One-Dimensional Quantum Walks

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ABSTRACT

We define and analyze quantum computational variants of random walks on one-dimensional lattices. In particular, we analyze a quantum analog of the symmetric random walk, which we call the *Hadamard walk*. Several striking differences between the quantum and classical cases are observed. For example, when unrestricted in either direction, the Hadamard walk has position that is nearly uniformly distributed in the range $[-t/\sqrt{2}, t/\sqrt{2}]$ after t steps, which is in sharp contrast to the classical random walk, which has distance $O(\sqrt{t})$ from the origin with high probability. With an absorbing boundary immediately to the left of the starting position, the probability that the walk exits to the left is $2/\pi$, and with an additional absorbing boundary at location n, the probability that the walk exits to the left actually increases, approaching $1/\sqrt{2}$ in the limit. In the classical case both values are 1.

1. INTRODUCTION

Classical random walks are very well-studied processes. In the simplest variation, a single particle moves on a two-way infinite, one-dimensional lattice. At each step, the particle moves one position left or right, depending on the flip of a fair coin. Such random walks may be generalized to more complicated lattices and to finite or infinite graphs, and have had several interesting applications in computer science (see, for instance, [3, 8, 20, 22], as well as the discussion below). We refer the reader to Kemeny and Snell [21] for basic facts regarding random walks.

In this paper we consider quantum variations of random walks on one-dimensional lattices—we refer to such processes as *quantum walks*.

In direct analogy to classical random walks, one may naïvely try to define quantum walks on the line as follows: at every time step, the particle moves, in superposition, both left and right with equal amplitudes (perhaps with a relative phase difference). However, such a walk is physically impossible, since the global process is necessarily non-unitary. It is also easy to verify that the only possible translationally invariant unitary processes on the line allowing only transitions between adjacent lattice sites are the left and right shift operators, up to an overall phase [24]. These processes simply correspond to motion in a single direction.

If the particle has an extra degree of freedom that assists in its motion, however, then it is possible to construct more interesting translation invariant local unitary processes. Consider a quantum particle that moves freely on the integer points on the line, and has an additional degree of freedom, its *chirality*, that takes values RIGHT and LEFT. A walk on the line by such a particle may be described as follows: at every time step, its chirality undergoes a unitary transformation and then the particle moves according to its (new) chirality state. Figure 1 depicts this two-stage move in a quantum walk where the chirality undergoes a Hadamard transformation. We call this particular walk the *Hadamard walk*.

Although the Hadamard walk looks similar to the classical random walk, its behavior is in fact strikingly different. The reason for this is quantum interference. Whereas there cannot be destructive interference in a classical random walk, in a quantum walk two separate paths leading to the same point may be out of phase and cancel one another.

Our motivation for studying quantum walks is two-fold. First, we believe that quantum walks have the potential to offer new tools for quantum algorithms, and second, we believe that techniques developed for analyzing quantum walks may yield techniques for analyzing discrete quantum processes (and quantum algorithms in particular) more generally.

Quantum walks on graphs have the potential for offering a systematic way of speeding up classical algorithms based on random walks. Well-known examples of algorithms based on random walks include algorithms for 2-Satisfiability, Graph Connectivity, and probability amplification (see, e.g., [25]). Recently, Schöning [29] discovered a random walk based al-

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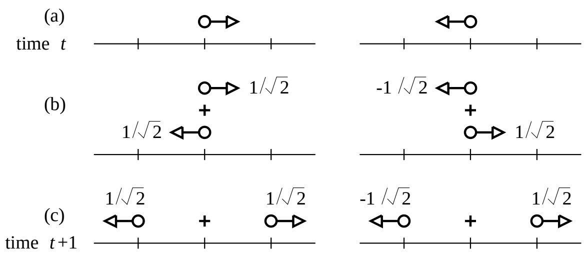

Figure 1: *The dynamics of the Hadamard walk. In (a) we begin at time t with a particle in chirality state* RIGHT *or* LEFT*. The result of the Hadamard transformation is shown in (b), the particle is now in an equal superposition of* LEFT *and* RIGHT *chirality states (with the amplitudes indicated) and then moves accordingly (c) to generate the state at time $t+1$.*

gorithm similar to that of Papadimitriou [27] that gives a the most efficient known solution to 3SAT. In general, Markov chain simulation has emerged as a powerful algorithmic tool and has had a profound impact on random sampling and approximate counting [18]. Among its numerous applications are estimating the volume of convex bodies [10] (see also [23] for recent progress on this problem) and approximating the permanent [17]. Very recently, Jerrum, Sinclair and Vigoda [19] used this approach to solve the long standing open problem of approximating the permanent for non-negative matrices.

Despite the fact that our quantum walks are easy to describe, certain variants (in particular the case where the walk has absorbing boundaries) seem to be quite difficult to analyze. Standard techniques for analyzing classical random walks are apparently of little use. Analysis of more complicated quantum processes, such as certain natural definitions for quantum walks on arbitrary finite graphs, seem to be out of our reach at the present time. However, as quantum algorithm design becomes more sophisticated, we believe it will be inevitable to develop methods for accurately analyzing discrete quantum processes. This paper represents one step toward this goal.

Overview of results

In this paper, we analyze in detail the dynamics of the Hadamard walk on the line. We study two basic variations of the Hadamard walk, which correspond to walks with and without absorbing boundaries. Both cases illustrate surprising behavior that underscores the differences between quantum and classical processes.

Our most accurate analyses are for quantum walks without absorbing boundaries. In the classical case, it is well-known that a random walk on a (two-way infinite) line has expected distance $\Theta(\sqrt{t})$ from the origin at time t, and the probability of being at a distance $\Omega(t)$ from the origin is exponentially small. In contrast, observation of a quantum particle doing a Hadamard walk on the line after t steps yields an expected distance $\Theta(t)$ from the origin. Moreover, the location of the particle is almost uniformly distributed over the interval $[-t/\sqrt{2}, t/\sqrt{2}]$, so that the quantum walk spreads quadratically faster than the classical random walk.

This also implies that the analogously defined walk on the circle *mixes* in linear time. This is in contrast with the classical random walk, which mixes in quadratic time. In this paper, by the *δ-mixing time* of a walk we mean the *first* time (independent of the initial position) at which the distribution induced by the walk is δ-close to uniform in total variation distance.

The presence of absorbing boundaries apparently complicates the analysis of the associated quantum walks considerably. For the case of quantum walks with boundaries, we focus on the question of determining exit probabilities of the walks.

First, we consider the case where we have a single absorbing boundary one location to the left of the origin—the process is terminated if the particle reaches this location. It is well known that in the classical case the random walk exits with probability 1. In contrast, the quantum walk exits with probability $2/\pi$. Thus, a considerable part of the quantum state keeps going infinitely in the other direction (to the right) without ever returning to the origin.

We then consider the case where there is a second absorbing boundary n positions to the right of the origin for some arbitrary n. The process is terminated if the particle reaches either absorbing boundary. Naturally, the presence of the second boundary decreases the probability of reaching the left boundary in the classical case: the walk exits from the left with probability $n/(n+1)$. Again surprisingly, in the quantum case, adding the second boundary on the right actually *increases* the chance of reaching the boundary on the left (so long as the second boundary allows the particle at least two non-boundary locations on which to walk). In the limit for large n, the probability of reaching the left boundary tends to $1/\sqrt{2}$ (and **not** $2/\pi$). The reason for this strange behavior is, again, the quantum interference. Adding a right boundary removes a part of the quantum state (the part that reaches the right boundary), which would otherwise have interfered destructively with another part of the state reaching the left boundary. Thus, removing a part of the quantum state at the right boundary *increases* the chance of reaching the left boundary.

Overview of methods

We will rely on two general ideas for analyzing the quantum processes in this paper, the *path integral approach* and the *Schrödinger approach*. Each approach has its advantages.

To use the path integral approach, one expresses the amplitude of a given state as a sum or integral, over all possible paths leading to that state, of the amplitude of taking that path. In our case, since the processes we consider involve discrete quantum systems, the amplitude is given as a combinatorial sum.

In practice, however, there are still difficulties, because the sums involve heavy cancellation. We get around these difficulties in various ways. For the infinite walk, we use a method due to Gosper and Zeilberger to obtain a recurrence relation for the sum, which leads to useful approximations. We also relate the sums to classical orthogonal polynomials, from which their asymptotic values can be derived. For the finite walks, we study the generating functions of the amplitudes. This requires methods from real and complex analysis, including a (possibly new) nonlinear version of the Riemann-Lebesgue lemma.

The Schrödinger approach takes advantage of the time and space homogeneity of the quantum walk. The crucial observation is that because of its translational invariance, the walk has a simple description in Fourier space. The Fourier transform of the amplitude is thus easily analyzed, and transformed back to the spatial domain. It is noteworthy that this technique is standard in the analysis of classical random walks [9].

A key advantage of the Schrödinger approach is that the Fourier integrals for the amplitudes are amenable to analysis in standard ways. There is a well-developed theory of the asymptotic expansion of integrals that allows us to determine the behavior of the wave function in the limit [4, 5]. This gives another asymptotic form for the probability distribution. The Schrödinger approach is also quite general and could be potentially applied to quantum walks on any Cayley graph.

Related work

Various quantum variants of random walks have previously been studied by a few authors [6, 12, 24, 32], but their results are, for the most part, unrelated to ours.

The first study of quantum walks is apparently due to Meyer [24]. Meyer's model (quantum lattice gas automata or QLGA) is equivalent to our two-way infinite Hadamard walk, but he addresses different questions than the ones we consider. After obtaining a formula for the amplitudes of the walk as a sum of binomial coefficients (which we state as Lemma 4), Meyer proceeds to analyzing the continuous-time limit of QLGA and shows that this limit is given by the Dirac equation [13]. The results about the continuous-time limit apparently do not imply anything for the discrete case that we study in this paper.

Farhi and Gutmann [12] and Childs, Farhi and Gutmann [6] analyze quantum walks on trees and exhibit collections of graphs on which the quantum process hits one particular node exponentially faster than the corresponding classical process. The definition for quantum walks considered in these papers is completely different from ours.

One of us [32] has considered unitary processes based on quantum walks on regular graphs in the context of space-bounded computation. In that paper the quantum processes considered are much different from those we study, as they were designed to suppress quantum effects (in order to closely approximate classical random walks on graphs) rather than take advantage of the quantum effects.

Finally, Aharonov, Ambainis, Kempe and Vazirani [2] have recently studied quantum walks on graphs and their mixing behavior. They consider a different notion of mixing for quantum walks, and show that a quantum walk on an n-cycle mixes in time $O(n \log n)$ (with respect to their notion of mixing). They also show a lower bound of $1/d\Phi$ for this mixing time for general graphs, where d is the maximum degree of a vertex in the graph and Φ is its conductance.

Organization of the paper

The rest of this paper is organized as follows. Section 2 contains formal definitions of the quantum walks we study. Section 3 states the results of our paper in detail. Section 4 gives proofs of our results on unrestricted quantum walks, and Section 5 does the same for quantum walks with boundaries. We conclude with Section 6, which mentions a few directions for further work.

2. DEFINITIONS

In this section we formally define our notion of quantum walks.

Let $\mathbb{Z}$ denote the integers and let $\Sigma = \{\mathrm{R}, \mathrm{L}\}$. We make the identification $\mathrm{R} = \textsc{right}$, $\mathrm{L} = \textsc{left}$. The quantum systems we consider will have the underlying classical state set $\mathbb{Z} \times \Sigma$. We view a state $(n, d) \in \mathbb{Z} \times \Sigma$ as consisting of a location n and a direction d.

The (pure) quantum states of our systems may be identified with unit vectors in the Hilbert space $\ell_2(\mathbb{Z}) \otimes \ell_2(\Sigma)$, for which the set $\{|n\rangle|d\rangle : n \in \mathbb{N},\ d \in \Sigma\}$ forms an orthonormal basis. Each state $|n\rangle|d\rangle$ is identified with the classical state (n, d).

The quantum walk we focus on is the Hadamard walk, which was discussed informally in the previous section. The Hadamard walk is based on the Hadamard transform, which is denoted H and acts on $\ell_2(\Sigma)$ as follows:

$$H : |\mathrm{R}\rangle \mapsto \frac{1}{\sqrt{2}}(|\mathrm{R}\rangle + |\mathrm{L}\rangle), \quad H : |\mathrm{L}\rangle \mapsto \frac{1}{\sqrt{2}}(|\mathrm{R}\rangle - |\mathrm{L}\rangle).$$

(Here and throughout this paper, when we describe a transformation on basis elements, it is assumed to be extended to the entire space by linearity.) To apply the Hadamard transform to the direction component of a particle (its *chirality*) means that we tensor with the identity:

$$(I \otimes H) : |n\rangle|\mathrm{R}\rangle \mapsto \frac{1}{\sqrt{2}}|n\rangle(|\mathrm{R}\rangle + |\mathrm{L}\rangle)$$
$$(I \otimes H) : |n\rangle|\mathrm{L}\rangle \mapsto \frac{1}{\sqrt{2}}|n\rangle(|\mathrm{R}\rangle - |\mathrm{L}\rangle)$$

Next, define the translation operator T by the following action on basis states:

$$T : |n\rangle|\mathrm{R}\rangle \mapsto |n+1\rangle|\mathrm{R}\rangle,$$
$$T : |n\rangle|\mathrm{L}\rangle \mapsto |n-1\rangle|\mathrm{L}\rangle.$$

The operator T simply corresponds to moving a particle one step left or right according to its chirality. Finally, define W as $W = T(I \otimes H)$. Clearly W is unitary. The operator W represents one step of a Hadamard walk.

In order to discuss quantum walks further in a physically meaningful way, we must consider measurements of the particle doing the quantum walk. Consider first the situation where our particle starts in the state $|0\rangle|\mathrm{R}\rangle$ and we alternate the following two steps: (i) apply the operator W, and (ii) measure the location of the particle. It is easy to see that we obtain precisely a classical unbiased random walk. However, without such observations that serve to "collapse" the state of the system after each application of W, the behavior of the walk is much different (since different paths will interfere with one another).

We will consider three different processes based on the Hadamard walk, which represent the cases where we have zero, one, or two absorbing boundaries. Precise descriptions of these processes follow.

Two-way infinite timed Hadamard walk

The simplest process we consider is the *two-way infinite timed Hadamard walk*. The process is as follows.

1. Initialize the system in classical state $|0\rangle|\mathrm{R}\rangle$.
2. For any chosen number of steps t, apply W to the system t times, then observe the location.

Semi-infinite Hadamard walk

For the second process we introduce an absorbing boundary. This is done by considering a measurement that corresponds to the question "Is the system at location n?". This measurement may be described as corresponding to the projection operators $\Pi^n_{yes} = |n\rangle\langle n| \otimes I_\Sigma$ (where I_Σ is the identity on $\ell_2(\Sigma)$ and $\Pi^n_{no} = I - \Pi^n_{yes}$ (where I denotes the identity on $\ell_2(\mathbb{Z}) \otimes \ell_2(\Sigma)$). For example, suppose a system is in the state

$$\frac{1}{2}|0\rangle|\mathrm{R}\rangle - \frac{1}{2}|0\rangle|\mathrm{L}\rangle + \frac{1}{2}|2\rangle|\mathrm{R}\rangle + \frac{1}{2}|4\rangle|\mathrm{L}\rangle$$

and is observed using the above measurement for $n = 0$. The answer obtained is "yes" with probability

$$\left\| \Pi^0_{yes} \left(\frac{1}{2}|0\rangle|\mathrm{R}\rangle - \frac{1}{2}|0\rangle|\mathrm{L}\rangle + \frac{1}{2}|2\rangle|\mathrm{R}\rangle + \frac{1}{2}|4\rangle|\mathrm{L}\rangle \right) \right\|^2 = \left\| \frac{1}{2}|0\rangle|\mathrm{R}\rangle - \frac{1}{2}|0\rangle|\mathrm{L}\rangle \right\|^2 = \frac{1}{2},$$

in which case the state of the system collapses to

$$\frac{1}{\sqrt{2}}(|0\rangle|\mathrm{R}\rangle - |0\rangle|\mathrm{L}\rangle),$$

and the answer is "no" with probability $1/2$, in which case the system collapses to state

$$\frac{1}{\sqrt{2}}(|2\rangle|\mathrm{R}\rangle + |4\rangle|\mathrm{L}\rangle).$$

Now we are ready to define our second quantum process:

1. Initialize the system in classical state $|1\rangle|\mathrm{R}\rangle$.
2. a. Apply W.

   b. Observe the system according to $\{\Pi^0_{yes}, \Pi^0_{no}\}$ (i.e., measure the system to see whether it is or is not at location 0).
3. If the result of the measurement was "yes" (i.e., revealed that the system was at location 0), then terminate the process, otherwise repeat step 2.

Finite Hadamard walk

The third and final process we consider is similar to the second, except that two absorbing boundaries are present rather than one. Specifically, using the same measurements as defined for the semi-infinite quantum walk, we consider the following process:

1. Initialize the system in classical state $|1\rangle|\mathrm{R}\rangle$.
2. a. Apply W.

   b. Observe the system according to $\{\Pi^0_{yes}, \Pi^0_{no}\}$

   c. Observe the system according to $\{\Pi^n_{yes}, \Pi^n_{no}\}$ (for some fixed $n > 1$).
3. If the result of either measurement was "yes" (i.e., revealed that the system was either at location 0 or location n), then terminate the process, otherwise repeat step 2.

Mixing times

One of the properties of quantum walks we will study is how fast the particle "diffuses" in space. This is traditionally done by analyzing the *mixing time.*

Consider an ergodic Markov chain $\mathcal{M}$ on the state space V, starting at state $u \in V$, which induces a probability distribution $P_u(\cdot, t)$ on the states at time t. Let $\pi(\cdot)$ denote the stationary distribution of the chain $\mathcal{M}$. The mixing time τ_ϵ is defined as follows:

$$\tau_\epsilon \quad = \quad \max_u \min_t \{t : \| P_u(\cdot, t') - \pi \| \le \epsilon \ \ \forall t' \ge t\}.$$

In other words, it is the first time t such that $P_u(\cdot, t')$ stays within total variation distance ϵ (i.e., ℓ_1 distance 2ϵ) of π at all subsequent time steps $t' \ge t$, irrespective of the initial state.

In the case of *unitary* Markov chains on a finite state space, such as finite graph analogues of the quantum walk we consider, no stationary distribution exists. In fact, the process is (approximately) periodic, since it corresponds to repeated transformation of the state by a fixed a unitary matrix. In this context, a more appropriate definition for mixing time is the following, where we measure distance from a desired target distribution π on the state space, and relax the condition that the probability distribution be close to it at all future time steps:

$$\tau_\epsilon \quad = \quad \max_u \min_t \{t : \| P_u(\cdot, t) - \pi \| \le \epsilon\}.$$

We use this notion of mixing in our paper. (See [2] for other possible notions of mixing.)

3. STATEMENT OF RESULTS

Results for two-way infinite timed quantum walks

To study the properties of quantum walks, we consider the wave function describing the position of the particle and analyze how it evolves with time. Let

$$\Psi(n,t) = \begin{pmatrix} \psi_{\mathrm{L}}(n,t) \\ \psi_{\mathrm{R}}(n,t) \end{pmatrix}$$

be the two component vector of amplitudes of the particle being at point n at time t, with the chirality being LEFT (upper component) or RIGHT (lower component). Similarly, let

$$P(n,t) = p_{\mathrm{L}}(n,t) + p_{\mathrm{R}}(n,t)$$

be the probability of being at position n at time t. For the initial condition we will focus on $\Psi(0,0) = (0,1)^\intercal$ and $\Psi(n,0) = (0,0)^\intercal$ for $n \ne 0$. We will let $\alpha = n/t$ throughout the paper.

The asymptotics reveal the following properties of the probability distribution. The wave function is almost uniformly spread over the region for which α is in the interval $[-1/\sqrt{2}, 1/\sqrt{2}]$, and shrinks quickly outside this region. This behavior is described in detail by the following theorems. In these theorems, we assume $n \equiv t \bmod 2$, since the amplitudes are 0 otherwise.

THEOREM 1. *Let $n = \alpha t \to \infty$ with α fixed. In case $-1 < \alpha < -1/\sqrt{2}$ or $1/\sqrt{2} < \alpha < 1$, there is a $c > 1$ for which $p_{\mathrm{R}}(n,t) = O(c^{-n})$ and $p_{\mathrm{L}}(n,t) = O(c^{-n})$.*

THEOREM 2. *Let $\epsilon > 0$ be any constant, and α be in the interval $(\frac{-1}{\sqrt{2}}+\epsilon, \frac{1}{\sqrt{2}}-\epsilon)$. Then, as $t \to \infty$, we have (uniformly in n)*

$$p_{\mathrm{L}}(n,t) \sim \frac{2}{\pi\sqrt{1-2\alpha^2}\,t}\cos^2\Big(-\omega t + \frac{\pi}{4} - \rho\Big),$$

$$p_{\mathrm{R}}(n,t) \sim \frac{2(1+\alpha)}{\pi(1-\alpha)\sqrt{1-2\alpha^2}\,t}\cos^2\Big(-\omega t + \frac{\pi}{4}\Big),$$

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

This theorem has several consequences. First, by integrating the expression of Theorem 2, we can see that almost all of the probability $(1 - \frac{2\epsilon}{\pi} - \frac{O(1)}{t})$ is concentrated in the interval $[(-1/\sqrt{2}+\epsilon)t, (1/\sqrt{2}-\epsilon)t]$. Second, we see that there are $\Omega(t)$ locations at which the cosine-squared in Theorem 2 is close to 1, and therefore p_L or p_R is $\Omega(\frac{1}{t})$. This implies that the quantum walk on the line is mixing in linear time.

THEOREM 3. *Let π_t denote the uniform distribution on $\mathbb{Z} \cap [-t/\sqrt{2}, t/\sqrt{2}]$. There is a constant $\delta < 1$ such that for all t sufficiently large, $\|P(\cdot,t) - \pi_t\| \le \delta$.*

Methods for two-way infinite timed quantum walks

The results described above can be obtained by two methods. These methods are discrete counterparts of the *path integral* and *Schrödinger* approaches in quantum mechanics. The two approaches differ in power, but each has its advantage. The path integral approach gives Theorem 1 and a version of Theorem 2 with a weaker convergence guarantee. The Schrödinger approach gives Theorem 2 and a weaker version of Theorem 1 (with $O(1/n^d)$ for all d instead of $O(c^{-n})$). It would be interesting to try to refine these approaches so that both give the stronger versions of the results.

We first sketch the path integral approach. The fastest way to compute the amplitudes is to determine the signed path counts, by a recurrence relation reminiscent of Pascal's triangle, and then divide by the appropriate power of $\sqrt{2}$. This determines all $\Psi(n,t')$ for $t' \le t$ with $O(t^2)$ operations. To analyze these amplitudes, however, it is better to start from an explicit formula.

LEMMA 4. *[24] Let $-n \le t < n$. Define $\ell = \frac{t-n}{2}$. The amplitudes of position n after t steps of the Hadamard walk are:*

$$\psi_{\mathrm{L}}(n,t) = \frac{1}{\sqrt{2^t}}\sum_k \binom{\ell-1}{k}\binom{t-\ell}{k}(-1)^{\ell-k-1} \quad (1)$$

$$\psi_{\mathrm{R}}(n,t) = \frac{1}{\sqrt{2^t}}\sum_k \binom{\ell-1}{k-1}\binom{t-\ell}{k}(-1)^{\ell-k}. \quad (2)$$

The boundary case $t = n$ requires a separate handling (the formulas (1) and (2) do not work) but is easy.

The sums of binomial coefficients in (1) and (2) are discrete counterparts of path integrals in quantum mechanics. The amplitudes in Lemma 4 can be expressed using values of classical orthogonal polynomials. Let $J_\nu^{(a,b)}(z)$ be the normalized degree ν Jacobi polynomial as in [30, p. 29] and $J_\nu^{(a,b)}$ its constant term.

LEMMA 5. *Let $n > 0$ and $\nu = (t-n)/2 - 1$. We have*

$$p_{\mathrm{L}}(n,t) = 2^{-n-2}\left(J_\nu^{(0,n+1)}\right)^2$$

$$p_{\mathrm{R}}(n,t) = \left(\frac{t+n}{t-n}\right)^2 2^{-n-2}\left(J_\nu^{(1,n)}\right)^2.$$

The Jacobi polynomial representation immediately gives the following symmetries, which allow us to consider values of n with one sign only.

THEOREM 6. *We have*

$$p_{\mathrm{L}}(-n,t) = p_{\mathrm{L}}(n-2,t)$$

$$p_{\mathrm{R}}(-n,t) = \left(\frac{t-n}{t+n}\right)^2 p_{\mathrm{R}}(n,t).$$

We then find asymptotic approximations to the amplitudes via large-parameter asymptotics for Jacobi polynomials [7]. This uses the Darboux method, starting from a generating function for J_ν.

The second approach we consider is a Fourier analysis of the Hadamard walk. It is a counterpart of the Schrödinger approach in quantum mechanics. The basic result is the following lemma.

LEMMA 7. *We have*

$$\psi_{\mathrm{L}}(n,t) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\,\frac{-ie^{ik}}{\sqrt{1+\cos^2 k}}\,e^{-i(\omega_k t - kn)},$$

$$\psi_{\mathrm{R}}(n,t) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right)e^{-i(\omega_k t - kn)},$$

where $\omega_k = \sin^{-1}\frac{\sin k}{\sqrt{2}} \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.

Using the Method of Stationary Phase [4, 5], it is possible to derive the asymptotic form of the amplitudes from their integral representation, and hence also the form of the probability distribution $P(n,t)$.

Results for semi-infinite and finite Hadamard walks

While there are several questions one could ask about about the semi-infinite and finite Hadamard walks, we will restrict our attention to the following simple question: *What are the exit probabilities of the walks?*

For the semi-infinite walk, there is just one exit probability, which is the probability that the measurement of whether the particle is at location 0 eventually results in the answer "yes". Let p_∞ denote this probability. We have

THEOREM 8. *$p_\infty = 2/\pi$.*

This theorem is in sharp contrast with the classical case, for which it is well-known that the probability of eventually exiting to the left is 1.

Now we consider the finite Hadamard walk. For each $n > 1$, let p_n be the probability that the process eventually exits to the left, i.e., the measurement in step 2b of the description of the process eventually results in "yes". Also define q_n to be the probability that the process exits to the right.

PROPOSITION 9. *For all $n > 1$, $p_n + q_n = 1$.*

The asymptotic behavior of p_n is as follows.

THEOREM 10. $\lim_{n\to\infty} p_n = 1/\sqrt{2}$.

Once again, this result is in sharp contrast to the classical case, for which the probability of exiting from the left is $1 - 1/n$.

When comparing this situation to the semi-infinite quantum walk, it is interesting to note that $1/\sqrt{2} > 2/\pi$. This means that for sufficiently large n, terminating the walk at location n actually *increases* the probability of reaching location 0. (Indeed, since p_3 is easily shown to be $2/3$, this holds already for the case $n = 3$.)

We are not yet able to derive a closed form for p_n. We conjecture the following.

CONJECTURE 11. *The probabilities p_n obey the following recurrence.*

$$\begin{aligned} p_1 &= 0, \\ p_{n+1} &= \frac{1+2p_n}{2+2p_n}, \quad n \geq 1. \end{aligned}$$

4. TWO-WAY INFINITE TIMED HADAMARD WALKS

We now analyze in detail the state of a particle doing a Hadamard walk in the two-way infinite case. We begin with the path integral approach.

Path integral analysis of the Hadamard walk

We wish to study the amplitudes of $|n\rangle|\mathrm{R}\rangle$ and $|n\rangle|\mathrm{L}\rangle$ in the superposition $W^t|0\rangle|\mathrm{R}\rangle$. Since these are real, the corresponding probabilities are obtained by squaring, and it will suffice to analyze the amplitudes.

To reach $|n\rangle|\mathrm{R}\rangle$ or $|n\rangle|\mathrm{L}\rangle$ in t steps, there must be $\ell = \frac{t-n}{2}$ moves left and $r = \frac{t+n}{2}$ $(= t - \ell)$ moves right. By counting such paths, one gets Lemma 4.

This gives the amplitudes of $|n\rangle|\mathrm{R}\rangle$ and $|n\rangle|\mathrm{L}\rangle$ for any n. However, formulas (1) and (2) involve the difference of two numbers that are both much bigger than the amplitudes. For this reason, they cannot be directly used to bound the amplitudes.

If n is close to 0, a simple manipulation with binomial coefficients gives nice formulas for $|n\rangle|\mathrm{R}\rangle$ and $|n\rangle|\mathrm{L}\rangle$.

LEMMA 12. *The amplitudes of $|0\rangle|\mathrm{R}\rangle$ and $|0\rangle|\mathrm{L}\rangle$ after t steps are:*

1. *0 if t is odd,*
2. $\frac{1}{2^u}(-1)^{\frac{u}{2}}\binom{u-1}{u/2}$ *if $t = 2u$, u even,*
3. $\frac{1}{2^u}(-1)^{\frac{u-1}{2}}\binom{u-1}{(u-1)/2}$ *and* $\frac{1}{2^u}(-1)^{\frac{u+1}{2}}\binom{u-1}{(u-1)/2}$ *if $t = 2u$, u odd.*

By Stirling's approximation, $\binom{u}{u/2} \sim \frac{2^u}{\sqrt{\pi u}}$. Therefore, the amplitudes of $|0\rangle|\mathrm{R}\rangle$ and $|0\rangle|\mathrm{L}\rangle$ after $t = 2u$ steps are $\frac{1}{2^u}\binom{u-1}{(u-1)/2} \approx \frac{1}{2^u}\frac{2^{u-1}}{\sqrt{\pi u}} = \frac{1}{2\sqrt{\pi u}} = \frac{1}{\sqrt{2\pi t}}$ and the probabilities of measuring them are approximately $\frac{1}{2\pi t}$.

However, for an arbitrary n, applying the idea of Lemma 12 still gives a difference of two very large numbers. To understand the asymptotics of these sums, one needs a different approach. We have two approaches. The first is by transforming the sum into a recurrence relation and solving the recurrence. The second is by describing the sum by Jacobi polynomials.

Combinatorial sums and recurrences

Consider the sums

$$S_{\mu,\nu} = \sum_k \binom{\mu}{k}\binom{\nu}{k}(-1)^k \tag{3}$$

and

$$T_{\mu,\nu} = \sum_k \binom{\mu}{k}\binom{\nu}{k+1}(-1)^k \tag{4}$$

By Lemma 4, calculating Ψ is equivalent to calculating these sums.

We will focus on $\psi_L(n,t)$. By Lemma 4, it corresponds to $S_{\mu,\nu}$ for $\mu = \frac{t-n}{2} - 1$, $\nu = \frac{t+n}{2}$. Using the Gosper-Zeilberger method [14, 15, 33] for generating recurrences from sums of binomial coefficients, we obtain the following lemma.

LEMMA 13. *[15] We have*

$$(\nu+2)S_{\mu,\nu+2} = (3\nu+4-\mu)S_{\mu,\nu+1} - (2\nu+2)S_{\mu,\nu}. \tag{5}$$

Together with Lemma 4, this relates the amplitudes of $|n\rangle|\mathrm{L}\rangle$ at time t, $|n-1\rangle|\mathrm{L}\rangle$ at time $t+1$, and $|n-2\rangle|\mathrm{L}\rangle$ at time $t+2$. We can also obtain a similar (but more complicated) recurrence that relates $S_{\mu-1,\nu+1}$, $S_{\mu,\nu}$ and $S_{\mu+1,\nu-1}$ (or, equivalently, amplitudes of $|n-1\rangle|\mathrm{R}\rangle$, $|n\rangle|\mathrm{R}\rangle$ and $|n+1\rangle|\mathrm{R}\rangle$ at time t).

Solving the recurrences

If we fix μ, the recurrence (5) becomes a recurrence in one variable ν. The simplest way to solve (5) is by approximating it by a recurrence with constant coefficients:

$$(\nu_0+2)A_{\mu,\nu+2} = (3\nu_0+4-\mu_0)A_{\mu,\nu+1} - (2\nu_0+2)A_{\mu,\nu},$$

where ν_0, μ_0 are particular values of ν and μ. This recurrence can be solved in a standard way. The form of the solution depends on ν_0 and μ_0. If the ratio $\frac{\mu_0}{\nu_0}$ belongs to the interval $[3-2\sqrt{2}, \frac{1}{3-2\sqrt{2}}]$ (which corresponds to $-t/\sqrt{2} \leq n \leq t/\sqrt{2}$), the solutions are of the form

$$a\left(\frac{2\nu_0+2}{\nu_0+2}\right)^{\nu/2}\sin(\nu\theta+\alpha) \tag{6}$$

where $\theta = \arccos\frac{3\nu_0+4-\mu_0}{2\sqrt{2}(\nu_0+1)}$. However, the error introduced by replacing ν and μ by ν_0 and μ_0 turns out to be too big. So, this simple approach fails, but also suggests a better approximation

$$A_{\mu,\nu} = a2^{\nu/2}\sin\left(\sum_{j=\mu}^{\nu-1}\theta_{\mu,j}+\alpha\right) \tag{7}$$

where $\theta_{\mu,j} = \arccos\frac{3j+4-\mu}{2\sqrt{2}(j+1)}$. The reason why this approximation works is as follows. If we look at the values $A_{\mu,\nu+2}$, $A_{\mu,\nu+1}$ and $A_{\mu,\nu}$, we have

$$\begin{aligned} A_{\mu,\nu} &= a2^{\nu/2}\sin(\Theta), \\ A_{\mu,\nu+1} &= a2^{(\nu+1)/2}\sin(\Theta+\theta_{\mu,\nu}), \\ A_{\mu,\nu+2} &= a2^{(\nu+2)/2}\sin(\Theta+\theta_{\mu,\nu}+\theta_{\mu,\nu+1}). \end{aligned} \tag{8}$$

where $\Theta = \alpha + \sum_{j=\mu}^{\nu-1} \theta_{\mu,j}$. If we consider (6) with $a2^{\nu/2}$ and Θ instead of a and α, we get

$$
\begin{aligned}
A_{\mu,\nu} &= a2^{\nu/2} \sin(\Theta), \\
A_{\mu,\nu+1} &= a2^{nu/2} \left(\frac{2\nu_0 + 2}{\nu_0 + 2}\right) \sin(\Theta + \theta_{\mu,\nu}), \\
A_{\mu,\nu+2} &= a2^{(\nu+2)/2} \left(\frac{2\nu_0 + 2}{\nu_0 + 2}\right)^2 \sin(\Theta + 2\theta_{\mu,\nu}). \quad (9)
\end{aligned}
$$

The expressions (8) and (9) are almost the same, except that (8) has 2 instead of $(\frac{2\nu_0+2}{\nu_0+2})$ and $\theta_{\mu,\nu} + \theta_{\mu,\nu+1}$ instead of $2\theta_{\mu,\nu}$. In both of those cases, the terms differ only by $O(\frac{1}{\nu})$. This can be used to show

LEMMA 14. *Let A be the approximation of the equation (7). If $A_{\mu,\nu} = S_{\mu,\nu}$ and $A_{\mu,\nu+1} = S_{\mu,\nu+1}$, then*

$$A_{\mu,\nu+2} = S_{\mu,\nu+2} + \Delta \quad (10)$$

where $|\Delta| = O(\frac{1}{\nu}) 2^{(\nu+2)/2} a$.

Thus, one step of the approximation introduces error at most $O(\frac{1}{\nu})$ of the possible value $(2^{(\nu+2)/2})$. By applying the argument of Lemma 14 $\nu - \mu - 1$ times (first to $A_{\mu,\mu}$, $A_{\mu,\mu+1}$, $A_{\mu,\mu+2}$, then to $A_{\mu,\mu+1}$, $A_{\mu,\mu+2}$ and $A_{\mu,\mu+3}$ and so on, until we get to $A_{\mu,\nu}$), we get

LEMMA 15. *Let $d < \frac{1}{3-2\sqrt{2}}$. If a and α are such that $S_{\mu,\mu} = A_{\mu,\mu}$ and $S_{\mu,\mu+1} = A_{\mu,\mu+1}$, then, for any ν satisfying $\nu < \mu < d\nu$,*

$$|S_{\mu,\nu} - A_{\mu,\nu}| \le \left(\left(1 + \frac{D}{\nu}\right)^{\nu-\mu-1}\right) 2^{\nu/2} a.$$

where D is a constant that depends on d.

Each approximation step has introduced a multiplicative error factor of $(1 + \frac{D}{\nu})$, which gives the total error factor of $(1 + \frac{D}{\nu})^{\nu-\mu-1}$.

Then, we use the method of Lemma 12 to obtain the precise values of $S_{\mu,\mu}$ and $S_{\mu,\mu+1}$ and use $S_{\mu,\mu}$ and $S_{\mu,\mu+1}$ to determine a_0 and α.

This gives an $O(\delta)$-good approximation of amplitudes of $|n\rangle|\mathrm{L}\rangle$ for $-\delta t < n < \delta t$. This approximation can be then used to show that, for any t and $\epsilon > 0$, $\Omega(t)$ amplitudes of $|n\rangle|\mathrm{L}\rangle$ must be at least $(1-\epsilon)$ times the amplitude of $|0\rangle|\mathrm{L}\rangle$, i.e., at least $(1-\epsilon)\frac{1}{\sqrt{2\pi t}}$. This implies Theorem 3.

However, Lemma 15 is not sufficient to prove Theorems 1 and 2, although, as we see, it is sufficient to show some of their important consequences. (In particular, it implies Theorem 3.) To obtain Theorems 1 and 2, one needs a different approach.

Connections to orthogonal polynomials

Our second approach relates the sums (3) and (4) to Jacobi polynomials.

The first sum is symmetric so for it we assume $\mu \ge \nu$. Then, it can be expressed in terms of the Gauss hypergeometric function. Using [1, 15.3.4] we have

$$S_{\mu,\nu} = {}_2F_1 \left[\begin{matrix} -\nu, -\mu \\ 1 \end{matrix}; -1\right] = 2^\nu \; {}_2F_1 \left[\begin{matrix} -\nu, \mu+1 \\ 1 \end{matrix}; 1/2\right].$$

Let $b = \mu - \nu$. Then from [1, 15.4.6] we see that

$$S_{\mu,\nu} = 2^\nu J_\nu^{(0,b)}.$$

(Recall that $J_\nu^{(0,b)}$ denotes the constant term of the degree ν Jacobi polynomial.) Using Lemma 4 we can now express the wave function for chirality L as follows. When $n \equiv t \mod 2$, $\psi_L(n,t)$ is

$$(-1)^{(t-n)/2} \times \begin{cases} 2^{-n/2-1} J_{\frac{t-n}{2}-1}^{(0,n+1)}, & \text{if } 0 \le n < t \\ 2^{n/2} J_{\frac{t+n}{2}}^{(0,-n-1)}, & \text{if } -t \le n < 0 \end{cases}$$

By similar arguments, we have for $\mu \ge \nu$

$$T_{\mu,\nu} = 2^{\nu-1} J_{\nu-1}^{(1,\mu-\nu+1)}$$

and for $\mu < \nu$

$$T_{\mu,\nu} = \frac{\nu}{\mu+1} 2^\mu J_\mu^{(1,\nu-\mu-1)}.$$

Then $\psi_R(n,t)$ is

$$(-1)^{(t-n)/2} \times \begin{cases} \left(\frac{t+n}{t-n}\right) 2^{-n/2-1} J_{\frac{t-n}{2}-1}^{(1,n)}, & \text{if } 0 \le n < t; \\ 2^{n/2-1} J_{\frac{t+n}{2}-1}^{(1,-n)}, & \text{if } -t \le n < 0. \end{cases}$$

From these representations of the wave function we obtain Lemma 5 and Theorem 6. Chen and Ismail [7] have analyzed the asymptotics for values of Jacobi polynomials whose parameters are linear functions of the degree. Using their ideas, we obtain, after some work, Theorems 1 and 2. (The results as stated in [7] have some minor errors. In particular, to obtain Theorem 1 one must take t_0 in (2.17) to have the larger absolute value.)

Fourier analysis of the Hadamard walk

We now turn to the Schrödinger approach for studying quantum walks. As mentioned in Section 1, the Hadamard walk has, due to translational invariance, a simple description in the Fourier domain. We therefore cast the problem of time evolution in this basis, where it can easily be solved, and at the end revert back to the real space description by inverting the Fourier transformation. This and the following two subsections represent a preliminary exposition of an analysis of the two-way infinite timed Hadamard walk to be given in more detail in [26].

The dynamics for Ψ in the Hadamard walk is given by the following transformation (cf. Figure 1):

$$
\begin{aligned}
&\Psi(n, t+1) \\
&= \begin{bmatrix} 0 & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \Psi(n-1, t) + \begin{bmatrix} \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{bmatrix} \Psi(n+1, t) \\
&= M_+ \Psi(n-1, t) + M_- \Psi(n+1, t),
\end{aligned}
$$

for matrices M_+, M_- defined appropriately. Since the particle starts at the origin with chirality state RIGHT, we have the initial conditions, $\Psi(0,0) = (0,1)^\mathsf{T}$, and $\Psi(n,0) = (0,0)^\mathsf{T}$ if $n \ne 0$.

With the above formulation, the analysis of the Hadamard walk reduces to solving a two dimensional linear recurrence. We now show how this recurrence may be analyzed.

The spatial Fourier transform $\tilde{\Psi}(k,t)$ (for $k \in [-\pi, \pi]$) of the wave function $\Psi(n,t)$ over $\mathbb{Z}$ is given by [11]:

$$\tilde{\Psi}(k,t) = \sum_n \Psi(n,t) e^{ikn}.$$

In particular, we have $\tilde{\Psi}(k,0) = (0,1)^\mathsf{T}$ for all k.

From the dynamics of Ψ, we may deduce the following.

$$\begin{aligned}\tilde{\Psi}(k,t+1) &= \sum_n \left(M_+\Psi(n-1,t) + M_-\Psi(n+1,t)\right) e^{ikn} \\ &= e^{ik} M_+ \sum_n \Psi(n-1,t)\, e^{ik(n-1)} \\ &\quad + e^{-ik} M_- \sum_n \Psi(n+1,t)\, e^{ik(n+1)} \\ &= \left(e^{ik}M_+ + e^{-ik}M_-\right)\tilde{\Psi}(k,t).\end{aligned}$$

Thus, we have,

$$\begin{aligned}\tilde{\Psi}(k,t+1) &= M_k\,\tilde{\Psi}(k,t) \quad \text{where} \qquad (11)\\ M_k &= e^{ik}M_+ + e^{-ik}M_-. \qquad (12)\end{aligned}$$

In the case of the Hadamard walk,

$$M_k = \frac{1}{\sqrt{2}}\begin{bmatrix} -e^{-ik} & e^{-ik} \\ e^{ik} & e^{ik}\end{bmatrix}. \qquad (13)$$

(More generally, we have that $M_k = \Lambda_k U^{\mathsf{T}}$, where Λ_k is the diagonal matrix with entries e^{-ik}, e^{ik} and U^T is the transpose of the unitary matrix U that acts on the chirality state of the particle.)

The recurrence in Fourier space thus takes the simple form $\tilde{\Psi}(k,t+1) = M_k\,\tilde{\Psi}(k,t)$, leading to

$$\tilde{\Psi}(k,t) = M_k^t\,\tilde{\Psi}(k,0). \qquad (14)$$

We may calculate M_k^t (and thus $\tilde{\Psi}(k,t)$) by diagonalizing the matrix M_k, which is readily done since it is a 2×2 unitary matrix. If M_k has eigenvectors $(|\Phi_k^1\rangle, |\Phi_k^2\rangle)$ and corresponding eigenvalues $(\lambda_k^1, \lambda_k^2)$, we can write:

$$M_k = \lambda_k^1\,|\Phi_k^1\rangle\langle\Phi_k^1| \;+\; \lambda_k^2\,|\Phi_k^2\rangle\langle\Phi_k^2|,$$

and then immediately we obtain the time evolution matrix as:

$$M_k^t = (\lambda_k^1)^t\,|\Phi_k^1\rangle\langle\Phi_k^1| \;+\; (\lambda_k^2)^t\,|\Phi_k^2\rangle\langle\Phi_k^2|. \qquad (15)$$

The eigenvalues of M_k are $\lambda_k^1 = e^{i\omega_k}$ and $\lambda_k^2 = e^{i(\pi-\omega_k)}$, where $\omega_k \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ satisfies $\sin(\omega_k) = \frac{\sin k}{\sqrt{2}}$. The corresponding eigenvectors are also easily calculated:

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

where the normalization factor is given by

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

In the Fourier basis the initial state is represented by $\tilde{\Psi}(k,0) = (0,1)^{\mathsf{T}}$ for all k. Using the relations (14) and (15) above, the wave function at time t may now be written as:

$$\begin{aligned}\tilde{\psi_{\mathrm{R}}}(k,t) &= \frac{1}{2}\Big(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\Big)\,e^{i\omega_k t} \\ &\quad + \frac{(-1)^t}{2}\Big(1 - \frac{\cos k}{\sqrt{1+\cos^2 k}}\Big)\,e^{-i\omega_k t} \\ \tilde{\psi_{\mathrm{L}}}(k,t) &= \frac{e^{-ik}}{2\sqrt{1+\cos^2 k}}\left(e^{i\omega_k t} - (-1)^t e^{-i\omega_k t}\right)\end{aligned}$$

We now invert the Fourier transformation, to return to the basis in real space. This gives us the representation of the wave functions in real space given in Lemma 7.

Asymptotic form of the wave function

In the previous subsection, we obtained a closed form solution for the time evolved wave function of the Hadamard walk. We now consider the behavior of the wave function for large t. Fortunately, the problem of analyzing integrals as in Lemma 7 is considerably simplified in this asymptotic limit. We use extensively the Method of Stationary Phase [4] to extract the asymptotic properties of the resulting wave function. This allows us to accurately derive several useful results.

The asymptotic analysis for ψ_{L} and ψ_{R} is essentially the same. They can both be written as a sum of integrals of the type $I(\alpha,t)$ as below (where $\alpha = n/t$ as usual):

$$I(\alpha,t) = \int_{-\pi}^{\pi}\frac{dk}{2\pi}\,g(k)\,e^{i\,\phi(k,\alpha)\,t}.$$

Here $g(k)$ is an analytic, periodic function of period 2π taken to be either even or odd, $\phi(k,\alpha) = -\omega_k + \alpha k$, and $\alpha \in [-1,1]$. Below, we describe a coarse analysis of the behavior of I as we vary α.

First, we consider $|\alpha|$ larger than $\frac{1}{\sqrt{2}}$ by a constant. For this range of α, ϕ does not have any stationary points, and we can use integration by parts to show that it decays faster than any inverse polynomial in t. Next, we look at the points $\alpha = 1/\sqrt{2}, -1/\sqrt{2}$. At these points, ϕ has a stationary point of order 2 at $k = 0, \pi$, respectively, as may readily be verified. Using the method of stationary phase, we thus get the following leading term for I at these points:

$$\begin{aligned}I\Big(\frac{-1}{\sqrt{2}},t\Big) &\sim \frac{g(\pi)}{3\pi}\sqrt{2}\,\Gamma(1/3)\left[\frac{6}{t}\right]^{1/3}\cos\left(\frac{\pi}{\sqrt{2}}t + \frac{\pi}{6}\right) \\ I\Big(\frac{1}{\sqrt{2}},t\Big) &\sim \frac{g(0)}{3\pi}\sqrt{\frac{3}{2}}\,\Gamma(1/3)\left[\frac{6}{t}\right]^{1/3}.\end{aligned}$$

Finally, we turn to the interval of most interest to us, $[\frac{-1}{\sqrt{2}}+\epsilon, \frac{1}{\sqrt{2}}-\epsilon]$. When α lies in this region, ϕ has two stationary points $k_\alpha, -k_\alpha$, where $k_\alpha \in [0,\pi]$ and

$$\cos k_\alpha = \frac{\alpha}{\sqrt{1-\alpha^2}}.$$

We can again employ the method of stationary phase to get the following dominant term in the expansion of $I(\alpha,t)$:

$$\frac{g(k_\alpha)}{\sqrt{2\pi t\,|\omega''_{k_\alpha}|}} \times \begin{cases} 2\cos(\phi(k_\alpha,\alpha)\,t + \pi/4) & \text{if } g \text{ is even} \\ 2i\sin(\phi(k_\alpha,\alpha)\,t + \pi/4) & \text{if } g \text{ is odd}\end{cases}$$

It is now straightforward to derive the asymptotic expression for $\Psi(n,t)$, and hence also for the probability distribution $P(n,t)$, for $|n/t|$ bounded away from $1/\sqrt{2}$. Theorem 2 summarizes this calculation. (In deriving this, it is helpful to note that $\theta = \omega_{k_\alpha}$ and $\rho = \pi - k_\alpha$. We also have $\theta + \rho - \chi = \pi$.)

The (approximate) probability distribution P compares very well with numerical results even for small t, as is evident from Figure 2. The bias to the right in the probability distribution plotted in the figure is an artifact of the choice of initial chirality state (it was chosen to be RIGHT). If the particle begins in the chirality state $\frac{1}{\sqrt{2}}(|\mathrm{L}\rangle + i|\mathrm{R}\rangle)$, the distribution at any time can be shown to be symmetric. Indeed, the Hadamard walk is an *unbiased* walk.

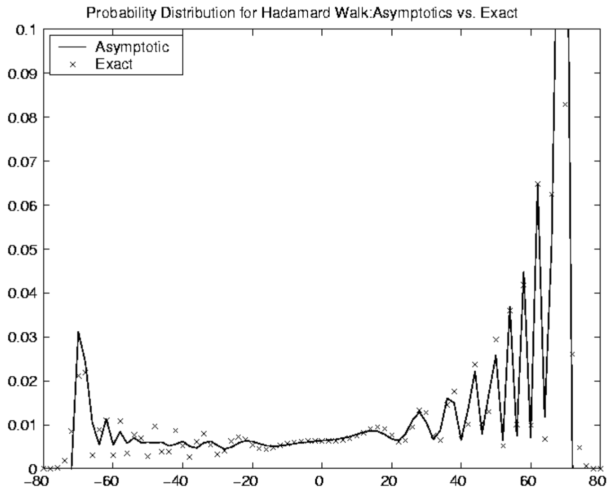

Figure 2: *A comparison of two probability distributions, one obtained by numerical integration of Lemma 7 and the other from an asymptotic analysis of the walk. The number of steps in the walk was taken to be* 100*. Only the probability at the* even *points is plotted, since the odd points have probability zero.*

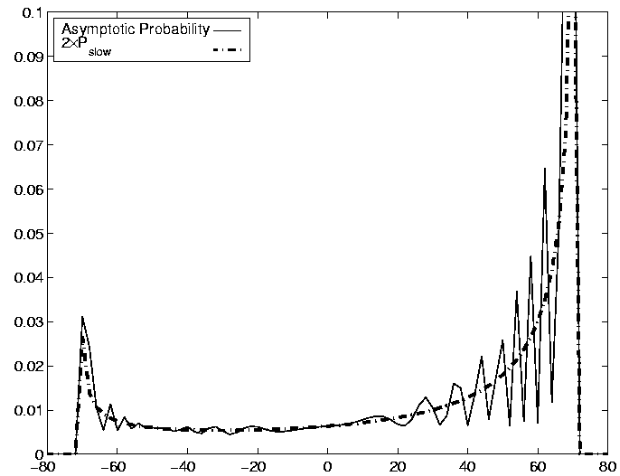

Figure 3: *A comparison of the distributions P and $P_{\rm slow}$ for $t = 100$. Only the probability at the* even *points is plotted, and $P_{\rm slow}$ is scaled by a factor of 2 because it has support on the odd points as well.*

	$p(\alpha)$ approx.	exact
$\langle \alpha \rangle$	$1 - 1/\sqrt{2} = 0.293$	0.293
$\langle \lvert\alpha\rvert \rangle$	$1/2$	0.500
$\langle \alpha^2 \rangle$	$1 - 1/\sqrt{2} = 0.293$	0.293

Figure 4: *A table of moments calculated with the approximation by the density function $p(\alpha)$, which are compared with exact results (obtained by numerical integration) with $t = 80$. As mentioned before, the particle has a constant speed to the right, as indicated by its mean position, which is a result of its biased initial state. For an unbiased initial state, the mean would be zero.*

Properties of the distribution

The net probability of the points n with α between $-1/\sqrt{2}+\epsilon$ and $1/\sqrt{2}-\epsilon$, where ϵ is an arbitrarily small constant, is $1 - \frac{2\epsilon}{\pi} - \frac{O(1)}{t}$, so the rest of the points do not contribute to any global properties of the distribution. Henceforth, we restrict ourselves to this interval.

For the purposes of studying its properties, it is convenient to decompose P as

$$P(n,t) \;=\; P_{\rm slow}(n,t) + P_{\rm fast}(n,t), \tag{16}$$

where

$$P_{\rm slow}(\alpha t, t) \;=\; \frac{1+\alpha}{\pi t\,|\omega''_{k_\alpha}|} \tag{17}$$

is a slowly varying (non-oscillating) function in α, and $P_{\rm fast}$ is the remaining (quickly oscillating) component. One can show that any contribution to a moment from the "fast" component $P_{\rm fast}$ is of lower order in t than the contribution from $P_{\rm slow}$. In Figure 3, we compare $P_{\rm slow}$ with P.

For example, the calculation of moments is simplified by the following observation. Let $p(\alpha) = tP_{\rm slow}(\alpha t, t)$. Then p is a probability density function over $[-1/\sqrt{2}, 1/\sqrt{2}]$: it is clearly non-negative, and we show below that it integrates to 1. This observation allows us to approximate the sums in the moment calculations by a *Riemann integral*, and the error so introduced is again a lower order term.

To see that $p(\alpha)$ integrates to 1, note that $\frac{\partial\phi}{\partial k}(k_\alpha,\alpha) = 0 = -\omega'_{k_\alpha} + \alpha$, so

$$|\omega''_{k_\alpha}| \;\equiv\; -\omega''_{k_\alpha} \;=\; -\frac{d\alpha}{dk_\alpha}.$$

Now,

$$\begin{aligned}\int_{-1/\sqrt{2}}^{1/\sqrt{2}} p(\alpha)\,d\alpha &= \frac{1}{\pi}\int_{1/\sqrt{2}}^{-1/\sqrt{2}} (1+\alpha)\frac{dk_\alpha}{d\alpha}\,d\alpha \\ &= \frac{1}{\pi}\int_0^{\pi}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right)dk \\ &= 1,\end{aligned}$$

since $\cos k/\sqrt{1+\cos^2 k}$ is anti-symmetric about the point $\pi/2$.

Moments for the density function p are now readily calculated by standard methods from complex analysis. Some of these are listed in Figure 4 for comparison with numerical results. This gives us the leading term for the moments for the distribution P.

We now look at the mixing behavior of the Hadamard walk. Figure 3 clearly suggests that the probability distribution P is almost uniform over the interval $(-t/\sqrt{2}, t/\sqrt{2})$, i.e., it spreads in linear time, *quadratically* faster than the classical random walk. We argue this formally below.

Recall that the δ-mixing time (τ_δ) of a randomized process is defined as the first time t such that the distribution at time t is at total variation distance (which is half the ℓ_1 distance) at most δ from the uniform distribution. We claim that there is a constant $\delta < 1$ such that at time t, P is δ-close to the uniform distribution on the integer points between $\mp t/\sqrt{2}$. For classical random walks, the corresponding mixing time is *quadratic* in t.

In order to show that the Hadamard walk is "mixed" at time t (in the sense described above), it suffices to show that a constant fraction $\beta > 0$ of the points in the said interval have probability between $c/\sqrt{2}\,t$ and $1/\sqrt{2}\,t$ for a constant $c > 0$. A straightforward calculation shows that this implies that the ℓ_1 distance from uniform over $[-t/\sqrt{2},\, t/\sqrt{2}]$ is at most $2(1-\beta c)$, so that $\delta = 1 - \beta c < 1$ is a constant.

As in the preceding discussion, we restrict ourselves to the interval where $\alpha \in [-1/\sqrt{2}+\epsilon,\ 1/\sqrt{2}-\epsilon]$ (with ϵ chosen to be a suitable constant) such that $P(\alpha, t)$ is at most $1/\sqrt{2}t$ within the interval. Recall that the probability mass within this interval is $1 - \frac{2\epsilon}{\pi} - \frac{O(1)}{t}$, which is a constant greater than 0. Clearly, this cannot hold unless at least a constant fraction $\beta = 1 - \frac{2\epsilon}{\pi} - c$ of the points within this interval have probability at least some constant $0 < c < 1 - \frac{2\epsilon}{\pi}$ over $\sqrt{2}\,t$. This proves Theorem 3, which shows of the mixing nature of the Hadamard walk.

5. SEMI-INFINITE AND FINITE HADAMARD WALKS

Now we turn to the case where a particle does a Hadamard walk in the presence of one or two absorbing boundaries.

For the semi-infinite (one boundary) case, note that the probability p_∞ may be expressed as

$$p_\infty = \sum_{t \ge 1} \left\| (\Pi^0_{yes} W)^t |1\rangle|\mathrm{R}\rangle \right\|^2 .$$

(Renormalizations do not appear in this expression because we are calculating an unconditional probability.) The sum will be evaluated by counting paths.

Let A_t be the set of t-tuples $(a_1, \ldots, a_t) \in \{-1, 1\}^t$ for which (i) $\sum_{i \le j} a_i \ge 0$, for all $j < t$, and (ii) $\sum_{i \le t} a_i = -1$. The set A_t is in one-to-one correspondence with the set of all paths starting in state $|1\rangle|\mathrm{R}\rangle$ and entering location 0 for the first time at time t (each a_i indicates $(-1)^{d_i}$ for d_i the direction after i applications of W). Let A_t^+ denote the subset of A_t for which

$$\#\{i \,|\, 1 \le i < t,\, a_i = a_{i+1} = -1\}$$

is even and let A_t^- denote the subset of A_t for which this number is odd. Now, the amplitude associated with each path in A_t^+ is $2^{-t/2}$, and the amplitude associated with each path in A_t^- is $-2^{-t/2}$. It follows that

$$p_\infty = \sum_{t \ge 1} \left(\#\left(A_t^+\right) - \#\left(A_t^-\right) \right)^2 2^{-t}. \tag{18}$$

We will evaluate the sum in (18) by defining a generating function for $\#\left(A_t^+\right) - \#\left(A_t^-\right)$. Let

$$f(z) = \sum_{t \ge 1} \left(\#\left(A_t^+\right) - \#\left(A_t^-\right) \right) z^t .$$

The function $f(z)$ obeys the equation

$$\begin{aligned} f(z) &= z - z\left(zf(z) + (zf(z))^2 + (zf(z))^3 + \cdots\right) \\ &= z - \frac{z^2 f(z)}{1 - zf(z)}, \end{aligned} \tag{19}$$

which follows from the fact that $-z(zf(z))^k$ is a generating function similar to f, but restricted to paths that pass through location 1 exactly k times, $k \ge 1$. Solving for $f(z)$ we obtain

$$f(z) = \frac{1 + 2z^2 - \sqrt{1 + 4z^4}}{2z}. \tag{20}$$

Equation (20) is similar in form to the generating function for the Catalan numbers. We have

$$\#\left(A_t^+\right) - \#\left(A_t^-\right) = \begin{cases} 1 & t = 1 \\ (-1)^{k+1} C_k & t = 4k + 3 \\ 0 & \text{otherwise} \end{cases}$$

where $C_k = \frac{1}{k+1}\binom{2k}{k}$ is the kth Catalan number. Thus

$$p_\infty = 1/2 + \big(\sum_{k \ge 0} C_k^2\, 2^{-4k}\big)/8.$$

Using induction, it is straightforward to prove that

$$\sum_{k \le N} C_k^2\, 2^{-4k} = (16\,N^3 + 36\,N^2 + 24\,N + 5)\, C_N^2\, 2^{-4N} - 4,$$

and hence

$$p_\infty = \frac{1}{2} + \frac{1}{8}\left(\frac{16}{\pi} - 4\right) = \frac{2}{\pi}.$$

Next, we consider the case of two absorbing boundaries. We show that p_n, the probability of exit to the left for the walk on $\{1, \ldots, n-1\}$, has the limiting value $1/\sqrt{2}$. The idea is to express p_n as an oscillatory integral, whose limit is a two-dimensional integral we can evaluate exactly.

As in the semi-infinite case, we count paths. Define A_t^+ and A_t^- as above, and let $A_{t,n}^+$ and $A_{t,n}^-$ denote the subsets of A_t^+ and A_t^-, respectively, for which paths are restricted to locations $1, \ldots, n-1$ before reaching location 0 on the last step. Defining

$$f_n(z) = \sum_{t \ge 0} \left(\#\left(A_{t,n}^+\right) - \#\left(A_{t,n}^-\right) \right) z^t, \tag{21}$$

we have for $n > 1$ that

$$p_n = \sum_{t \ge 0} \left(\#\left(A_{t,n}^+\right) - \#\left(A_{t,n}^-\right) \right)^2 2^{-t} = (f_n \odot f_n)(1/2),$$

where $\odot$ denotes the Hadamard product [31, p. 157]. The generating functions f_n satisfy

$$f_n(z) = z\left(\frac{1 - 2zf_{n-1}}{1 - zf_{n-1}}\right) \tag{22}$$

with $f_1(z) = 0$. The reasoning is similar to the semi-infinite case. We will let $z = e^{i\theta}/\sqrt{2}$ in the analysis that follows.

Integrals for exit probabilities

LEMMA 16. *We have*

$$p_n = \frac{2}{\pi} \int_0^{\pi/2} |f_n(e^{i\theta}/\sqrt{2})|^2\, d\theta.$$

Proof. By the integral representation of the Hadamard product [31, p. 157] we have

$$p_n = (f_n \odot f_n)(1/2) = \frac{1}{2\pi}\int_0^{2\pi} |f_n(e^{i\theta}/\sqrt{2})|^2 \, d\theta. \qquad (23)$$

Using (22) we see that f_n is odd and satisfies $f_n(\bar{z}) = \overline{f_n(z)}$. Using these symmetries we get the result. ∎

Lemma 17. *For $n \geq 1$ and $|z| = 1/\sqrt{2}$, we have $|f_n| \leq 1$.*

Proof. It is more convenient to work with $g_n = z f_n(z/\sqrt{2})$, which satisfies the recurrence relation

$$g_n = z^2 \left(\frac{1 - \sqrt{2} g_{n-1}}{\sqrt{2} - g_{n-1}} \right) \qquad (24)$$

with $g_1(z) = 0$. The map

$$w \mapsto \frac{1 - \sqrt{2} w}{\sqrt{2} - w}$$

maps the unit disk to itself. (Observe that it maps the unit circle to itself and apply the maximum modulus principle.) Using induction on n, (24) implies that $|g_n| \leq 1$ on the unit disk. ∎

Lemma 18. *Let*

$$\lambda_{1,2} = \frac{(2z^2 - 1) \pm \sqrt{1 + 4z^4}}{2} \qquad (25)$$

(subscript 1 for +; principal branch taken) and

$$\mu_{1,2} = \frac{(2z^2 + 1) \pm \sqrt{1 + 4z^4}}{2z^2} \qquad (26)$$

(ditto). Then for $n \geq 1$ we have (with $m = n - 1$)

$$h_n := \frac{f_n}{z} = \mu_1 \mu_2 \frac{(\lambda_1/\lambda_2)^m - 1}{\mu_2 (\lambda_1/\lambda_2)^m - \mu_1}.$$

Proof. Let φ_z denote the Möbius transformation $w \mapsto \frac{2z^2 w - 1}{z^2 w - 1}$, so that h_n is the m-th iterate of φ_z, starting from 0. By diagonalizing the matrix of φ_z, we obtain a formula for this. (This technique comes from [28, p. 182].) ∎

Lemma 19. *We have:*

(i) $|\lambda_1/\lambda_2| = 1$ *for* $0 < \theta < \pi/4$;
(ii) $|\lambda_1/\lambda_2| < 1$ *for* $\pi/4 < \theta < \pi/2$;
(iii) $|\mu_2|^2 = 2$ *for* $\pi/4 < \theta < \pi/2$; *and*
(iv) $\mu_1/\mu_2 = 1 + 2\cos 2\theta + 2\cos\theta\sqrt{2\cos 2\theta} \in \mathbb{R}$ *for* $0 < \theta < \pi/4$.

Proof. We prove (i) and (ii) together. From the relation $|a + b|^2 = |a|^2 + |b|^2 + 2\Re(\bar{a}b)$, we find

$$|\lambda_1|^2 - |\lambda_2|^2 = 4\Re\left(\overline{(2z^2 - 1)}\sqrt{1 + 4z^4}\right).$$

Since $z = e^{i\theta}/\sqrt{2}$, we have

$$\left(\overline{(2z^2 - 1)}\sqrt{1 + 4z^4}\right)^2 = (e^{-2i\theta} - 1)^2 (1 + e^{4i\theta})$$

$$= 8(\cos^2\theta - 1/2)(\cos^2\theta - 1).$$

This is negative for $0 < \theta < \pi/4$ and positive for $\pi/4 < \theta < \pi/2$. Hence its square root is pure imaginary in the first case, making $|\lambda_1|^2 - |\lambda_2|^2 = 0$. In the second case, the square root is a real number that we determine to be negative, making $|\lambda_1|^2 - |\lambda_2|^2 < 0$.

Now consider (iii). Since $|2z^2| = 1$ it will suffice to consider

$$\nu = (2z^2 + 1) - \sqrt{1 + 4z^4}$$

and show that $\nu\bar{\nu} = 2$. Substituting $z = e^{i\theta}/\sqrt{2}$ and rationalizing the denominator, we find that

$$2/\nu = 1 + e^{-2i\theta} + e^{-2i\theta}\sqrt{1 + e^{4i\theta}}$$

whereas

$$\bar{\nu} = 1 + e^{-2i\theta} - \sqrt{1 + e^{4i\theta}}.$$

These are equal precisely when

$$e^{-2i\theta}\sqrt{1 + e^{4i\theta}} = -\sqrt{1 + e^{4i\theta}},$$

which is true for $\pi/4 < \theta < 3\pi/4$.

To prove (iv), observe that

$$a + bi := \frac{\mu_1}{\mu_2} = \frac{2z^2 + 1 + \sqrt{1 + 4z^4}}{2z^2 + 1 - \sqrt{1 + 4z^4}}$$

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

Since $2z^2 = e^{2i\theta}$ and we are taking the principal branch of the square root this is

$$(e^{2i\theta} + e^{-2i\theta}) + 1 + (1 + e^{-2i\theta})e^{i\theta}\sqrt{e^{2i\theta} + e^{-2i\theta}}$$

$$= 1 + 2\cos 2\theta + 2\cos\theta\sqrt{2\cos 2\theta}.$$

Since $0 \leq 2\theta \leq \pi/2$, this is real, so

$$a = 1 + 2\cos 2\theta + 2\cos\theta\sqrt{2\cos 2\theta}, \qquad b = 0.$$

∎

A nonlinear Riemann-Lebesgue lemma

For a smooth function on the cylinder $T = \{|z| = 1\} \times \{|u| \leq \pi\}$, the following result is physically plausible. Our application motivates the precise assumptions.

Lemma 20. *Let $F : T \to \mathbb{R}$ be C^2 for $|u| < \pi$, bounded when $z = e^{iu}$, with radial average*

$$G(u) := \frac{1}{2\pi}\int_0^{2\pi} F(e^{i\phi}, u) d\phi$$

bounded and Riemann integrable on $|u| < \pi$. Then

$$\lim_{m\to\infty} \int_{-\pi}^{\pi} F(e^{imu}, u) du = \int_{-\pi}^{\pi} G(u) du.$$

Proof: Choose $\epsilon > 0$. We let $a = -\pi$, $b = \pi$ and $h = 2\pi/m$ so that the m intervals

$$I_k = [a + kh, a + (k+1)h], \qquad k = 0, \ldots, m-1$$

cover $[a, b]$. Let $J_\epsilon = [a + \epsilon, b - \epsilon]$. Since F is bounded and $[a, b] - J_\epsilon$ is covered by $2\epsilon/h + O(1)$ intervals we have

$$\int_a^b F(e^{imu}, u) du$$

$$= \sum_{I_k \subset J_\epsilon} \int_{I_k} F(e^{imu}, u) du + O(\epsilon + 1/m) \qquad (27)$$

If $u \in [c, c+h] \subset J_\epsilon$ then

$$F(e^{imu}, u) - F(e^{imu}, c) = \int_c^u \frac{\partial F}{\partial \xi}(e^{imu}, \xi)\, d\xi = O(h).$$

Therefore

$$\int_c^{c+h} F(e^{imu}, u) du = \int_c^{c+h} F(e^{imu}, c) du + O(1/m^2)$$

$$= \frac{1}{m} \int_0^{2\pi} F(e^{i\phi}, c) d\phi + O(1/m^2).$$

Substituting this in (27) we get

$$\int_a^b F(e^{imu}, u) du = \frac{2\pi}{m} \sum_{I_k \subset J_\epsilon} G(a + kh) + O(\epsilon + 1/m).$$

The sum is $2\epsilon/h + O(1)$ evaluation points shy of being a Riemann sum, so by our assumption on G,

$$\limsup_{m\to\infty} \int_a^b F(e^{imu}, u) du \leq \int_a^b G(u) du + O(\epsilon).$$

Similarly,

$$\liminf_{m\to\infty} \int_a^b F(e^{imu}, u) du \geq \int_a^b G(u) du - O(\epsilon).$$

Since ϵ is arbitrary the result follows. ■

The limiting exit probability.

In this section we prove Theorem 10. It follows from the two lemmas below.

LEMMA 21. *We have*

$$\lim_{n\to\infty} p_n = \frac{1}{2} + \frac{4}{\pi} \int_0^{\pi/4} \frac{d\theta}{\mu_1/\mu_2 + 1}.$$

Proof. From Lemma 16 we have, since $|f_n|$ is even,

$$p_n = \frac{1}{\pi} \int_{-\pi/4}^{\pi/4} |f_n|^2 d\theta + \frac{1}{\pi} \int_{\pi/4}^{\pi/2} |f_n/z|^2 d\theta. \qquad (28)$$

By Lemma 17 and (ii)-(iii) of Lemma 19, the second term has the limit 1/2 as $n \to \infty$.

In the first term, we consider θ to be a function of $u = \arg(\lambda_1/\lambda_2)$ (this is real by Lemma 19), choosing the branch that maps 0 to 0. This gives

$$\frac{1}{\pi} \int_{-\pi/4}^{\pi/4} |f_n|^2 d\theta = \frac{2}{\pi} \int_{-\pi}^{\pi} \left| \frac{(\lambda_1/\lambda_2)^m - 1}{\mu_2(\lambda_1/\lambda_2)^m - \mu_1} \right|^2 \frac{d\theta}{du} du,$$

with $m = n - 1$. Applying Lemma 20 with

$$F(z, u) = |(z-1)/(\mu_2 z - \mu_1)|^2 \, d\theta/du$$

and undoing the substitution, we find its limit is

$$\frac{4}{\pi^2} \int_0^{\pi/4} d\theta \int_0^{2\pi} \frac{1 - \cos\phi}{|\mu_2 e^{i\phi} - \mu_1|^2} d\phi$$

$$= \frac{4}{\pi^2} \int_0^{\pi/4} \frac{d\theta}{|\mu_2|^2} \int_0^{2\pi} \frac{1 - \cos\phi}{(\mu_1/\mu_2 - \cos\phi)^2 + (\sin\phi)^2} d\phi.$$

Now apply Poisson's integral formula [31, p. 124] to the inner integral and observe that $\mu_1 \overline{\mu_2} = 2$. ■

LEMMA 22. *We have*

$$\int_0^{\pi/4} \frac{d\theta}{\mu_1/\mu_2 + 1} = \frac{\pi}{4}\left(\frac{1}{\sqrt{2}} - \frac{1}{2}\right).$$

Proof. Use of (iv) of Lemma 19, followed by an orgy of substitutions ($\psi = 2\theta$, then $t = \tan\psi/2$, $\rho = \sin^{-1} t$, finally $u = \tan\rho/2$) reduces the integral to an arctangent. We omit the details. ■

6. CONCLUSION

In this paper we have defined and studied quantum walks on one-dimensional lattices, and noted several striking differences from classical random walks.

There are many interesting questions regarding quantum walks that we leave open. In particular, for the case of quantum walks with absorbing boundaries, a more complete analysis remains to be done. We have restricted our attention to the question of determining exit probabilities, and even here there are apparently difficult problems remaining such as proving Conjecture 11 (assuming it is true).

It is yet unclear whether quantum walks are interesting from an algorithmic point of view. Any speed-up of a known classical algorithm based on random walks (such as those mentioned in Section 1) seems to involve the analysis of quantum walks on graphs much more complex than the line. The recent work of [2] represents a step forward in this direction.

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