} F^l zA]_{13}\} \delta_3(j) \\
& + \{za_{i1}(zA)_{12} + za_{i1} [\sum_{l=1}^{\infty} F^l zA]_{12}\} \delta_2(j) e^{ik} \\
& + \{za_{i4}(zA)_{42} + za_{i4} [\sum_{l=1}^{\infty} F^l zA]_{42}\} \delta_2(j) \\
& + \{za_{i4}(zA)_{43} + za_{i4} [\sum_{l=1}^{\infty} F^l zA]_{43}\} \delta_3(j) e^{-ik}
\end{aligned}$$

So we have

$$f_j^i(k, z) = za_{i1} [(I - F)^{-1} zA]_{13} \delta_3(j) + za_{i1} [(I - F)^{-1} zA]_{12} \delta_2(j) e^{ik}$$

$$+za_{i4}[(I - F)^{-1}zA]_{42}\delta_2(j) + za_{i4}[(I - F)^{-1}zA]_{43}\delta_3(j)e^{-ik}.$$

This implies the theorem.

Note that for $n \geq 1$, $f_j^{i,n}(k, z) = 0$, for both $j = 1$ and $j = 4$. By a similar argument as that in the proof of Theorem 3.6, we have

Proposition 3.5

$$f_j^{i,1}(k, z) = ([I - F]^{-1}zA)_{i3}\delta_3(j) + ([I - F]^{-1}zA)_{i2}e^{ik}\delta_2(j).$$

$$f_2^{i,0}(k, z) = za_{i1}f_2^{1,1}(k, z) + za_{i4}e^{-ik}f_2^{4,1}(k, z).$$

$$f_3^{i,0}(k, z) = za_{i1}f_3^{1,1}(k, z) + za_{i4}e^{-ik}f_3^{4,1}(k, z).$$

In particular, if $a_{ij} = \frac{1}{4}$, for all i and j , then we have

$$f_2^{i,0}(k, z) = \left(\frac{1}{4} + \frac{1}{4}e^{-ik}\right)f_2^{1,1}(k, z). \quad (3.7)$$

$$f_3^{i,0}(k, z) = \left(\frac{1}{4} + \frac{1}{4}e^{-ik}\right)f_3^{1,1}(k, z). \quad (3.8)$$

Using sample path analysis, we also obtain

Theorem 3.7 *We have*

$$(a) \quad f_2^{i,n}(k, z) = f_2^{i,1}(k, z)f_2^{2,n-1}(k, z) + f_3^{i,1}(k, z)f_2^{3,n-1}(k, z), \text{ for } n \geq 1.$$

$$(b) \quad f_3^{i,n}(k, z) = f_2^{i,1}(k, z)f_3^{2,n-1}(k, z) + f_3^{i,1}(k, z)f_3^{3,n-1}(k, z), \text{ for } n \geq 1.$$

In particular, if $a_{ij} = \frac{1}{4}$, for all i and j , then we have

$$f_2^{i,n}(k, z) = (f_2^{1,1}(k, z) + f_3^{1,1}(k, z))^{n-1}f_2^{1,1}(k, z).$$

$$f_3^{i,n}(k, z) = (f_2^{1,1}(k, z) + f_3^{1,1}(k, z))^{n-1}f_3^{1,1}(k, z).$$

The hitting probability of half-space is related to the green function for amplitudes in half-space:

For $n \geq 1$, the probability that the random walk ever exists from the right half-space is

$$P^{i,n} = P_2^{i,n} + P_3^{i,n} = f_2^{i,n}(0, 1) + f_3^{i,n}(0, 1).$$

Notation 3.9 Let $Y_n = Y_n(w)$ be a random variable defined by $w_\tau = (Y_n(w), Y_n(w))$, for a path w with initial position $w_0 = (0, n)$. Let E^{in} denote the expectation with respect to the distribution P^{in} .

We are interested in the following problems.

Problem 1. Find $P^{i,n}$, $P_2^{i,n}$ and $P_3^{i,n}$.

Problem 2. Find $\lim_{n \rightarrow \infty} P^{i,n}$, if it exists.

Problem 3. Find α such that the scaling limit $\lim_{n \rightarrow \infty} E^{in}[e^{it \frac{Y_n}{n^\alpha}} | \tau < \infty]$ exists and find its limit.

3.3.2 Applications to classical symmetric random Walk.

For this walk in 2 dimensions, we put

$$A = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix},$$

in the equation of Theorem 3.6 and solve. We have

$$f_2^{1,0}(k, z) = \frac{2e^{ik} - \sqrt{4e^{2ik} - z^2 e^{ik}(e^{ik} + 1)^2}}{4(e^{ik} + 1)}.$$

$$f_3^{1,0}(k, z) = \frac{2e^{ik} - \sqrt{4e^{2ik} - z^2 e^{ik}(e^{ik} + 1)^2}}{4e^{ik}(e^{ik} + 1)}.$$

By (3.7) and (3.8), we have

$$f_2^{1,1}(k, z) = \frac{2e^{ik} - \sqrt{4e^{2ik} - z^2 e^{ik}(e^{ik} + 1)^2}}{z(1 + e^{-ik})(e^{ik} + 1)}.$$

$$f_3^{1,1}(k, z) = \frac{2e^{ik} - \sqrt{4e^{2ik} - z^2 e^{ik}(e^{ik} + 1)^2}}{z(1 + e^{-ik})e^{ik}(e^{ik} + 1)}.$$

Proposition 3.6 We have

- (a) $P_2^{i,n} = \frac{1}{2}$, for all $i \geq 1$.
- (b) $P_3^{i,n} = \frac{1}{2}$, for all $i \geq 1$.
- (c) $P^{i,n} = 1$.

Proof.

- (a) $P_2^{i,n} = f_2^{i,n}(0, 1) = (f_2^{1,1}(0, 1) + f_3^{1,1}(0, 1))^{n-1} f_2^{1,1}(0, 1) = \frac{1}{2}$.
- (b) $P_3^{i,n} = f_3^{i,n}(0, 1) = (f_2^{1,1}(0, 1) + f_3^{1,1}(0, 1))^{n-1} f_3^{1,1}(0, 1) = \frac{1}{2}$.
- (c) $P^{i,n} = P_2^{i,n} + P_3^{i,n} = 1$.

Theorem 3.8 *Given that $\tau < \infty$, the conditional expectation of $\frac{y_n}{n}$ has the following limit.*

$$\lim_{n \rightarrow \infty} E[e^{it \frac{y_n}{n}} | \tau < \infty] = e^{-\frac{|t|}{2} + \frac{t}{2}i}.$$

Proof. By the definition of $E[e^{it \frac{y_n}{n}} | \tau < \infty]$ and Theorem 3.7, we have

$$\begin{aligned} E[e^{it \frac{y_n}{n}} | \tau < \infty] &= \sum_{y \in Z} e^{i \frac{y}{n} t} P^{1,n}(y) \\ &= f_2^{1,n}\left(\frac{t}{n}, 1\right) + f_3^{1,n}\left(\frac{t}{n}, 1\right) = (f_2^{1,1}\left(\frac{t}{n}, 1\right) + f_3^{1,1}\left(\frac{t}{n}, 1\right))^n \\ &= \left(\frac{2}{1 + e^{-i \frac{t}{n}}} - \frac{\sqrt{-e^{-i \frac{t}{n}}(e^{i \frac{t}{n}} - 1)^2}}{e^{i \frac{t}{n}} + 1}\right)^n \\ &= \left(\frac{2}{1 + e^{-\frac{t}{n}i}}\right)^n \left(1 - \frac{1 + e^{-\frac{t}{n}i}}{2} \frac{\sqrt{-e^{-i \frac{t}{n}}(e^{i \frac{t}{n}} - 1)^2}}{e^{i \frac{t}{n}} + 1}\right)^n \end{aligned}$$

Note that

$$\lim_{n \rightarrow \infty} \left(\frac{2}{1 + e^{-\frac{t}{n}i}}\right)^n = e^{\frac{t}{2}i}.$$

$$\lim_{n \rightarrow \infty} \left(1 - \frac{1 + e^{-\frac{t}{n}i}}{2} \frac{\sqrt{-e^{-i \frac{t}{n}}(e^{i \frac{t}{n}} - 1)^2}}{e^{i \frac{t}{n}} + 1}\right)^n = e^{-\frac{|t|}{2}}.$$

So the theorem follows.

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