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A path integral formula with applications to quantum random walks in Z^d

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Abstract

We consider general quantum random walks in a d-dimensional half-space. We first obtain a path integral formula for general quantum random walks in a d-dimensional space. Our path integral formula is valid for general quantum random walks on Cayley graphs as well. Then the path integral formula is applied to obtain the scaling limit of the exit distribution, the expectation of exit time and the asymptotic behaviour of the exit probabilities, for general quantum random walks in a half-space under some conditions on amplitude functions. The conditions are shown to be satisfied by both the Hadamard and Grover quantum random walks in two-dimensional half-spaces. For the two-dimensional case, we show that the critical exponent for the scaling limit of the hitting distribution is 1 as the lattice spacing tends to zero, i.e. the natural magnitude of the hitting position is of order $O(1)$ if the lattice spacing is set to be $1/n$. We also show that the rate of convergence of the total hitting probability has lower bound n^{-2} and upper bound $n^{-2+\epsilon}$ for any $\epsilon > 0$. For a quantum random walk with a fixed starting point, we show that the probability of hitting times at the hyperplane decays faster than that of the classical random walk. In both one and two dimensions, given the event of a hit, the conditional expectation of hitting times is finite, in contrast to being infinite for the classical case. In the one-dimensional case, we also obtain an exact order of the probability distribution of the hitting time at 0.

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1. Introduction

Discrete time quantum random walks were first used by Feynman in [10] for discretizing the Dirac equation. The term ‘quantum random walks’ was first given by Aharonov *et al* in [2]. Motivated by quantum information and quantum computing, quantum random walks were again studied by Meyer in [22, 23]. Recently, Aharonov *et al* [1] studied quantum random walks on general graphs with rigorous proofs. In [3], Ambainis *et al* also gave a detailed study of quantum random walks on a line with rigorous proofs. Subsequently, several rigorous results for quantum random walks on either d-dimensional whole lattice spaces or one-dimensional half-spaces were obtained [4, 6, 13, 19–21]. We refer to Kempe [16] for an excellent overview.

For the mathematical results obtained so far, the most commonly used techniques are diagonalization of the shift operator, path integrals, combinatorial methods and the 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 Z^d. So far the path integral has been formulated in a combinatorial form which is particularly simple for applications to one-dimensional quantum random walks.

In this paper, we consider general quantum random walks in a d-dimensional half-space. We first obtain a path integral formula for the case of d-dimensional general quantum random walks (proposition 1.1). Under some conditions on amplitude functions (A.1)–(A.6) in section 1.3, we then apply the path integral formula to obtain a scaling limit of the exit distribution, the expectation of exit time and the asymptotic behaviour of the exit probabilities, for general quantum random walks in a half-space (theorems 1.1–1.4). The conditions are shown to be satisfied by both Hadamard and Grover's quantum random walks in two-dimensional half-spaces (theorem 1.5). Our path integral formula works for general quantum random walks on Cayley graphs as well. Using the same method, we also prove an asymptotic property for the absorbing probability for the one-dimensional Hadamard quantum random walk on half-line (theorem 1.6). It is well known that the expectation of the hitting time at 0 is infinite for the one-dimensional classical random walk starting at position $n > 0$. For the quantum case, we show that the corresponding probability distribution of the hitting time at 0 decays faster than the classical case and if it hits, the conditional expectation of hitting time is finite.

1.1. Notations and definitions

In this paper, we consider quantum random walks on a d-dimensional half-space. 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 $\{|x\rangle, x \in Z^d\}$. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j\rangle, j = 1, 2, \ldots, 2d.\}$. The state space is defined by $H = H_p \otimes H_c$.

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

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

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 the initial state ψ_0. In this paper, we will mainly consider Hadamard walks and Grover's walks defined as follows.

The one-dimensional Hadamard walk is the quantum random walk on Z^1 with $A = H_2$, where H_2 is the 2×2 Hadamard matrix

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

The two-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 two 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 $|x\rangle \otimes |j\rangle$ and Π_x the orthogonal projection of H onto the linear span of $\{|x\rangle \otimes |j\rangle;\ j = 1, 2, \ldots, 2d\}$. The position operators $X = (X_1, \ldots, X_d)$ are unbounded linear operators on H such that

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

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

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

Computer simulations show that the probability distribution of a 1D Hadamard walk at time $t = 100$ with the initial state $\psi_0 = |0\rangle \otimes |2\rangle$ has a leftward drift, see e.g., [16]. So the quantum random walk is asymmetric with respect to the initial state $\psi_0 = |0\rangle \otimes |j\rangle$ with $j = 1$ (right) and 2 (left). Unlike the classical random walk with a Gaussian character, it is bimodal and spread out through the whole interval $[-100, 100]$. It spreads out faster than the classical random walk. The variance for the classical random walk is $\sigma^2(t) = t$, while $\sigma^2(t) = t^2$ is expected for the quantum random walk. For a symmetrized initial state $\psi_0 = |0\rangle \otimes \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$, the distribution at time $t = 100$ is symmetric with respect to 0. It is also bimodal and spread out through the whole interval $[-100, 100]$.

In [3], Ambainis *et al* obtained the results (a)–(d). Suppose that the initial state is $\psi_0 = |0\rangle \otimes |1\rangle$.

(a) Let $x = \alpha t \to \infty$ 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.

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

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

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

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

$$\tau_\epsilon = \max_u \min_t \{t; \|p_u(., t') - \pi\| \leqslant \epsilon, \ \forall t' \geqslant t\},$$

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

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

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

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

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

In [3], a 1D Hadamard walk on half-space $[0, \infty)$, called a semi-infinite walk, 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.

(c) Let p_∞ be the probability that the process is eventually terminated. Then

$$p_\infty = \frac{2}{\pi} = 0.6366.$$

It is well known that $p_\infty = 1$, for a one-dimensional classical random walk.

One-dimensional Hadamard walk on a finite interval $[0, n]$, $n > 1$, is also considered in [3]. It is defined by the following.

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.

(d) Let p_n be the probability that a quantum random walk on $[0, n]$ is eventually terminated at 0. Then,

$$\lim_{n\to\infty} p_n = \frac{1}{\sqrt{2}} = 0.7071.$$

Since $\frac{1}{\sqrt{2}} > \frac{2}{\pi}$, $\lim_{n\to\infty} p_n > p_\infty$. This is interesting because for classical random walks, $p_n \leqslant p_\infty$, for all $n > 0$.

For the problem of the scaling limit of a quantum random walk, we consider the position operator at time t, $X_t = U^{*t} X U^t$. Grimmett *et al* [12] obtained the weak scaling limit of $\frac{1}{t} X_t$ as $t \to \infty$. Konno [19, 20] also obtained the scaling limit, but with a different description of the distribution.

The method used in [13] is to diagonalize the shift operator S in the Fourier space. Then the asymptotic behaviour of moments can be easily determined. The proofs of (a) and (b) in [3] also depend on the diagonalization of S in Fourier space. Diagonalization of S in Fourier space does not work for a quantum random walk in a restricted space, for example, a half-space. The proofs of (c) and (d) in [3] depend on a path integral formula in terms of combinatorics which is special for one-dimensional Hadamard walks. This special combinatorial form of path integral does not work for general quantum random walks. Since we consider quantum random walks in dimensions >1 and in half-spaces, we will develop a form of path integral for general quantum random walks in the following subsection.

1.2. The path integral

Our formulation of path integral is described as follows. A path w is defined by $w = (w_0, w_1, \ldots, w_n)$, 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 the ith step of w. Then $w = (w_0, w_1, \ldots, w_n)$ can be 1-1 identified with $\left(w_0; e_{j_1}, \ldots, e_{j_n}\right)$. Let $\Omega^n = \{w; |w| = n\}$.

Definition 1.1. *(Amplitude function) For $1 \leqslant i, j \leqslant 2d$, $x \in Z^d$, the amplitude function is defined for $w \in \Omega^n$,*

$$\Psi_j^{i,x}(w) = \delta_j(j_n) a_{j_n j_{n-1}} a_{j_{n-1} j_{n-2}} \ldots a_{j_1 i}, \tag{1.1}$$

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

$$\Psi_j^{i,x}(w) = b_{i j_1} b_{j_1 j_2} \ldots b_{j_{n-1} j_n} \delta_j(j_n). \tag{1.2}$$

Definition 1.2. *Let $\Gamma \subseteq \Omega^n$. The amplitude of Γ is defined by*

$$\Psi_j^{i,x}(\Gamma) = \sum_{w \in \Gamma} \Psi_j^{i,x}(w). \tag{1.3}$$

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

$$\Psi_j^{i,x}(\Gamma) = \sum_{n=0}^{\infty} \Psi_j^{i,x}(\Gamma_n), \tag{1.4}$$

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

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

Proposition 1.1. *(a) Suppose $\psi_t = U^t|x\rangle|i\rangle$, then*

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

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

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

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

Remark 1.1. Proposition 1.1. 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 $i = 1, \dots, 2d$.

Remark 1.2. The above proposition works for general quantum random walks on Cayley graph as well. Let G be a group with group operation. 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 $\{|x\rangle, x \in G\}$. The coin Hilbert space H_c is spanned by an orthonormal basis $\{|j\rangle, e_j \in E\}$. The state space is $H = H_p \otimes H_c$.

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

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

for all j. The coin operator $A : H_c \to H_c$ 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 the initial state ψ_0. Then proposition 1.1 holds for quantum random walks on (G, E)

1.3. Quantum random walks in half-spaces

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 $D = \{(x, y) \in Z^2, x \leqslant 0\}$ 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 defined 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 (1.12) and (1.13)). Therefore, the Green function is absolutely convergent for $|z| < 1$. It exists in the sense of $L^2(\theta)$, for $z = \mathrm{e}^{\mathrm{i}\theta}$ and satisfies

$$\left\| \Psi_j^{in}(w_t = (0, y), \tau = t) \right\|_{L^2(t)}^2 = \frac{1}{2\pi} \int_0^{2\pi} \mathrm{d}\theta f_j^{i,n}(y, \mathrm{e}^{\mathrm{i}\theta}) f_j^{i,n}(y, \mathrm{e}^{-\mathrm{i}\theta}). \qquad (1.5)$$

Similarly, let

$$f_j^{i,n}(k, z) = \sum_y \mathrm{e}^{\mathrm{i}ky} f_j^{i,n}(y, z), \qquad 0 \leqslant k \leqslant 2\pi,$$

and

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

be the Fourier transforms (throughout this paper, we use $f_j^{i,n}(k, z)$ instead of $\hat{f}_j^{i,n}(k, z)$; the Fourier transform is understood by the variables). Then

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

Therefore, for a.e. k,

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

This implies $\sum_t \left| f_j^{i,n}(k,t)\right|^2 < \infty$ and $f_j^{i,n}(k,z)$ is analytic in $|z| < 1$, for a.e. k, and $f_j^{i,n}(k, r\,\mathrm{e}^{\mathrm{i}\theta}) \to f_j^{i,n}(k, \mathrm{e}^{\mathrm{i}\theta})$ 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. We obtain the following proposition.

Proposition 1.2. *For each fixed k, there exists $\delta > 0$ such that for all $|z| < \delta$, the Green functions satisfy*

$$F = z\tilde{A}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathrm{e}^{\mathrm{i}k} & 0 & 0 \\ 0 & 0 & ([1-F]^{-1}zA)_{13} & 0 \\ 0 & 0 & 0 & \mathrm{e}^{-\mathrm{i}k} \end{pmatrix}. \tag{1.6}$$

To simplify notation, we put

$$([1-F]^{-1}zA)_{13} = g(k,z) \quad \text{for} \quad |z| < \delta. \tag{1.7}$$

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

$$f_3^{i,1}(k,z) = ([1-F]^{-1}zA)_{i3} \quad \text{for} \quad |z| < \delta. \tag{1.8}$$

In particular,

$$f_3^{1,1}(k,z) = ([1-F]^{-1}zA)_{13} = g \quad \text{for} \quad |z| < \delta. \tag{1.9}$$

$$f_3^{1}(k,z) = za_{11} f_3^{1,1}(k,z) = za_{11} g \quad \text{for} \quad |z| < \delta. \tag{1.10}$$

We also obtain

Corollary 1.1. *For $n \geqslant 1$, $|z| < \delta$,*

(a) $f_3^{i,n}(k) = f_3^{i,1}(k)\left(f_3^{3,1}(k)\right)^{n-1}$.
(b) $f_3^{3,n}(k) = \left(f_3^{3,1}(k)\right)^n$ *and* $f_3^{3,1}(k) = ([1-F]^{-1}zA)_{33}$.

We will obtain results for general quantum random walks in two dimensions under the following conditions. We will show in theorem 1.5 that all the conditions (A.1–A.6) are satisfied for both Hadamard walk and Grover's walk in two dimensions.

A.1. *Equation (1.6) 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 $|z| \leqslant 1$ and equal to $f_j^i(k,z)$ for $|z| < \delta$.*

A.2. *For every k, $f_3^{31}(k,z)$ is analytic in the unit disc $|z| < 1$ and continuous in the closed unit ball $|z| \leqslant 1$. Moreover, $\left|f_3^{31}(k,\mathrm{e}^{\mathrm{i}\theta})\right| \leqslant 1$, a.e. $k, \theta \in [0, 2\pi]$, and the set $L = \{k, \theta \in [0,2\pi];\, |f_3^{31}(k,\mathrm{e}^{\mathrm{i}\theta})| = 1\}$ has a positive Lebesgue measure.*

A.3. *For every fixed θ, there exists a set $D_\theta = [0,2\pi]\backslash\{k_1(\theta), k_2(\theta), \ldots, k_l(\theta)\}$ such that the partial derivative $\partial_k f_3^{31}(k, \mathrm{e}^{-\mathrm{i}\theta})$ exists and is continuous in D_θ.*

A.4. *For every k, there exists a set $D_k = [0, 2\pi]\backslash\{\theta_1(k), \theta_2(k), \ldots, \theta_m(k)\}$ such that the partial derivative $\partial_r f_3^{31}(k, r\,\mathrm{e}^{-\mathrm{i}\theta})$ 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*

$$\left|\partial_r f_3^{31}(k, r\,\mathrm{e}^{\mathrm{i}\theta})\right| \leqslant C \sum_{i=1}^{m} \frac{1}{\sqrt{|\theta - \theta_i|}},$$

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

A.5. *There exist $0 \leqslant \xi_1 < \xi_2 < \cdots < \xi_t \leqslant 2\pi$, such that for every $\xi_i < \theta < \xi_{i+1}$, L^c is a finite union of open intervals, $\cup_j I_j$, with disjoint closures. Let $I_j = (a_j, b_j)$. Let $c_j = \frac{a_j+b_j}{2}$. 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. Moreover,*

$$1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \leqslant C\sqrt{|k - a_j|},$$

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

$$1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \leqslant C\sqrt{|k - b_j|},$$

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

A.6. *For a fixed k, let $\theta_1 = \theta_1(k)$ such that $\xi_i < \theta_1 < \xi_{i+1}$ and (θ_1, k) is on the boundary of L. For $\eta > 0$, let $\Omega_1 = \{\xi_i < \theta < \xi_{i+1} - -\eta, a_j < k < c_j\}$ and $\Omega_2 = \{\xi_{i+1} - 2\eta < \theta < \xi_{i+1}, a_j < k < c_j\}$. There exist positive constants η and C such that either both of the following inequalities hold:*

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_1$$

$$C\sqrt{|\theta_1 - \theta|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_2,$$

or both of the following inequalities hold:

$$C\sqrt{|\theta - \xi_{i+1}|}\sqrt{|k - a_j|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_2$$

$$C\sqrt{|\theta_1 - \theta|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_1.$$

Moreover, similar lower bounds hold for the other side of the interval $c_j < k < b_j$, with a_j replaced by b_j.

In order to apply proposition 1.2 to obtain an exact formula for $f_j^i(k, z)$ over $|z| < 1$ and extend it to $|z| = 1$, we use the following lemma.

Lemma 1.1. *Suppose (A.1) holds. Then for a.e. $k, h_j^i(k, z) = f_j^i(k, z)$, for $|z| < 1$, and $h_j^i(k, z)$ is a version of $f_j^i(k, z)$ for $|z| = 1$, i.e. $h_j^i(k, \mathrm{e}^{\mathrm{i}\theta})$ is the Fourier transform of $\Psi_j^{in}(w_t = (0, y), \tau = t)$.*

We will show that for both Hadamard walk and Grover's walk in two dimensions, condition (A.1) holds. Therefore by solving the equation, we have an exact formula for $f_j^i(k, z)$, extended up to $|z| \leqslant 1$. We will continue to use the same notation, $f_j^i(k, z)$, $|z| \leqslant 1$, for the extended function. Similarly, we will obtain an exact formula for $f_3^{in}(k, z)$ so that (1.6)–(1.10) and corollary 1.1 hold for all z up to $|z| \leqslant 1$.

1.4. The first hitting probabilities of D

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

$$f_j^{i,n}(y,z) = \sum_{t=1}^{\infty} \Psi_j^{in}(w_t = (0,y), \tau = t) z^t. \tag{1.11}$$

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

$$P_3^{i,n}(y) = \sum_{t=1}^{\infty} \left|\Psi_3^{in}(w_t = (0,y), \tau = t)\right|^2 = \left\|\Psi_3^{in}(w_t = (0,y), \tau = t)\right\|^2_{L^2(t)}. \tag{1.12}$$

By (1.12), $\Psi_3^{in}(w_t = (0,y), \tau = t)$ is in $L^2(t)$; therefore $f_3^{i,n}(y,z)$ is in $L^2(\theta)$, for $z = \mathrm{e}^{\mathrm{i}\theta}$. For $n \geqslant 1$, the probability that the quantum random walk ever exits from the right half-space is

$$P_3^{i,n} = \sum_y \sum_{t=1}^{\infty} \left|\Psi_3^{in}(w_t = (0,y), \tau = t)\right|^2 = \left\|\Psi_3^{in}(w_t = (0,y), \tau = t)\right\|^2_{L^2(y,t)}. \tag{1.13}$$

By Fourier transform, we have

$$P_j^{i,n}(k) = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \frac{1}{2\pi}\int_0^{2\pi} f_j^{i,n}(k-k_1, \mathrm{e}^{\mathrm{i}\theta}) f_j^{i,n}(k_1, \mathrm{e}^{-\mathrm{i}\theta})\, \mathrm{d}k_1 \tag{1.14}$$

and

$$P_j^{i,n} = P_j^{i,n}(k)|_{k=0} = \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \frac{1}{2\pi}\int_0^{2\pi} f_j^{i,n}(-k_1, \mathrm{e}^{\mathrm{i}\theta}) f_j^{i,n}(k_1, \mathrm{e}^{-\mathrm{i}\theta})\, \mathrm{d}k_1. \tag{1.15}$$

In this paper, we consider the following problems.

Problem 1. *Suppose that the quantum random walk starts with the initial state $|(n,0)\rangle \otimes |i\rangle$. Let $P_3^{i,n}$ be the probability that there is ever an exit from the right half-space. Find $\lim_{n\to\infty} P_3^{i,n}$.*

Problem 2. *Let $Y_n = Y_n(w)$ be the position on the y-axis that a quantum random walk hits the left half-space the first time, with the initial position at $(n, 0)$. Our problem is to find the critical exponent α such that Y_n/n^α has a non-trivial scaling limit, as n goes to infinity. By the well-known Levy–Cramer theorem, this is equivalent to the scaling limit of its characteristic function (Fourier transform), i.e. show that the scaling limit $\lim_{n\to\infty} \frac{1}{P_3^{i,n}} P_3^{i,n}\left(\frac{k}{n^\alpha}\right)$ exists.*

Problem 3. *Let τ be the first hitting time at the left half-space. It is well known that the expectation of τ is infinity for classical random walks. Our problem is to show that for a quantum random walk, if it hits, then the conditional expectation of τ is finite.*

Problem 4. *Determine the asymptotic behaviour of $P_3^{i,n}$ as $n \to \infty$.*

1.5. Main results

The following theorem gives the solution to problem 1.

Theorem 1.1. *For a quantum random walk in two dimensions, if (A.1) holds, then P_3^{3n} decreases as n increases, and*

$$\lim_{n\to\infty} P_3^{3n} = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \chi_L(k,\theta)\, \mathrm{d}k\, \mathrm{d}\theta,$$

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

Let $P_3^{3\infty} = \lim_{n\to\infty} P_3^{3n}$. We will prove in section 4 that for the Hadamard walk in two dimensions, $P_3^{3\infty} \approx 0.556$ and for Grover's walk, $P_3^{3\infty} \approx 0.387\,129$. For Grover's walk in two dimensions, theorem 1.4 gives an estimate of the rate of convergence for P_3^{3n}, as $n \to \infty$.

The following theorem is our result on the scaling limit of the hitting distribution, stated in problem 2. Let $Y_n = Y_n(w)$ be a random variable defined by $w_\tau = (0, Y_n(w))$, for a path w with the initial position $w_0 = (n, 0)$. Let E^{in} denote the expectation with respect to the distribution P_3^{in}.

Theorem 1.2. *Suppose (A.1)–(A.3) hold; then the critical exponent* $\alpha = 1$ *and the conditional distribution of* $\frac{Y_n}{n}$ *given that* $\tau < \infty$ *has the following limit:*

$$\lim_{n\to\infty} E^{3n}\left[\mathrm{e}^{\mathrm{i}t\frac{Y_n}{n}}\middle|\tau < \infty\right] = \frac{1}{P_3^{3\infty}(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} \chi_L(k,\theta)\,\mathrm{e}^{t\partial_k f_3^{31}(k,\mathrm{e}^{-\mathrm{i}\theta})[f_3^{31}(k,\mathrm{e}^{-\mathrm{i}\theta})]^{-1}}\,\mathrm{d}k\,\mathrm{d}\theta, \tag{1.16}$$

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

Remark 1.3. It is well known that for a classical random walk on Z^2, Y_n/n converges to a Cauchy distribution with parameter 1 (characteristic function $\mathrm{e}^{-|t|}$), as n goes to infinity.

The next theorem solves problem 3.

Theorem 1.3. *Suppose (A.1)–(A.4) hold; then given that* τ *is finite, the conditional expectation of* τ*, with respect to* E^{3n}*, is finite.*

Remark 1.4. For a classical random walk on Z^2, given that the initial position is $(n, 0)$, the expectation of τ is infinite.

The next theorem improves theorem 1.1 and solves problem 4.

Theorem 1.4. *Suppose (A.1–A.6) hold. Then for any* $\epsilon > 0$,

$$c_1 n^{-2} \leqslant P_3^{3n} - P_3^{3\infty} \leqslant c_2(\epsilon) n^{-2+\epsilon}, \tag{1.17}$$

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

For applications of proposition 1.1–theorem 1.4, we show

Theorem 1.5. *For both Hadamard walk and Grover's walk in two dimensions, (A.1–A.6) hold.*

We also obtain the following result on the exiting probability for Hadamard walk on a half-line. Let $p(t)$ be the probability that t is the first hitting time at 0 by a Hadamard walk with the initial state $|1\rangle \otimes |1\rangle$.

Theorem 1.6. *We have* $p(t) = \frac{1}{2}$*, for* $t = 1$*;* $p(t) = \frac{8}{\pi}t^{-3} + O(t^{-4})$*, for* $t = 4k + 3, k = 1, 2, \ldots$*, as* $t \to \infty$*; and* $p(t) = 0$*, otherwise.*

Since given $\tau < \infty$ with $\psi_0 = |1\rangle \otimes |1\rangle$, the conditional expectation $E^{11}[\tau|\tau < \infty] = \sum_{t=1}^{t=\infty} tp(t)$, we have

Corollary 1.2. *For the Hadamard walk in one dimension, we have* $E^{11}[\tau|\tau < \infty] < \infty$.

To compare quantum random walks and classical random walks on half-line, using the same metxprochod as that in theorem 1.6, we also obtain the well-known.

Theorem 1.7. *Let $(S_n)_0^\infty$ be a simple random walk on Z^1 starting at 1. Let $p_c(t)$ be the probability that the first hitting time at 0 by $(S_n)_0^\infty$ is t. Then*

$$p_c(t) = \sqrt{\frac{2}{\pi}} t^{-\frac{3}{2}} + O(t^{-2}),$$

for $t = 2k+1, k = 1, 2, \ldots,$ *as* $t \to \infty$; $p_c(t) = 0$, *otherwise.*

It follows from theorem 1.7 that the expectation of hitting time at 0 is infinite for the classical case. For the quantum case, theorem 1.6 and corollary 1.2 show that the hitting probability decays faster than the classical case and given $\tau < \infty$, the conditional expectation of τ is finite.

2. Proofs of proposition 1.1–corollary 1.1 and lemma 1.1

Proof of proposition 1.1. Proof of (a). By definition of U,

$$\begin{aligned} U^t|x\rangle|i\rangle &= U^{t-1}\left(\sum_j a_{ji}|x+e_j\rangle|j\rangle\right) \\ &= U^{t-2}\left(\sum_{j_2}\sum_{j_1} a_{j_2j_1}a_{j_1i}|x+e_{j_1}+e_{j_2}\rangle|j_2\rangle\right). \end{aligned}$$

By induction, the above

$$= \sum_{j_t,\ldots,j_1} a_{j_tj_{t-1}}\ldots a_{j_2j_1}a_{j_1i}\big|x+e_{j_1}+e_{j_2}+\ldots+e_{j_t}\big\rangle|j_t\rangle$$

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

by definition. This proves (a).

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

Proof of proposition 1.2. We first show that

$$\lim_{z\to 0}\sum_y \left|f_j^i(y,z)\right| = 0. \tag{2.1}$$

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

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

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

$$M\sum_{y\neq 0}\sum_{t=|y|}^\infty |z|^t + M\sum_{t=1}^\infty |z|^t \leqslant \left[\frac{2M}{1-|z|}+M\right]\frac{|z|}{1-|z|},$$

which goes to 0 as $|z| \to 0$.

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

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

The infinite series of the above sum is bounded by $\sum_l 4^l C^l$, where $C = \max_{i,j} \left\| f_j^i(y,z) \right\|_{L^1(y)}$ and $\left\| f_j^i(y,z) \right\|_{L^1(y)} = \sum_y \left| f_j^i(y,z) \right|$. By (2.1), $C < 1$ if $|z|$ is sufficiently small. Therefore, the series is convergent for sufficiently small $|z|$.

Applying the Fourier transform, we have

$$f_j^i(k,z) = zb_{i2}\delta_2(j)\,\mathrm{e}^{\mathrm{i}k} + zb_{i4}\delta_4(j)\,\mathrm{e}^{-\mathrm{i}k} \\ + \left[zb_{i1}zb_{13} + zb_{i1}\sum_{l=1}^{\infty}\sum_{j_1 j_2 \ldots j_l} f_{j_1}^1(k,z) f_{j_2}^{j_1}(k,z)\ldots f_{j_l}^{j_{l-1}}(k,z) zb_{j_l 3} \right]\delta_3(j) \\ = zb_{i2}\delta_2(j)\,\mathrm{e}^{\mathrm{i}k} + zb_{i4}\delta_4(j)\,\mathrm{e}^{-\mathrm{i}k} + \left\{ zb_{i1}(zB)_{13} + zb_{i1}\left[\sum_{l=1}^{\infty} F^l zB\right]_{13} \right\}\delta_3(j).$$

So we have

$$f_j^i(k,z) = zb_{i2}\,\mathrm{e}^{\mathrm{i}k}\delta_2(j) + zb_{i4}\,\mathrm{e}^{-\mathrm{i}k}\delta_4(j) + zb_{i1}\left[\frac{I}{I-F}zB\right]_{13}\delta_3(j).$$

Note that by (2.1), the above series is convergent for sufficiently small $|z|$ and $I - F$ is invertible. This implies the theorem. □

Proof of corollary 1.1. Corollary 1.1 is proved by using a similar argument as in the proof of proposition 1.2. □

Proof of lemma 1.1. Since for a.e. k, $f_j^i(k,z)$ is analytic in $|z| < 1$ and by assumption, $h_j^i(k,z) = f_j^i(k,z)$ for $|z| < \delta$. They must equal in $|z| < 1$, for a.e. k.

Since for $0 < r < 1$, $f_j^i(k, r\,\mathrm{e}^{\mathrm{i}\theta})$ is the Fourier transform of $\Psi_j^{i0}(w_t = (0,y), \tau = t)r^t$ and $\Psi_j^{i0}(w_t = (0,y), \tau = t)r^t$ goes to $\Psi_j^{i0}(w_t = (0,y), \tau = t)$ in $L^2(y,t)$, we have $f_j^i(k, r\,\mathrm{e}^{\mathrm{i}\theta})$ goes to $f_j^i(k, \mathrm{e}^{\mathrm{i}\theta})$ in $L^2(k,\theta)$, as $r \to 1$, which is the Fourier transform of $\Psi_j^{i0}(w_t = (0,y), \tau = t)$. On the other hand, $f_j^i(k, r\,\mathrm{e}^{\mathrm{i}\theta}) = h_j^i(k, r\,\mathrm{e}^{\mathrm{i}\theta})$ and $h_j^i(k,z)$ is continuous in $|z| \leqslant 1$; therefore, $h_j^i(k, \mathrm{e}^{\mathrm{i}\theta})$ is a version for $f_j^i(k, \mathrm{e}^{\mathrm{i}\theta})$. □

3. Proofs of theorems 1.1–1.4

Proof of theorem 1.1. Since for every k, $f_3^{3n}(k,z)$ is analytic in $|z| < 1$, for all $n = 1, 2, 3, \ldots$, corollary 1.1 holds for $|z| < 1$. Moreover, since $f_3^{31}(k,z)$ is relatively continuous in closed unit ball, $f_3^{3n}(k,z)$ is also relatively continuous in the closed unit ball and corollary 1.1 holds for $|z| \leqslant 1$.

By (1.15),

$$P_3^{3n} = P_3^{3n}(k)\big|_{k=0} \\ = \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi} f_3^{3n}(-k_1, \mathrm{e}^{\mathrm{i}\theta}) f_3^{3n}(k_1, \mathrm{e}^{-\mathrm{i}\theta})\,\mathrm{d}k_1\,\mathrm{d}\theta$$

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left(f_3^{31}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\right)^n\left(f_3^{31}(k_1,\mathrm{e}^{-\mathrm{i}\theta})\right)^n \mathrm{d}k_1\,\mathrm{d}\theta$$

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left[f_3^{31}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\bar{f}_3^{31}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\right]^n \mathrm{d}k_1\,\mathrm{d}\theta$$

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left|f_3^{31}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\right|^{2n} \mathrm{d}k_1\,\mathrm{d}\theta, \tag{3.1}$$

for all $n = 1, 2, \ldots$.

Since $P_3^{3n} \leqslant 1$, for all n, we have $0 \leqslant \left|f_3^{13}(-k,\mathrm{e}^{\mathrm{i}\theta})\right| \leqslant 1$, for a.e. $k, \theta \in [0, 2\pi]$. Therefore, P_3^{3n} decreases as n increases. The limit exists as n goes to ∞. Moreover, by the dominated convergence theorem, we have

$$\lim_{n\to\infty} P_3^{3n} = \lim_{n\to\infty}\frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left|f_3^{31}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\right|^{2n} \mathrm{d}k_1\,\mathrm{d}\theta \tag{3.2}$$

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\lim_{n\to\infty}\left|f_3^{1,3}(-k_1,\mathrm{e}^{\mathrm{i}\theta})\right|^{2n} \mathrm{d}k_1\,\mathrm{d}\theta$$

$$= \frac{1}{(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\chi_L(k,\theta)\,\mathrm{d}k_1\,\mathrm{d}\theta, \tag{3.3}$$

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

Proof of theorem 1.2. By definition,

$$E^{3n}[\mathrm{e}^{\mathrm{i}t\frac{Y_n}{n}}|\tau < \infty] = \frac{1}{p_3^{3n}}\sum_{y\in Z}\mathrm{e}^{\mathrm{i}\frac{y}{n}t}p_3^{3n}(y)$$

$$= \frac{1}{p_3^{3n}(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}f_3^{3n}(-k,\mathrm{e}^{\mathrm{i}\theta})f_3^{3n}\left(k+\frac{t}{n},\mathrm{e}^{-\mathrm{i}\theta}\right)\mathrm{d}k\,\mathrm{d}\theta$$

$$= \frac{1}{p_3^{3n}(2\pi)^2}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\left[f_3^{31}(-k,\mathrm{e}^{\mathrm{i}\theta})\right]^n\left[f_3^{31}(k,\mathrm{e}^{-\mathrm{i}\theta})+\frac{t}{n}\frac{\partial f_3^{31}(\eta_{k\theta},\mathrm{e}^{-\mathrm{i}\theta})}{\partial k}\right]^n\mathrm{d}k\,\mathrm{d}\theta, \tag{3.4}$$

by the mean-value theorem. By (A.3), the above integrand goes to

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

as n goes to ∞. By the dominated convergence theorem, we have thus proved the theorem. □

Proof of theorem 1.3. We shall use the following theorem to prove theorem 1.3. □

Theorem 3.1. *Let μ be a probability measure supported in $[0, \infty)$. Let $\rho(s) = \int_0^\infty \mathrm{e}^{-st}\,\mathrm{d}\mu(t)$ be the Laplace transform of μ. For all $n = 1, 2, \ldots$, the following statements hold.*

(a) If $\int_0^\infty t^n\,\mathrm{d}\mu(t) < \infty$, then $(-1)^n\frac{d^n\rho(s)}{\mathrm{d}s^n} = \int_0^\infty t^n\,\mathrm{e}^{-st}\,\mathrm{d}\mu(t) < \infty$.
(b) If $(-1)^n\frac{d^n\rho(s)}{\mathrm{d}s^n}\big|_0$ exists, then $\int_0^\infty t^n\,\mathrm{d}\mu(t) < \infty$.

The proof of theorem 3.1 is given in the appendix. To prove theorem 1.3, let

$$P_j^{i,n}(t) = \sum_{y\in Z}\left|\Psi_j^{in}(w_t = (0,y), \tau = t)\right|^2 = \left\|\Psi_j^{in}(w_t = (0,y), \tau = t)\right\|_{L^2(y)}^2 \tag{3.5}$$

be the probability that a two-dimensional quantum random walk in the right half-space D^c, with the initial position at $(n, 0)$ and type i, exists from D^c at time t. Let

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

be the Laplace transform. By the same argument as that in (1.15), we have

$$\begin{aligned}\rho(s) &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \frac{1}{2\pi}\int_0^{2\pi} f_j^{i,n}(-k, \mathrm{e}^{-s+\mathrm{i}\theta}) f_j^{i,n}(k, \mathrm{e}^{-\mathrm{i}\theta})\,\mathrm{d}k \\ &= \frac{1}{2\pi}\int_0^{2\pi} \mathrm{d}\theta \frac{1}{2\pi}\int_0^{2\pi} \left[f_j^{i,1}(-k, \mathrm{e}^{-s+\mathrm{i}\theta}) f_j^{i,1}(k, \mathrm{e}^{-\mathrm{i}\theta})\right]^n \mathrm{d}k. \end{aligned} \tag{3.6}$$

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

$$\begin{aligned}&\partial_s\left[f_3^{3,1}(-k, \mathrm{e}^{-s+\mathrm{i}\theta}) f_3^{3,1}(k, \mathrm{e}^{-\mathrm{i}\theta})\right]^n \\ &\qquad = n\left[f_3^{3,1}(-k, \mathrm{e}^{-s+\mathrm{i}\theta})\right]^{n-1} \partial_s f_3^{3,1}(-k, \mathrm{e}^{-s+\mathrm{i}\theta})\left[f_3^{3,1}(k, \mathrm{e}^{-\mathrm{i}\theta})\right]^n.\end{aligned}$$

By (A.2) and (A.6), $\left|f_3^{3,1}\right| \leqslant 1$ and for every k, there exists a set $D_k = [0, 2\pi]\backslash\{\theta_1(k), \theta_2(k), \ldots, \theta_m(k)\}$ such that the partial derivative $\partial_r f_3^{31}(k, r\,\mathrm{e}^{-\mathrm{i}\theta})$ exists and is continuous in $0 < r < 1, \theta \in D_k$. Moreover there exists a constant, independent of k, θ, r such that

$$\left|\partial_r f_3^{31}(k, r\,\mathrm{e}^{\mathrm{i}\theta})\right| \leqslant C\sum_{i=1}^{m} \frac{1}{\sqrt{|\theta - \theta_i|}},$$

for all $k \in [0, 2\pi]$, $\frac{1}{2} < r < 1$ and $\theta \in D_k$. Therefore, the derivative of the integrand in (3.6) 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. By theorem 3.1, $\sum_{t=1}^{\infty} t P_3^{3,n}(t) < \infty$. This implies the theorem.

Proof of theorem 1.4. To prove theorem 1.4, we use the following lemma [9, p. 37]. □

Lemma 3.1. *Let g and h be functions on interval (α, β) such that the integral $f(n) = \int_\alpha^\beta g(u)\,\mathrm{e}^{nh(u)}\,\mathrm{d}u$ exists for all sufficiently large positive n. Suppose h is a real-valued function, continuous at $u = \alpha$, continuously differentiable for $\alpha < u \leqslant \alpha + \eta$, with $\eta > 0$. Suppose further that $h' < 0$, for $\alpha < u \leqslant \alpha + \eta$, and $h(u) \leqslant h(\alpha) - \epsilon$, with $\epsilon > 0$, for $\alpha + \eta \leqslant u \leqslant \beta$. 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*

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

as $n \to \infty$.

By theorem 1.1,

$$\begin{aligned} P_3^{3n} - P_3^{3\infty} &= \frac{1}{(2\pi)^2}\int_{L^c} |f|^{2n}\,\mathrm{d}\theta\,\mathrm{d}k \\ &= \frac{1}{(2\pi)^2}\sum_{i=1}^{t-1}\sum_j \int_{\xi_i}^{\xi_{i+1}}\int_{I_j} |f|^{2n}\,\mathrm{d}k\,\mathrm{d}\theta. \end{aligned} \tag{3.7}$$

Let $I_j = (a_j, b_j)$ and $c_j = \frac{a_j+b_j}{2}$. We write $\int_{I_j} = \int_{a_j}^{c_j} + \int_{c_j}^{b_j}$. Then (3.7) is a finite sum of integrals. To prove theorem 1.4, it is then sufficient to show that each term has the desired asymptotic behaviour.

Let

$$Q = \frac{1}{(2\pi)^2} \int_{\xi_i}^{\xi_{i+1}} \int_{a_j}^{c_j} |f|^{2n} \, \mathrm{d}k \, \mathrm{d}\theta. \tag{3.8}$$

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

By (A.3), 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 (A.5), there is a sufficiently small positive constant ϵ, independent of θ such that

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

has a positive Lebesgue measure,

$$1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \leqslant C\sqrt{|k - a_j|}, \qquad C\sqrt{|k - a_j|} \leqslant \tfrac{1}{2}, \tag{3.9}$$

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

$$|f|^2 \leqslant \alpha < 1, \tag{3.10}$$

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

For the lower bound of Q, we have

$$Q \geqslant \frac{1}{(2\pi)^2} \int_{O_{ij}} \int_{a_j}^{(a_j+\epsilon)} \left|1 - C(k - a_j)^{\frac{1}{2}}\right|^n \mathrm{d}k \, \mathrm{d}\theta.$$

Applying lemma 3.1, with

$$h(k) = \ln\left[1 - C(k - a_j)^{\frac{1}{2}}\right],$$
$$g(k) = 1, \qquad \lambda = 1, \qquad \nu = \tfrac{1}{2},$$

we have

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

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

For the upper bound, let $Q_1 = \frac{1}{(2\pi)^2} \int_{\Omega_1} |f|^{2n} \, \mathrm{d}k \, \mathrm{d}\theta$ and $Q_2 = \frac{1}{(2\pi)^2} \int_{\Omega \setminus \Omega_1} |f|^{2n} \, \mathrm{d}k \, \mathrm{d}\theta$. 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 $\Omega_{13} = \Omega_1 \setminus (\Omega_{11} \cup \Omega_{12})$. By (A.6), if γ is sufficiently small, then

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_{11}, \tag{3.11}$$

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_{12}, \tag{3.12}$$

$$\left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \leqslant \alpha < 1 \qquad \text{in} \quad \Omega_{13}, \tag{3.13}$$

and

$$C\sqrt{|\theta - \xi_i|}\sqrt{|k - a_j|} \leqslant \tfrac{1}{2}.$$

We have

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

where

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

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

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

By (3.13), $Q_{13} = O(\mathrm{e}^{-cn})$, as $n \to \infty$, for some $c > 0$. For the upper bound of Q_{11}, by (3.11), for any $\delta > 0$,

$$Q_{11} \leqslant \frac{1}{(2\pi)^2} \int_{\xi_i}^{\xi_{i+1}-\eta} \int_{a_j}^{(a_j+\gamma)} \left|1 - C(\theta - \xi_i)^{\frac{1}{2}} (k - a_j)^{\frac{1}{2}+\delta}\right|^n \mathrm{d}k \, \mathrm{d}\theta.$$

Applying lemma 3.1, with

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

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

we have

$$\frac{1}{(2\pi)^2} \int_{\xi_i}^{\xi_{i+1}-\eta} \int_{a_j}^{(a_j+\gamma)} \left|1 - C(\theta - \xi_i)^{\frac{1}{2}} (k - a_j)^{\frac{1}{2}+\delta}\right|^n \mathrm{d}k \, \mathrm{d}\theta$$
$$\sim \int_{\xi_i}^{\xi_{i+1}-\eta} \left(\frac{1}{C(\theta - \xi_i)^{\frac{1}{2}} n} \right)^{\left(\frac{1}{2}+\delta\right)^{-1}} \mathrm{d}\theta \sim O(n^{-2+\epsilon}),$$

as $n \to \infty$. Here ϵ can be chosen arbitrary small if δ is chosen small enough.

Similarly, $Q_{12} \leqslant O(n^{-2+\epsilon})$, as $n \to \infty$.

For Q_2, let $\Omega_{21} = \{k_1(\xi_{i+1} - \eta) < k < c_j, \theta_1 - \gamma < \theta < \theta_1\}$, $\Omega_{22} = (\Omega \backslash \Omega_1) \backslash \Omega_{21}$. By (A.6), if γ is sufficiently small, then

$$C\sqrt{|\theta - \theta_1|} \leqslant 1 - \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \qquad \text{in} \quad \Omega_{21}, \tag{3.14}$$

$$\left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right|^2 \leqslant \alpha < 1 \qquad \text{in} \quad \Omega_{22}, \tag{3.15}$$

and

$$C\sqrt{|\theta - \theta_1|} \leqslant \tfrac{1}{2}.$$

Let

$$Q_{21} = \frac{1}{(2\pi)^2} \int_{\Omega_{21}} |f|^{2n} \, \mathrm{d}k \, \mathrm{d}\theta, \qquad Q_{22} = \frac{1}{(2\pi)^2} \int_{\Omega_{22}} |f|^{2n} \, \mathrm{d}k \, \mathrm{d}\theta.$$

Then $Q_2 = Q_{21} + Q_{22}$. By (3.15), $Q_{22} = O(\mathrm{e}^{-cn})$, as $n \to \infty$, for some $c > 0$. By a similar argument as that in the lower bound, $Q_{21} \leqslant O(n^{-2})$, as $n \to \infty$.

4. Proof of theorems 1.5

Proof of (A.6). For Grover's walk in two 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 equation (1.6) and solve. We get $g(z) = 0$ if $z = 0, -\mathrm{e}^{\mathrm{i}k}$ or $-\mathrm{e}^{-\mathrm{i}k}$. For $0 < |z| < \delta, z \neq -\mathrm{e}^{\mathrm{i}k}, -\mathrm{e}^{-\mathrm{i}k}, 0,$

$$g(z) = \frac{z^4 + z^3 \cos k + z \cos k + 1 - R(z)}{z(z + \mathrm{e}^{\mathrm{i}k})(z + \mathrm{e}^{-\mathrm{i}k})}, \tag{4.1}$$

where

$$R(z) = \sqrt{(-1 + z^2)^2[1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2 \cos^2 k]}. \tag{4.2}$$

By proposition B.1 in the appendix, a branch of $R(z)$ can be chosen such that $R(z)$ is analytic in $|z| < 1$, relatively continuous in $|z| \leqslant 1$ and $R(0) = 1$. Let $h(k, z)$ be the right-hand side of (4.1). To show (A.6), it is sufficient to show that for every k, $h(k, z)$ is analytic in $|z| < 1$ and continuous in $|z| \leqslant 1$.

Since $R(z)$ is analytic in $|z| < 1$ and relatively continuous in $|z| \leqslant 1$, the numerator of h is analytic in the unit disc and thus h is meromorphic. The denominator of $h(z)$ on the boundary of the unit disc is 0 only if $z = -\mathrm{e}^{\mathrm{i}k}$ or $z = -\mathrm{e}^{-\mathrm{i}k}$ and in either case, the numerator is also zero. We note that $z^4 + z^3 \cos k + z \cos k + 1 + R(z)$ at $z = -\mathrm{e}^{\mathrm{i}k}$ or $z = -\mathrm{e}^{-\mathrm{i}k}$ is not 0. Multiplying $z^4 + z^3 \cos k + z \cos k + 1 + R(z)$ to the numerator and the denominator of $h(z)$, the numerator becomes $z^2(z + \mathrm{e}^{\mathrm{i}k})^2(z + \mathrm{e}^{-\mathrm{i}k})^2$. This implies that the numerator is a zero of order 2 at $z = -\mathrm{e}^{\mathrm{i}k}$ or $z = -\mathrm{e}^{-\mathrm{i}k}$. This implies that $h(z) = 0$ at $z = -\mathrm{e}^{\mathrm{i}k}$ or $z = -\mathrm{e}^{-\mathrm{i}k}$. Therefore h is relatively continuous in the closed unit ball, if h is analytic inside the unit disc. Therefore, it remains to show that h is analytic in $|z| < 1$.

To this end, recall that $f_3^{11}(k, z)$ is analytic in $\{|z| < 1\}$ and, by (1.9), equals to h in $\{|z| < \delta\}$. Let z_0 be the pole of h with the 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 disc. We have thus proved that both h and g are analytic inside the unit disc and relatively continuous in the closed unit ball.

We now consider the case of Hadamard walk. For Hadamard walk in two 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 (1.6) and solve. We get $g(z) = 0$ for $z = 0, \mathrm{e}^{\mathrm{i}k}, \mathrm{e}^{-\mathrm{i}k}$. For $0 < |z| < \delta, z \neq 0, \mathrm{e}^{\mathrm{i}k}, -\mathrm{e}^{-\mathrm{i}k}$,

$$g = \frac{-z^4 + \mathrm{i}z^3 \sin k + \mathrm{i}z \sin k + 1 - R(z)}{z(-z + \mathrm{e}^{\mathrm{i}k})(z + \mathrm{e}^{-\mathrm{i}k})}, \tag{4.3}$$

where

$$R(z) = \sqrt{(-1 + z^2)(-1 + z^6 - 2\mathrm{i}z \sin k - 2\mathrm{i}z^5 \sin k + z^2 \sin^2 k - z^4 \sin^2 k)}. \tag{4.4}$$

To show (A.6) for Hadamard walk, by (1.6), it is sufficient to show that for every k, $g(k, z)$ is analytic in $|z| < 1$ and continuous in $|z| \leqslant 1$. Let $h(k, z)$ be the right-hand side of (4.3).

We shall first show that for every k, $h(k, z)$ is analytic in $|z| < 1$ and continuous in $|z| \leqslant 1$. Let

$$K = (-1 + z^2)(-1 + z^6 - 2\mathrm{i}z \sin k - 2\mathrm{i}z^5 \sin k + z^2 \sin^2 k - z^4 \sin^2 k).$$

Then $R^2(z) = K$.

Consider K on the unit circle,

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

Also,

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

This is a quadratic equation for $\sin k$. For every θ, there is only one solution for $\sin k$ (the other solution has an absolute value greater than 1).

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. By the same argument as that used for Grover's walk, we can choose a branch cut for $R(z)$ such that it is analytic in the unit disc and $R(0) = 1$. This implies that h is meromorphic inside the unit disc. By the same argument as that used for Grover's walk, h is analytic inside the unit disc and relatively continuous in the closed unit ball.

Proof of (A.2). For Hadamard walk, by solving equation (1.6), we have $f_3^{31}(k, 0) = 0$, and for $0 < |z| < \delta$,

$$f_3^{31}(k, z) = \frac{z(-1 + z^2 + z\cos k - \mathrm{i}z \sin k)}{1 - z^2 + z^4 - \mathrm{i}z(-1 + z^2)\sin k + R(z)}. \tag{4.5}$$

By the same argument as that for g in the proof of (A.6), the above expression for $f_3^{31}(k, z)$ can be extended to $|z| < 1$. Since both the 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

$$N = z(-1 + z^2 + z\cos k - \mathrm{i}z \sin k),$$
$$T = 1 - z^2 + z^4 - \mathrm{i}z(-1 + z^2)\sin k,$$
$$R^2(z) = K,$$
$$K = (-1 + z^2)(-1 + z^6 - 2\mathrm{i}z \sin k - 2\mathrm{i}z^5 \sin k + z^2 \sin^2 k - z^4 \sin^2 k).$$

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

$$T^2 - K = 0$$

if and only if

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

However,

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

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 $f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})$ is never zero.

From the proof of theorem 1.1, since $P_3^{3n} \leqslant 1$, for all n, we have $0 \leqslant \left|f_3^{13}(-k, \mathrm{e}^{\mathrm{i}\theta})\right| \leqslant 1$, for a.e. $k, \theta \in [0, 2\pi]$. For Hadamard walk, to show $L = \left\{k, \theta \in [0, 2\pi]; \left|f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})\right| = 1\right\}$ has a positive Lebesgue measure, we first show

$$|f(k, \mathrm{e}^{\mathrm{i}\theta})| = 1 \qquad \Longleftrightarrow \qquad \sin\theta(\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta) \leqslant 0. \tag{4.6}$$

By direct calculation, we have

$$\begin{aligned}
&|T^2 - K| = |N|^4,\\
&|N|^2 = 1 + 4\sin\theta(\sin\theta - \sin k),\\
&|R(z)|^2 = |4\sin\theta(\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta)|,\\
&|T|^2 = (1 - 4\sin^2\theta + 2\sin\theta \sin k)^2.
\end{aligned}$$

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.

$$\begin{aligned}
-4&\sin\theta(\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta)\\
&= |4\sin\theta(\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta)|,
\end{aligned}$$

which holds only when the left-hand side is non-negative. This implies (4.6) and $L = \{\theta, k; \sin\theta(\sin\theta \sin^2 k + 2\cos 2\theta \sin k - \sin 3\theta) \leqslant 0\}$.

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

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

see figure 1. This implies that L has a positive Lebesgue measure. The numerical value of the Lebesgue measure of $L \approx 0.556$.

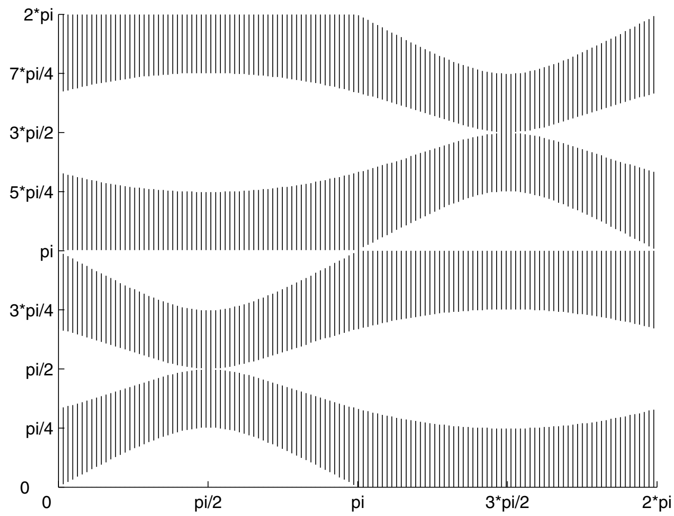

Figure 1. The shaded area is L for the Hadamard walk in two dimensions. The k-axis is the horizontal axis and the θ-axis is the vertical axis.

For Grover's walk, solving equation (1.6) we get $f_3^{31}(k, 0) = 0$ and for $0 < |z| < \delta$,

$$f_3^{31}(k, z) = \frac{z - z^3}{-1 + z^4 + z(-1 + z^2)\cos k - R(z)}, \tag{4.7}$$

where

$$R(z) = \sqrt{(-1 + z^2)^2(1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2\cos^2 k)}. \tag{4.8}$$

By the same argument as that for the case of the Hadamard walk, the above expression for $f_3^{31}(k, z)$ can be extended to $|z| < 1$.

We write

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

where

$$\begin{aligned} N &= z - z^3, \\ T &= -1 + z^4 + z(-1 + z^2)\cos k, \\ R^2(z) &= K, \\ K &= (-1 + z^2)^2[1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2\cos^2 k]. \end{aligned}$$

Simplifying, we get

$$f_3^{31}(k, z) = \frac{z}{-1 - z^2 - z\cos k - R_s(z)} = \frac{N_s}{T_s - R_s(z)},$$

with $R_s^2(z) = 1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2\cos k$. The branch cut for $R_s(z)$ is defined similarly as in $R(z)$. By direct calculation, $T_s^2 - R_s = z^2$. Hence, $T_s - R_s(z) \neq 0$ on the unit circle. Therefore for every k, $f_3^{31}(k, z)$ is relatively continuous in the closed unit ball.

A similar argument as in the case of the Hadamard walk shows

$$|f(k, \mathrm{e}^{\mathrm{i}\theta})| = 1 \quad \Longleftrightarrow \quad (2\cos\theta + \cos k)^2 - 1 \leqslant 0. \tag{4.9}$$

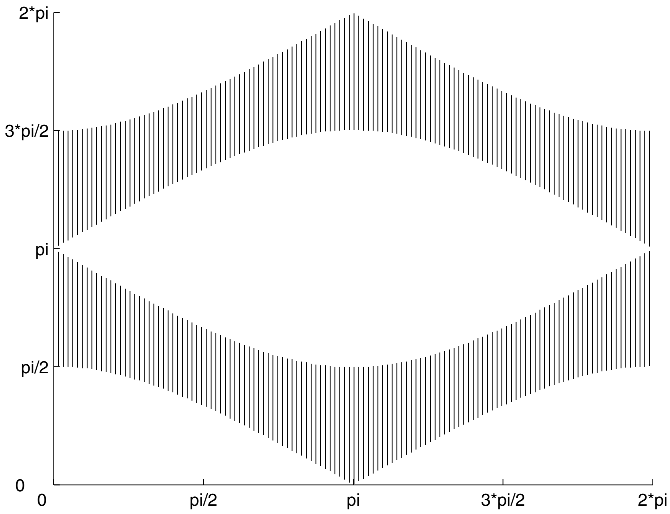

Figure 2. The shaded area is L for Grover's walk in two dimensions. The k-axis is the horizontal axis and the θ-axis is the vertical axis.

Therefore, L equals the region defined by the right-hand side of (4.9). Then the region L^c in the square $(\theta, k) \in [0, \pi] \times [0, \pi]$ is

$$\{k \in [0, \pi], \theta \in (0, \theta_1) \cup (\theta_2, \pi)\},$$

here $\theta_1 = \arccos\left(\frac{1-\cos k}{2}\right)$, $\theta_2 = \arccos\left(\frac{-1-\cos k}{2}\right)$, see figure 2. Therefore, L has a positive Lebesgue measure; we have thus proved (A.2) for Grover's walk. The numerical value for the Lebesgue measure of $L \approx 0.387\,129$.

Proof of (A.3). From the proof of proposition B.1 in the appendix, for every fixed k, all the zeros of K is on the unit circle. Fix θ, let $k_i(\theta)$, $i = 1, 2, \ldots, l$, be the solutions of $K(k, \mathrm{e}^{\mathrm{i}\theta}) = 0$. For Hadamard walk, from the proof of (A.2),

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

where N and T are smooth functions of k and θ respectively. Then

$$\frac{\partial f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})}{\partial k} = \frac{(\partial_k N)(T + R(z)) - N\left(\partial_k T + \partial_k K \frac{1}{2R(z)}\right)}{(T + R(z))^2}.$$

From the proof of (A.2), the denominator can never be zero on the unit circle. Therefore, $\frac{\partial f_3^{31}(k, \mathrm{e}^{\mathrm{i}\theta})}{\partial k}$ exists and is continuous in D_θ.

For Grover's walk, we get from the proof of (A.2),

$$f_3^{31}(k, z) = \frac{z}{-1 - z^2 - z\cos k - R_s(z)} = \frac{N_s}{T_s - R_s(z)},$$

with $R_s^2(z) = 1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2 \cos k$. The denominator can never be zero on the unit circle. By the same argument as for the Hadamard case, (A.3) holds for Grover's walk as well.

Proof of (A.4). For the Hadamard walk, from the proof of proposition B.1, for every fixed k, all the zeros of K are on the unit circle. Let $\theta_1(k), \theta_2(k), \ldots, \theta_8(k)$ be the angles of the zeros of K.

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

$$\left|\frac{\partial f}{\partial s}\right| = |\partial_z f \partial_s z| \\ = \left|\frac{\partial_z N(T + R(z)) - N(\partial_z T + \partial_z R(z))}{(T + R(z))^2}(-\mathrm{e}^{-s}\,\mathrm{e}^{\mathrm{i}\theta})\right|.$$

Note that $T + R(z)$ is non-zero on the unit circle. Also, N and T are polynomials in z. Hence, we only need to estimate $\partial_z R(z)$.

From the proof of proposition B.1, $R(z) = \prod_{j=1}^{8} h_{\theta_j}$, and properties (c)–(e) in there, we have

$$\left|h'_{\theta_j}(z)\right| = \left|R'_{\pi+\theta_j}(\mathrm{e}^{\mathrm{i}\theta_j} - z)(-1)\right| = \left|\frac{1}{2R_{\pi+\theta_j}(\mathrm{e}^{\mathrm{i}\theta_j} - z)}\right| \\ = \frac{1}{2\sqrt{|\mathrm{e}^{\mathrm{i}\theta_j} - z|}} \leqslant \frac{C}{\sqrt{|\theta_j - \theta|}},$$

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

By property (e) in the proof of proposition B.1,

$$\left|h_{\theta_j}(z)\right| = \left|R_{\pi+\theta_j}(\mathrm{e}^{\mathrm{i}\theta_j} - z)\right| \\ = \sqrt{|\mathrm{e}^{\mathrm{i}\theta_j} - z|} \leqslant C,$$

for all $|z| \leqslant 1$. By the product rule, (A.4) follows.

For Grover's walk, we use the simplified formula from the proof of (A.2),

$$f_3^{31}(k, z) = \frac{z}{-1 - z^2 - z\cos k - R_s(z)} = \frac{N_s}{T_s - R_s(z)},$$

with $R_s^2(z) = 1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2\cos k$. The denominator can never be zero on the unit circle. By the same argument as that for the Hadamard case, (A.4) holds for Grover's walk as well.

Proof of (A.5). For simplicity, we write f for f_3^{31}. We first consider the Hadamard walk. 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 $p_1(\theta) < p_2(\theta) < \cdots < p_l(\theta)$ 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 $\theta \in \left(0, \frac{\pi}{4}\right)$, $p_1(\theta) = k_1(\theta)$ and $p_2(\theta) = \pi - k_1(\theta)$. Let $\Omega = \left\{\theta \in \left(0, \frac{\pi}{4}\right), k \in (k_1, \pi/2)\right\}$. We will consider the behaviour of $|f|^2$ over Ω only, since the other regions can be treated similarly.

In Ω, we have

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

Hence,

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

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

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

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

$$1 - |f|^2 \sim O(\sqrt{K_0}). \tag{4.10}$$

Now we show the upper bound. For a fixed θ, we have

$$\partial_k K_0 = \cos k(2\sin\theta\sin k + 2\cos 2\theta)\sin\theta. \tag{4.11}$$

Since the right side of (4.11) is less than a positive constant for all (θ, k) in Ω, by the mean-value theorem, we have

$$K_0(\theta, k) \leqslant C_1(k - k_1), \tag{4.12}$$

for all (θ, k) in Ω. By (4.10), we then have

$$1 - |f|^2 \leqslant C_1\sqrt{k - k_1}, \tag{4.13}$$

for all (θ, k) in Ω.

For Grover's walk, for convenience we will prove (A.5) by interchanging the role of k and θ, which is essentially the same. Also by symmetry, we only need to consider $0 \leqslant \theta \leqslant \pi$ and $0 \leqslant k \leqslant \pi$. Let $\xi_1 = 0$ and $\xi_2 = \pi$. For fixed $0 < k < \pi$, let $p_1(k) < p_2(k) < \cdots < p_l(k)$ be the endpoints of the intervals in L^c. For $k \in (0, \pi)$, $p_1(k) = 0$, $p_2(k) = \theta_1(k)$, $p_3(k) = \theta_2(k)$ and $p_4(k) = \pi$, where $\theta_1 = \arccos\left(\frac{1-\cos k}{2}\right)$, $\theta_2 = \arccos\left(\frac{-1-\cos k}{2}\right)$. We shall consider the behaviour of $|f|^2$ on $\Omega = \{(\theta, k) | k \in (0, \pi), \theta \in (0, \theta_1(k))\}$ only since the rest of the region can be treated similarly.

In Ω, we have

$$\begin{aligned}|f|^2 &= [-2\cos\theta - \cos k + \sqrt{(2\cos\theta + \cos k)^2 - 1}]^2\\ &= [-M(\theta, k) + \sqrt{M^2(\theta, k) - 1}]^2,\end{aligned}$$

where $M(\theta, k) = 2\cos\theta + \cos k$. Note that on $\theta = \theta_1$, $M(\theta, k) = 1$; therefore,

$$1 - |f|^2 = 1 - (-M + \sqrt{M^2 - 1})^2 = 2(1 - M^2) + 2M\sqrt{M^2 - 1} \sim O(\sqrt{M^2 - 1}), \tag{4.14}$$

as $M \to 1$. Since

$$\partial_\theta(M^2 - 1) = -2M\sin\theta,$$

and $|M| \leqslant 3$ in Ω, we have

$$M^2 - 1 \leqslant C(\theta_1 - \theta),$$

in Ω, by the mean-value theorem. This implies (A.5) for Grover's walk.

Proof of (A.6). We shall consider $\Omega = \left\{\theta \in \left(0, \frac{\pi}{4}\right), k \in (k_1, \pi/2)\right\}$ only since the rest can be treated similarly. Let $\Omega_1 = \left\{\theta \in \left(0, \frac{\pi}{4} - \eta\right), k \in (k_1, \pi/2)\right\}$ and $\Omega_2 = \left\{\theta \in \left(\frac{\pi}{4} - 2\eta, \frac{\pi}{4}\right), k \in (k_1, \pi/2)\right\}$. For fixed k, let θ_1 be such that $k_1(\theta_1) = k$. We shall show

$$1 - |f|^2 \geqslant C_2\sqrt{\theta - \theta_1}, \tag{4.15}$$

for all (θ, k) in Ω_2, and

$$1 - |f|^2 \geqslant C_2\sqrt{\theta}\sqrt{k - k_1}, \tag{4.16}$$

for all (θ, k) in Ω_1.

By

$$\partial_\theta K_0 = \cos\theta(\sin\theta + 2\cos 2\theta - \sin 3\theta) + \sin\theta(\cos\theta - 4\sin 2\theta - 3\cos 3\theta), \tag{4.17}$$

we have

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

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

$$-\partial_\theta K_0 \geqslant C_2 > 0, \tag{4.18}$$

for all (θ, k) in Ω_2. By the mean-value theorem,

$$K_0 \geqslant C_2(\theta - \theta_1), \tag{4.19}$$

for all (θ, k) in Ω_2. By (4.10), we have thus proved (4.15).

To prove (4.16), we take the partial derivative in k. By (4.11),

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

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 $0 \leqslant \theta \leqslant \pi/4 - \eta$, and $C_2\theta < \sin\theta$, for some $C_2 > 0$; there exists a sufficiently small γ such that

$$\partial_k K_0 \geqslant C_2\theta, \tag{4.20}$$

for all $0 < \theta < \pi/4 - \eta$, $k_1 < k < k_1 + \gamma$. By the mean-value theorem and (4.10), we have

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

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 $0 < \theta < \pi/4 - \eta$, $k_1 + \gamma \leqslant k \leqslant \pi/2$, we have proved (4.16) by choosing a sufficiently small $C_2 > 0$.

Now we prove (A.6) for Grover's walk. We shall consider the behaviour of $|f|^2$ on $\Omega = \{(\theta, k) | k \in (0, \pi), \theta \in (0, \theta_1(k))\}$ only since the rest of the region can be treated similarly. By (4.14), we have

$$1 - |f|^2 \sim O(\sqrt{M^2 - 1}), \qquad \text{as} \quad M \to 1.$$

Here $M^2 - 1 = (2\cos\theta + \cos k)^2 - 1$, and

$$\partial_\theta(M^2 - 1) = -2M\sin\theta. \tag{4.21}$$

Let $\Omega_1 = \{(\theta, k), 0 < k < \pi - \eta, 0 < \theta < \theta_1\}$ and $\Omega_1' = \{(\theta, k), 0 < k < \pi - \eta, \theta_1 - \gamma < \theta < \theta_1\}$. Note that M is strictly positive bounded away from zero in Ω, and $\sin\theta$ is bounded away from zero in Ω_1'; therefore, by the mean-value theorem, there exist positive constants η and γ such that

$$1 - |f|^2 \geqslant C\sqrt{\theta_1 - \theta} \qquad \text{in} \quad \Omega_1'. \tag{4.22}$$

Since $1 - |f|^2$ is strictly positive and relatively continuous in the closure of $\Omega_1 \backslash \Omega_1'$, we have

$$1 - |f|^2 \geqslant C\sqrt{\theta_1 - \theta} \qquad \text{in} \quad \Omega_1, \tag{4.23}$$

if C is sufficiently small.

Let $\Omega_2 = \{(\theta, k), \pi - 2\eta < k < \pi, 0 < \theta < \theta_1\}$ and $\Omega_2' = \{(\theta, k), 0 < \theta < \theta_0, k_1 - \gamma < k < k_1\}$, where $0 < \theta_0 < \pi/2$ such that $(\theta_0, \pi - 2\eta)$ is on the boundary of L.

We have

$$\partial_k(M^2 - 1) = -2\sin k Z(\theta, k),$$

where $Z(\theta,k)=\cos k+2\cos\theta$. Note that $Z(0,\pi)=1$ and is continuous. This implies that there exist positive constants γ and η such that

$$Z(\theta,k)>C>0 \qquad \text{in} \quad \Omega_2'.$$

If $\pi/2<k<k_1<\pi$, then

$$\sin k \geqslant \sin k_1=\sqrt{1-(1-2\cos\theta)^2}$$
$$=\sqrt{4\cos\theta(1-\cos\theta)}=\sqrt{8\cos\theta}\sin\frac{\theta}{2}\geqslant C_2>0 \qquad \text{in} \quad \Omega_2'.$$

This implies that

$$1-|f|^2\geqslant C\sqrt{\theta}\sqrt{k_1-k} \qquad \text{in} \quad \Omega_2'.$$

Since $1-|f|^2$ is continuous strictly positive in the closure of $\Omega_2\backslash\Omega_2'$, we have thus proved

$$1-|f|^2\geqslant C\sqrt{\theta}\sqrt{k_1-k} \qquad \text{in} \quad \Omega_2,$$

for a sufficiently small constant C. This proves (A.6) for Grover's walk.

5. One-dimensional walks, proof of theorem 1.6

For the one-dimensional Hadamard walk, the equation analogous to proposition 1.2 is

$$F=z\widetilde{A}\begin{pmatrix}0 & 0\\ 0 & ([1-F]^{-1}zA)_{12}\end{pmatrix}. \tag{5.1}$$

Solving the equation, we get

$$f_2^{1,1}(0)=0, \qquad f_2^{1,1}(z)=g(z)=\frac{1+z^2-\sqrt{1+z^4}}{\sqrt{2}z}. \tag{5.2}$$

Note that the solution is analytic in $|z|<1$ and relatively continuous in the closed unit ball. Therefore, it is a version of $f_2^{1,1}(z)$ on the closed unit ball.

Remark 5.1. Equation (5.2) has been obtained in [3].

Proof of theorem 1.6. Let

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

By the Fourier inverse transform, we have

$$p(t)=\left|\Psi_2^{11}(w_t=0,\tau=t)\right|^2=|A(t)|^2.$$

We write $A(t)=B(t)-C(t)$, where

$$B(t)=\frac{1}{2\pi}\int_0^{2\pi}\sqrt{2}\cos\theta\,\mathrm{e}^{\mathrm{i}t\theta}\,\mathrm{d}\theta,$$

$$C(t)=\frac{\sqrt{2}}{4\pi}\int_0^{2\pi}\sqrt{1+\mathrm{e}^{-4\mathrm{i}\theta}}\,\mathrm{e}^{\mathrm{i}(t+1)\theta}\,\mathrm{d}\theta.$$

We have

$$B(t)=\frac{\sqrt{2}}{\pi}\int_0^{\pi}\cos(\theta)\cos(t\theta)\,\mathrm{d}\theta=0,$$

if $t\geqslant 2$, and $\sqrt{2}/2$ if $t=1$.

To estimate $C(t)$, we shall use the following lemma [9, p. 49, (11)]. □

Lemma 5.1. *If $\phi(\theta)$ is N times continuously differentiable for $\alpha \leqslant \theta \leqslant \beta$, and $0 < \lambda \leqslant 1, 0 < \mu \leqslant 1$, then*
$\int_\alpha^\beta \mathrm{e}^{\mathrm{i}t\theta}(\theta-\alpha)^{\lambda-1}(\beta-\theta)^{\mu-1}\phi(\theta)\,\mathrm{d}\theta = B_N(t) - A_N(t) + O(t^{-N})$ *as* $t \to \infty$, *where*

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

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

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

We note that for $0 < \theta < \pi$, $\sqrt{-\mathrm{e}^{2\mathrm{i}\theta}} = -\mathrm{i}\,\mathrm{e}^{\mathrm{i}\theta}$ and $\sqrt{-\mathrm{e}^{-2\mathrm{i}\theta}} = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\theta}$; for $0 < \theta < \pi/2$, $\sqrt{\mathrm{e}^{2\mathrm{i}\theta}} = \mathrm{e}^{\mathrm{i}\theta}$ and $\sqrt{\mathrm{e}^{-2\mathrm{i}\theta}} = \mathrm{e}^{-\mathrm{i}\theta}$; for $\pi/2 < \theta < \pi$, we have $\sqrt{\mathrm{e}^{2\mathrm{i}\theta}} = -\mathrm{e}^{\mathrm{i}\theta}$ and $\sqrt{\mathrm{e}^{-2\mathrm{i}\theta}} = -\mathrm{e}^{-\mathrm{i}\theta}$.

Therefore, we have

$$\begin{aligned}
\frac{4\pi}{\sqrt{2}}C(t) &= \int_0^{2\pi} \sqrt{1+\mathrm{e}^{-4\mathrm{i}\theta}}\,\mathrm{e}^{\mathrm{i}(t+1)\theta}\,\mathrm{d}\theta \\
&= \int_0^{\pi} \sqrt{1+\mathrm{e}^{-4\mathrm{i}\theta}}\,\mathrm{e}^{\mathrm{i}(t+1)\theta}\,\mathrm{d}\theta + \int_0^{\pi} \sqrt{1+\mathrm{e}^{4\mathrm{i}\theta}}\,\mathrm{e}^{-\mathrm{i}(t+1)\theta}\,\mathrm{d}\theta \\
&= \int_0^{\pi/4} \sqrt{2\cos(2\theta)}\,\mathrm{e}^{\mathrm{i}t\theta}\,\mathrm{d}\theta + \int_{\pi/4}^{\pi/2} \mathrm{i}\sqrt{-2\cos(2\theta)}\,\mathrm{e}^{\mathrm{i}t\theta}\,\mathrm{d}\theta \\
&\quad + \int_{\pi/2}^{3\pi/4} \mathrm{i}\sqrt{-2\cos(2\theta)}\,\mathrm{e}^{\mathrm{i}t\theta}\,\mathrm{d}\theta + \int_{3\pi/4}^{\pi} -\sqrt{2\cos(2\theta)}\,\mathrm{e}^{\mathrm{i}t\theta}\,\mathrm{d}\theta \\
&\quad + \int_0^{\pi/4} \sqrt{2\cos(2\theta)}\,\mathrm{e}^{-\mathrm{i}t\theta}\,\mathrm{d}\theta + \int_{\pi/4}^{\pi/2} -\mathrm{i}\sqrt{-2\cos(2\theta)}\,\mathrm{e}^{-\mathrm{i}t\theta}\,\mathrm{d}\theta \\
&\quad + \int_{\pi/2}^{3\pi/4} -\mathrm{i}\sqrt{-2\cos(2\theta)}\,\mathrm{e}^{-\mathrm{i}t\theta}\,\mathrm{d}\theta + \int_{3\pi/4}^{\pi} -\sqrt{2\cos(2\theta)}\,\mathrm{e}^{-\mathrm{i}t\theta}\,\mathrm{d}\theta \\
&= \int_0^{\pi/4} 2\cos(t\theta)\sqrt{2\cos(2\theta)}\,\mathrm{d}\theta + \int_{\pi/4}^{\pi/2} -2\sin(t\theta)\sqrt{-2\cos(2\theta)}\,\mathrm{d}\theta \\
&\quad + \int_{\pi/2}^{3\pi/4} -2\sin(t\theta)\sqrt{-2\cos(2\theta)}\,\mathrm{d}\theta + \int_{3\pi/4}^{\pi} -2\cos(t\theta)\sqrt{2\cos(2\theta)}\,\mathrm{d}\theta \\
&= 8\int_0^{\pi/4} \cos(t\theta)\sqrt{2\cos(2\theta)}\,\mathrm{d}\theta,
\end{aligned}$$

for $t = 4k+3$, k is a non-negative integer; it is equal to 0, otherwise.

Note that

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

Applying lemma 5.1 to the above integral, with $\lambda = 1, \mu = \frac{1}{2}$, and $\phi(\theta) = \left(\frac{\pi}{4} - \theta\right)^{\frac{1}{2}}\sqrt{2\cos(2\theta)}$, we get

$$\int_0^{\pi/4} \cos(t\theta)\sqrt{2\cos(2\theta)}\,\mathrm{d}\theta = -2\Gamma(3/2)\,\mathrm{e}^{\mathrm{i}\pi(t+1)/4}t^{-3/2} + O(t^{-2}),$$

as $t \to \infty$. Therefore, we have

$$A(t) = \frac{2\sqrt{2}}{\sqrt{\pi}} t^{-\frac{3}{2}} + O(t^{-2}),$$

as $t \to \infty$, for $t = 4k + 3$, where k is an integer; $A(t) = \frac{\sqrt{2}}{2}$, for $t = 1$ and 0, otherwise. This implies the theorem.

Since theorem 1.7 is well known, we skip the proof.

6. Conclusion

The hitting probabilities of a classical random walk have many applications such as for solving elliptic partial differential equations, see e.g. [7], mathematical finance, e.g. [30], and in the area of computing. In computing, examples include solving hard problems such as estimating the volume of a convex set [8] and approximation of the permanent [13]. For solving partial differential equations, since the probability distribution of a quantum random walk behaves like a wave, the hitting probabilities of a quantum random walk should be useful in solving hyperbolic partial differential equations. In the area of computing, several results have shown that a quantum algorithm exhibits speedup over the classical algorithm, see e.g., [13, 29]. Therefore, we expect that a quantum random walk may be useful in providing algorithms that have speedups over those done by classical random walks. In fact, some results have shown that a quantum random walk can do the same job and sometimes faster than the classical ones. For examples, Shenvi *et al* [28] show that a quantum random walk can be used to do the same task as Grover's search algorithm [13] and Childs *et al* [5] give a quantum algorithm based on quantum random walks for travelling through a graph with an exponential speedup over the classical one.

A faster convergence to the hitting distribution means that a more efficient algorithm is possible for the task. In this paper, we mainly deal with the hitting probabilities of the hyperplane by quantum random walks on Z^d. For the two-dimensional case, we obtained the scaling limit of the hitting probabilities as the lattice spacing tends to zero. We showed that the critical exponent for the scaling limit is 1, i.e. the natural magnitude of the hitting position is of the order $O(1)$ if the lattice spacing is set to be $1/n$. We also showed that the rate of convergence of the hitting probability has lower bound n^{-2} and upper bound $n^{-2+\epsilon}$ for any $\epsilon > 0$. For a quantum random walk with a fixed starting point, we showed that the probability of hitting times at the hyperplane decays faster than that of the classical random walk. In both one and two dimensions, given that if it hits, the conditional expectation of hitting times is finite, in contrast with being infinite for the classical case. In the one-dimensional case, we also obtained an exact order of the probability distribution of the hitting time at 0. Along the same lines, it would be interesting to investigate the properties of the hitting distributions and the rate of convergence for other types of domains for quantum random walks on general graphs.

Another interesting question is about the decoherence of quantum random walks. Decoherence of a quantum random walk results from the interaction between a quantum random walk and its environment. A decoherence random walk should behave like its classical counterpart. For example, if a classical random walk is ergodic then the corresponding quantum random walk with a small effect of decoherence should be also ergodic. If a classical random walk on a regular lattice is diffusive, then the corresponding quantum random walk with even a very small decoherence should be also diffusive. Therefore we expect that a decoherence quantum random walk will provide a useful tool for simulating the limiting distribution for the classical analogue, but with faster convergence to the limiting distribution.

In [17], a computer simulation shows that the behaviour of a decoherent quantum random walk in Z^1 is diffusive, i.e. the variance at time t is of the order $O(t)$. An interesting problem is to prove that the limiting distribution of the decoherence random walk is normal as $t \to \infty$ and estimate the rate of convergence. The idea of our path integral formula is applicable to the decoherence case as well. It seems that this type of path integral formula will be an analytical tool and provide an insight to the problem.

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Appendix A

Proof of theorem 3.1. We shall prove by induction. Let $n = 1$.

(a) By definition,

$$\frac{\rho(s+h)-\rho(s)}{h} = \int_0^\infty \frac{1}{h}[\mathrm{e}^{-(s+h)t} - \mathrm{e}^{-st}]\,\mathrm{d}\mu(t).$$

Since $\frac{1}{h}[\mathrm{e}^{-(s+h)t} - \mathrm{e}^{-st}] \to -t\,\mathrm{e}^{st}$ as $h \to 0$ and $\left|\frac{1}{h}[\mathrm{e}^{-(s+h)t} - \mathrm{e}^{-st}]\right| \leqslant t$ which is integrable with respect to μ, (a) follows by the dominated convergence theorem.

(b) We have

$$\int_0^\infty t\,\mathrm{d}\mu(t) = \int_0^\infty \liminf_{s\downarrow 0} \frac{1}{s}[1-\mathrm{e}^{-st}]\,\mathrm{d}\mu(t).$$

By Fatou's lemma, the above

$$\leqslant \liminf_{s\downarrow 0} \int_0^\infty \frac{1}{s}[1-\mathrm{e}^{-st}]\,\mathrm{d}\mu(t) = \liminf_{s\downarrow 0}(-1)\frac{\rho(s)-\rho(0)}{s} = (-1)\frac{\mathrm{d}\rho(s)}{\mathrm{d}s}|_{s=0} < \infty.$$

Now assume that both statements (a) and (b) hold for $n-1$. Assume that $\int_0^\infty t^n\,\mathrm{d}\mu(t) < \infty$. By (a) for $n-1$,

$$\frac{\rho^{(n-1)}(s+h)-\rho^{(n-1)}(s)}{h} = \int_0^\infty t^{n-1}\frac{1}{h}[\mathrm{e}^{-(s+h)t} - \mathrm{e}^{-st}]\,\mathrm{d}\mu(t).$$

The absolute value of the above integrand is bounded by t^n which is integrable, (a) follows by the dominated convergence theorem with $h \to 0$.

(b) Assume that $(-1)^n \frac{d^n\rho(s)}{\mathrm{d}s^n}\Big|_0$ exists. Then $(-1)^{n-1}\frac{d^{n-1}\rho(s)}{\mathrm{d}s^{n-1}}\Big|_0$ exists. By (b) with $n-1$, $\int_0^\infty t^{n-1}\,\mathrm{d}\mu(t) < \infty$. By (a) with $n-1$,

$$(-1)^{n-1}\frac{d^{n-1}\rho(s)}{\mathrm{d}s^{n-1}} = \int_0^\infty t^{n-1}\,\mathrm{e}^{-st}\,\mathrm{d}\mu(t)$$

for all s. If $\int_0^\infty t^{n-1}\,\mathrm{d}\mu(t) = 0$, then μ is supported at 0 and (b) holds for all n. Suppose $\int_0^\infty t^{n-1}\,\mathrm{d}\mu(t) > 0$. Let ν be the probability measure defined by

$$\nu(t) = \frac{t^{n-1}\,\mathrm{d}\mu(t)}{\int_0^\infty t^{n-1}\,\mathrm{d}\mu(t)}$$

and

$$\phi(s) = \frac{\int_0^\infty t^{n-1}\,\mathrm{e}^{-st}\,\mathrm{d}\mu(t)}{\int_0^\infty t^{n-1}\,\mathrm{d}\mu(t)}$$

be the Laplace transform of ν. Since $(-1)^n \frac{d^n\rho(s)}{\mathrm{d}s^n}\big|_0$ exists, ϕ is differentiable at 0. By (b) with $n = 1$, $\int_0^\infty t\,\mathrm{d}\nu(t) < \infty$. Therefore, $\int_0^\infty t^n\,\mathrm{d}\mu(t) < \infty$. End of proof of theorem 3.1. □

Appendix B

Proposition B.1. *Let $R(z)$ be given by (4.2). A branch of $R(z)$ can be chosen such that $R(z)$ is analytic in $|z| < 1$, relatively continuous in $|z| \leqslant 1$ and $R(0) = 1$.*

Proof. Let $R_\phi(z) = \sqrt{r}\,\mathrm{e}^{\frac{\mathrm{i}\theta}{2}}$ for $z = r\,\mathrm{e}^{\mathrm{i}\theta}, \phi - 2\pi < \theta \leqslant \phi$. Then we have the following properties: (a) $x = \pm R_\phi(c)$ is the solution to $x^2 = c$, (b) $R_\phi(z)$ is analytic in $\{z|\arg z \neq \phi + 2k\pi\}\backslash\{0\}$, (c) $R'_\phi(z) = \frac{1}{2R_\phi(z)}$, (d) $R^2_\phi(z) = z$, (e) $|R_\phi(z)| = \sqrt{|z|}$.

Note that $R^2(z) = K$, where

$$K = (-1 + z^2)^2[1 + z^2 + z^4 + 2(z + z^3)\cos k + z^2\cos^2 k].$$

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

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

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 $\{\mathrm{e}^{\mathrm{i}\theta_j}\}, \theta_j = \theta_j(k)$, such that $\sum_{j=1}^8 \theta_j = 0$. For each j, set $h_{\theta_j}(z) = R_{\pi+\theta_j}(\mathrm{e}^{\mathrm{i}\theta_j} - z)$. We then have the following properties: (1) $h_{\theta_j}(z)$ is analytic except $\{z; |z| \geqslant 1, \arg z = \theta_j\}$; (2) $h_{\theta_j}(z)$ is analytic in $\{z; |z| < 1\}$ and relatively continuous in $|z| \leqslant 1$; (3) $h_{\theta_j}(0) = \mathrm{e}^{\frac{\mathrm{i}\theta_j}{2}}$. If we define $R(z) = \prod_{j=1}^8 h_{\theta_j}$, then $R^2(z) = K$ and $R(0) = 1$. Therefore, $R(z)$ is the desired branch. □

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