# Absorption Probabilities for the Two-Barrier Quantum Walk 

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#### Abstract

Let $p_{j}^{(n)}$ be the probability that a Hadamard quantum walk, started at site $j$ on the integer lattice $\{0, \ldots, n\}$, is absorbed at 0 . We give an explicit formula for $p_{j}^{(n)}$. Our formula proves a conjecture of John Watrous, concerning an empirically observed linear fractional recurrence relation for the numbers $p_{1}^{(n)}$.


Key words: Quantum walks, quantum random walks, discrete quantum processes, quantum computation.

## 1 Introduction

Consider a Hadamard quantum walk on the sites $0,1, \ldots, n$, as defined in [1]. The boundary sites, 0 and $n$, are absorbing, so any walk is certain to be absorbed. Let $p_{j}^{(n)}$ denote the probability that the walk ends at location 0 .

The main result of this paper is an explicit formula for this probability. Let $A=2+\sqrt{2}$, and $B=2-\sqrt{2}$. We will prove that when $n \geq 1$ and $1 \leq j \leq n$, we have

$$
\begin{equation*}
p_{j}^{(n)}=\frac{\sqrt{2}}{4} \frac{\left(A^{n-j}-B^{n-j}\right)\left(A^{j-1}+B^{j-1}\right)}{A^{n-1}+B^{n-1}}, \tag{1.1}
\end{equation*}
$$

[^0]In particular, when $j=1$,

$$
\begin{equation*}
p_{1}^{(n)}=\frac{\sqrt{2}}{2} \frac{A^{n-1}-B^{n-1}}{A^{n-1}+B^{n-1}} \tag{1.2}
\end{equation*}
$$

and this satisfies the recurrence relation

$$
\begin{equation*}
p_{1}^{(n)}=\frac{1+2 p_{1}^{(n-1)}}{2+2 p_{1}^{(n-1)}} \tag{1.3}
\end{equation*}
$$

This recurrence relation, conjectured by Watrous from numerical data, appears in [1]. It is a consequence of (1.2) that

$$
\lim _{n \rightarrow \infty} p_{1}^{(n)}=\frac{1}{\sqrt{2}}
$$

a result that was proved with some effort in [1].
The absorption probability values are interrelated in many interesting ways. In the two-dimensional table of $p_{j}^{(n)}$, there is a linear fractional recurrence relation, similar to (1.3), for each column and each diagonal. This "numerology" was first observed empirically, and then led us to conjecture (1.1). There is also a linear recurrence relation common to all rows: if $1 \leq j \leq n-3$, we have

$$
p_{j}^{(n)}-7 p_{j+1}^{(n)}+7 p_{j+2}^{(n)}-p_{j+3}^{(n)}=0
$$

Two other relations, which we discuss later, have combinatorial interpretations.

It is interesting to consider the implications of (1.1) for starting sites in the "interior" of the lattice. For $j=\alpha n, \alpha$ fixed and $n \rightarrow \infty, p_{j}^{(n)}$ will be close to the limit $\frac{\sqrt{2}}{4}=0.35355 \ldots$. Thus, from the interior region, the probabilities for absorption at the left and right are almost constant, approximately $35 \%$ and $65 \%$. On the other hand, for the classical random walk, with equal probability of moving left and right, the probability that the walk, starting from $j$, is absorbed at the left, decreases linearly with $j$, from 1 at the left barrier to 0 at the right barrier. (One proof of this appears in [3].) This gives another example of the idea that quantum walks "spread out" more evenly than classical walks do.

## 2 Some Generating Functions.

Our work will be based on the path count generating function approach which was employed in [1] and [2].

Recall that for our walk, each site $j$ has two states, corresponding to the walker facing left and facing right. The one-step evolution matrix is a Hadamard transformation, i.e. starting from state $|n, R\rangle$ the particle can go next to

$$
\begin{array}{cc}
|n+1, R\rangle & \text { with amplitude } 1 / \sqrt{2} \\
|n-1, L\rangle & \text { w. a. } 1 / \sqrt{2}
\end{array}
$$

and from $|n, L\rangle$ it can go to

$$
\begin{aligned}
& |n+1, R\rangle \quad \text { w.a. } 1 / \sqrt{2} \\
& |n-1, L\rangle \text { w.a. }-1 / \sqrt{2}
\end{aligned}
$$

The initial state of the particle is $|j, R\rangle$, with $0<j<n$.
We define the path count generating function to be

$$
\begin{equation*}
f_{j}^{(n)}(z)=\sum_{m \geq 1}\left(\sum_{P} \sigma(P)\right) z^{m} \tag{2.1}
\end{equation*}
$$

where the $m$-th sum is over paths $P$ of length $m$ that are absorbed at the left (0) state, and the sign, $\sigma(P)$, is $(-1) \#$ of $L L$ blocks. In computing the sign, overlaps count, for example, the sign of $L L L$ is +1 .

The probability of absorption at 0 is given by the formula

$$
\begin{equation*}
p_{j}^{(n)}=\frac{1}{2 \pi i} \int_{|z|=1 / \sqrt{2}}\left|f_{j}^{(n)}(z)\right|^{2} z^{-1} d z \tag{2.2}
\end{equation*}
$$

In [1] it was shown that

$$
\begin{equation*}
f_{1}^{(2)}=z \tag{2.3}
\end{equation*}
$$

and for $n>1$,

$$
\begin{equation*}
f_{1}^{(n)}=z \frac{1-2 z f_{1}^{(n-1)}}{1-z f_{1}^{(n-1)}} \tag{2.4}
\end{equation*}
$$

We now complement this with another recurrence relation that allows (2.1) to be computed for $j>1$. Observe that any path from $j$ that is absorbed at 0 must go through 1 . Hence any such absorbed path breaks up into: a) a path from $j$ to 1 reaching 1 only once; and b) a path from 1 to 0 . Part a) is of the same shape as a path from $j-1$ to 0 on a lattice with absorption at $n-1$, and part b) is just a path from 1 to 0 . The path of part b), if it immediately moves left, must be preceded by an $L$ move, so we must correct the sign for
this case (and this case only). This gives

$$
\begin{equation*}
f_{j}^{(n)}=f_{j-1}^{(n-1)}\left(f_{1}^{(n)}-2 z\right), \quad 2 \leq j<n \tag{2.5}
\end{equation*}
$$

Here are few of these functions.

$$
\begin{gathered}
f_{1}^{(3)}=\frac{z\left(2 z^{2}-1\right)}{(z-1)(z+1)}, \quad f_{2}^{(3)}=\frac{z^{2}}{(z-1)(z+1)} ; \\
f_{1}^{(4)}=\frac{z\left(4 z^{4}-3 z^{2}+1\right)}{2 z^{4}-2 z^{2}+1}, \quad f_{2}^{(4)}=\frac{z^{2}\left(2 z^{2}-1\right)}{2 z^{4}-2 z^{2}+1}, \quad f_{3}^{(4)}=\frac{z^{3}}{2 z^{4}-2 z^{2}+1} ; \\
f_{1}^{(5)}=\frac{z\left(2 z^{2}-1\right)\left(4 z^{4}-2 z^{2}+1\right)}{\left(2 z^{3}+z^{2}-z-1\right)\left(2 z^{3}-z^{2}-z+1\right)}, f_{2}^{(5)}=\frac{z^{2}\left(4 z^{4}-3 z^{2}+1\right)}{\left(2 z^{3}+z^{2}-z-1\right)\left(2 z^{3}-z^{2}-z+1\right)}, \\
f_{3}^{(5)}=\frac{z^{3}\left(2 z^{2}-1\right)}{\left(2 z^{3}+z^{2}-z-1\right)\left(2 z^{3}-z^{2}-z+1\right)}, f_{4}^{(5)}=\frac{z^{4}}{\left(2 z^{3}+z^{2}-z-1\right)\left(2 z^{3}-z^{2}-z+1\right)} .
\end{gathered}
$$

We note that for each $n$, the $f_{j}^{(n)}$ have the same denominator. This can be proved as follows. We first observe that the power series for $f_{j}$ begins with $\pm z^{j}$, so that $f_{j}=z^{j} u$, with $u(0) \neq 0, \infty$. In particular, we have $f_{1}=z a(z) / b(z)$, where $a$ and $b$ are polynomials. Next, we group paths according to the location of the first $R$ move and find the relation

$$
f_{j}=z f_{j+1}+\sum_{k=2}^{j}(-)^{k} z^{k} f_{j+2-k}+(-)^{j-1} z^{j}
$$

valid for $1 \leq j<n-1$. From this it follows that $b f_{j+1}$ is a polynomial, using induction on $j$.

It is interesting that the path sign is essentially the same as the Rudin-Shapiro coefficient. This coefficient $a_{n}$ is determined by the parity of the number of " 11 " blocks in the binary notation of the positive integer $n$. The Rudin-Shapiro coefficient has many applications, including the solution of extremal problems in classical Fourier analysis. For a survey of this topic, see [4].

## 3 Some Combinatorial Results.

It is interesting to see how much can be determined by purely combinatorial arguments, without relying on integration. We begin with two interesting relations.

Theorem 3.1 We have

$$
p_{1}^{(n)}+p_{n-1}^{(n)}=1
$$

That is, in any row, the outer entries sum to 1.

Proof. Let $P$ be a path that starts from 1 and is absorbed at $n$. Its complement $\bar{P}$, obtained by interchanging $L$ and $R$, is a path that starts at $n-1$ and is absorbed at 0 . We note that $P$ must begin and end with $R$ moves. Let $P$ contain $\ell L$ moves, $r R$ moves, and have $k$ occurrences of $R L$. Then the sign of $P$ is $(-1)^{\ell-k}$. However,

$$
k=\# \text { of } R L \text { in } \bar{P}=\# \text { of } L R \text { in } \bar{P}
$$

since $\bar{P}$ begins and ends with $L$ moves. Therefore we have

$$
\sigma(P)=(-1)^{\ell-k}, \quad \sigma(\bar{P})=(-1)^{r-k}
$$

which implies

$$
\sigma(P) \sigma(\bar{P})=(-1)^{\ell+r}=(-1)^{r-\ell}=(-1)^{n-1}
$$

This tells us that if we complement all paths, the probability is unchanged, since it is a sum of squares of quantities (signed path counts) that individually change only by a sign. So

$$
\begin{aligned}
& 1-p_{1}^{(n)}=\operatorname{Pr}[\text { a walk from } 1 \text { is absorbed at } n] \\
= & \operatorname{Pr}[\text { a walk from } n-1 \text { is absorbed at } 0]=p_{n-1}^{(n)} .
\end{aligned}
$$

If we let $q_{j}^{(n)}=1-p_{j}^{(n)}$ be the probability that the walk reaches site $n$, then Theorem 3.1 looks like an "obvious" symmetry relation that should also hold for $j>1$. However, this is not so. (See Table 1 at the end of this paper.)

Theorem 3.2 We have

$$
2 p_{1}^{(n)}=p_{2}^{(n)}+1
$$

In words, doubling the first number in any row is the same as increasing the second by 1.

Proof. Observe that

$$
f_{1}^{(n)}(z)=z+z f_{2}^{(n)}(z)
$$

Now take the Hadamard square of both sides, and evaluate at $1 / 2$. The two terms in the right side do not interfere because $f_{2}^{(n)}(z)$ is a multiple of $z^{2}$.

For $n=2,3$, the absorption probabilities can be obtained by combinatorial reasoning, without any integration. First, for $n=2$, we have

$$
p_{1}^{(2)}=1 / 2,
$$

since there are only two possible paths, each absorbed after one step. To compute $p_{1}^{(3)}$, observe that for $t=1,3,5, \ldots$, there is precisely one path that
reaches site 0 after $t$ steps. Therefore, the signs are irrelevant, and we have

$$
p_{1}^{(3)}=\frac{1}{2}+\frac{1}{8}+\frac{1}{32}+\cdots=\frac{2}{3} .
$$

Using Theorem 3.1, we find

$$
p_{2}^{(3)}=\frac{1}{3} .
$$

## 4 Proof of the Explicit Formula.

In this section we prove that (1.1) holds. What we would like to do is integrate (2.2) by residues, and expose the dependence of $p_{j}^{(n)}$ on $n$. With the original integral, this is probably impossible, since we do not know where the poles inside the circle of integration actually are. However, we can express $p_{j}^{(n)}$ using the integral of a new rational function, with the same mysterious poles inside, but with only one pole outside. Since the sum of the residues of any rational function vanishes, we can just as well evaluate the residue outside the circle, and this leads to a formula for $p_{j}^{(n)}$.

Let us begin with another formula for the path count generating function. Let $\alpha, \beta$ be the two roots of

$$
T^{2}-\left(1-2 z^{2}\right) T-z^{2}=0 .
$$

These will always be used symmetrically so we do not care which is which. Explicitly,

$$
\alpha, \beta=\frac{1-2 z^{2} \pm \sqrt{1+4 z^{4}}}{2} .
$$

Also there is a recurrence relation

$$
\begin{equation*}
\alpha^{k}=\left(1-2 z^{2}\right) \alpha^{k-1}+z^{2} \alpha^{k-2} \tag{4.1}
\end{equation*}
$$

and similarly for $\beta$.
Lemma 4.1 If $1 \leq j<n$, then

$$
f_{j}^{(n)}=z^{j} \frac{\alpha^{n-j}-\beta^{n-j}}{\alpha^{n}-\beta^{n}+2 z^{2}\left(\alpha^{n-1}-\beta^{n-1}\right)},
$$

Proof. This can be proved by induction. First, let $j=1$ and increase $n$, using (2.4). Then, for each $n$ in turn, let $j=2, \ldots, n-1$, and use (2.5).

It will be convenient to allow let $j=n$, and define $f_{n}^{(n)}=0$, so that $p_{n}^{(n)}=0$. This is consistent with the above formula, as well as (2.5).

As a function of $z, f_{j}(n)$ is odd or even according as $j$ is. We now write $f_{j}^{(n)}=z^{j} g_{j}^{(n)}$, and $t=z^{2}$. Then,

$$
g_{j}^{(n)}(t)=\frac{r_{n-j}}{r_{n}-2 t r_{n-1}},
$$

where

$$
r_{k}=\frac{\alpha^{k}-\beta^{k}}{\alpha-\beta}
$$

Since $r_{k+2}-(\alpha+\beta) r_{k+1}+\alpha \beta r_{k}=0$, we have $r_{0}=0, r_{1}=1$, and

$$
\begin{equation*}
r_{k+2}-(1-2 t) r_{k+1}-t r_{k}=0 \tag{4.2}
\end{equation*}
$$

Consequently, the $r_{k}$ are polynomials in $t$.
On the circle $|z|=1 / \sqrt{2}$, we have $\bar{z}=1 /(2 z)$, and $\bar{t}=1 /(4 t)$. Making this substitution into $\bar{g}_{j}$, clearing denominators, and observing that $\alpha \beta=-t$, we get

$$
\left|g_{j}^{(n)}\right|^{2}=(-)^{j} 2^{j} t^{j} \frac{r_{n-j}^{2}}{\left(r_{n}+2 t r_{n-1}\right)\left(r_{n}-r_{n-1}\right)}
$$

Since $f_{j}^{(n)}=z^{j} g_{j}^{(n)}$, we get from this

$$
\begin{equation*}
p_{j}^{(n)}=\frac{(-1)^{j}}{2 \pi i} \int_{|t|=1 / 2} \frac{t^{j-1} r_{n-j}^{2}}{\left(r_{n}+2 t r_{n-1}\right)\left(r_{n}-r_{n-1}\right)} d t \tag{4.3}
\end{equation*}
$$

The next task is to study the poles of the integrand.
Lemma 4.2 The zeroes of $r_{n+1}-r_{n}$ are inside the circle $|t|=1 / 2$, and the zeroes of $r_{n+1}+2 t r_{n}$ are outside it.

Proof. The rational function $f_{1}^{(n)}$ is analytic for $|z| \leq 1 / \sqrt{2}$ (this is implicit in the proof of Lemma 17 of [1]), and this holds for $f_{j}^{(n)}$ as well, since it has the same denominator as $f_{1}^{(n)}$. The result is a consequence of this and the computations used to derive (4.3).

As a consequence of this lemma, we can choose an $\epsilon>0$ so that $p_{j}^{(n)}$ is given as in (4.3), but with the contour of integration now $|t|=1 / 2-\epsilon$.

Lemma 4.3 Let $n \geq 2$. If $1 \leq j \leq n, H_{j}=t^{j-1}(1+2 t) r_{n-j}+(-1)^{j}\left(r_{j}-\right.$ $\left.r_{j-1}\right)\left(r_{n}+2 t r_{n-1}\right)$ is a polynomial in $t$, divisible by $r_{n}-r_{n-1}$.

Proof. The recurrence relation on $r_{j}$ implies that $H_{j+2}=(1-2 t) H_{j+1}+H_{j}$, so it suffices to check the statement for $j=1$ and $j=2$. It is easy to check that $H_{1}=r_{n-1}-r_{n}$, and the recurrence relation on $r_{n}$ implies that $H_{2}=r_{n}-r_{n-1}$.

The above proof has the consequence that $H_{j} /\left(r_{n}-r_{n-1}\right)$ depends on $j$ only.
Theorem 4.4 Let $n \geq 2$ and $1 \leq j \leq n$. Then (1.1) holds.
Proof. Using Lemma 4.3 to rewrite $t^{j-1} r_{n-j}$, we have for $1 \leq j \leq n$

$$
p_{j}^{(n)}=-\frac{1}{2 \pi i} \int_{|t|=\frac{1}{2}-\epsilon} \frac{r_{n-j}\left(r_{j}-r_{j-1}\right) d t}{(1+2 t)\left(r_{n}-r_{n-1}\right)}+\frac{1}{2 \pi i} \int_{|t|=\frac{1}{2}-\epsilon} \frac{R_{j}(t) d t}{\left(r_{n}+2 t r_{n-1}\right)(1+2 t)},
$$

for some polynomial $R_{j}$. The second integral is zero, because all the poles of the rational function are outside the integration contour. In the first integral, the integrand

$$
\frac{r_{n-j}\left(r_{j}-r_{j-1}\right)}{(1+2 t)\left(r_{n}-r_{n-1}\right)},
$$

as a function on the Riemann sphere, has a unique singularity outside the contour, which is a pole of order 1 at $t=-\frac{1}{2}$. Indeed, the degree of $r_{k}$ is $k-1$ so the degree of the denominator is two plus the degree of the numerator, which assures that there is no pole at infinity.

Since the residues of a rational function sum to zero, we get

$$
\begin{equation*}
p_{j}^{(n)}=\operatorname{Res}_{t=-\frac{1}{2}} \frac{r_{n-j}\left(r_{j}-r_{j-1}\right)}{(1+2 t)\left(r_{n}-r_{n-1}\right)}=\frac{1}{2} \frac{r_{n-j}\left(r_{j}-r_{j-1}\right)}{\left(r_{n}-r_{n-1}\right)}\left(-\frac{1}{2}\right) . \tag{4.4}
\end{equation*}
$$

To derive the explicit formula, observe that $\alpha(-1 / 2)=\frac{2+\sqrt{2}}{2}$ and $\beta(-1 / 2)=$ $\frac{2-\sqrt{2}}{2}$, so (with $A, B=2 \pm \sqrt{2}$ )

$$
r_{k}\left(-\frac{1}{2}\right)=\frac{A^{k}-B^{k}}{2^{k+1 / 2}}, \quad\left(r_{k}-r_{k-1}\right)\left(-\frac{1}{2}\right)=\frac{A^{k-1}-B^{k-1}}{2^{k}} .
$$

Then, substitute these values into (4.4) and simplify.
It is natural to extend our notation so that $p_{0}^{(n)}=1$ for $n \geq 2$. The explicit formula does not work there, but the above proof indicates a reason for this. We could use (4.2) to extend $r_{j}$ to $j=-1$, but then $r_{-1}$ would not be a polynomial, invalidating our arguments.

Using the recurrence relation for $r_{k}$, we can prove that when $n \geq 1$, the polynomial $r_{n}-r_{n-1}$ has distinct roots. However, the computations for this are not very enlightening, so we leave verification of this to the reader.

## 5 Remarks.

Initially, we had arrived at the formula (1.1) after numerical calculations that were done by a different method, which we believe to be of independent interest. In this section, we discuss how these calculations were done. The idea is to combine numerical approximation of the residues with a bound on the denomininator.

Suppose we want a value for

$$
\begin{equation*}
p:=\frac{1}{2 \pi i} \int_{|z|=a}|f(z)|^{2} \frac{d z}{z}, \tag{5.1}
\end{equation*}
$$

in which $f \in \mathbf{Q}(z)$, and $a \in \mathbf{Q}$. Let $a$ be large enough that all the poles of $f$ are inside the circle $|z|=a$. On this circle, $\bar{z}=a^{2} / z$, and if we use this to get an expression for $\bar{f}$, we can bring (5.1) into the form

$$
p=\frac{m_{1}}{m_{2}} \cdot \frac{1}{2 \pi i} \int_{|z|=a} \frac{b(z) d z}{c(z) d(z)},
$$

in which $m_{1}, m_{2} \in \mathbf{Z}, b, c, d \in \mathbf{Z}[v]$, and $c, d$ are monic. The zeroes of $c$ and $d$ are algebraic integers, and we choose notation so that those of $c$ and $d$ are outside and inside the circle, respectively.

In the cases of interest to us, $c$ and $d$ had distinct roots, so let us make this simplifying assumption. Then, evaluating $(2 \pi i)^{-1} \int b(c d)^{-1} d z$ by residues produces

$$
\begin{equation*}
\sum_{\xi} \frac{b(\xi)}{\prod_{\eta}(\xi-\eta)} \cdot \frac{1}{\prod_{\xi^{\prime} \neq \xi}\left(\xi-\xi^{\prime}\right)} \tag{5.2}
\end{equation*}
$$

In this expression, $\xi$ and $\xi^{\prime}$ range over zeroes of $d$, and $\eta$ ranges over zeroes of $c$. The denominators are algebraic integers, and

$$
\begin{gathered}
\prod_{\eta}(\xi-\eta) \mid \operatorname{resultant}(c, d):=R \\
\prod_{\xi^{\prime} \neq \xi}\left(\xi-\xi^{\prime}\right) \mid \operatorname{discriminant}(d):=D
\end{gathered}
$$

Since $b$ has integral coefficients, we conclude that (5.1) is an integral multiple of $\Delta^{-1}$, where

$$
\Delta=m_{2} R D
$$

In particular (by Galois theory), $p$ is a rational number.
To obtain (5.1) exactly, then, it will suffice to compute the integer $\delta$, and then evaluate (5.2) using numerical approximations to the zeroes, with enough accuracy to determine (5.1) to the nearest integer.

Using this method, we were able to compute absorption probabilities exactly up to $n=20$ in a couple of minutes on a workstation. Straight numerical integration would have been much slower, and would not have given us exact results.

We end this paper with a short table of the $p_{j}^{(n)}$. The numerators of $p_{1}$ are Sequence A084068 in [5].

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## References

[1] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, J. Watrous, One-dimensional quantum walks, in: Proceedings of the Thirty-Third Annual ACM Symposium on Theory of Computing, 2001, pp. 60-69.
[2] E. Bach, S. Coppersmith, M. Paz Goldschen, R. Joynt, and J. Watrous, Onedimensional quantum walks with absorbing boundaries, J. Comp. Sys. Sci., 69, 2004, 562-592.
[3] P. G. Doyle and J. L. Snell, Random Walks and Electrical Networks, MAA, 1984.
[4] M. Mendès France, The Rudin-Shapiro sequence, Ising chain, and paperfolding, in B. C. Berndt et al., eds., Analytic Number Theory: Proceedings of a Conference in Honor of Paul Bateman, Birkhäuser, 1990, pp. 367-382.
[5] N. J. A. Sloane, On-Line Encyclopedia of Integer Sequences.


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