

One-dimensional quantum walks with absorbing boundaries

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Abstract

In this paper we analyze the behavior of quantum random walks. In particular we present several new results for the absorption probabilities in systems with both one and two absorbing walls for the one-dimensional case. We compute these probabilities both by employing generating functions and by use of an eigenfunction approach. The generating function method is used to determine some simple properties of the walks we consider, but appears to have limitations. The eigenfunction approach works by relating the problem of absorption to a unitary problem that has identical dynamics inside a certain domain, and can be used to compute several additional interesting properties, such as the time dependence of absorption. The eigenfunction method has the distinct advantage that it can be extended to arbitrary dimensionality. We outline the solution of the absorption probability problem of a $(D - 1)$ -dimensional wall in a D -dimensional space.

1 Introduction

Several recent papers have studied the properties of *quantum walks*, which are quantum computational variants of discrete-time random walks [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. The behavior of quantum walks differs from that of ordinary random walks in several striking ways, due to the fact that quantum walks exhibit interference patterns whereas ordinary random walks do not. For instance, mixing times, hitting times, and exit probabilities of quantum walks can differ significantly from analogously defined random walks [1, 2, 3, 9]. One-dimensional quantum walks are also relevant to quantum chaos [12]. In this paper we investigate the behavior of a class of one-dimensional quantum walks that are very simple generalizations of the quantum walks introduced in Refs. [6, 2].

Continuous-time variants of quantum walks have also been proposed and exhibit significant differences from classical continuous random walks [13, 14]. However, we will not discuss this model of quantum walks in this paper.

Ordinary random walks have had many applications in computer science, particularly as algorithmic tools. Examples include randomized algorithms for graph connectivity, 2SAT, and approximating the permanent (see, for instance, Lovász [15] for several examples of algorithmic

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applications of random walks). Quantum walks have the potential to offer new tools for the design of quantum algorithms, which is one of the primary motivations for studying their behavior. For example, given that quantum walks on certain simple structures mix faster or have faster hitting times than random walks, there is the potential that they will admit quantum speed-ups for algorithms based on random walks on more complicated structures.

One-dimensional quantum walks are not likely to be directly applicable to algorithm design. Although there has been some work on quantum walks on general graphs [1], many questions about quantum walks on general graphs appear to be quite difficult to answer at the present time. Thus it is important to extend techniques developed to analyze one-dimensional quantum walks to quantum walks on general graphs. To this end, we also investigate the behavior of quantum walks in D dimensions.

Ref. [2] demonstrates that one-dimensional quantum walks differ qualitatively from classical random walks. For example, this walk spreads with time as t instead of \sqrt{t} . Moreover, if the walk is evolved in a system with one absorbing boundary, the probability of eventual absorption by the wall is less than unity (in contrast to a classical unbiased one-dimensional random walk, where this probability is unity). In this paper we generalize and extend the results of Ref. [2] and calculate the absorption probabilities of one-dimensional quantum walks in systems with one and two absorbing walls. We use a combinatorial method as well as an eigenfunction expansion method. The combinatorial method is similar to that used in Ref. [2], and the eigenfunction method has been used by others to address periodic systems [1, 2, 7, 8, 16, 12] as well as systems with potential steps [7, 8]. Naturally the two methods agree perfectly in all cases in which results have been obtained using both methods. We extend the eigenfunction method to general dimensionality.

1.1 Summary of results

First, for one-barrier systems, we obtain exact expressions for the probability of absorption by the barrier, as a function of the initial distance to the barrier. Complementing these formulas gives the probability of escape to infinity. These expressions involve integrals of different forms coming from our two methods of analysis. Both forms allow asymptotic analysis of the absorption probabilities; in particular, we compute the limiting probabilities when the initial distance to the barrier is large. We do this both for Hadamard walks and for walks based on general unitary transformations.

Next, for the two-barrier Hadamard system, we compute the long-time limit of the probability of absorption by each barrier when the walker starts off very far from one barrier but an arbitrary distance from the other barrier. Again, the expressions involve integrals whose asymptotic limits are easily analyzed, so that we can compute the limiting probabilities when the initial distance to both barriers is large. We then outline how the eigenfunction method can be used to analyze the behavior in small systems. Then we use the eigenfunction method to analyze the time dependence of the absorption in the limit of long times for walks with both one and two walls. We find that the approach to the asymptotic limit is much slower when there are two walls, where the probability remaining to be absorbed at time t decays as $1/\sqrt{t}$, than when the system has one wall, where the probability remaining to be absorbed at time t is proportional to $1/t^2$.

Finally, we study D -dimensional walks, and show that the region over which most of the probability is distributed by time t has volume proportional to t^D . We indicate how to solve the problem of the absorption of a $(D - 1)$ -dimensional wall without giving explicit results.

1.2 Organization of the paper

In Section 2 we give definitions for one-dimensional quantum walks and for the specific processes based on quantum walks that we consider. Section 3 presents our results based on the combinatorial approach and Section 4 presents our results based on the eigenfunction method. Finally, in Section 5 we analyze generalizations of one-dimensional quantum walks to higher dimensions.

2 Definitions

2.1 One-dimensional quantum walks

For any finite or countable set S we may denote by $\mathcal{H}(S)$ the Hilbert space of all square-summable functions from S to the complex numbers \mathbb{C} , along with the usual inner product. Using the Dirac notation, the space $\mathcal{H}(S)$ has a *standard basis* $\{|s\rangle : s \in S\}$, which is orthonormal. One-dimensional quantum walks are discrete-time quantum processes on the space $\mathcal{H}(\mathbb{Z} \times \{L, R\})$. The standard basis for this space therefore consists of elements of the form $|n, d\rangle$, where $n \in \mathbb{Z}$ is the *location* and $d \in \{L, R\}$ is the *direction* component of such an element.

Given any unitary operator U on $\mathcal{H}(\{L, R\})$, define a unitary operator W_U acting on $\mathcal{H}(\mathbb{Z} \times \{L, R\})$ by

$$W_U |n, d\rangle = \langle L|U|d\rangle |n-1, L\rangle + \langle R|U|d\rangle |n+1, R\rangle$$

for each standard basis state $|n, d\rangle$, and extending to all of $\mathcal{H}(\mathbb{Z} \times \{L, R\})$ by linearity. Alternately we may define $W_U = T(I \otimes U)$, where T is defined by

$$T |n, L\rangle = |n-1, L\rangle, \quad T |n, R\rangle = |n+1, R\rangle.$$

We use the term *one-dimensional quantum walk* to refer generally to any process involving the iteration of W_U , since such processes are reminiscent of a particle doing a random walk on a one-dimensional lattice.

We will also consider quantum walks on higher dimensional lattices in the final section of this paper—definitions for this type of walk appear in that section.

2.2 Absorbing boundaries and exit probabilities

In this paper we will be interested in the situation in which our system is initialized to some state and we alternately apply the operator W_U and perform some measurement of the system. The type of measurements we focus on are as follows. For each $n \in \mathbb{Z}$, consider the projections Π_{yes}^n and Π_{no}^n defined as

$$\Pi_{\text{yes}}^n = |n, L\rangle \langle n, L| + |n, R\rangle \langle n, R|, \quad \Pi_{\text{no}}^n = I - \Pi_{\text{yes}}^n.$$

These projections describe a projective measurement that corresponds to asking the question “is the particle at location n ?”. Given a system in state $|\psi\rangle$, the answer is “yes” with probability $\|\Pi_{\text{yes}}^n |\psi\rangle\|^2$, in which case the state of the system becomes $\Pi_{\text{yes}}^n |\psi\rangle$ (renormalized) and the answer is “no” with probability $\|\Pi_{\text{no}}^n |\psi\rangle\|^2$, in which case the state of the system becomes $\Pi_{\text{no}}^n |\psi\rangle$ (renormalized).

The first type of process we consider is the one-boundary quantum walk, which is as follows. The system being considered is initialized to some state $|0\rangle$ ($\alpha |L\rangle + \beta |R\rangle$), which corresponds to a particle at location 0 and having direction component in state ($\alpha |L\rangle + \beta |R\rangle$). Fix an integer $M > 0$, which will be the location of our absorbing boundary. For given U , we alternately apply

W_U and the measurement described by $\{\Pi_{yes}^M, \Pi_{no}^M\}$, which gives result “yes” if the particle has reached location M and “no” otherwise. The process is repeated until the result “yes” is obtained. The probability that the result “yes” is obtained is the *exit probability* for this walk. For fixed U and given M, α , and β , we will denote this exit probability by $r_M(\alpha, \beta)$. We also write $p_M = r_M(1, 0)$ and $q_M = r_M(0, 1)$ for short, i.e., p_M is the exit probability for starting in state $|0, L\rangle$ and q_M is the exit probability for starting in state $|0, R\rangle$.

We also consider two-boundary quantum walks. In this case, the particle is initialized in some state $|0\rangle (\alpha |L\rangle + \beta |R\rangle)$ and we alternately apply W_U and the (commuting) measurements described by

$$\{\Pi_{yes}^{-M_L}, \Pi_{no}^{-M_L}\} \quad \text{and} \quad \{\Pi_{yes}^{M_R}, \Pi_{no}^{M_R}\}$$

for $0 < M_L, M_R$. The quantities of interest in this case are the probability of exiting from the left (i.e., measuring the particle at location $-M_L$) and the probability of exiting from the right (measuring the particle at location M_R). Again, in this case the boundaries are absorbing, since the process is terminated when either measurement gives result “yes”.

2.3 Statement of results

In this paper, we give a complete description of the exit probabilities for one-boundary quantum walks in one-dimension for arbitrary unitary U , any starting state of the form $|0\rangle (\alpha |L\rangle + \beta |R\rangle)$, and any boundary location $M > 0$. This includes integrals for computing exact exit probabilities, closed form solutions for the exit probabilities in the limit of large M (one of which proves a recent conjecture of Yamasaki, Kobayashi and Imai [11]), and several other results concerning the behavior of these probabilities. It is proved that it is enough to consider only real unitary U for the purposes of analyzing such walks.

For two-boundary Hadamard quantum walks in one dimension, we present integrals for the exact exit probabilities when the particle starts out an arbitrary distance from one wall and an asymptotically large distance from the other. These integrals are evaluated to yield closed form solutions for the exit probabilities when the distance from the first wall is small and when the particle starts out very far from both walls. We then calculate the time-dependence of the absorption probability at long times for both one- and two-wall walks.

Finally, for D -dimensional walks, we generalize some of the results of [2] on one-dimensional walks, including a derivation of the asymptotic form for the amplitudes associated with the walk and a demonstration that the amplitude spreads nearly uniformly. For D -dimensional quantum walks with a $(D - 1)$ -dimensional barrier an integral for the absorption probability is derived.

3 Combinatorial analysis

3.1 Generating functions

As described in Section 2, we consider the case where our system is initialized in some state

$$|0\rangle (\alpha |L\rangle + \beta |R\rangle)$$

and we alternately apply the unitary operator W_U and perform the measurement described by $\{\Pi_{yes}^M, \Pi_{no}^M\}$ for some choice of $M > 0$. This process is repeated until the measurement gives result “yes”, at which time the process is terminated.

We begin with two special cases: the first is the case that the starting state is $|0, L\rangle$ and the absorbing boundary is at $M = 1$, and the second is the case that the starting state is $|0, R\rangle$ and

the boundary is at $M = 1$. We will define generating functions for these cases that are used to determine exit probabilities for all starting states and boundary positions. For given unitary U define two generating functions f and g as follows:

$$f_u(z) = \sum_{t=1}^{\infty} \langle 1, R | W_u (\Pi_{\text{no}}^1 W_u)^{t-1} | 0, L \rangle z^t,$$

$$g_u(z) = \sum_{t=1}^{\infty} \langle 1, R | W_u (\Pi_{\text{no}}^1 W_u)^{t-1} | 0, R \rangle z^t.$$

The coefficient of z^t in $f_u(z)$ is therefore the (non-normalized) amplitude with which the system is in state $|1, R\rangle$ after t time steps, assuming the system starts in state $|0, L\rangle$, and $g_u(z)$ is similar except we start in state $|0, R\rangle$. We will simply write f and g to denote f_u and g_u when U is understood. Thus, for example, the probability that a particle starting in state $|0, L\rangle$ is eventually observed at location 1 is

$$p_1 = \sum_{t \geq 0} |[z^t]f(z)|^2,$$

where $[z^t]f(z)$ denotes the coefficient of z^t in $f(z)$, and similarly the probability that a particle starting in state $|0, R\rangle$ is eventually observed at location 1 is

$$q_1 = \sum_{t \geq 0} |[z^t]g(z)|^2.$$

The reason that the generating functions f and g are useful for analyzing exit probabilities for all boundary positions is as follows. For given $M \geq 2$ consider a generating function defined similarly to f , except for the boundary at location M rather than location 1. Then this generating function is simply $f(z)(g(z))^{M-1}$, which follows from the fact that to get from location 0 to location M , the particle needs to effectively move right M times, and for each move after the first, the starting direction component is R . Similarly, the generating function corresponding to starting in state $|0, R\rangle$ is simply $(g(z))^M$.

Given arbitrary generating functions u and v , their *Hadamard product* is $u \odot v$, defined by

$$(u \odot v)(z) = \sum_{t \geq 0} ([z^t]u(z))([z^t]v(z)) z^t.$$

Thus, $p_1 = (f \odot \bar{f})(1)$ and $q_1 = (g \odot \bar{g})(1)$. In general we have

$$(u \odot v)(1) = \frac{1}{2\pi} \int_0^{2\pi} u(e^{i\theta})v(e^{-i\theta})d\theta, \quad (1)$$

provided $\sum_{t \geq 0} ([z^t]u(z))([z^t]v(z))$ converges. A proof of this fact follows from results in Section 4.6 of Titchmarsh [17].

3.2 Hadamard Walk

The most common choice for U in recent papers on one-dimensional quantum walks has been (or is equivalent to) the following:

$$U |L\rangle = \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle), \quad U |R\rangle = \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle), \quad (2)$$

i.e., U is the Hadamard transform where we identify $|L\rangle = |0\rangle$ and $|R\rangle = |1\rangle$. The resulting walk has been called the *Hadamard walk*. It turns out that the general behavior of this walk is not specific to the Hadamard transform, as we will show shortly. (Nayak and Vishwanath [16] have also claimed results concerning the generality of the Hadamard walk.) However, it is helpful to first consider the Hadamard transform because it is simple and we can reduce the behavior of general quantum walks to the Hadamard walk.

It can be shown that for U as in Eq. (2) we have

$$f(z) = \frac{1 + z^2 - \sqrt{1 + z^4}}{\sqrt{2}z}, \quad (3)$$

$$g(z) = \frac{1 - z^2 - \sqrt{1 + z^4}}{\sqrt{2}z} = f(z) - \sqrt{2}z. \quad (4)$$

We will not argue this here, since later we will derive generating functions for arbitrary U that give these generating functions in the case of the Hadamard transform.

Define $F(\theta) = f(e^{i\theta})$ and $G(\theta) = g(e^{i\theta})$. Then by Eq. (1)

$$p_1 = \frac{1}{2\pi} \int_0^{2\pi} |F(\theta)|^2 d\theta = \frac{2}{\pi}$$

$$q_1 = \frac{1}{2\pi} \int_0^{2\pi} |G(\theta)|^2 d\theta = \frac{2}{\pi},$$

as proved in Ref. [2]. Thus, in this case a particle starting at location 1 has a $1 - 2/\pi \approx 0.3634$ probability of “escaping” the absorbing boundary at location 0, which contrasts with the classical unbiased random walk, for which the probability of escape is 0.

Suppose now that the boundary is at location M for any $M \geq 1$. Then from the discussion in the previous subsection we conclude that

$$p_M = \frac{1}{2\pi} \int_0^{2\pi} |F(\theta)|^2 |G(\theta)|^{2M-2} d\theta \quad (5)$$

$$q_M = \frac{1}{2\pi} \int_0^{2\pi} |G(\theta)|^{2M} d\theta. \quad (6)$$

These expressions make it very easy to calculate the exit probabilities in the limit for large M . We will prove shortly that $|G(\theta)| \leq 1$ for all $\theta \in [0, 2\pi]$, with strict inequality for $\theta \in (\pi/4, 3\pi/4) \cup (5\pi/4, 7\pi/4)$. This gives

$$\begin{aligned} \lim_{M \rightarrow \infty} p_M &= \lim_{M \rightarrow \infty} \frac{1}{2\pi} \int_0^{2\pi} |F(\theta)|^2 |G(\theta)|^{2M-2} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi/4}^{\pi/4} |F(\theta)|^2 d\theta + \frac{1}{2\pi} \int_{3\pi/4}^{5\pi/4} |F(\theta)|^2 d\theta \\ &= \frac{2}{\pi} - \frac{1}{2} \approx .1366 \end{aligned}$$

and

$$\lim_{M \rightarrow \infty} q_M = \lim_{M \rightarrow \infty} \frac{1}{2\pi} \int_0^{2\pi} |G(\theta)|^{2M} d\theta = \frac{1}{2\pi} \int_{-\pi/4}^{\pi/4} d\theta + \frac{1}{2\pi} \int_{3\pi/4}^{5\pi/4} d\theta = \frac{1}{2}.$$

The estimate for $|G|$ can be verified as follows. Substituting $z = e^{i\theta}$ in (4), we find

$$G(\theta) = \frac{-2i \sin \theta \pm \sqrt{2 \cos 2\theta}}{\sqrt{2}}. \quad (7)$$

So $|G(\theta)|^2 = 2 \sin^2 \theta + \cos 2\theta = 1$ whenever $\cos 2\theta \geq 0$. On the other hand, if $\cos 2\theta < 0$, then

$$|G(\theta)|^2 = \frac{(2 \sin \theta \pm \sqrt{-2 \cos 2\theta})^2}{2}. \quad (8)$$

The sign is negative when $\theta \in (\pi/4, 3\pi/4)$, making

$$|G(\theta)|^2 = 2 \sin^2 \theta + \cos 2\theta - 2 \sin \theta \sqrt{-2 \cos 2\theta} < 1.$$

In the other interval, the sign is positive, and we argue similarly.

Now let us calculate the exit probabilities in the limit for large M for arbitrary directional component in the starting state. Assume the particle starts in state

$$|0\rangle (\alpha |L\rangle + \beta |R\rangle).$$

Recall that we denote the exit probability for starting in this state by $r_M(\alpha, \beta)$. The generating function for absorbed paths is now

$$\alpha f(z)g(z)^{M-1} + \beta g(z)^M = (\alpha f(z) + \beta g(z))g(z)^{M-1}.$$

The exit probability is therefore

$$\begin{aligned} r_M(\alpha, \beta) &= \frac{1}{2\pi} \int_0^{2\pi} |\alpha F(\theta) + \beta G(\theta)|^2 |G(\theta)|^{2M-2} d\theta \\ &\sim \frac{1}{2\pi} \int_{\Gamma} |\alpha F(\theta) + \beta G(\theta)|^2 d\theta \end{aligned}$$

where $\Gamma = (-\frac{\pi}{4}, \frac{\pi}{4}) \cup (\frac{3\pi}{4}, \frac{5\pi}{4})$. It will be helpful to note that

$$\frac{1}{2\pi} \int_{\Gamma} F(\theta)G(-\theta)d\theta = \frac{1}{2\pi} \int_{\Gamma} |F(\theta)|^2 d\theta - \frac{1}{2\pi} \int_{\Gamma} \sqrt{2}e^{-i\theta}F(\theta)d\theta = \frac{1}{\pi} - \frac{1}{2},$$

which follows from the fact that $g(z) = f(z) - \sqrt{2}z$. Therefore

$$\lim_{M \rightarrow \infty} r_M(\alpha, \beta) = |\alpha|^2 \left(\frac{2}{\pi} - \frac{1}{2} \right) + |\beta|^2 \left(\frac{1}{2} \right) + 2\Re(\alpha\bar{\beta}) \left(\frac{1}{\pi} - \frac{1}{2} \right). \quad (9)$$

The extreme values of this probability can be obtained as follows. First, note that it is enough to consider real values of α and β . Setting $\alpha = \cos \theta$, $\beta = \sin \theta$ and looking for critical points, one finds that the probability is maximized when $\alpha = \cos(5\pi/8)$ and $\beta = \sin(5\pi/8)$, giving

$$\lim_{M \rightarrow \infty} r_M(\alpha, \beta) = \frac{1}{\sqrt{2}} + \frac{1 - \sqrt{2}}{\pi} \approx .5753$$

and is minimized when $\alpha = \cos(\pi/8)$ and $\beta = \sin(\pi/8)$, giving

$$\lim_{M \rightarrow \infty} r_M(\alpha, \beta) = -\frac{1}{\sqrt{2}} + \frac{1 + \sqrt{2}}{\pi} \approx .0614.$$

3.3 Asymptotics of Exit Probabilities

It is clear from the integral representation of $r_M(\alpha, \beta)$ and the estimate $|G| \leq 1$ that these probabilities decrease with M , to the limits computed in the last section. In this subsection we investigate how quickly the limit $r_\infty = \lim_{M \rightarrow \infty} r_M(\alpha, \beta)$ is approached. We shall prove that

$$r_M(\alpha, \beta) = r_\infty + O(M^{-2}) \quad (10)$$

and show how to compute an asymptotic series for the remainder. The principal technique is Watson's lemma [18], which is suited for handling integrals of functions with branch points. The basic idea is to make a change of variables to eliminate the branch point and then integrate by parts.

Expanding the integral representation of the last section, we get

$$\begin{aligned} r_M(\alpha, \beta) &= \frac{|\alpha|^2}{2\pi} \int_0^{2\pi} |F|^2 |G|^{2M-2} d\theta \\ &\quad + \frac{|\beta|^2}{2\pi} \int_0^{2\pi} |G|^{2M} d\theta \\ &\quad + \frac{2\Re(\alpha\bar{\beta})}{2\pi} \int_0^{2\pi} \Re(F/G) |G|^{2M} d\theta. \end{aligned} \quad (11)$$

(The last term has no contribution from $\Im(\alpha\bar{\beta})$ because of symmetry.)

The coefficient of $|\alpha|^2$ is

$$p_M = \frac{1}{2\pi} \int_0^{2\pi} |F|^2 |G|^{2M-2} d\theta = \left(\frac{2}{\pi} - \frac{1}{2} \right) + 4I_M,$$

where

$$I_M = \frac{1}{2\pi} \int_{\pi/4}^{\pi/2} |F/G|^2 |G|^{2M} d\theta. \quad (12)$$

Here we have used the symmetry and periodicity of the integrand.

The functions appearing in the right hand side of (12) are analytic, with branch points at $\pi/4$. It will be useful to develop series expansions for them. When $\pi/4 < \theta < \pi/2$ we have from (8)

$$|G|^2 = \frac{(2 \sin \theta - \sqrt{-2 \cos 2\theta})^2}{2}.$$

Letting $\theta = \pi/4 + t$, this implies that

$$|G|^2 = 1 - 2\sqrt{2}s + 4s^2 - 2\sqrt{2}s^3 + \frac{5\sqrt{2}}{3}s^5 + O(s^6) \quad (13)$$

with $s = t^{1/2}$. We can derive a similar expression for $|F/G|^2$ as follows. Starting from (3) and (4) we get, after some algebra

$$\frac{f}{g} = z^2 - \sqrt{1+z^4} = z \left(z \pm \sqrt{z^2 + z^{-2}} \right).$$

When $z = e^{i\theta}$ and $\pi/4 < \theta < 3\pi/4$, the sign is positive, so

$$|F/G|^2 = \left| e^{i\theta} + i\sqrt{-2 \cos 2\theta} \right|^2 = 1 - 2 \cos 2\theta + 2 \sin \theta \sqrt{-2 \cos 2\theta}.$$

This implies

$$|F/G|^2 = 1 + 2\sqrt{2}s + 4s^2 + 2\sqrt{2}s^3 - \frac{5\sqrt{2}}{3}s^5 + O(s^6). \quad (14)$$

We now return to the evaluation of I_M . The substitution $e^{-u} = |G(\theta)|^2$ produces

$$I_M = \frac{1}{2\pi} \int_{\pi/4}^{\pi/2} |F|^2 |G|^{2M-2} d\theta = \frac{1}{2\pi} \int_0^{\log(3+2\sqrt{2})} \phi(u) e^{-uM} du. \quad (15)$$

When M is large, the factor ϕ influences the value of I_M only locally, that is, only through its Taylor series expansion near $u = 0$. Our next task is to determine this expansion. Recall that

$$e^{-u} = 1 - u + \sum_{k=2}^{\infty} (-1)^k \frac{u^k}{k!}. \quad (16)$$

Since this equals (13), the implicit function theorem implies that there is a function r , analytic around 0, for which $s = r(u)$. The coefficients of r can be computed term by term. Doing this, we get

$$r(u) = \frac{\sqrt{2}}{4}u + \frac{\sqrt{2}}{96}u^3 + \frac{11\sqrt{2}}{7680}u^5 + O(u^6). \quad (17)$$

From $r = t^{1/2}$ we get $r'(u)du = (1/2)t^{-1/2}dt$, so

$$\phi(u) = 2r(u)r'(u)|F/G|_{s=r(u)}^2. \quad (18)$$

Combining this with (14) and (17), we get

$$\phi(u) = \frac{1}{4}u + \frac{1}{4}u^2 + \frac{1}{6}u^3 + \frac{1}{12}u^4 + \frac{79}{1920}u^5 + O(u^6). \quad (19)$$

Now, integrate (15) by parts $\nu + 1$ times. We find that

$$I_M = \sum_{k=0}^{\nu} \frac{\phi^{(k)}(0)}{M^{k+1}} + O(M^{-\nu-2}). \quad (20)$$

Taking $\nu = 5$ and computing the derivatives from (19) gives us the asymptotic series

$$p_M = \left(\frac{2}{\pi} - \frac{1}{2}\right) + \frac{1}{2\pi M^2} + \frac{1}{\pi M^3} + \frac{2}{\pi M^4} + \frac{4}{\pi M^5} + \frac{79}{8\pi M^6} + O(M^{-7}). \quad (21)$$

Aficionados of the ‘‘law of small numbers’’ will appreciate that one must develop this series to order 6 to obtain a coefficient that does not fit the initial pattern.

Applying similar reasoning, the coefficient of $|\beta|^2$ is

$$q_M = \frac{1}{2} + \frac{1}{2\pi M^2} + \frac{1}{2\pi M^4} + \frac{19}{8\pi M^6} + O(M^{-7}), \quad (22)$$

and the coefficient of $2\Re(\alpha\bar{\beta})$ is

$$(pq)_M = \left(\frac{1}{\pi} - \frac{1}{2}\right) - \frac{1}{2\pi M^3} - \frac{3}{4\pi M^4} - \frac{2}{\pi M^5} - \frac{15}{4\pi M^6} + O(M^{-7}). \quad (23)$$

Using these in (11), we get (10).

3.4 Other Transformations

In this section we argue that the exit probabilities of the Hadamard walk are not really specific to the Hadamard transform. The argument can be generalized to other properties of the Hadamard walk. More generally, we show that it suffices to analyze unitary transformations U with only real entries.

Suppose instead of using the Hadamard transform we let U be the general transformation defined by:

$$U|L\rangle = a|L\rangle + b|R\rangle, \quad U|R\rangle = c|L\rangle + d|R\rangle. \quad (24)$$

We will consider generating functions $f_u(z)$ and $g_u(z)$ defined in Section 3.2 for this general transformation U . It is easy to see that these generating functions must satisfy

$$\begin{aligned} f_u(z) &= bz + azf_u(z)g_u(z) \\ g_u(z) &= dz + czf_u(z)g_u(z). \end{aligned}$$

Solving these equations for $f_u(z)$ and $g_u(z)$ and taking the solutions that make sense for small powers of z gives

$$\begin{aligned} f_u(z) &= \frac{1 - (ad - bc)z^2 - \sqrt{1 - 2(ad + bc)z^2 + (ad - bc)^2z^4}}{2cz} \\ g_u(z) &= \frac{1 + (ad - bc)z^2 - \sqrt{1 - 2(ad + bc)z^2 + (ad - bc)^2z^4}}{2az}. \end{aligned}$$

The first few terms of these functions are as follows:

$$\begin{aligned} f_u(z) &= bz + abdz^3 + abd(ad + bc)z^5 + abd(a^2d^2 + 3abcd + b^2c^2)z^7 + \\ &\quad abd(a^3d^3 + 6ab^2c^2d + 6a^2bcd^2 + b^3d^3)z^9 + \dots \\ g_u(z) &= dz + bcdz^3 + bcd(ad + bc)z^5 + bcd(a^2d^2 + 3abcd + b^2c^2)z^7 + \\ &\quad bcd(a^3d^3 + 6ab^2c^2d + 6a^2bcd^2 + b^3d^3)z^9 + \dots \end{aligned}$$

Letting $X = ad$ and $Y = bc$, we see that

$$\begin{aligned} f_u(z) &= \frac{1 - (X - Y)z^2 - \sqrt{1 - 2(X + Y)z^2 + (X - Y)^2z^4}}{2cz} \\ g_u(z) &= \frac{1 + (X - Y)z^2 - \sqrt{1 - 2(X + Y)z^2 + (X - Y)^2z^4}}{2az}. \end{aligned}$$

Next, we can simplify matters by taking into account that U is unitary. An arbitrary 2×2 unitary matrix can be written

$$e^{i\eta} \begin{pmatrix} e^{i(\phi+\psi)}\sqrt{\rho} & e^{i(-\phi+\psi)}\sqrt{1-\rho} \\ e^{i(\phi-\psi)}\sqrt{1-\rho} & -e^{i(-\phi-\psi)}\sqrt{\rho} \end{pmatrix} \quad (25)$$

where η, ϕ, ψ are real and $0 \leq \rho \leq 1$. The global phase of η will not affect the behavior of the walk in any way, so for simplicity we may set $\eta = 0$ without loss of generality. We will write $U_{\rho, \phi, \psi}$ to denote this transformation in order to stress the dependence on ρ, ϕ , and ψ . This leaves us with

$$\begin{aligned} X &= -\rho \\ Y &= 1 - \rho. \end{aligned}$$

Since $X - Y = -1$ and $-(X + Y) = 2\rho - 1$, we may write

$$f_{U_{\rho,\phi,\psi}}(z) = \frac{1 + z^2 - \sqrt{1 + 2(2\rho - 1)z^2 + z^4}}{2e^{i(-\phi+\psi)}\sqrt{1-\rho}z} \stackrel{\text{def}}{=} f_{\rho,\phi,\psi}(z)$$

$$g_{U_{\rho,\phi,\psi}}(z) = \frac{1 - z^2 - \sqrt{1 + 2(2\rho - 1)z^2 + z^4}}{2e^{i(\phi+\psi)}\sqrt{\rho}z} \stackrel{\text{def}}{=} g_{\rho,\phi,\psi}(z).$$

Thus,

$$|F_{\rho,\phi,\psi}(\theta)|^2 = \frac{1}{4(1-\rho)} \left| 1 + e^{2i\theta} - \sqrt{1 + 2(2\rho - 1)e^{2i\theta} + e^{4i\theta}} \right|^2$$

$$|G_{\rho,\phi,\psi}(\theta)|^2 = \frac{1}{4\rho} \left| 1 - e^{2i\theta} - \sqrt{1 + 2(2\rho - 1)e^{2i\theta} + e^{4i\theta}} \right|^2,$$

and as a result we see that, for instance, the quantities

$$p_M = \frac{1}{2\pi} \int_0^{2\pi} |F_{\rho,\phi,\psi}(\theta)|^2 |G_{\rho,\phi,\psi}(\theta)|^{2M-2} d\theta$$

$$q_M = \frac{1}{2\pi} \int_0^{2\pi} |G_{\rho,\phi,\psi}(\theta)|^{2M} d\theta$$

depend only on M and ρ . Therefore, the exit probabilities for the Hadamard walk would have been the same had we taken $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$ or $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$ rather than the Hadamard transform.

For arbitrary starting states, the exit probabilities may depend on ϕ and ψ in addition to ρ , but this change can be compensated for by considering slightly different starting states. Consider the starting state $|0\rangle (\alpha |L\rangle + \beta |R\rangle)$ and transformation $U_{\rho,\phi,\psi}$. Then the exit probability for this walk is

$$r_M(\alpha, \beta) = \frac{1}{2\pi} \int_0^{2\pi} |\alpha F_{\rho,\phi,\psi}(\theta) + \beta G_{\rho,\phi,\psi}(\theta)|^2 |G_{\rho,\phi,\psi}(\theta)|^{2M-2} d\theta.$$

But since $e^{i(-\phi+\psi)} f_{\rho,\phi,\psi} = f_{\rho,0,0}$ and $e^{i(\phi+\psi)} g_{\rho,\phi,\psi} = g_{\rho,0,0}$, we see that the exit probability is precisely the same as the exit probability for the walk given by unitary transformation $U_{\rho,0,0}$ and starting state $\alpha e^{i(\phi-\psi)} |0, L\rangle + \beta e^{i(-\phi-\psi)} |0, R\rangle$.

Consequently, it suffices to study the simpler type of transformation $U_{\rho,0,0}$, i.e., transformations of the form

$$|L\rangle \rightarrow \sqrt{\rho} |L\rangle + \sqrt{1-\rho} |R\rangle \quad \text{and} \quad |R\rangle \rightarrow \sqrt{1-\rho} |L\rangle - \sqrt{\rho} |R\rangle \quad (26)$$

for $\rho \in [0, 1]$ to determine the properties of more general walks. Such transformations have been considered by Yamasaki, Kobayashi and Imai [11]. In this case we get

$$f_U(z) = \frac{1 + z^2 - \sqrt{1 + 2(2\rho - 1)z^2 + z^4}}{2\sqrt{1-\rho}z}$$

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

Then

$$p_M = \frac{1}{2\pi} \int_0^{2\pi} |F_U(\theta)|^2 |G_U(\theta)|^{2M-2} d\theta$$

$$q_M = \frac{1}{2\pi} \int_0^{2\pi} |G_U(\theta)|^{2M} d\theta.$$

Letting $\theta_\rho = \frac{\cos^{-1}(1-2\rho)}{2}$, and $\Gamma_\rho = (-\theta_\rho, \theta_\rho) \cup (\pi - \theta_\rho, \pi + \theta_\rho)$, we see (after some algebra) that $|G_u(\theta)| = 1$ for $\theta \in \Gamma_\rho$ and $|G_u(\theta)| < 1$ for $\theta \notin \Gamma_\rho$. This gives

$$q_M \sim \frac{1}{2\pi} \int_{\Gamma_\rho} d\theta = \frac{\cos^{-1}(1-2\rho)}{\pi} = \frac{\sin^{-1}(2\rho-1)}{\pi} + \frac{1}{2}. \quad (27)$$

This agrees with Conjecture 1 of [11] and Eq. (45) below, obtained by the eigenvalue method (since $\cos^{-1}(1-2\rho) = 2 \sin^{-1} \sqrt{\rho}$). We also have

$$p_M \sim \frac{2}{\pi\sqrt{1/\rho-1}} + \frac{\rho}{(1-\rho)\pi} \cos^{-1}(1-2\rho) - \frac{\rho}{(1-\rho)}. \quad (28)$$

This can be computed as $1/(2\pi) \int_{\Gamma_\rho} |F/G|^2 d\theta$, but we leave this integration job to the interested reader. This value also follows from Eq. (45) below.

4 Eigenfunction method

In this section we present an eigenfunction method for computing absorption probabilities of quantum walks. We present the method for the quantum random walk introduced in Ref. [11]; the calculation for the general quantum walk corresponding to the transformation of Eq. (24) is straightforward but involves slightly more complicated notation. Letting $L(n, t)$ denote the amplitude of state $|n, L\rangle$ at time t and $R(n, t)$ denote the amplitude of state $|n, R\rangle$ at time t , the dynamical equations are

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} \sqrt{\rho} L(n+1, t-1) + \sqrt{1-\rho} R(n+1, t-1) \\ \sqrt{1-\rho} L(n-1, t-1) - \sqrt{\rho} R(n-1, t-1) \end{pmatrix}, \quad (29)$$

where we are ignoring boundaries for now. The Hadamard walk corresponds to the choice $\rho = 1/2$.

Though our main interest here is in studying systems with one or two absorbing boundaries, it will be very useful to have at our disposal the eigenfunctions for systems with no boundaries and for periodic systems. Therefore, we compute them first.

4.1 Systems with no boundaries

If one looks for solutions of the form

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} A_k \\ B_k \end{pmatrix} e^{i(kn - \omega_k t)},$$

then to satisfy Eq. (29) one must have

$$e^{-i\omega_k} \begin{pmatrix} A_k \\ B_k \end{pmatrix} = U_k \begin{pmatrix} A_k \\ B_k \end{pmatrix},$$

with

$$U_k = \begin{pmatrix} \sqrt{\rho} e^{ik} & \sqrt{1-\rho} e^{ik} \\ \sqrt{1-\rho} e^{-ik} & -\sqrt{\rho} e^{-ik} \end{pmatrix}.$$

The characteristic polynomial of U_k is $\lambda^2 - \sqrt{\rho} (e^{ik} - e^{-ik}) \lambda - 1$, so its eigenvalues are

$$\lambda_{k\pm} = \sqrt{\rho} \left[i \sin k \pm \sqrt{\cos^2 k + (-1 + 1/\rho)} \right]. \quad (30)$$

Since U_k is unitary we may write $\lambda_{k\pm} = e^{-i\omega_{k\pm}}$ with

$$\begin{aligned} \omega_{k+} &= -\sin^{-1}(\sqrt{\rho} \sin k) \\ \omega_{k-} &= \pi - \omega_{k+}. \end{aligned} \quad (31)$$

The corresponding eigenfunctions have the form (4.1) with

$$\begin{aligned} A_{k\pm} &= \frac{1}{\sqrt{2N}} \sqrt{1 \pm \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}}}, \\ B_{k\pm} &= \pm \frac{e^{-ik}}{\sqrt{2N}} \sqrt{1 \mp \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}}}. \end{aligned} \quad (32)$$

We have normalized these eigenfunctions so that $|A_{k,\sigma}|^2 + |B_{k,\sigma}|^2 = 1/N$, which makes the probabilities over any N consecutive lattice sites sum to 1. We have also chosen the arbitrary phase to ensure that the $A_{k\pm}$ are real and positive. The group velocity is

$$v_{\pm} \equiv \frac{d\omega_{\pm}}{dk} = \mp \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}}; \quad (33)$$

v_- is positive for $-\pi/2 < k < \pi/2$, and $v_+ = -v_-$ is positive for $-\pi < k < -\pi/2$ and for $\pi/2 < k < \pi$.

4.2 Model with periodic boundary conditions

We now consider a system whose boundary conditions are periodic with period N . Any wavefunction of this system can be written as a linear superposition of the eigenstates computed above:

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \sum_{\substack{k \in (-\pi, \pi) \\ \sigma = \pm}} C_{k,\sigma} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \end{pmatrix} e^{ikn - i\omega_{k,\sigma} t}. \quad (34)$$

For an initial condition of the form

$$\begin{pmatrix} L(n, 0) \\ R(n, 0) \end{pmatrix} = \delta_{n0} \begin{pmatrix} \alpha \\ \beta \end{pmatrix},$$

the $C_{k\pm}$ satisfy

$$\begin{pmatrix} A_{k+} & A_{k-} \\ B_{k+} & B_{k-} \end{pmatrix} \begin{pmatrix} C_{k+} \\ C_{k-} \end{pmatrix} = \frac{1}{N} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

Solving for the $C_{k\pm}$ yields

$$C_{k\pm} = A_{k\pm} \alpha + \overline{B_{k\pm}} \beta. \quad (35)$$

In the sequel we will consider periodic systems with N large compared to the physical feature of interest (i.e., $M \ll N$), with the idea of letting $N \rightarrow \infty$. As an alternative to this procedure, one could also average over the continuous variable k from the start.

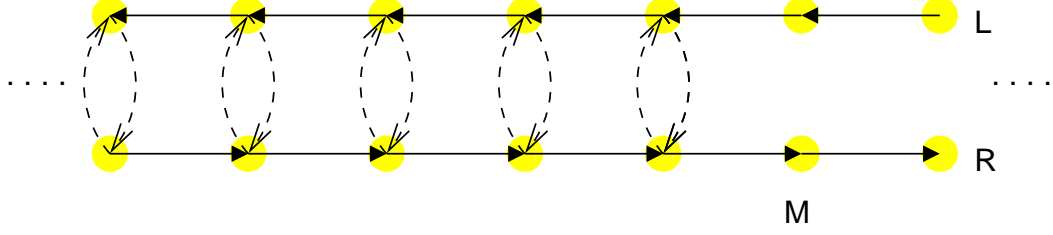


Figure 1: Diagram of system with unitary time evolution with dynamics that for all $n < M$ are identical to those of a quantum walk with an absorbing wall at position $n = M$.

4.3 Model with one absorbing boundary

Now consider a system with an absorbing wall at location $n = M$, where for definiteness we will take $M > 0$. For our purposes it is useful to think of the wall as a boundary through which right-movers can be transmitted, so that the problem remains unitary and probability is conserved. We extend the problem so that inside the domain the dynamics are identical to the original model, and outside the domain right-movers move right and left-movers move left, as shown in figure 1. Specifically, the model is as follows.

For $n < M - 1$:

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} \sqrt{\rho} L(n+1, t-1) + \sqrt{1-\rho} R(n+1, t-1) \\ \sqrt{1-\rho} L(n-1, t-1) - \sqrt{\rho} R(n-1, t-1) \end{pmatrix},$$

for $n \geq M$:

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L(n+1, t-1) \\ R(n-1, t-1) \end{pmatrix},$$

and finally, for the boundary condition:

$$\begin{pmatrix} L(M-1, t) \\ R(M-1, t) \end{pmatrix} = \begin{pmatrix} L(M, t-1) \\ \sqrt{1-\rho} L(M-2, t-1) - \sqrt{\rho} R(M-2, t-1) \end{pmatrix}. \quad (36)$$

There are no left-movers outside the domain, and once the right-movers go through the barrier they are no longer converted to left-movers, so one must have $L(M, t) = 0$ at all times t . The boundary condition Eq. (36) then implies that $L(M-1, t) = 0$ also at all times t .

Thus, our system evolves according to Eq. (29) and must satisfy $L(M-1, t) = 0$ at all times t . The eigenstates of the periodic system discussed above clearly do not satisfy this condition. The only way that $L(M-1, t)$ can vanish at all times t is for contributions from different k that have the same value of ω to interfere destructively (otherwise the contributions can cancel at some but not all times). From the dispersion relation Eq. (30), we see that $\omega_{k\pm} = \omega_{(\pi-k)\pm}$, and that there are no other degeneracies. Thus one is led to look for eigenfunctions of the form

$$\begin{pmatrix} \mathcal{L}_{k\pm}(n, t) \\ \mathcal{R}_{k\pm}(n, t) \end{pmatrix} = \mathcal{N}_{k\pm} \left[\begin{pmatrix} A_{k\pm} \\ B_{k\pm} \end{pmatrix} e^{ikn} + \zeta_{k\pm} \begin{pmatrix} A_{(\pi-k)\pm} \\ B_{(\pi-k)\pm} \end{pmatrix} e^{i(\pi-k)n} \right] e^{-i\omega_{k\pm}t}, \quad (37)$$

where the $\mathcal{N}_{k\pm}$ are normalization constants. The coefficients $\zeta_{k\pm}$ are fixed by requiring $\mathcal{L}(M-1, t) = 0$ for all t , or

$$A_{k\pm} e^{ik(M-1)} + \zeta_{k\pm} A_{(\pi-k)\pm} e^{i(\pi-k)(M-1)} = 0, \quad (38)$$

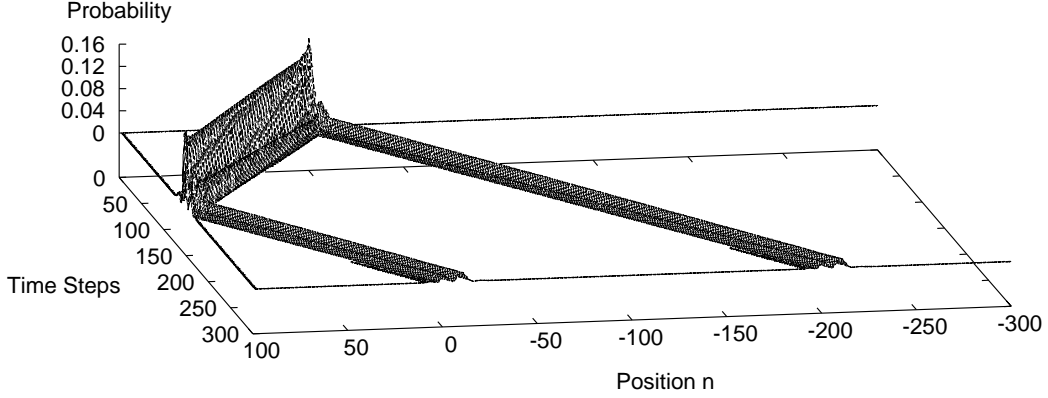


Figure 2: Probability $|L(n,t)|^2 + |R(n,t)|^2$ as a function of n and t of a Hadamard walk in one-dimension with one absorbing wall started from the initial condition $L(n,0) = 0$ and $R(n,0) \propto \exp(-n^2/100) \cos(\pi n/10)$, which is overwhelmingly composed of values of k very close to $\pi/10$. Two wavepackets propagate with group velocities $\pm v \approx 0.689$ (Eq. 33; both $+v$ and $-v$ are seen because the two bands propagate in opposite directions for a given k); one reflects from the absorbing boundary at position $n = 100$ with reflection probability $P_r \approx 0.184$ (Eq. 40).

yielding (using the $A_{k\pm}$ determined in Eq. (32))

$$\zeta_{k\pm} = - \left(\sqrt{1 + \frac{\cos^2 k}{-1 + 1/\rho}} \pm \frac{\cos k}{\sqrt{-1 + 1/\rho}} \right) e^{-i(\pi - 2k)(M-1)}.$$

This situation is analogous to what one finds when one considers the scattering of a particle by a potential step, as discussed in many elementary quantum mechanics texts (see, e.g., [19]; also see [8]). A rightmoving wave hits the step; the reflected wave is leftgoing. Figure 2, which shows the time evolution of a Hadamard walk starting from an initial condition that is a superposition of a small band of k 's, shows that an absorbing wall indeed acts in this manner.

We know that in the $-$ band the wavefunctions proportional to e^{ikn} with wavevectors k in the range $(-\pi/2, \pi/2)$ are rightgoing, and we interpret with component at wavevector $\pi - k$ as the leftgoing piece generated by reflection off the boundary. The probability that a wave is reflected, $P_r(k)$, is just (for $k \in (-\pi/2, \pi/2)$)

$$P_r(k) = |\zeta_{k-}|^2 = \left(\sqrt{1 + \frac{\cos^2 k}{-1 + 1/\rho}} - \frac{\cos k}{\sqrt{-1 + 1/\rho}} \right)^2. \quad (39)$$

Similar calculations for the reflection coefficient of rightmoving wavepackets in the other band and also for leftmoving waves that are reflected at a boundary at which $R(-M+1, t) = 0$ at all times t yields that the probability of reflection at wavevector k in all cases is

$$P_r(k) = |\zeta_{k-}|^2 = \left(\sqrt{1 + \frac{\cos^2 k}{-1 + 1/\rho}} - \frac{|\cos k|}{\sqrt{-1 + 1/\rho}} \right)^2. \quad (40)$$

These reflection coefficients agree well with the results of our numerical simulations.

We now need to write the initial condition as a superposition of eigenfunctions. Perhaps the simplest way to do this is to use the method of images. Thus, we consider a system with no boundary; one introduces an image outside the domain that is adjusted to enforce the appropriate boundary condition, which here is $L(M-1, t) = 0$ for all t . We consider initial conditions in which the ‘‘physical’’ particle is at the origin,

$$\begin{pmatrix} L(n, 0) \\ R(n, 0) \end{pmatrix} = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \delta_{n0}.$$

The form of the unnormalized wavefunction derived above suggests that it will be useful to consider together the pairs of wavevectors $k, \pi - k$. Thus we write

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} \delta_{n,0} = \sum_{\substack{k \in (-\pi/2, \pi/2) \\ \sigma = \pm}} \left\{ C_{k,\sigma} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \end{pmatrix} e^{ikn} + C_{\pi-k,\sigma} \begin{pmatrix} A_{\pi-k,\sigma} \\ B_{\pi-k,\sigma} \end{pmatrix} e^{i(\pi-k)n} \right\},$$

where the $C_{k,\sigma}$ are given in Eq. (35). We now attempt to place an image so that the condition $L(M-1, t) = 0$ holds at all t . We guess that the image particle should be at $n = 2(M-1)$ (again, this is suggested by the form of Eq. (37)) and try writing

$$\begin{aligned} \begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} &= \sum_{\substack{k \in (-\pi/2, \pi/2) \\ \sigma = \pm}} e^{-i\omega_{k,\sigma}t} \left[\left\{ C_{k,\sigma} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \end{pmatrix} e^{ikn} + C_{\pi-k,\sigma} \begin{pmatrix} A_{\pi-k,\sigma} \\ B_{\pi-k,\sigma} \end{pmatrix} e^{i(\pi-k)n} \right\} \right. \\ &+ \left. \left\{ D_{k,\sigma} \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \end{pmatrix} e^{ik(n-2(M-1))} + D_{\pi-k,\sigma} \begin{pmatrix} A_{\pi-k,\sigma} \\ B_{\pi-k,\sigma} \end{pmatrix} e^{i(\pi-k)(n-2(M-1))} \right\} \right], \end{aligned} \quad (41)$$

where once again we have used the fact that $\omega_{k,\sigma} = \omega_{\pi-k,\sigma}$. Again, since $L(M-1, t) = 0$ for all times, we must have for each $k \in (-\pi/2, \pi/2)$:

$$\begin{aligned} &C_{k,\sigma} A_{k,\sigma} e^{ik(M-1)} + C_{\pi-k,\sigma} A_{\pi-k,\sigma} e^{i(\pi-k)(M-1)} \\ &+ D_{k,\sigma} A_{k,\sigma} e^{-ik(M-1)} + D_{\pi-k,\sigma} A_{\pi-k,\sigma} e^{-i(\pi-k)(M-1)} = 0. \end{aligned}$$

It is straightforward to verify that this equation is satisfied if we choose

$$D_{k,\sigma} = -e^{i\pi(M-1)} C_{\pi-k,\sigma} \frac{A_{\pi-k,\sigma}}{A_{k,\sigma}}.$$

Hence, inside the domain ($n < M$) the time-dependent wavefunction is

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \sum_{\substack{k \in (-\pi/2, \pi/2) \\ \sigma = \pm}} e^{-i\omega_{k,\sigma}t} \left\{ \begin{pmatrix} A_{k,\sigma} \\ B_{k,\sigma} \end{pmatrix} e^{ikn} \mathcal{F}_{k,\sigma} + \begin{pmatrix} A_{\pi-k,\sigma} \\ B_{\pi-k,\sigma} \end{pmatrix} e^{i(\pi-k)n} \mathcal{G}_{k,\sigma} \right\}, \quad (42)$$

with

$$\begin{aligned} \mathcal{F}_{k,\sigma} &= \left[C_{k,\sigma} - e^{i(\pi-2k)(M-1)} C_{\pi-k,\sigma} \frac{A_{\pi-k,\sigma}}{A_{k,\sigma}} \right] \\ \mathcal{G}_{k,\sigma} &= \left[C_{\pi-k,\sigma} - e^{-i(\pi-2k)(M-1)} C_{k,\sigma} \frac{A_{k,\sigma}}{A_{\pi-k,\sigma}} \right]. \end{aligned} \quad (43)$$

As expected, this wavefunction satisfies Eq. (38).

The wavefunction of Eq. (42) is a superposition of wavefunctions proportional to e^{ikn} , which describe free particles propagating with constant velocity $d\omega/dk$ (often called plane waves, since in higher dimensions the surfaces of constant phase are planes). In the limit of long times, the only components that are in the physical domain are leftgoing, which for $k \in (-\pi/2, \pi/2)$ are $((k, +)$ and $(\pi - k, -)$. Therefore, Λ_M , the probability that the particle escapes to $n \rightarrow -\infty$ when the absorbing wall is at M , is

$$\Lambda_M = \sum_{k \in (-\pi/2, \pi/2)} |\mathcal{F}_{k,+}(M)|^2 + |\mathcal{G}_{k,-}(M)|^2.$$

Using Eqs. (43), (35), and (32), we see that $\mathcal{G}_{k,-}(M) = \overline{\mathcal{F}_{k,+}(M)}$, so

$$\Lambda_M = 2 \sum_{k \in (-\pi/2, \pi/2)} |\mathcal{F}_{k,+}(M)|^2,$$

with

$$\mathcal{F}_{k,+}(M) = \frac{\alpha}{A_{k+}} \left(A_{k+}^2 - e^{i(\pi-2k)(M-1)} A_{k-}^2 \right) + \beta A_{k-} \left(e^{ik} + e^{i(\pi-2k)(M-1)} e^{-ik} \right).$$

Converting the sum to an integral, and noting that the integrals of terms that are odd in k vanish, we find that

$$\Lambda_M = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} dk \mathcal{L}_M(k),$$

with

$$\begin{aligned} \mathcal{L}_M(k) = & \ell^2 \left(1 - \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}} \right) \left(\frac{1/\rho + \cos(2k)}{1/\rho - 1} + \cos(\pi M) \cos(2k(M-1)) \right) \\ & + r^2 \left(1 - \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}} \right) (1 - \cos(\pi M) \cos(2kM)) \\ & + 2\ell r \cos \Phi \left(\frac{\cos k}{\sqrt{1/\rho - 1}} \right) \left(1 - \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}} \right) (\cos k - \cos(\pi M) \cos(k(2M-1))), \end{aligned} \quad (44)$$

where we have written $\alpha = \ell e^{i\phi_l}$, $\beta = r e^{i\phi_r}$, and $\Phi = \phi_l - \phi_r$. We obtain

$$\begin{aligned} \Lambda_M(\rho) = & \ell^2 \left(-\frac{2}{\pi \sqrt{1/\rho - 1}} + \frac{1}{1-\rho} \left(1 - \frac{2\rho}{\pi} \sin^{-1} \sqrt{\rho} \right) \right. \\ & \left. - \frac{1}{\pi} (-1)^M \int_{-\pi/2}^{\pi/2} dk \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}} \cos(2k(M-1)) \right) \\ & + r^2 \left(1 - \frac{2}{\pi} \sin^{-1} \sqrt{\rho} + \frac{1}{\pi} (-1)^M \int_{-\pi/2}^{\pi/2} dk \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}} \cos(2kM) \right) \\ & + \ell r \cos \Phi \left(\frac{1}{\sqrt{1/\rho - 1}} - \frac{2}{\pi} \left(1 + \frac{1-2\rho}{\sqrt{\rho(1-\rho)}} \sin^{-1} \sqrt{\rho} \right) \right. \\ & \left. + \frac{2}{\pi} \frac{(-1)^M}{\sqrt{1/\rho - 1}} \int_{-\pi/2}^{\pi/2} dk \frac{\cos^2 k}{\sqrt{1/\rho - \sin^2 k}} \cos(k(2M-1)) \right). \end{aligned} \quad (45)$$

M	\mathcal{C}_ℓ	\mathcal{C}_r	$\mathcal{C}_{\ell r}$
1	$1 - \frac{2}{\pi} \approx 0.36338$	$1 - \frac{2}{\pi} \approx 0.36338$	$2 - \frac{4}{\pi} \approx 0.72676$
2	$2 - \frac{4}{\pi} \approx 0.72676$	$3 - \frac{8}{\pi} \approx 0.45352$	$3 - \frac{8}{\pi} \approx 0.45352$
3	$4 - \frac{10}{\pi} \approx 0.816901$	$13 - \frac{118}{3\pi} \approx 0.479811$	$11 - \frac{100}{3\pi} \approx 0.38967$
4	$14 - \frac{124}{3\pi} \approx 0.843191$	$65 - \frac{608}{3\pi} \approx 0.489196$	$53 - \frac{496}{3\pi} \approx 0.372765$
5	$66 - \frac{614}{3\pi} \approx 0.852577$	$341 - \frac{16046}{15\pi} \approx 0.493304$	$277 - \frac{13036}{15\pi} \approx 0.367488$
∞	$\frac{3}{2} - \frac{2}{\pi} \approx 0.86338$	$\frac{1}{2}$	$1 - \frac{2}{\pi} \approx 0.36338$

Table 1: Coefficients characterizing the probability of escape to $-\infty$ of the Hadamard walk started in the initial state $\alpha |0, L\rangle + \beta |0, R\rangle$ by an absorbing wall at M . Here, $\alpha = \ell e^{i\phi_l}$, $\beta = r e^{i\phi_r}$, and $\Phi = \phi_l - \phi_r$. The quantity Λ_M , the probability of escape to $-\infty$ when the wall is located at M , is given by $\Lambda_M = \ell^2 \mathcal{C}_\ell(M) + r^2 \mathcal{C}_r(M) + \ell r \cos \Phi \mathcal{C}_{\ell r}(M)$. The probability of absorption by the wall is $1 - \Lambda_M$.

If instead of Eq. (26) we use the more general transformation of Eq. (25), one finds that the only change in Eq. (45) is that $\cos \Phi \rightarrow \cos(\Phi + 2\phi)$. Thus, as noted in Sec. 3.4, the absorption probabilities do not depend on η or ψ , and the ϕ dependence can be removed by suitable adjustment of the initial condition.

Eq. (45) only applies when $M > 1$, because when $M = 1$ the initial condition is inconsistent with the boundary condition unless $\alpha = 0$. This complication for $M = 1$ is easily handled by evolving the walk for one time step by hand; for the initial condition $\alpha |L, 0\rangle + \beta |R, 0\rangle$ the probability of escape to $-\infty$ when $M = 1$ is related to Λ_{2L} , the probability that a walk starting in the state $|L, 0\rangle$ escapes to $n \rightarrow -\infty$ when the wall is at $M = 2$, by

$$\Lambda_1 = |\alpha\sqrt{\rho} + \beta\sqrt{1-\rho}|^2 \Lambda_{2L}.$$

For the special case of the Hadamard walk ($\rho = 1/2$, $\phi = 0$), we find $\Lambda_1 = (1 + 2\ell r \cos \Phi)(1 - 2/\pi)$. Values for other finite values of M are easily obtained by evaluation of the integrals in Eq. (45); a few values for the Hadamard walk are listed in Table 1.

In the limit $M \rightarrow \infty$ all the M -dependent terms vanish because of the oscillating integrands. The coefficient of the r^2 term in the limit $M \rightarrow \infty$ has been correctly conjectured by Yamasaki et al. [11] on the basis of numerical results. In the limit $M \rightarrow \infty$, the probability that a particle undergoing a Hadamard walk escapes to $n \rightarrow -\infty$ is

$$\Lambda_\infty = \ell^2 \left(\frac{3}{2} - \frac{2}{\pi} \right) + \frac{r^2}{2} + \ell r \cos \Phi \left(1 - \frac{2}{\pi} \right). \quad (46)$$

As expected, this agrees with Eq. (9). Integration by parts of the integrals in Eq. (45) may be used to find the behavior at large but finite M (c.f., Eqs. (21–23)).

4.4 Model with two absorbing boundaries

Now we discuss the situation in which there are two absorbing walls, so the domain of the quantum walk is finite. We restrict consideration to the Hadamard walk ($\rho = 1/2$, $\eta = \psi = \phi = 0$), but

no essential complications are introduced when η , ϕ , ψ , or ρ take on different values. We place the walls at $+M_R$ and $-M_L$ and again start the walker out at position $n = 0$.

By exploiting the results obtained above for the single wall case, it is rather simple to compute the absorption probabilities when M_L is very large. This can be seen by noting that because when the walls are very far apart, the evolution can be viewed as a succession of reflections off the two walls followed by a single transmission. From Eq. (40), we know that the reflection probability is $P_r = (\sqrt{1 + \cos^2 k} - |\cos k|)^2$. Let us denote by $\mathcal{T}_{LM_R}(k)$ the probability of transmission through (or, in other words, absorption by) the left boundary of the component at wavevector k when the right wall is at M_R . Because the wavepacket can be absorbed at $-M_L$ the first time it hits that boundary, or it can be reflected at both the left and right boundaries and then absorbed at the left boundary, etc., we have

$$\begin{aligned}\mathcal{T}_{LM_R}(k) &= \mathcal{L}_{M_R}(k) [(1 - P_r) + P_r P_r (1 - P_r) + P_r P_r P_r (1 - P_r) + \dots] \\ &= \mathcal{L}_{M_R}(k) \frac{1}{1 + P_r} \\ &= \frac{1}{2} \mathcal{L}_{M_R}(k) \left(1 + \frac{\cos k}{\sqrt{1 + \cos^2 k}} \right),\end{aligned}$$

where $\mathcal{L}_{M_R}(k)$ is defined in Eq. (44).

When $M_R > 1$, the transmission through the left wall when the right wall is located at M_R , T_{LM_R} , is thus

$$T_{LM_R} = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} dk \mathcal{T}_{LM_R}(k),$$

with

$$\begin{aligned}\mathcal{T}_{LM_R}(k) &= \frac{1}{2} \ell^2 \frac{1}{1 + \cos^2 k} (2 + \cos(2k) + \cos(\pi M) \cos(2k(M - 1))) \\ &\quad + \frac{r^2}{2} \frac{1}{1 + \cos^2 k} (1 - \cos(\pi M) \cos(2kM)) \\ &\quad + \ell r \cos \Phi \cos k \frac{1}{1 + \cos^2 k} (\cos k - \cos(\pi M) \cos(k(2M - 1))).\end{aligned}$$

Once again the $M_R = 1$ case is done by evolving the system by hand for one time step. The results for some finite values of M_R are listed in Table 2. The result for $M_R = 1$ was obtained previously in Ref. [2].

As $M_R \rightarrow \infty$, the absorption by the left wall, $T_{L\infty}$ is

$$T_{L\infty} = \ell^2 \left(1 - \frac{1}{2\sqrt{2}} \right) + r^2 \left(\frac{1}{2\sqrt{2}} \right) + \ell r \cos \Phi \left(1 - \frac{1}{\sqrt{2}} \right)$$

The minimum value of $T_{L\infty}$ is when $\Phi = \pi$, $\ell = \sin(\pi/8)$, where $T_{L\infty} = 1 - 1/\sqrt{2} \approx 0.292893$, and the maximum value of $T_{L\infty}$ occurs when $\Phi = 0$, $\ell = \sin(3\pi/8)$, where $T_{L\infty} = 1/\sqrt{2} \approx 0.707107$.

When the two walls are close together, the calculations are straightforward in principle but tedious in practice. The overall strategy of the calculation in this case is exactly the same as in all the calculations above—instead of considering a problem with absorbing barriers, one considers a unitary problem whose time evolution is identical within the physical domain. Here we embed the walk in a large periodic domain; the model is as follows.

For $-M_L + 1 < n < M_R - 1$:

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} L(n+1, t-1) + R(n+1, t-1) \\ L(n-1, t-1) - R(n-1, t-1) \end{pmatrix}$$

M	D_ℓ	D_r	D_{lr}
1	$1 - \frac{1}{\sqrt{2}} \approx 0.292893$	$1 - \frac{1}{\sqrt{2}} \approx 0.292893$	$2 - \sqrt{2} \approx 0.585786$
2	$2 - \sqrt{2} \approx 0.585786$	$6 - 4\sqrt{2} \approx 0.343146$	$6 - 4\sqrt{2} \approx 0.343146$
3	$7 - \frac{9}{\sqrt{2}} \approx 0.636039$	$35 - \frac{49}{\sqrt{2}} \approx 0.351768$	$30 - 21\sqrt{2} \approx 0.301515$
4	$36 - 25\sqrt{2} \approx 0.64461$	$204 - 144\sqrt{2} \approx 0.353247$	$170 - 120\sqrt{2} \approx 0.294373$
5	$205 - \frac{289}{\sqrt{2}} \approx 0.64614$	$1189 - \frac{1681}{\sqrt{2}} \approx 0.353501$	$986 - 697\sqrt{2} \approx 0.293147$
∞	$1 - \frac{1}{2\sqrt{2}} \approx 0.646447$	$\frac{1}{2\sqrt{2}} \approx 0.353553$	$1 - \frac{1}{\sqrt{2}} \approx 0.292893$

Table 2: Coefficients characterizing the probability of escape through the left barrier to $-\infty$ of the quantum walk started in the initial state $\alpha |0, L\rangle + \beta |0, R\rangle$ with absorbing walls at M and at $-M_L$, when $M_L \rightarrow \infty$. Here, $\alpha = \ell e^{i\phi_l}$, $\beta = r e^{i\phi_r}$, and $\Phi = \phi_l - \phi_r$. The quantity $\mathcal{T}_L(M)$, the probability of escape to $-\infty$, is given by $\mathcal{T}_L(M) = \ell^2 D_\ell(M) + r^2 D_r(M) + \ell r \cos \Phi D_{lr}(M)$. The probability of absorption by the right wall at M is $1 - \mathcal{T}_L(M)$.

for $n \geq M_R$ and $n \leq -M_L$:

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L(n+1, t-1) \\ R(n-1, t-1) \end{pmatrix}$$

and for the boundary points:

$$\begin{pmatrix} L(M_R - 1, t) \\ R(M_R - 1, t) \end{pmatrix} = \begin{pmatrix} L(M_R, t-1) \\ \frac{1}{\sqrt{2}} (L(M_R - 2, t-1) - R(M_R - 2, t-1)) \end{pmatrix}$$

$$\begin{pmatrix} L(-M_L + 1, t) \\ R(-M_L + 1, t) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} (L(-M_L + 2, t-1) + R(-M_L + 2, t-1)) \\ R(-M_L, t-1) \end{pmatrix}$$

We wish to find the energy eigenstates that satisfy

$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L_\omega(n) \\ R_\omega(n) \end{pmatrix} e^{-i\omega t}$$

and are consistent with the boundary conditions $L(M_R + N) = L(-M_L)$, $R(M_R + N) = R(-M_L)$.

The eigenvalues and eigenfunctions of the model are specified by these conditions and can be found similarly to those of systems with a finite square well potential [7]. In the ‘‘outer’’ region, the eigenfunctions take the form

$$\begin{pmatrix} u_\omega e^{-i\omega n} \\ v_\omega e^{i\omega n} \end{pmatrix} e^{-i\omega t},$$

where the periodic boundary condition is enforced by requiring $e^{i\omega(M_L+N)} = e^{-i\omega M_R}$; the u and v will be fixed by matching to the inner region. Since we wish to take $N \rightarrow \infty$, there will be a continuum of values of ω . Finding the wavefunction for all M_L and M_R is rather involved; for every ω one must match the inner and outer wavefunctions, keeping in mind that in the inner region there are ranges of ω for which there are no solutions proportional to e^{ikn} with k real and

instead the wavefunctions have the form $e^{\kappa n}$ with κ real. When the inner region is small, the eigenfunctions can be found by brute force matching to the outer region. For $M_L = 1, M_R = 1$, we have $L_\omega(0) = u_\omega$ and $R_\omega(0) = v_\omega$. The wavefunction must satisfy the initial condition, so $u_\omega = \alpha$ and $v_\omega = \beta$. Thus, for this case, as expected, the probability of absorption at the right and barriers are $|\beta|^2$ and $|\alpha|^2$, respectively. When $M_L = 1, M_R = 2$, the coefficients $L_\omega(n)$ in the ‘‘inner’’ region satisfy the following:

$$\begin{aligned} L_\omega(0) &= \frac{1}{\sqrt{2}} e^{i\omega} (L_\omega(1) + R_\omega(1)), \\ L_\omega(1) &= u_\omega, \\ R_\omega(1) &= \frac{1}{\sqrt{2}} e^{i\omega} (L_\omega(0) - R_\omega(0)), \\ R_\omega(0) &= v_\omega. \end{aligned}$$

These equations can be solved to yield $L_\omega(0)$ and $R_\omega(1)$ in terms of u_ω and v_ω , which are in turn fixed by enforcing the initial condition. However, the algebra is complicated and will not be given here.

4.5 Arithmetic properties of exit probabilities

In this subsection we discuss what can be said about the exact exit probabilities for the Hadamard walk.

Examination of Table 1 above suggests that the coefficients $\mathcal{C}_\ell(M)$, $\mathcal{C}_r(M)$, and $\mathcal{C}_{\ell r}(M)$ are all rational numbers plus rational multiples of $1/\pi$. This can be proved as follows. Taking $\rho = 1/2$ in Eq. (45) we get for $M > 1$

$$\mathcal{C}_\ell(M) = \left(\frac{3}{2} - \frac{2}{\pi} \right) - \frac{(-1)^M}{\pi} \int_{-\pi/2}^{\pi/2} \frac{\cos k \cos(2(M-1)k)}{\sqrt{1 + \cos^2 k}} dk, \quad (47)$$

$$\mathcal{C}_r(M) = \frac{1}{2} + \frac{(-1)^M}{\pi} \int_{-\pi/2}^{\pi/2} \frac{\cos k \cos(2Mk)}{\sqrt{1 + \cos^2 k}} dk,$$

and

$$\mathcal{C}_{\ell r}(M) = 1 - \frac{2}{\pi} + \frac{2}{\pi} (-1)^M \int_{-\pi/2}^{\pi/2} \frac{\cos^2 k \cos((2M-1)k)}{\sqrt{1 + \cos^2 k}} dk.$$

In the notation of section 3, these are $1 - p_M$, $1 - q_M$, and $-2(pq)_M$, respectively.

The integrals can be evaluated by observing that $\cos(mk) = T_m(\cos k)$, where T_m is the degree m Chebyshev polynomial of the first kind. The polynomial T_m has integral coefficients, and is even or odd depending on whether m is even or odd. Making the substitution $u = \cos k$, we see (since we started with even integrands) that each of the integrals is a linear combination, with rational coefficients, of expressions of the form

$$\int_0^1 \frac{u^j}{\sqrt{1-u^4}} du = \frac{\sqrt{\pi}}{4} \cdot \frac{\Gamma((j+1)/4)}{\Gamma((j+3)/4)}$$

with j odd. For such j , one of $\{(j+1)/4, (j+3)/4\}$ is an integer and the other is a half integer. Thus one of the Γ values is an integer and the other is a rational multiple of $\sqrt{\pi}$, giving the desired form.

A similar argument can be used to prove that the coefficients D_ℓ , D_r , and $D_{\ell r}$ of Table 2 are rational numbers plus rational multiples of $\sqrt{2}$. For this one needs the integral

$$\int_0^1 \frac{u^{2j}}{(1+u^2)\sqrt{1-u^2}} du.$$

If we substitute $u^2 = t$ and use Theorem 2.2.2 of [20], we see it equals

$$\frac{\sqrt{\pi}}{2} \cdot \frac{\Gamma(j+1/2)}{\Gamma(j+1)} {}_2F_1 \left[\begin{matrix} 1, j+1/2 \\ j+1 \end{matrix}; -1 \right],$$

where ${}_2F_1$ is the Gaussian hypergeometric function. It then follows from (15.3.5) and (15.4.11) of [21] that the coefficients have the desired form.

These observations allow us to generalize a result of [2]. Suppose we start both walks at the same distance from the right barrier, in the state $\alpha = 1, \beta = 0$. Then the escape probability for the 1-barrier walk is never equal to the limit (as the left barrier recedes to $-\infty$) of the corresponding probability for the 2-barrier walk. This is so because π is not an algebraic number, and the coefficient of $1/\pi$ in $C_\ell(M)$ is nonzero. (This last point can be verified as follows. From the explicit form of T_m given in (22.3.6) of [21] we see that the nonzero coefficients of T_m alternate in sign, and when m is even, T_m has constant term $(-1)^{m/2}$. From this it follows that every term that the integral in (47) contributes to the coefficient $1/\pi$ is negative, so that $2/\pi$ in (47) cannot be cancelled out.) The physical interpretation of this result is that no matter how far away the second wall is, it reflects probability back to the first wall.

The precise arithmetic properties of these numbers are interesting to contemplate. We can show, for example, that when $C_\ell(M) = c_{M,1} + c_{M,2}/\pi$, the denominator of $c_{M,2}$ divides the product of the odd numbers in $\{1, \dots, M-1\}$. The first coefficient $c_{M,1}$ is always an integer, as suggested by Table 1.

4.6 Time dependence of absorption

The eigenfunction method can be used to calculate the time evolution of the absorption by the boundaries. We consider here the situation when the walker starts off far from any boundary (M large). We also specialize to $\rho = 1/2$; once again, generalization to other transformations is straightforward.

When there are two walls, the approach to the asymptotic behavior is quite slow. This is because the reflection coefficient tends to unity as $k \rightarrow \pi/2$, and the group velocity v_g also vanishes as $k \rightarrow \pi/2$. Therefore, it takes a very long time for all the probability to be absorbed at the walls—the fast-moving wavepackets are absorbed quickly, but as the evolution proceeds one is left with components that move slower and slower and are absorbed less and less. The fraction of the probability at wavevector k that is absorbed per unit time is

$$\frac{[\text{fraction of probability absorbed per collision}]}{[\text{time between collisions}]} = \frac{1 - P_r(k)}{2M/v_g(k)} = \frac{1 - \left(\sqrt{1 + \cos^2 k} - \cos k\right)^2}{2M\sqrt{1 + \cos^2 k} / \cos k} \equiv \gamma_k,$$

where we have used the forms for the reflection coefficient $P_r(k)$ and the group velocity $v_g(k)$ from Eqs. (40) and (33), respectively. Thus, the change in probability \mathcal{P}_k at wavevector k in a time Δt is approximately

$$(\mathcal{P}_k(t + \Delta t) - \mathcal{P}_k(t)) / \Delta t \approx -\gamma_k \mathcal{P}_k(t), \quad (48)$$

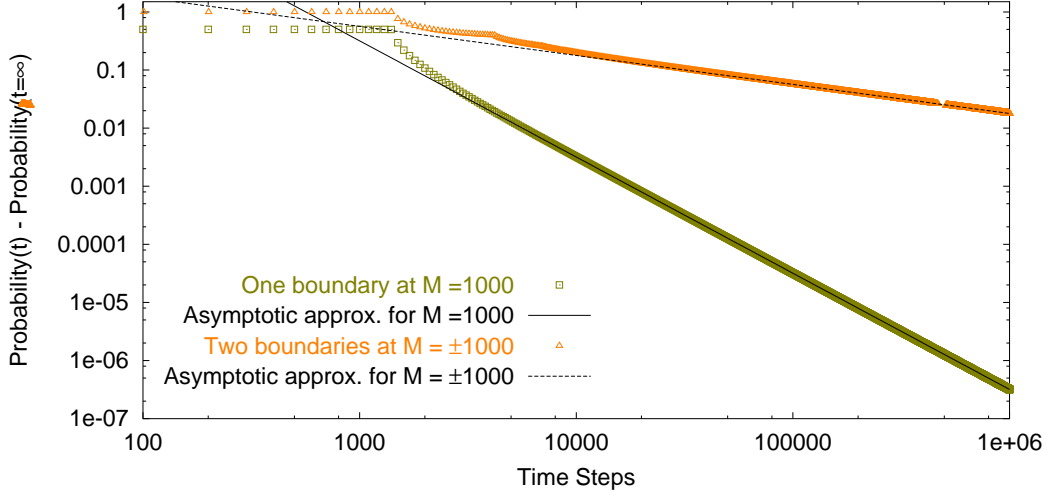


Figure 3: The time dependence of $\mathcal{P}(t)$, the probability that the particle has not been absorbed, is different in systems with one and two absorbing boundaries. With one boundary, $\mathcal{P}(t) \propto \mathcal{P}(\infty) + \text{constant}/t^2$ (Eq. (51)), while with two boundaries, $\mathcal{P}(t) \propto 1/\sqrt{t}$ (Eq. (50)). The faster approach to the asymptotic value for systems with one boundary is because there are no repeated reflections, while the constant probability at short times for both systems is because no probability has yet reached the boundary at position M . Simulations and the analytic forms are all obtained using the initial conditions $\ell = 0$ and $r = 1$. The probability at $t = \infty$ for one boundary is given by Eq. (45), and for two boundaries it is zero.

which in limit of slow variation, which is appropriate at long times, yields the differential equation

$$\frac{d\mathcal{P}_k}{dt} \sim -\gamma_k \mathcal{P}_k(t), \quad (49)$$

so that $\mathcal{P}_k(t) = \mathcal{P}_k(0)e^{-\gamma_k t}$. The total probability that the particle is inside the region at time t , $\mathcal{P}(t)$, is the integral over wavevectors k of the probabilities $\mathcal{P}_k(t)$. At long times the probability is dominated by k 's near $\pm\pi/2$ (since the decay rate tends to zero there); expanding for k 's near $\pm\pi/2$ yields

$$\mathcal{P}(t) = \frac{2}{\pi} \int_0^{\pi/2} dk (\mathcal{P}_{\pi/2}(0) + \mathcal{P}_{-\pi/2}(0)) e^{-(\pi/2-k)^2 t/M},$$

where the choice of initial condition determines $\mathcal{P}_{\pm\pi/2}(0)$. The leading asymptotic behavior as $t \rightarrow \infty$, obtained by evaluating this integral, is

$$\mathcal{P}(t) \propto \sqrt{\frac{M}{t}}. \quad (50)$$

When there is one wall that is far from the origin, the approach of the absorption probability to the asymptotic value is faster because there is no possibility of repeated reflections. The behavior can be characterized using Eq. (41) by calculating the total left-going probability from the physical particle,

$$\int_{-\pi/2}^{\pi/2} dk (|C_{k,+}|^2 + |C_{\pi-k,-}|^2),$$

the fraction of right-going probability from the physical particle that has yet to reach the wall position $n = M$,

$$\int_{\cos^{-1}\left(\frac{M/t}{\sqrt{1-(M/t)^2}}\right)}^{\pi/2} dk (|C_{k,+}|^2 + |C_{\pi-k,-}|^2),$$

and the fraction of left-going probability from the image particle that has already passed the wall position $n = M$,

$$\int_{-\cos^{-1}\left(\frac{M/t}{\sqrt{1-(M/t)^2}}\right)}^{\cos^{-1}\left(\frac{M/t}{\sqrt{1-(M/t)^2}}\right)} dk (|D_{k,+}|^2 + |D_{\pi-k,-}|^2),$$

as a function of time. The C 's and D 's represent probability amplitudes of plane waves emanating from the physical and image particle, respectively, as indicated in Eq. (41), and the limits of integration take into account that at time T , only the k 's for which $v_g T < M$ have yet to reach the wall. This gives the asymptotic time dependence for the probability as

$$\mathcal{P}(t) = \mathcal{P}(\infty) + \frac{M^2}{\pi t^2} + O\left(\frac{M^3}{t^3}\right), \quad (51)$$

where $\mathcal{P}(\infty) = \Lambda_M(\rho = 1/2)$ is given in Eq. (45). Figure 3 demonstrates that the asymptotic forms (50) and (51) provide an excellent description of the time dependence for times greater than a few times the system size.

5 Quantum walks in general dimensionality

5.1 Introduction

A quantum walk on a D -dimensional lattice $\vec{n} \in \mathbb{Z}^D$ may be defined in several ways. We shall adopt the following definition. One-dimensional quantum walks are discrete-time quantum processes on the space

$$\mathcal{H}(\mathbb{Z}^D \times \{L_1, R_1, L_2, R_2, \dots, L_D, R_D\}).$$

The standard basis for this space therefore consists of elements of the form $|n_1, d_1\rangle \otimes |n_2, d_2\rangle \otimes \dots \otimes |n_D, d_D\rangle$, where $\vec{n} = (n_1, n_2, \dots, n_D) \in \mathbb{Z}^d$ is the *location* and $d_i \in \{L_i, R_i\}$ is the *direction* component corresponding to the i th spatial dimension. Given an arbitrary unitary coin-toss operator $C^{(i)}$ on the two-dimensional space $\mathcal{H}(\{L^{(i)}, R^{(i)}\})$, define a unitary operator W_u by $W_u = \prod_{i=1}^d T^{(i)}(I \otimes C^{(i)})$, where the translation $T^{(i)}$ in the i th dimension is defined by

$$T^{(i)} |n_i, L_i\rangle = |n_i - 1, L_i\rangle, \quad T^{(i)} |n_i, R_i\rangle = |n_i + 1, R_i\rangle,$$

A D -dimensional quantum walk is a process involving the iteration of W_u . The quantum state at time t is given by

$$\sum_{\vec{n}, \vec{d}} \Psi(\vec{n}, d_1, \dots, d_D, t) |n_1, d_1\rangle \otimes |n_2, d_2\rangle \otimes \dots \otimes |n_D, d_D\rangle$$

In physics terms, one would say that there is a 2-dimensional “internal degree of freedom” for each spatial dimension on each site of the hypercubic lattice, and $\Psi(\vec{n}, d_1, \dots, d_D, t)$ is the time-dependent wavefunction. In our definition, there is a separate coin toss in each dimension, since the 2×2 matrices $C^{(i)}$ act only on the vector $\{L_i, R_i\}$, and this vector is normalized for each value

of the index i . Each $C^{(i)}$ is unitary and therefore preserves the normalization. In our definition, it is not necessary that $C^{(i)} = C^{(j)}$ for $i \neq j$, so the dynamics of the walk may be different in the different spatial directions. The normalization of the wavefunction is

$$\sum_{\vec{n}, \vec{d}} |\Psi(\vec{n}, d_1, \dots, d_D, t)|^2 = D.$$

We shall abbreviate $\Psi(\vec{n}, d_1, \dots, d_D, t)$ by $\Psi(\vec{n}, \vec{d}, t)$.

A second more general definition would allow mixing of $\{L_i, R_i\}$ and $\{L_j, R_j\}$ with $i \neq j$ at the coin toss step. Yet a third definition is that adopted by Mackay *et al.* [5]. These authors introduce d qubits at each site, resulting in a $2^d \times 2^d$ coin-toss matrix. The second and third models can also be treated by the eigenfunction method, but the results are more cumbersome.

It is important to realize that our definition of the D -dimensional walk is not trivial. Physically, it is a fully D -dimensional analog of propagation of electrons on a lattice of atoms, just as the 1-dimensional walk represents propagation of electrons on a line of atoms. Mathematically, the crucial point is that the paths which interfere to give the probability amplitudes are also D -dimensional. The wavefunction spreads in all dimensions at each iteration of W_U .

In this section, we give the formal eigenfunction expansion solution for the asymptotic behavior of our D -dimensional quantum walk (first model) and the survival probability in this model when a $D - 1$ -dimensional absorbing wall is present.

5.2 No boundaries

The problem of finding $\Psi(\vec{n}, \vec{d}, t) = W_U^t \Psi(\vec{n}, \vec{d}, 0)$ with given $\Psi(\vec{n}, \vec{d}, 0)$ in the absence of absorbing walls may be solved by an eigenfunction expansion. We make the Ansatz

$$\Psi(\vec{n}, \vec{d}, t) = \psi_{\vec{k}}(\vec{d}) e^{i(\vec{k} \cdot \vec{n} - \omega_{\vec{k}} t)},$$

where $\psi_{\vec{k}}(\vec{d})$ are the eigenfunctions of $C_k^{ss'}$:

$$\sum_{s'=1}^{2D} U_k^{ss'} \psi_{\vec{k}}(s') = e^{-i\omega_{\vec{k}}} \psi_{\vec{k}}(s), \quad (52)$$

and s and $s' \in \{1, 2, \dots, 2D\}$ label the components of \vec{d} . The matrix $U_k^{ss'}$ is given by

$$U_k^{ss'} = \begin{pmatrix} C_{11}^{(1)} e^{ik_1} & C_{12}^{(1)} e^{ik_1} & 0 & 0 & \dots \\ C_{21}^{(1)} e^{-ik_1} & C_{22}^{(1)} e^{-ik_1} & 0 & 0 & \dots \\ 0 & 0 & C_{11}^{(2)} e^{ik_2} & C_{12}^{(2)} e^{ik_2} & \dots \\ 0 & 0 & C_{21}^{(2)} e^{-ik_2} & C_{22}^{(2)} e^{-ik_2} & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Each submatrix is unitary. The wavevector variable $\vec{k} = (k_1, k_2, \dots, k_D)$ lies in the hypercubic region $|k_i| \leq \pi, i = 1 \dots D$. (It is convenient to envision the hypercubic lattice to be extended periodically in all dimensions, and then taking the period to infinity.) There are in fact $2D$ solutions to the eigenvalue equations 52 at a fixed value of \vec{k} . Let us index the eigenvalues $\omega_{\vec{k}}^\alpha$ and the eigenfunctions $\psi_{\vec{k}}^\alpha$ by $\alpha = 1 \dots 2D$. This ‘‘band’’ index α replaces the $(+, -)$ labels of the previous section.

The eigenvalues of the operator U have degeneracies that are important for the solution of problems involving boundaries.

Let us first consider the 2×2 submatrix u_1 :

$$u_1^{ss'}(k_1) = \begin{pmatrix} C_{11}^{(1)} e^{ik_1} & C_{12}^{(1)} e^{ik_1} \\ C_{21}^{(1)} e^{-ik_1} & C_{22}^{(1)} e^{-ik_1} \end{pmatrix}.$$

This is unitary and satisfies $\det u_1 = \pm 1$. A determinant of -1 for a submatrix characterizes the Hadamard transformation, but a general 2×2 coin-toss operator could also have a positive determinant. One can show that u_1 satisfies the identity $Ru_1(k_1)R^{-1} = \det(u_1)u_1(-k_1)$, where R is the matrix

$$R = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Thus $u_1(k_1)$ is unitarily equivalent to $u_1(-k_1)$ up to a sign. If we denote the reflection

$$(k_1, k_2, \dots, k_D) \rightarrow (-k_1, k_2, \dots, k_D)$$

by $\vec{k} \rightarrow \vec{k}_R$ we have $\omega_k^\alpha = \omega_{k_R}^\alpha$ if $\det u_1(k) = 1$ and $\omega_k^\alpha = \omega_{(\pi-k_1, k_2, \dots, k_D)}^\alpha$ if $\det u_1(k) = -1$

For a general coin toss matrix $C_{ss'}$ no such simple description of the degeneracies exists.

A quantum walk that starts at the origin $\vec{n} = (0, 0, \dots, 0)$ with arbitrary internal state satisfies

$$\Psi(\vec{n}, \vec{d}, t = 0) = \delta_{\vec{n}, \vec{0}} \Psi_0(s) = \int \sum_{\alpha=1}^{2D} a_\alpha(\vec{k}) \psi_k^\alpha(s) e^{i\vec{k} \cdot \vec{n}} \mathcal{D}k, \quad (53)$$

so that the coefficients a_α are determined by the initial conditions. We shall employ the shorthand notation

$$\int f \mathcal{D}k \equiv \left(\frac{1}{2\pi} \right)^D \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} f dk_1 dk_2 \cdots dk_D,$$

and note that

$$\int e^{i\vec{k} \cdot \vec{n}} \mathcal{D}k = \delta_{\vec{n}, \vec{0}}.$$

Thus, given the initial condition, we find the $a_\alpha(\vec{k})$ by inverting a set of linear equations at each value of \vec{k} :

$$\Psi_0(s) = \sum_{\alpha=1}^{2D} a_\alpha(\vec{k}) \psi_k^\alpha(s).$$

The full solution at all times is then

$$\Psi(\vec{n}, \vec{d}, t) = \sum_{\alpha=1}^{2D} \int a_\alpha(\vec{k}) \psi_k^\alpha(s) e^{i(\vec{k} \cdot \vec{n} - \omega_k^\alpha t)} \mathcal{D}k.$$

To understand the asymptotic properties of this wavefunction at long times, consider a point that moves at constant velocity $\vec{n} = \vec{c}t$ away from the origin. After this substitution, the behavior of the integral as $t \rightarrow \infty$ may be obtained by the stationary phase method. The neighborhood(s) of the point or points in k -space $\vec{k}_r^\alpha(n)$ where $\nabla_{\vec{k}} \omega_k^\alpha - \vec{c} = 0$ dominate the integral. The subscript r

labels the roots of this equation and may range over several values. The result is

$$\begin{aligned}\Psi(\vec{n}, s, t) &= \sum_{\alpha=1}^{2D} \int a_{\alpha}(\vec{k}) \psi_{\vec{k}}^{\alpha}(s) e^{i(\vec{k} \cdot \vec{c} - \omega_{\vec{k}}^{\alpha})t} \mathcal{D}k \\ &\rightarrow \left(\frac{i\pi}{2}\right)^{D/2} \sum_{\alpha=1}^{2D} \sum_r a_{\alpha}(\vec{k}_r^{\alpha}) \psi_{\vec{k}_r}^{\alpha}(s) \exp \left[(i\vec{k}_r^{\alpha} \cdot \vec{c} - i\omega_{\vec{k}_r}^{\alpha})t \right] \\ &\quad \times |J_r^{\alpha}|^{-1/2} t^{-D/2} + \mathcal{O}(t^{-D/2-1}),\end{aligned}$$

where J_r^{α} is the Jacobian of the function $\omega_{\vec{k}}^{\alpha}$ at the point \vec{k}_r^{α} . If there are no solutions to the zero-gradient condition, then the asymptotic behavior of $|\Psi(\vec{n}, \vec{d}, t)|$ is generically determined by contributions from the boundary of the region of integration and one finds $|\Psi(\vec{n}, \vec{d}, t)| = \mathcal{O}(t^{-D})$.

From this expression, we deduce that the probability $|\Psi(\vec{n}, \vec{d}, t)|^2$ spreads linearly with time from the origin. The square of the wavefunction at a fixed point \vec{n} falls off asymptotically in time as t^{-D} . However, the overall probability is normalized:

$$1 = \sum_{\vec{n}s} |\Psi(\vec{n}, s, t)|^2 \rightarrow t^{-D} \times \sum_{|\vec{n}| < t} cst. \sim t^{-D} \Omega,$$

where Ω is the volume occupied by the wavepacket. Hence $\Omega \sim t^D$ and the radius $\Omega^{1/D} \sim t$. This arises from the fact that the initial wavepacket is a superposition of waves at various values of \vec{k} with various group velocities $\vec{v}_k^{\alpha} = \nabla_{\vec{k}} \omega_{\vec{k}}^{\alpha}$. Each such component moves according to the ballistic equation $\vec{n} = \vec{v}_k^{\alpha} t$. Because of the limited range of $|\vec{k}|$, there is a maximum group velocity in each spatial direction. This maximum velocity defines the wavefront in that direction. Even though the boundary of the wavefunction may have a very irregular shape, that shape is maintained and the object expands linearly in all directions.

5.3 (D-1)-dimensional absorbing wall

We now generalize the absorption problem to a $(D-1)$ -dimensional wall located at

$$\vec{n} = (M, 0, 0, \dots, 0),$$

with $M > 0$. We shall treat only the case where $\det u_1 = +1$, as the other case has been treated in detail in one dimension.

In fact, many of the results from Sec.4 generalize immediately. We again extend the problem to the full space, stipulating that there is no motion to the left in the region $n_1 \geq M$. Then it is sufficient to solve for the wavefunctions $\Psi(\vec{n}, \vec{d}, t) = \Psi(n_1, n_2, \dots, n_D, \vec{d}, t)$ in the region $n_1 < M$ that satisfy $\Psi(M-1, n_2, \dots, n_D, 1, t) = 0$, which means we have solutions of the form

$$\Psi(\vec{n}, \vec{d}, t) = \sum_{\alpha=1}^{2D} \int_{k_1 \geq 0} \left[A_{\alpha}(\vec{k}, M) \psi_{\vec{k}}^{\alpha}(s) e^{i\vec{k} \cdot \vec{n}} + A_{\alpha}(\vec{k}_R, M) \psi_{\vec{k}_R}^{\alpha}(s) e^{i\vec{k}_R \cdot \vec{n}} \right] e^{-i\omega_{\vec{k}}^{\alpha} t} \mathcal{D}k.$$

Enforcing the boundary condition leads to the relation

$$\sum_{\alpha=1}^{2D} A_{\alpha}(\vec{k}_R, M) \psi_{\vec{k}_R}^{\alpha}(1) = - \sum_{\alpha=1}^{2D} A_{\alpha}(\vec{k}, M) e^{2ik_1(M-1)} \psi_{\vec{k}}^{\alpha}(1)$$

between an expansion coefficient and its reflected counterpart. As seen already in Sec.4, this relation is consistent with the initial conditions, if it is kept in mind that the wavefunction is only needed in the half-space $n_1 < M$. The initial condition is

$$\Psi(\vec{n}, \vec{d}, t = 0) = \delta_{\vec{n}, \vec{0}} \Psi_0(\vec{d}) = \sum_{\alpha=1}^{2D} \int A_{\alpha}(\vec{k}, M) \psi_{\vec{k}}^{\alpha}(s) e^{i\vec{k} \cdot \vec{n}} \mathcal{D}k.$$

Using the method of images or otherwise, we invert this expression to determine the $A_{\alpha}(\vec{k}, M)$ and the final solution for $n_1 < M$ is

$$\Psi(\vec{n}, s, t) = \sum_{\alpha=1}^{2D} \int A_{\alpha}(\vec{k}, M) \psi_{\vec{k}}^{\alpha}(s) e^{i\vec{k} \cdot \vec{n}} e^{-i\omega_{\vec{k}}^{\alpha} t} \mathcal{D}k.$$

To obtain the survival probability Λ_M , we note that at long times only leftmoving waves ($v_1^{\alpha}(\vec{k}) = \partial\omega_{\vec{k}}^{\alpha}/\partial k_1 < 0$) will be present in the physical domain:

$$\Lambda_M = \frac{1}{D} \sum_{\alpha=1}^{2D} \sum_{s=1}^{2D} \int_{v_1^{\alpha}(\vec{k}) < 0} \left| A_{\alpha}(\vec{k}, M) \psi_{\vec{k}}^{\alpha}(s) \right|^2 \mathcal{D}k.$$

An application of Parseval's theorem shows that $0 < \Lambda_M < 1$, except for special choices of the initial condition. This is in sharp distinction to the classical random walk, for which the survival probability vanishes for all D and M .

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