

Continuous-Time Quantum Walk on Integer Lattices and Homogeneous Trees

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Received: 15 January 2010 / Accepted: 10 May 2010 / Published online: 20 May 2010
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Abstract This paper is concerned with the continuous-time quantum walk on \mathbb{Z} , \mathbb{Z}^d , and infinite homogeneous trees. By using the generating function method, we compute the limit of the average probability distribution for the general isotropic walk on \mathbb{Z} , and for nearest-neighbor walks on \mathbb{Z}^d and infinite homogeneous trees. In addition, we compute the asymptotic approximation for the probability of the return to zero at time t in all these cases.

Keywords Quantum walk · Tree · Limit theorem

1 Introduction

The concept of quantum walk has its origin in the field of quantum computation where the notion of classical random walk has been adapted to the quantum-mechanical setting in an attempt to improve the performance of random walk algorithms. Since its origination in the middle of 90s, this new concept has drawn a lot of attention in physical and mathematical literature.

The early papers that formulated the main ideas of quantum walk are [3] and [14]. From the numerous later papers, we would like to mention [6] where the continuous-time quantum walk was defined and [2] which defined and studied the discrete-time quantum walk on finite graphs. An introductory review of quantum walks can be found in [9]. For recent developments the reader can also consult [12].

In general, a quantum walk is described by a triple (G, ψ, U_t) , where G is a graph, ψ is a unit-length complex vector function on this graph, i.e., $\psi \in \mathcal{H} = L^2(G) \otimes \mathbb{C}^N$, $\|\psi\| = 1$, and U_t is a family of unitary operators on \mathcal{H} .

The interpretation is that the state of a particle at time t is completely described by function $U_t\psi$. Upon measurement at time t , the particle is found at vertex v in state $s \in \{1, 2, \dots, N\}$ with probability $p(v, s, t) = |(U_t\psi)(v, s)|^2$. (By probability we mean a collection of non-negative numbers $p(v, s, t)$ that sum to 1, $\sum_{v \in V} \sum_{s=1}^N p(v, s, t) = 1$.)

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There are two types of quantum walk on graph G . The first type is the discrete-time walk. Time is discrete, $t \in \mathbb{Z}$, and a step of the quantum walk is given by a unitary transformation U , so that $\psi_{t+1} = U\psi_t$. This one-step transformation U has some special properties, one of which is locality: $U_{iv,ju} = 0$ if the graph-theoretical distance between vertices v and u is sufficiently large. The discrete-time quantum walks on \mathbb{Z} and \mathbb{Z}^d have been studied in [10] and [8] who found that their asymptotic behavior is significantly different from the behavior of classical random walks.

In this paper we are going to investigate continuous-time quantum walks [6] on infinite graphs. We assume that function ψ depends only on the position of the particle and time (hence $N = 1$), that $t \in \mathbb{R}$, and that the evolution operators U_t are given by the following expression:

$$U_t = \exp(-iXt),$$

where X is a self-adjoint operator (“Hamiltonian”) on $L^2(G)$ that respects the structure of the graph. One example of such an operator is the discrete Laplacian of the graph. We also assume that the initial function ψ is concentrated on one of the vertices, the origin of the walk. As usual, the probability to find a particle at vertex v if the system is measured at time t is given by $|\psi(v, t)|^2$.

The continuous-time walk is not local and the relation between continuous-time and discrete-time walks is not yet clear [4]. However, the continuous-time has an advantage over the discrete-time model in being more tractable analytically.

For our study, we choose the simplest infinite graphs: the integer lattices \mathbb{Z} and \mathbb{Z}^d , and the homogeneous infinite tree \mathbb{T}_m , in which every vertex has valency m . The continuous-time walk on \mathbb{Z} has been previously investigated by several researchers. In particular, by using the Fourier inversion method, Gottlieb in [7] derived a formula for the limit probability distribution for a very general class of quantum walks on \mathbb{Z} . In our paper, an equivalent formula for the limit is obtained by using the generating series method instead of the Fourier inversion. The advantage of this method is that it is easier to generalize it to the case of homogeneous trees which is not considered in [7]. In addition, this method allows us to show that the probability distribution converges to zero faster than any polynomial in time in the regions sufficiently far away from the origin. This provides a simple large deviation estimate for quantum walks on \mathbb{Z} .

Let us start with graph $G = \mathbb{Z}$, let the initial function $\psi_l(0) = \delta_0$, where δ_0 is the delta-function concentrated on 0, and let $U_t = \exp(iXt)$, where X is an Hermitian operator on $L^2(\mathbb{Z})$. We are interested in computing

$$\psi_l(t) = \langle \delta_l | U_t \delta_0 \rangle.$$

We say that the quantum walk has *finite support* if there exists a constant L , such that $X_{ij} = 0$ if $|i - j| > L$. We call the walk *isotropic* if $X_{ij} = a_{i-j}$ and $a_{-l} = \overline{a_l}$, where a_l are certain constants. If $X_{ij} = \delta_{|i-j|-1}$, we say that the quantum walk is *nearest-neighbor*.

For a general isotropic quantum walk on \mathbb{Z} , define the *generating function* of the walk by the formula $P(\theta) = \sum_{-L}^L a_l e^{il\theta}$. For example, for the nearest-neighbor random walk, $P(\theta) = 2 \cos \theta$.

Theorem 1.1 *Let $P(\theta)$ be the generating function of an isotropic quantum walk with finite support on \mathbb{Z} . Assume that $\psi_l(0) = \delta_0$. Let $\alpha = l/t$ and suppose that equation $P'(\theta) = -\alpha$ has $K > 0$ real solutions $\theta_k(\alpha)$ in the interval $[0, 2\pi)$. Then, the transition amplitude from 0*

to l is given by the formula

$$\psi_l(t) = -\frac{1}{\sqrt{2\pi t}} \sum_{k=1}^K \frac{1}{\sqrt{|P''(\theta_k)|}} e^{it(P(\theta_k) + \alpha\theta_k) \pm \pi i/4} + O\left(\frac{1}{t}\right), \tag{1}$$

where the sign before $\pi i/4$ equals the sign of $P''(\theta_k)$. If equation $P'(\theta) = -\alpha$ has no real solutions, then

$$|\psi_l(t)| \leq c_n t^{-n}$$

for all n and appropriately chosen c_n .

We will prove this theorem in Sect. 2.

Next, define the rescaled probability distribution as $p(\alpha, t) = t|\psi_{[\alpha t]}(t)|^2$, and define the average rescaled probability as

$$\bar{p}(\alpha, T) = \frac{1}{\sqrt{T}} \int_T^{T+\sqrt{T}} p(\alpha, t) dt. \tag{2}$$

Corollary 1.2 *Suppose that equation $P'(\theta) = -\alpha$ has $K > 0$ real solutions $\theta_k(\alpha)$ in the interval $[0, 2\pi)$, and that numbers*

$$\omega_k := P(\theta_k) + \alpha\theta_k$$

are all different. Then

$$\lim_{T \rightarrow \infty} \bar{p}(\alpha, T) = \frac{1}{2\pi} \sum_{k=1}^K \frac{1}{|P''(\theta_k)|}. \tag{3}$$

If equation $P'(\theta) = -\alpha$ has no real solutions, then

$$\lim_{T \rightarrow \infty} \bar{p}(\alpha, T) = 0.$$

In the case, when some of ω_k coincide, (3) needs a small adjustment which takes into account the positive interference of the exponents with the same frequency.

Proof of Corollary 1.2 From Theorem 1.1, it follows that

$$\begin{aligned} p(\alpha, t) &= \frac{1}{2\pi} \sum_{k=1}^K \frac{1}{|P''(\theta_k)|} \\ &+ \frac{1}{2\pi} \sum_{k \neq l} \frac{\exp[it(\omega_k - \omega_l) + [\text{sgn}(P''(\theta_k)) - \text{sgn}(P''(\theta_l))]\pi i/4]}{\sqrt{|P''(\theta_k)||P''(\theta_l)|}} \\ &+ O\left(\frac{1}{t}\right). \end{aligned}$$

After averaging over t , we get

$$\bar{p}(\alpha, T) = \frac{1}{2\pi} \sum_{k=1}^K \frac{1}{|P''(\theta_k)|} + O\left(\frac{1}{\sqrt{T}}\right).$$

□

In particular, we obtain the following formula for the probability of return to zero.

Corollary 1.3 *Let equation $P'(\theta) = 0$ have $K > 0$ real solutions θ_k in the interval $[0, 2\pi)$ and assume that $P(\theta_k)$ are all different. Then the average probability of the return to zero is*

$$\overline{p_0}(t) = \frac{1}{2\pi t} \sum_{k=1}^K \frac{1}{|P''(\theta_k)|} + O\left(\frac{1}{t^{3/2}}\right).$$

A somewhat different expression for the limit of the average rescaled probability distribution was obtained in [7]. Namely, by using the Fourier inversion methods Gottlieb obtained the following formula for the limit:

$$p_\psi(X) = \frac{1}{2\pi} \int_{\{\theta: -P'(\theta) \in X\}} |(\mathcal{F}^* \psi)(\theta)|^2 d\theta.$$

Here, $p_\psi(X)$ denotes the limit of the probability to find the particle in the set $\{l; l/t \in\}$ at time t , provided that the initial wave function is ψ . The function $(\mathcal{F}^* \psi)(\theta)$ is defined as $\sum_{n \in \mathbb{Z}} \psi_n e^{in\theta}$. In our case, the random walk is started from the origin and therefore $(\mathcal{F}^* \psi)(\theta) = 1$. Then, by using Gottlieb’s formula, it is easy to compute

$$\lim_{d\alpha} \frac{p_\psi([\alpha, \alpha + d\alpha])}{d\alpha} = \frac{1}{2\pi} \sum_{\{\theta: -P'(\theta) = \alpha\}} \frac{1}{|P''(\theta_k)|},$$

which is (3). We obtain (3) by the method of generating functions which we will also use for quantum walks on trees.

For a particular example, consider the nearest-neighbor quantum walk on \mathbb{Z} . That is, assume that $X_{ij} = \delta_{|i-j|-1}$. Then, $P'(\theta) = -2 \sin \theta$ and there are two solutions $\theta_k(\alpha)$ for $\alpha < 2$: $\theta_1 = \arcsin(\alpha/2)$ and $\theta_2 = \pi - \theta_1$. Hence, we can compute $|P''(\theta_k)| = \sqrt{4 - \alpha^2}$, and the average rescaled distribution has the following limit:

$$\overline{p}(\alpha, T) \xrightarrow{T \rightarrow \infty} \frac{1}{\pi} \frac{1}{\sqrt{4 - \alpha^2}}. \tag{4}$$

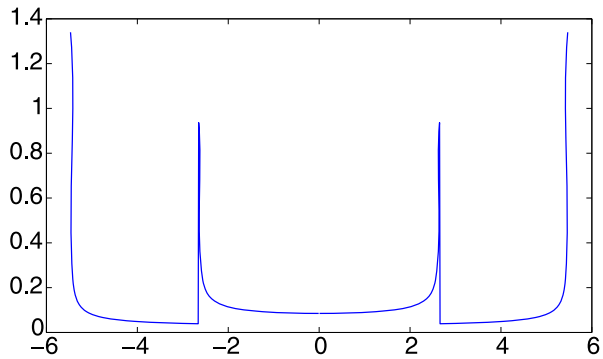
In other words, the average rescaled distribution converges to the arcsine law. (This result is the first limit theorem for continuous-time quantum walks, which was obtained in [11] by using the asymptotics of Bessel functions.)

Consider another example with $P(\theta) = e^{-i2\theta} + e^{-i\theta} + e^{i\theta} + e^{i2\theta}$. The limit probability distribution can be computed numerically by using Theorem 1.1. It is shown in Fig. 1. Note that the points where the probability distribution has singularities correspond to local maxima of the function $P'(\theta) = -2(2 \sin 2\theta + \sin \theta)$.

Let us summarize the main features of quantum walks on the integer lattice. First of all, the length of the interval where the distribution of quantum walk is essentially supported is of order t instead of \sqrt{t} as in the classical case. Then, the probability of the return to the origin at time t is of order t^{-1} instead of $t^{-1/2}$. Finally, unlike the classical case, the limit distribution is not Gaussian and its shape depends on the generator of the quantum walk.

What can be said about the continuous-time quantum walk on \mathbb{Z}^d ? We consider here only the nearest-neighbor walk. It turns out that in this case the quantum walk on \mathbb{Z}^d factorizes provided it was started from the origin. That is, every transition amplitude of the walk on \mathbb{Z}^d can be written as a product of transition amplitudes of the walk on \mathbb{Z} .

Fig. 1 The limit average probability distribution for the quantum walk on \mathbb{Z} with $P(\theta) = e^{-i2\theta} + e^{-i\theta} + e^{i\theta} + e^{i2\theta}$



For simplicity of notation we consider only the case of \mathbb{Z}^2 . The general case is similar. Let $\psi_{(i,j)}(t)$ be the transition amplitude of the transition from vertex $(0, 0)$ to vertex (i, j) . (That is, $\psi_{(i,j)}(t) = \langle \delta_{(i,j)} | U_t \delta_{(0,0)} \rangle$, where $\delta_{(0,0)}$ and $\delta_{(i,j)}$ denote the delta-functions concentrated on vertices $(0, 0)$ and (i, j) , respectively.)

Theorem 1.4 *Let the nearest-neighbor quantum walk on \mathbb{Z}^2 be started from the origin, i.e., $\psi(0) = \delta_{(0,0)}$. Then,*

$$\psi_{(i,j)}(t) = \psi_i(t)\psi_j(t),$$

where $\psi_i(t)$ is the transition amplitude for the nearest-neighbor quantum walk on \mathbb{Z} started from the origin.

We prove this result in Sect. 2. Previously, this fact was observed without proof in Appendix of [1].

Let us now turn to continuous-time quantum walks on homogeneous trees. (The previous studies of this topic include [6] and [15].) We restrict our investigations to the case of the nearest-neighbor walk.

Let $G = \mathbb{T}_m$, the m -valent infinite tree with $m \geq 3$, the initial ψ be δ_e , where e is the root of the tree, and let $U_t = \exp(iXt)$, where X is the adjacency matrix of the tree. Let $r := 2\sqrt{m-1}$. (This is the spectral radius of the operator X .) Finally, let us define the following functions of parameter α :

$$\begin{aligned} \omega_1(\alpha) &= \alpha \arctan \frac{\alpha}{\sqrt{r^2 - \alpha^2}} + \sqrt{r^2 - \alpha^2}, \\ \omega_2(\alpha) &= \alpha\pi - \omega_1, \end{aligned}$$

and

$$\begin{aligned} \varphi_1(\alpha) &= -\arctan \left[\frac{m}{m-2} \frac{\alpha}{\sqrt{r^2 - \alpha^2}} \right] - \frac{\pi}{4}, \\ \varphi_2(\alpha) &= -\pi - \varphi_1. \end{aligned}$$

Theorem 1.5 *Consider the nearest-neighbor quantum walk on the regular infinite tree of valency m . Assume $\psi(0) = \delta_e$, and let $\psi_i(t)$ be the amplitude of transition from the root to*

a vertex w which is located at distance l from the root. Let $\alpha = l/t$. Then

$$e^{\frac{\alpha t}{2} \log(m-1)} \psi_l(t) = \frac{1}{\sqrt{2\pi t}} \frac{1}{(r^2 - \alpha^2)^{1/4}} \sqrt{\frac{(m-1)\alpha^2}{\alpha^2 + (m-2)^2}} \left[\sum_{k=1}^2 e^{it\omega_k(\alpha) + i\varphi_k(\alpha)} \right] + O\left(\frac{1}{t}\right), \quad \text{if } 0 < \alpha < r.$$

In addition, there is a constant $c > 0$, which depends only on m , such that

$$e^{\frac{\alpha t}{2} \log(m-1)} |\psi_l(t)| \leq \frac{c}{t} \quad \text{if } \alpha > r.$$

We will prove this theorem in Sect. 3.

Next, define

$$p(\alpha, t) = m(m-1)^{[\alpha t]-1} \cdot t |\psi_{[\alpha t]}(t)|^2, \tag{5}$$

and

$$\bar{p}(\alpha, T) = \frac{1}{\sqrt{T}} \int_T^{T+\sqrt{T}} p(\alpha, t) dt. \tag{6}$$

The factor $m(m-1)^{[\alpha t]-1}$ in (5) equals the number of vertices in the tree at the distance $[\alpha t] \geq 1$ from the root. Intuitively, $\bar{p}(\alpha, T)$ is the average probability density of the event that we find a particle at the distance approximately αt from the root if we measure its position at time approximately equal to T . Then, we have the following corollary of Theorem 1.5.

Corollary 1.6 *Suppose that $\omega_1(\alpha) \neq \omega_2(\alpha)$. Then*

$$\lim_{T \rightarrow \infty} \bar{p}(\alpha, T) = \frac{1}{\pi} \frac{1}{\sqrt{r^2 - \alpha^2}} \frac{m\alpha^2}{\alpha^2 + (m-2)^2}, \quad \text{if } 0 < \alpha < r, \\ = 0, \quad \text{if } \alpha > r.$$

The proof of this corollary is similar to the proof of Corollary 1.2 and is omitted.

The limit distribution is similar to the arcsine distribution (4), except it has a weighting factor, which is different for every m . A plot of the limit average distribution is shown in Fig. 2 for $m = 4$ and $m = 20$. For the purposes of comparison we have additionally rescaled the support of the distribution so that supports are the same for both m . It can be seen that the walk on the tree of higher valency has higher density next to the border of the support.

Note that the quantum walk on trees behaves (perhaps non-surprisingly) quite different from the classical random walk on trees. In the latter case, it is possible to show that the distribution of the particle distance from the root is asymptotically Gaussian with mean ct and standard deviation $\sigma\sqrt{t}$ where $c, \sigma > 0$ (see [16] and [13]). This result is very different from what we find in the quantum case.

Consider now the amplitude of the return to zero at time t .

Theorem 1.7 *Let $\psi_0(t)$ denote the transition amplitude of the return to the root at time t for the nearest-neighbor quantum walk on the m -valent infinite tree started at the root. Suppose that $m \geq 3$. Then, for large t the following asymptotic approximation is valid:*

$$\psi_0(t) = -\frac{1}{\sqrt{\pi t^{3/2}}} \frac{m(m-1)^{1/4}}{(m-2)^2} \sin\left[(2\sqrt{m-1})t - \pi/4\right] + O\left(\frac{1}{t^2}\right).$$

Fig. 2 The limit average probability distribution for the quantum walk on a homogeneous tree with valency m . The *solid line* is for $m = 4$, and the *dashed line* is for $m = 20$. The support of the distribution is rescaled to $[0, 1]$ interval

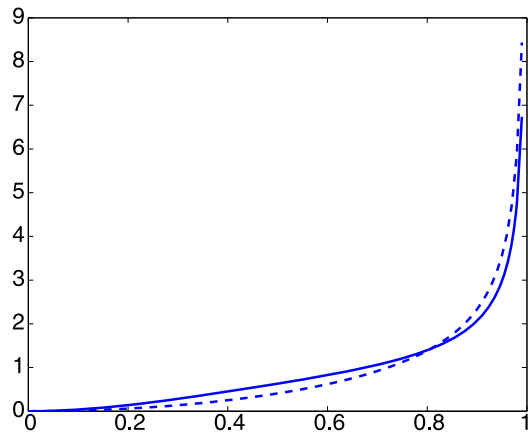
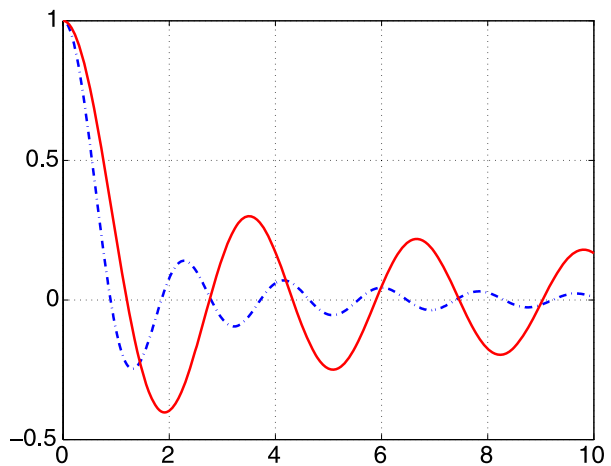


Fig. 3 The transition amplitude of the return to the root for the nearest-neighbor quantum walk. The *solid line* is for integer lattice \mathbb{Z} ; the *dash-dotted line* is for 4-valent infinite tree \mathbb{T}_4



The plot of $\psi_0(t)$ for $m = 4$ is shown in Fig. 3 by dash-dotted line. We can see that the frequency of oscillations in the return amplitude is higher than in the case $m = 2$. In addition, the absolute values of maxima decline faster.

As a corollary of Theorem 1.7, we can see that the probability of the return to zero has the following asymptotic approximation:

$$p_0(t) = \frac{m^2(m-1)^{1/2}}{\pi(m-2)^4} \frac{1}{t^3} \sin^2[(2\sqrt{m-1})t - \pi/4] + O(t^{-7/2}).$$

If we compare these results with the case of the classical random walk, we find two surprising facts. First, there is no exponential decay factor in the probability of return. The decay is polynomial of order t^{-3} . Second the exponent in this polynomial decay does not depend on the valency of the tree although the frequency of oscillations and the overall constant does depend on it.

The rest of the paper is organized as follows. Section 2 provides proofs for Theorems 1.1 and 1.4 concerning quantum walks on \mathbb{Z} and \mathbb{Z}^d . And Sect. 3 gives proofs for Theorems 1.5 and 1.7 concerning the nearest-neighbour quantum walk on homogeneous trees.

2 Quantum Walk on Integer Lattices

Proof of Theorem 1.1 It is convenient to introduce additional notation. Let G be a graph (V, E) . For $f, g \in L^2(V)$, we define

$$\langle f, g \rangle = \sum_{x \in V} \overline{f(x)}g(x).$$

Then, for $V = \mathbb{Z}$ we can write

$$\psi_l(t) = \langle \delta_l, e^{itX} \delta_0 \rangle = \sum_{k=0}^{\infty} (X^k)_{0l} \frac{(it)^k}{k!}$$

where S_{-l} is the shift operator that sends δ_k to δ_{k-l} .

Let $a_l^{(k)} := (X^k)_{0l}$. Then, it is easy to see that $\sum_{l=-\infty}^{\infty} a_l^{(k)} z^l = \phi(z)^k$, with $\phi(z) := \sum_{l=-L}^L a_l z^l$. Therefore,

$$a_l^{(k)} = \frac{1}{2\pi i} \oint \frac{\phi(z)^k}{z^{l+1}} dz,$$

where the integration is over a small contour around 0. Hence, the transition amplitude is given by the formula

$$\psi_l(t) = \sum_{k=0}^{\infty} a_l^{(k)} \frac{(it)^k}{k!} = \frac{1}{2\pi i} \oint \frac{e^{it\phi(z)}}{z^{l+1}} dz = -\frac{1}{2\pi} \int_0^{2\pi} e^{it(P(\theta)+\alpha\theta)} d\theta,$$

where we made the change of variables $z = e^{-i\theta}$ and where $\alpha = l/t$.

We can evaluate the asymptotic behavior of this integral by the method of stationary phase (Chap. 4 in [5]). The points of the stationary phase can be found from the equation:

$$P'(\theta) = -\alpha. \tag{7}$$

Suppose that this equations has $K > 0$ solutions $\theta_k(\alpha)$. Then, the asymptotic contribution of the stationary point θ_k to the integral above is given by the following formula:

$$-\frac{1}{\sqrt{2\pi t}} \frac{1}{\sqrt{|P''(\theta_k)|}} e^{it(P(\theta_k)+\alpha\theta_k) \pm \pi i/4} + o\left(\frac{1}{t}\right),$$

where the sign before $\pi i/4$ depends on whether $P''(\theta_k)$ is positive or negative. By adding these contributions we obtain the first claim of the theorem.

If (7) has no real solutions, then there are no points of stationary phase in interval $[0, 2\pi)$. In this case, we can apply the method of integration by parts. Usually, in this case the asymptotic approximation is of the order t^{-1} . However, in our case it is smaller due to special properties of function $P(\theta)$ and number α .

Indeed, let us denote $P(\theta) + \alpha\theta$ as $f_\alpha(\theta)$ for shortness. Note that the first derivative f'_α is periodic with period 2π and therefore all other derivatives are also periodic with period 2π . In addition, if αt is integer (which is exactly the case we consider, then $\exp(itf_\alpha(\theta))$ is periodic with period 2π .

Since $|f'(\theta)| \neq 0$ anywhere in interval $[0, 2\pi)$, hence we can use integration by parts in the following form:

$$\begin{aligned} \int_0^{2\pi} e^{itf_\alpha(\theta)} d\theta &= \frac{1}{it} \int_0^{2\pi} \frac{1}{f'(\theta)} \frac{d}{d\theta} (e^{itf_\alpha(\theta)}) d\theta \\ &= \frac{1}{it} \left[\frac{1}{f'(2\pi)} (e^{itf_\alpha(2\pi)}) - \frac{1}{f'(0)} (e^{itf_\alpha(0)}) \right] \\ &\quad - \frac{1}{it} \int_0^{2\pi} \frac{d}{d\theta} \left(\frac{1}{f'(\theta)} \right) e^{itf_\alpha(\theta)} d\theta. \end{aligned}$$

By using the special properties of the function $f_\alpha(\theta)$, we can conclude that the first term is zero and therefore

$$\int_0^{2\pi} e^{itf_\alpha(\theta)} d\theta = -\frac{1}{it} \int_0^{2\pi} \left(\frac{1}{f'(\theta)} \right)' e^{itf_\alpha(\theta)} d\theta.$$

In particular, this integral is $O(t^{-1})$. Since the function $(1/f'(\theta))'$ is periodic, hence the argument can be repeated. It is easy to see that it can be repeated indefinitely, and we obtain that the integral is less than $c_n t^{-n}$ for every n . □

Proof of Theorem 1.4 Let X be the adjacency matrix for \mathbb{Z}^2 and H and V be the adjacency matrices that take into account only horizontal and vertical bonds, respectively. In other words,

$$X = H + V,$$

and

$$\begin{aligned} H_{ij,kl} &= (\delta_{i-1,k} + \delta_{i+1,k})\delta_{jl}, \\ V_{ij,kl} &= \delta_{ik}(\delta_{j-1,l} + \delta_{j+1,l}). \end{aligned}$$

It is easy to see that

$$(HV)_{ij,kl} = (VH)_{ij,kl} = (\delta_{i-1,k} + \delta_{i+1,k})(\delta_{j-1,l} + \delta_{j+1,l}).$$

That is, H and V commute. This implies that

$$e^{itX} = e^{itH} e^{itV}.$$

After we apply e^{itV} to $\psi(0) = \delta_{(0,0)}$, the result at vertex (i, j) is $\delta_{0i} \psi_j(t)$ where δ_{0i} is the Kronecker delta and $\psi_j(t)$ is the wave function for the nearest-neighbor quantum walk at \mathbb{Z} started at 0. Next, after we apply e^{itH} , the result at vertex i, j is $\psi_i(t)\psi_j(t)$ since it equals the wave function of the nearest-neighbor walk on graph $\mathbb{Z} \times (0, j)$ started with the initial data $\psi_j(t)$. □

3 Nearest-Neighbor Quantum Walk on Trees

Proof of Theorem 1.5 First, note that

$$\begin{aligned} \psi_w(t) &= \langle \delta_w, e^{itX} \delta_e \rangle = \sum_{k=0}^{\infty} \langle \delta_w, X^k \delta_e \rangle \frac{(it)^k}{k!} \\ &= \sum_{k=0}^{\infty} c_k(|w|) \frac{(it)^k}{k!}, \end{aligned}$$

where $c_k(|w|)$ denotes the number of all possible paths with k edges that start at the root and end at vertex w .

Let A_k denote the number of paths from e to e that have length k and do not pass along a specific edge which is connected to e , say, do not pass along edge x_1 . Let B_k be the number of paths from e to e that have length k , without any additional restrictions. Let $A(z)$ and $B(z)$ denote the generating functions for A_k and B_k , respectively, that is,

$$A(z) = \sum_{k=0}^{\infty} A_k z^k, \quad \text{and} \quad B(z) = \sum_{k=0}^{\infty} B_k z^k,$$

where we set $A_0 = B_0 = 1$.

From Lemma 3.1 proved below, it follows that

$$\sum_{r=0}^{\infty} c_{l+r}(l) z^r = A(z)^l B(z).$$

Hence,

$$c_{l+r}(l) = \frac{1}{2\pi i} \oint \frac{A(z)^l B(z)}{z^{r+1}} dz,$$

where the integration is around a small circle around 0.

Let $|w| = l$, then for the transition amplitude from e to w , we can write

$$\begin{aligned} \psi_l(t) &= \sum_{k=l}^{\infty} \frac{(it)^k}{k!} c_k(l) \\ &= \sum_{r=0}^{\infty} \frac{(it)^{l+r}}{(l+r)!} \frac{1}{2\pi i} \oint \frac{A(z)^l B(z)}{z^{r+1}} dz, \end{aligned}$$

which we can re-write as follows:

$$\begin{aligned} \psi_l(t) &= \frac{1}{2\pi i} \oint A(z)^l B(z) z^{l-1} \left(\sum_{k=0}^{\infty} \frac{(it/z)^{l+k}}{(l+k)!} \right) dz \\ &= \frac{1}{2\pi i} \oint A(z)^l B(z) z^{l-1} \left[e^{it/z} - \sum_{k=0}^{l-1} \frac{(it/z)^k}{k!} \right] dz. \end{aligned}$$

The sum in the last line gives zero contribution to the integral since neither $A(z)$ nor $B(z)$ has any singularity at 0. Hence, we can write

$$\begin{aligned} \psi_l(t) &= \frac{1}{2\pi i} \oint A(z)^l B(z) z^{l-1} e^{it/z} dz = \frac{1}{2\pi i} \oint \left[\frac{A(1/u)}{u} \right]^l \frac{B(1/u)}{u} e^{itu} du \\ &= \frac{1}{2\pi i} \oint [F(u)]^l G(u) e^{itu} du, \end{aligned}$$

where we used the substitution $u = 1/z$, and

$$\begin{aligned} F(u) &:= \frac{1}{u} A\left(\frac{1}{u}\right), \\ G(u) &:= \frac{1}{u} B\left(\frac{1}{u}\right). \end{aligned}$$

The second and third integrals are taken over a sufficiently large circle around the zero which includes all of the singularities of $F(u)$ and $G(u)$.

We calculate $F(u)$ and $G(u)$ explicitly below (Lemmas 3.2 and 3.3). The function $G(u)$ is analytical at points $u = \pm m$, therefore the only singularities of the integrand are branch points of $F(u)$ and $G(u)$ at $u = \pm 2\sqrt{m-1}$.

We want to find out the asymptotic approximation for those values of l which are comparable with t . Let $l = \alpha t$ with $\alpha \geq 0$. Then we can write the transition amplitude as follows:

$$\psi_l(t) = \frac{1}{2\pi i} \oint e^{it[u - i\alpha \log F(u)]} G(u) du. \tag{8}$$

Recall that $r := 2\sqrt{m-1}$. Let us deform the contour of integration so that it goes first from $-r$ to r just below the real axis, and then goes back just above the real axis.

Let $f(u) := u - i\alpha \log F(u)$. For real $u \in [-r, r]$, we can compute $\text{Im} f(u) = (\alpha/2) \log(m-1)$, which is constant with respect to u . Hence, we can use the stationary phase approximation to this integral.

In order to find the points of stationary phase, we need to solve the equation $d(\text{Re} f(u))/du = 0$. Since $\text{Im} f(u)$ is constant, it is the same as solving

$$\frac{df(u)}{du} \equiv 1 - i\alpha \frac{F'(u)}{F(u)} = 0. \tag{9}$$

First, let us consider the case $0 < \alpha < r$.

For the part of the contour that lies in the upper part of the complex plane, we have: $F(u) = (u - i\sqrt{r^2 - u^2})/(2(m-1))$, hence $f'(u) = 1 + \alpha/\sqrt{r^2 - u^2}$ and (9) becomes $-\alpha = \sqrt{r^2 - u^2}$ which has no solutions in the interval $(-r, r)$ for any positive α . Hence, the contribution of this part of the contour is asymptotically negligible provided that the integral along the other part of the contour has stationary points.

For the part of the contour that lies in the lower part of the complex plane, we have $F(u) = (u + i\sqrt{r^2 - u^2})/(2(m-1))$, and (9) reduces to $\alpha = \sqrt{r^2 - u^2}$, which has two solutions $u_{1,2} = \pm\sqrt{r^2 - \alpha^2}$ for $\alpha < r$.

Recall that the method of stationary phase says that if \bar{u} is the only stationary point of function $f(u)$, located inside $[a, b]$, then

$$\int_a^b e^{itf(u)} G(u) du = \sqrt{\frac{2\pi}{tf''(\bar{u})}} G(\bar{u}) e^{itf(\bar{u}) \pm \pi i/4} + O(1/t),$$

where the sign before $\pi i/4$ is positive if $\operatorname{Re} f''(\bar{u}) > 0$ and negative if $\operatorname{Re} f''(\bar{u}) < 0$.

We compute $F(u_{1,2}) = (\pm\sqrt{r^2 - \alpha^2} + i\alpha)/(2(m - 1))$. The second derivative of $f(u)$ can be evaluated at $u_{1,2}$ as follows.

$$f''(u_{1,2}) = \mp \frac{\sqrt{r^2 - \alpha^2}}{\alpha^2}.$$

In addition, we have

$$G(u_{1,2}) = \frac{\pm(m - 2)\sqrt{r^2 - \alpha^2} - i m \alpha}{2(\alpha^2 + (m - 2)^2)},$$

and

$$|G(u_{1,2})| = \sqrt{\frac{m - 1}{\alpha^2 + (m - 2)^2}}.$$

Hence,

$$\begin{aligned} \psi_l(t) &= e^{-\frac{\alpha t}{2} \log(m-1)} \left\{ \left(\frac{\alpha^2}{2\pi t} \frac{1}{(r^2 - \alpha^2)^{1/2}} \right)^{1/2} \sqrt{\frac{m - 1}{\alpha^2 + (m - 2)^2}} \right. \\ &\quad \left. \times \left[\sum_{k=1}^2 e^{it\omega_k(\alpha) + i\varphi_k(\alpha)} \right] + O\left(\frac{1}{t}\right) \right\}. \end{aligned}$$

Here, the frequencies can be computed as

$$\omega_1 = \alpha \arctan \frac{\alpha}{\sqrt{r^2 - \alpha^2}} + \sqrt{r^2 - \alpha^2},$$

and

$$\omega_2 = \alpha\pi - \omega_1,$$

and the phases can be computed as

$$\varphi_1 = -\arctan \frac{m\alpha}{(m - 2)\sqrt{r^2 - \alpha^2}} - \frac{\pi}{4},$$

and

$$\varphi_2 = -\pi - \varphi_1.$$

Now, consider the case $\alpha > r$. In this case, neither part of the contour has a point of stationary phase and for the large t , the boundary points of the interval $[-r, r]$ contribute most to the integral. In this situation, we can estimate the integral by using integration by parts. Consider, for example, the integral

$$I_1(\varepsilon) = \int_{-r+\varepsilon}^{r-\varepsilon} e^{itf(u)} G(u) du,$$

where $f(u)$ and $G(u)$ are defined as continuous limits of the upper half-plane branches of $f(u)$ and $G(u)$. Then we can write:

$$\begin{aligned}
 I_1(\varepsilon) &= \frac{1}{it} \int_{-r+\varepsilon}^{r-\varepsilon} \left(\frac{d}{du} e^{itf(u)} \right) \frac{G(u)}{f'(u)} du \\
 &= e^{itf(u)} \frac{G(u)}{itf'(u)} \Big|_{-r+\varepsilon}^{r+\varepsilon} - \frac{1}{it} \int_{-r+\varepsilon}^{r-\varepsilon} e^{itf(u)} \left(\frac{G(u)}{f'(u)} \right)' du.
 \end{aligned}
 \tag{10}$$

Since $f'(u) = 1 + \alpha/\sqrt{r^2 - u^2}$, therefore $\frac{G(u)}{f'(u)} \rightarrow 0$ as $u \rightarrow \pm r$, which implies that the first part of (10) becomes zero as $\varepsilon \rightarrow 0$. For the second part, note that

$$G'(u) = A(u) + B(u)\sqrt{r^2 - u^2} + C(u) \frac{1}{\sqrt{r^2 - u^2}},$$

for some functions $A(u)$, $B(u)$, and $C(u)$ analytic on $[-r, r]$, which implies that

$$\left(\frac{G(u)}{f'(u)} \right)' = \frac{G'(u)}{f'(u)} - \frac{G(u)}{[f'(u)]^2} f''$$

has singularities $(u + r)^{-1/2}$ and $(r - u)^{-1/2}$ at $-r$ and r respectively. This implies that $(\frac{G(u)}{f'(u)})'$ is absolutely integrable at $[-r, r]$ and therefore

$$|\lim_{\varepsilon \rightarrow 0} I_1(\varepsilon)| \leq \frac{1}{t} e^{-t\text{Im}f} \int_{-r}^r \left| \left(\frac{G(u)}{f'(u)} \right)' \right| du \leq \frac{c}{t} e^{-(\alpha t/2) \log(m-1)}.$$

A similar estimate holds for the integral along the contour in the lower half-plane. This completes the proof of Theorem 1.5. □

Here are the auxiliary results that we used in the proof.

Lemma 3.1 *Suppose that graph G is an infinite homogeneous tree with root e . Let A_k be the number of paths in G from e to e that have length k and do not pass along a specific edge which is connected to e . Let B_k be the number of paths from e to e that have length k , without further restrictions, and let $c_k(|w|)$ be the number of paths from e to w that have length k . Then,*

$$c_k(|w|) = \sum_{k_0+k_1+\dots+k_{|w|}=k} A_{k_0} A_{k_1} \dots A_{k_{|w|-1}} B_{k_{|w|}}.$$

Proof Assume that each edge in the tree is oriented and has a label, x , which is chosen from the set $\{1, \dots, m\}$. It is assumed that the labels of edges around each vertex are all different. We write label x if we move in the direction of the orientation and x^{-1} if we move in the opposite direction. Let $x_i x_{i-1} \dots x_1$ be the shortest path from e to w . There is a one-to-one correspondence between the set of shortest paths and vertices so we can write $w = x_i x_{i-1} \dots x_1$. Also, let $w_i = x_i x_{i-1} \dots x_1$. This is one of the vertices on the shortest path from e to w . We write the edges in the path from right to left so that w_1 is a neighbor of the root.

Every path from e to w can be considered as the shortest path from e to w decorated with loops which can be attached at each of the points of the shortest path, w_i . In order to make sure that we do not double count the loops we forbid the loop attached at w_i to go along the edge that connects w_i to w_{i+1} . In this way, at every point of the path we know in which loop we are in: We are always in the loop attached at that w_i that has the largest length $|w_i|$ among all those vertices w_i that have already been visited.

Let $l = |w|$. The number of possible different loops that can be attached at w_0, w_1, \dots, w_{l-1} is counted by $A_{k_0}, A_{k_1}, \dots, A_{k_{l-1}}$, respectively, where k_0, k_1, \dots, k_{l-1} are the lengths of the loops. The number of different loops that can be attached at $w = w_l$ is counted by B_{k_l} . Then, the total length of the path is $k_0 + k_1 + \dots + k_l$ and by assumption it must be equal to k . Hence the total number of paths is

$$\sum_{k_0+k_1+\dots+k_l=k} A_{k_0}A_{k_1} \cdots A_{k_{l-1}}B_{k_l}. \quad \square$$

Lemma 3.2

$$G(z) := \frac{1}{z}B\left(\frac{1}{z}\right) = \frac{-(m-2)z + m\sqrt{z^2 - 4(m-1)}}{2(z^2 - m^2)}. \quad (11)$$

Proof The function $B(z)$ is related to the Green function of the nearest-neighbor random walk on an infinite tree, which is well-known. (See Dynkin and Maljutov for the seminal contribution, and Lemma 1.24 on p. 9 in [17].) Hence, we can compute

$$B(z) = \frac{-(m-2) + m\sqrt{1 - 4(m-1)z^2}}{2(1 - m^2z^2)}.$$

It follows that

$$G(z) = \frac{-(m-2)z + m\sqrt{z^2 - 4(m-1)}}{2(z^2 - m^2)}. \quad (12)$$

□

Note that we chose the branches of $G(z)$ in such a way that the function is analytical outside the cut $[-2\sqrt{m-1}, 2\sqrt{m-1}]$. In particular, this function does not have poles at $\pm m$.

More precisely, the sign before the square root is determined by the rule that for sufficiently small t ,

$$G(it) \approx -i \frac{\sqrt{m-1}}{m} \in \mathbb{C}^-$$

and

$$G(-it) \approx i \frac{\sqrt{m-1}}{m} \in \mathbb{C}^+.$$

Lemma 3.3

$$F(z) := \frac{1}{z}A\left(\frac{1}{z}\right) = \frac{z - \sqrt{z^2 - 4(m-1)}}{2(m-1)}.$$

Proof In order to compute $A(z)$, we note that the following recursive relation holds.

$$A_{2k} = (m-1) \sum_{l=0}^{k-1} A_{2l}A_{2(k-l-1)}. \quad (13)$$

Indeed, consider a path from e to e , that avoids the edge x_1 . There are $m-1$ possibilities to start the path. Suppose that the path starts with $x_i, i \neq 1$, so that the second point on the

path is the endpoint of x_i which we denote w_1 . Let r be the first time when the path returns to e . Then $w_{r-1} = w_1$ and the path from w_1 to w_{r-1} is one of the A_{r-2} paths from w_1 to w_1 that avoid passing through the edge labelled x_i . The remainder of the path goes from e to e and it is one of the A_{2k-r} paths that avoid the edge x_1 . The number r must be even, greater than 0 and less than $2k$. Hence we can write it as $r = 2l + 2$, where $0 \leq l \leq k - 1$. This implies the recursive (13).

Next, we can use the recursion formula for Catalan numbers,

$$C_k = \sum_{l=0}^{k-1} C_l C_{k-l-1},$$

and (13) in order to conclude that

$$A_{2k} = (m - 1)^k C_k.$$

By using the generating function for Catalan numbers, we obtain the following formula for $A(z)$:

$$A(z) = \frac{1 - \sqrt{1 - 4(m - 1)z^2}}{2(m - 1)z^2}.$$

It follows that

$$F(z) = \frac{z - \sqrt{z^2 - 4(m - 1)}}{2(m - 1)}. \quad \square$$

The sign of the square root in the expression for $F(z)$ is determined by the following rule: for all sufficiently small t ,

$$F(it) \approx -i/\sqrt{m - 1} \in \mathbb{C}^-,$$

and

$$F(-it) \approx i/\sqrt{m - 1} \in \mathbb{C}^+.$$

Proof of Theorem 1.7 By (8), we need to find asymptotics for

$$\psi_0(t) = \frac{1}{2\pi i} \oint e^{itu} G(u) du, \tag{14}$$

where

$$G(u) = \frac{-(m - 2)u + m\sqrt{u^2 - r^2}}{2(u^2 - m^2)}$$

and $r = 2\sqrt{m - 1}$. We can deform the contour so that it starts at $-r$, passes just below the real axis to r and then returns back to $-r$ just above the real axis. Then, we find that

$$\psi_0(t) = \frac{1}{\pi} \int_{-r}^r e^{itu} \frac{m\sqrt{r^2 - u^2}}{2(u^2 - m^2)} du.$$

The main contribution is produced by singular points $\pm r$. After integration by parts, we obtain the following formula

$$\psi_0(t) = -\frac{1}{2\pi i} \frac{m}{t} \left[\int_{-r}^r \frac{1}{\sqrt{r^2 - u^2}} \frac{-ue^{itu}}{u^2 - m^2} du + \int_{-r}^r \frac{-2u\sqrt{r^2 - u^2}}{(u^2 - m^2)^2} e^{itu} du \right].$$

We can apply van der Corput's results (see [5], p. 24) to the first integral in the brackets and obtain the following asymptotic approximation.

$$\int_{-r}^r \frac{1}{\sqrt{r^2 - u^2}} \frac{-ue^{itu}}{u^2 - m^2} du = \sqrt{\frac{\pi}{2rt}} \frac{r}{r^2 - m^2} (e^{-itr + \pi i/4} - e^{itr - \pi i/4}) + O(t^{-1}).$$

We can apply the integration by parts to the second integral and find that it is $O(t^{-1})$. It follows that

$$\begin{aligned} \psi_0(t) &= \frac{1}{\sqrt{2\pi} t^{3/2}} \frac{m\sqrt{r}}{r^2 - m^2} \sin(rt - \pi/4) + O(t^{-2}) \\ &= -\frac{1}{\sqrt{\pi} t^{3/2}} \frac{m(m-1)^{1/4}}{(m-2)^2} \sin(2\sqrt{m-1}t - \pi/4) + O(t^{-2}). \end{aligned} \quad \square$$

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