Grover walks on a line with absorbing boundaries

Kun Wang¹,² · Nan Wu¹,² · Parker Kuklinski³ · Ping Xu⁴ · Haixing Hu⁴ · Fangmin Song¹,²

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Abstract In this paper, we study Grover walks on a line with one and two absorbing boundaries. In particular, we present some results for the absorbing probabilities in both a semi-finite and finite line. Analytical expressions for these absorbing probabilities are presented by using the combinatorial approach. These results are perfectly matched with numerical simulations. We show that the behavior of Grover walks on a line with absorbing boundaries is strikingly different from that of classical walks and that of Hadamard walks.

Keywords Quantum walks · Grover walks · Three-state walks · Absorbing boundaries

1 Introduction

Since the seminal works by [1–3], quantum walks have been the subject of research for the past two decades. They were originally proposed as a quantum generalization of classical random walks [4]. Asymptotic properties such as mixing time, mixing rate and hitting time of quantum walks on a line and on general graphs have been studied extensively [5–9]. Applications of quantum walks for quantum information processing have also been investigated. Particularly, quantum walks can solve the element distinctness problem [10,11] and perform the quantum search algorithms...
In some applications, quantum walks based algorithms can even gain exponential speedup over all possible classical algorithms [13]. The discovery of their capability for universal quantum computations [14,15] indicates that understanding quantum walks is necessary for better understanding quantum computing itself. For a more comprehensive review, we refer the readers to [16,17] and the references within.

One-dimensional three-state quantum walks, first considered by Inui et al. [18], are variations of two-state quantum walks on a line. In the three-state walk, the walker is governed by a coin with three degrees of freedom. In each step, the walker is not only capable of moving left or right, but also able to stay at the same position. Three-state quantum walks have interesting differences from two-state quantum walks. Most notably, if the walker of a three-state quantum walk is initialized at one site, it is trapped with large probability near the origin after walking enough steps [19]. This phenomenon is previously found in quantum walks on square lattices [20] and is called localization. In fact, this model is the simplest model that exhibits localization, a quantum effect entirely absent from the corresponding classical random walk. Three-state random walks are essentially regarded as the same process as two-state random walks by scaling the time. A thorough understanding of the localization effect on this model becomes particularly relevant given the fact that this phenomenon is commonplace in higher-dimensional systems [17]. Recent researches showed that the localization effect happens with a broad family of coin operators in three-state quantum walks [21–23].

The presence of absorbing boundaries apparently complicates the analysis of quantum walks considerably. Two-state quantum walks with one or two boundaries have been investigated extensively [5,24]. The effects of general initial conditions and general coin operators have also been studied [25–27]. In this paper, we focus on the question of determining the absorbing probabilities in Grover walks with one or two boundaries.

First, we consider the case where we have a single absorbing boundary. The walk process is terminated if the walker reaches that boundary. We offer methods to calculate the absorbing probability for an arbitrary boundary. When the boundary is fixed at $-1$, it is known that in the classical case the walker is absorbed with probability 1 [28], while in Hadamard walks the walker has an absorption probability of $2/\pi$ [5]. Intuitively, as some probability amplitudes are trapped near origin due to the localization effect in Grover walks, the absorbing probability of Grover walks is smaller than that of Hadamard walks. However, the Grover walker is absorbed with probability 0.6693 which is larger than $2/\pi$. What’s more, when the boundary is moved from $-1$ to $-2$, the absorbing probabilities suffer an extreme fast decrease. To explain these strange behaviors, we numerically study the oscillating localization effect in Grover walks with one boundary. We find that the localization is occurred owing to the quantum state oscillating between $-1$ and 0. If the boundary is at $-1$, the localization effect disappears and the state is absorbed, resulting in a large absorbing probability. If the boundary is at $-2$, the localization effect revives and the absorbing probability plummets.

Then, we review the case where there are two boundaries—one is at site $-M$ ($M > 0$) to the walker’s left, and the other is at site $N$ ($N > 0$) to the walker’s right. The walk is terminated if the walker is trapped in either absorbing boundary.
Methods are designed to calculate the left and right absorbing probabilities to arbitrary accuracy for arbitrary left and right boundaries. In Hadamard walks, the left absorbing probability approaches $1/\sqrt{2}$ when the left boundary is at $-1$ and the right boundary approaches infinity. It is concluded that adding a second boundary on the right actually increases the probability of reaching the left. In Grover walks with two boundaries, we get the same left absorbing probability $1/\sqrt{2}$ under the same setting. The conclusion is still correct in Grover walks as $1/\sqrt{2} > 0.6693$. When the left boundary is at $-1$, the oscillating localization effect disappears. As position $-1$ is occupied, the part of quantum state, which would have otherwise localized, now is absorbed. When the left boundary is to the left of $-1$, the sum of the left and right absorbing probabilities is generally less than 1 due to oscillating localization. When studying the case where the left boundary is at $-2$, we show that the localization probabilities are exponentially decaying in Grover walks with two boundaries.

The rest of this paper is organized as follows. Section 2 gives formal definitions of Grover walks with one and two absorbing boundaries, and the absorbing probabilities which we study. Sections 3 and 4 present the methods and results on Grover walks with one and two boundaries. Finally, we conclude in Sect. 5.

2 Definitions

2.1 Grover walks

The three-state quantum walk (3QW) considered here is a kind of generalized two-state quantum walk on a line. The Hilbert space of the system is given by the tensor product $\mathcal{H} = \mathcal{H}_P \otimes \mathcal{H}_C$ of the position space

$$\mathcal{H}_P = \text{Span}\{ |m\rangle, m \in \mathbb{Z} \}$$

and the coin space $\mathcal{H}_C$. In each step, the walker has three choices—it can move to the left, move to the right or just stay at the current position. To each of these options, we assign a vector of the standard basis of the coin space $\mathcal{H}_C$, i.e., the coin space is three-dimensional

$$\mathcal{H}_C = \mathbb{C}^3 = \text{Span}\{ |L\rangle, |S\rangle, |R\rangle \}.$$  

The evolution operator realizing a single step of the three-state quantum walk is given by $U = S \cdot (I_P \otimes C)$ where $S$ is the position shift operator, $I_P$ is the identity operator of the position space $\mathcal{H}_P$, and $C$ is the coin flip operator. In the three-state quantum walk on a line, the position shift operator $S$ has the form of

$$S = \sum_{m=-\infty}^{+\infty} |m - 1\rangle \langle m| \otimes |L\rangle \langle L| + |m\rangle \langle m| \otimes |S\rangle \langle S| + |m + 1\rangle \langle m| \otimes |R\rangle \langle R|.$$  

As for the coin operator $C$, a common choice is the Grover operator $G$. The Grover operator is originally designed for Grover’s search algorithm [29], and now finds its
use in quantum walks. The Grover operator is defined as

\[
G = \frac{1}{3} \begin{pmatrix}
-1 & 2 & 2 \\
2 & -1 & 2 \\
2 & 2 & -1
\end{pmatrix}.
\] (1)

The state of the walker after evolving \( t \) steps is given by the successive applications of the evolution operator \( U \) on the initial state. Let \( |\psi(t)\rangle \) be the system state after walking \( t \) steps, then

\[
|\psi(t)\rangle = \sum_m |m\rangle \otimes (|\psi_L(t, m)\rangle |L\rangle + |\psi_S(t, m)\rangle |S\rangle + |\psi_R(t, m)\rangle |R\rangle) = U^t |\psi(0)\rangle,
\] (2)

where \( |\psi(0)\rangle \) is the initial state, \( \psi_L(t, m) \) is the probability amplitude of the walker being at position \( m \) with coin state \( |L\rangle \) after walking \( t \) steps. \( \psi_S(t, m) \) and \( \psi_R(t, m) \) are defined similarly. We will write \( |m, L\rangle \), \( |m, S\rangle \) and \( |m, R\rangle \) for short whenever there is no ambiguity. Let \( P(t, m) \) be the probability of finding the walker at position \( m \) after walking \( t \) steps, then

\[
P(t, m) = |\psi_L(t, m)|^2 + |\psi_S(t, m)|^2 + |\psi_R(t, m)|^2.
\]

In summary, the process of Grover walks on a line can be described as follows.

Step 1 Initialize the system state to \( |\psi_0\rangle = \alpha |0, L\rangle + \beta |0, S\rangle + \gamma |0, R\rangle \), where \( \alpha, \beta, \gamma \in \mathbb{C} \) and \( |\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1 \).

Step 2 For any chosen number of steps \( t \), apply \( U \) to the system \( t \) times.

Step 3 Measure the system state \( |\psi(t)\rangle \) to get the walker’s position probability distribution.

2.2 Grover walks with one boundary

In this process, we introduce an absorbing boundary into the line, resulting in Grover walks on a semi-infinite line. This can be done by setting a measurement device which corresponds to answering the question “Is the walker at position \( n \)?”. The measurement is implemented as two projection operators

\[
\Pi^n_{\text{yes}} = |n\rangle \langle n| \otimes I_C, \quad \Pi^n_{\text{no}} = I - \Pi^n_{\text{yes}},
\]

where \( I_C \) is the identity operator of the coin space \( \mathcal{H}_C \) and \( I \) is the identity operator of the Hilbert space \( \mathcal{H} \).

As an example of the measurement, suppose the system is now in state \( |\psi(t)\rangle = \frac{1}{\sqrt{3}} |0, L\rangle + \frac{1}{\sqrt{5}} |0, S\rangle + \frac{1}{\sqrt{5}} |0, R\rangle + \frac{1}{\sqrt{3}} |1, S\rangle + \frac{1}{\sqrt{5}} |2, R\rangle \), and is measured by the projection operator \( \Pi^n_{\text{yes}} \) (corresponding to the question “Is the walker at position \( 0 \)?”). The answer yes is obtained with probability

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\[
\|\Pi_{\text{yes}}^{0} |\psi(t)\rangle\|^2 = \|\Pi_{\text{yes}}^{0} \left( \frac{1}{\sqrt{5}} |0, L\rangle + \frac{1}{\sqrt{5}} |0, S\rangle \\
+ \frac{1}{\sqrt{5}} |0, R\rangle + \frac{1}{\sqrt{5}} |1, S\rangle + \frac{1}{\sqrt{5}} |2, R\rangle \right)\|^2 \\
= \left( \frac{1}{\sqrt{5}} |0, L\rangle + \frac{1}{\sqrt{5}} |0, S\rangle + \frac{1}{\sqrt{5}} |0, R\rangle \right)^2 = \frac{3}{5},
\]

in which case the system state collapses to \(|\psi(t)\rangle_{\text{yes}} = \frac{1}{\sqrt{3}} |0, L\rangle + \frac{1}{\sqrt{3}} |0, S\rangle + \frac{1}{\sqrt{3}} |0, R\rangle\). The answer is \text{no} with probability \(2/5\), in which case the system collapses to state \(|\psi(t)\rangle_{\text{no}} = \frac{1}{\sqrt{2}} |1, S\rangle + \frac{1}{\sqrt{2}} |2, R\rangle\).

Analogous to Grover walks on a line, Grover walks on a line with one boundary can be depicted as follows:

Step 1 Initialize the system state to \(|\psi_0\rangle = \alpha |0, L\rangle + \beta |0, S\rangle + \gamma |0, R\rangle\), where \(\alpha, \beta, \gamma \in \mathbb{C}\) and \(|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1\).

Step 2 For each step of the evolution

1. Apply \(U\) to the system.
2. Measure the system according to \(\{\Pi_{\text{yes}}^{-M}, \Pi_{\text{no}}^{-M}\}\) to test whether the walker is or not at \(-M\) (\(M > 0\)).

Step 3 If the measurement result is \text{yes} (i.e., the walker is at \(-M\)), then terminate the process, otherwise repeat Step 2.

We are interested in the probability that the measurement result is \text{yes} which is called the absorbing probability. Let \(P_{-M,0,\infty}(\alpha, \beta, \gamma)\) denote the absorbing probability, where \(-M, 0\) and \(\infty\) represent the left boundary, the walker’s initial position and the right boundary, respectively, and \(\alpha, \beta, \gamma\) are the probability amplitudes of the coin components \(|L\rangle, |S\rangle, |R\rangle\). To keep accordance with the two boundaries case in symbols, we assume there is a right boundary which is infinitely far away in the one boundary case. That’s why we have a rather confusing \(\infty\) here.

### 2.3 Grover walks with two boundaries

The third process is similar to Grover walks with one boundary, except that two boundaries are presented rather than one. Specifically, using the same measurement devices as defined for semi-infinite Grover walks, we describe the following process which is called Grover walks on a line with two boundaries, or the finite Grover walks.

Step 1 Initialize the system state to \(|\psi_0\rangle = \alpha |0, L\rangle + \beta |0, S\rangle + \gamma |0, R\rangle\), where \(\alpha, \beta, \gamma \in \mathbb{C}\) and \(|\alpha|^2 + |\beta|^2 + |\gamma|^2 = 1\).

Step 2 For each step of the evolution

1. Apply \(U\) to the system.
2. Measure the system according to \(\{\Pi_{\text{yes}}^{-M}, \Pi_{\text{no}}^{-M}\}\) to test whether the walker is or not at \(-M\) (\(M > 0\)). \(-M\) is the left absorbing boundary.
3. Measure the system according to \(\{\Pi_{\text{yes}}^{N}, \Pi_{\text{no}}^{N}\}\) to test whether the walker is or not at \(N\) (\(N > 0\)). \(N\) is the right absorbing boundary.
Step 3 If either of the measurement results is yes (i.e., the walker is either at \( -M \) or \( N \)), then terminate the process, otherwise repeat Step 2.

We are interested in the absorbing probabilities that the walker is eventually absorbed by the left or the right boundary. Let

- \( P_{-M,0,N}(\alpha, \beta, \gamma) \) be the left absorbing probability that the measurement of whether the walker is at position \( -M \) eventually results in yes.
- \( Q_{-M,0,N}(\alpha, \beta, \gamma) \) be the right absorbing probability that the measurement of whether the walker is at position \( N \) eventually results in yes.

In the above conventions, \( -M, 0 \) and \( N \) represent the left boundary, the walker’s initial position and the right boundary, respectively, and \( \alpha, \beta, \gamma \) are the probability amplitudes of the coin components \( |L\rangle, |S\rangle, |R\rangle \).

3 One boundary

We begin with three special initial cases: (1) The initial state is \( |0, L\rangle \); (2) the initial state is \( |0, S\rangle \); and (3) the initial state is \( |0, R\rangle \). The boundary is fixed at \(-1\) for above three cases. We will define generating functions for these simple cases which are used to determine absorbing probabilities for all boundaries. The methods applied in this section are inspired by [26]. We thank them for offering such elegant methods.

3.1 Generating functions

We first consider simple cases where the boundary is at \(-1\), and the initial state is \( |0, L\rangle \), \( |0, S\rangle \) and \( |0, R\rangle \), respectively. We define the following generating functions \( l(z) \), \( s(z) \) and \( r(z) \) for each of above three cases

\[
l(z) = \sum_{t=1}^{\infty} (-1, L | U \left( \prod_{t-1}^{-1} U \right) | 0, L \rangle z^t, \quad (3)
\]

\[
s(z) = \sum_{t=1}^{\infty} (-1, L | U \left( \prod_{t-1}^{-1} U \right) | 0, S \rangle z^t, \quad (4)
\]

\[
r(z) = \sum_{t=1}^{\infty} (-1, L | U \left( \prod_{t-1}^{-1} U \right) | 0, R \rangle z^t. \quad (5)
\]

\(<-1, L | U \left( \prod_{t-1}^{-1} U \right) | 0, L \rangle \) is the probability amplitude with which the walker first reaches the boundary \(-1\) after walking \( t \) steps when starting with state \( |0, L\rangle \). It’s easy to see that we encode all the probability amplitudes that lead the walker to \(-1\) into the coefficients of \( z^t \) in \( l(z) \). \( s(z) \) and \( r(z) \) are similarly defined except that the system is initialized to \( |0, S\rangle \) and \( |0, R\rangle \), respectively.

Recall that we denote \( P_{-1,0,\infty}(1, 0, 0), P_{-1,0,\infty}(0, 1, 0) \) and \( P_{-1,0,\infty}(0, 0, 1) \) as the probabilities that a walker starting in state \( |0, L\rangle \), \( |0, S\rangle \) or \( |0, R\rangle \) is eventually absorbed by the left or the right boundary.
absorbed by the boundary $-1$. These probabilities can be calculated by summing up the squared amplitudes encoded in the generating functions:

$$ P_{-1,0,\infty}(1,0,0) = \sum_{t=1}^{\infty} \left\| [z^t] l(z) \right\|^2, $$

$$ P_{-1,0,\infty}(0,1,0) = \sum_{t=1}^{\infty} \left\| [z^t] s(z) \right\|^2, $$

$$ P_{-1,0,\infty}(0,0,1) = \sum_{t=1}^{\infty} \left\| [z^t] r(z) \right\|^2, $$

where $[z^t] l(z)$ is the coefficient of $z^t$ in $l(z)$, and similarly for $[z^t] s(z), [z^t] r(z)$.

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

$$ (u \odot v)(z) = \sum_{t=1}^{\infty} \left( [z^t] u(z) \right) \left( [z^t] v(z) \right) z^t. $$

Thus, $P_{-1,0,\infty}(1,0,0) = (l \odot \bar{l})(1), P_{-1,0,\infty}(0,1,0) = (s \odot \bar{s})(1)$ and $P_{-1,0,\infty}(0,0,1) = (r \odot \bar{r})(1)$. In general, we have

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

provided that $\sum_{t=1}^{\infty} ([z^t] u(z)) ([z^t] v(z))$ converges. Let $L(\theta) = l(e^{i\theta}), S(\theta) = s(e^{i\theta}), R(\theta) = r(e^{i\theta})$, we can calculate the absorbing probabilities in analytical form using Eq. 6:

$$ P_{-1,0,\infty}(1,0,0) = \frac{1}{2\pi} \int_0^{2\pi} |L(\theta)|^2 \, d\theta $$

$$ P_{-1,0,\infty}(0,1,0) = \frac{1}{2\pi} \int_0^{2\pi} |S(\theta)|^2 \, d\theta $$

$$ P_{-1,0,\infty}(0,0,1) = \frac{1}{2\pi} \int_0^{2\pi} |R(\theta)|^2 \, d\theta. $$

The generating functions defined by Eqs. 4–5 can be solved. The solving procedure is detailed in “Appendix 1” section. We present the results in Theorem 1.

**Theorem 1** The generating functions $l(z), s(z)$ and $r(z)$ defined in Grover walks with one boundary satisfy the following recurrences

$$ l(z) = \frac{-3 - 4z - 3z^2 + (1 + z)\Delta}{2z}, $$

The generating functions defined by Eqs. 4–5 can be solved. The solving procedure is detailed in “Appendix 1” section. We present the results in Theorem 1.
Fig. 1 (Color online) Numerical simulations of the absorbing probabilities evolving with walking steps in Grover walks with one boundary. The boundary is fixed at $-1$. Solid lines represent the theoretical probabilities. Dashed lines represent the numerical probabilities.

\[
s(z) = \frac{-3 - z + \Delta}{2z},
\]

\[
r(z) = \frac{3 + 2z + 3z^2 + (-1 + z)\Delta}{4z},
\]

where $\Delta = \sqrt{9 + 6z + 9z^2}$.

Then by Eqs. 7–9, we can calculate the absorbing probabilities for these three special cases:

\[
P_{-1,0,\infty}(1, 0, 0) = \frac{1}{2\pi} \int_0^{2\pi} |L(\theta)|^2 \, d\theta = \frac{1}{2\pi} \int_0^{2\pi} |l(e^{i\theta})|^2 \, d\theta \approx 0.4248,
\]

\[
P_{-1,0,\infty}(0, 1, 0) = \frac{1}{2\pi} \int_0^{2\pi} |S(\theta)|^2 \, d\theta = \frac{1}{2\pi} \int_0^{2\pi} |s(e^{i\theta})|^2 \, d\theta \approx 0.5255,
\]

\[
P_{-1,0,\infty}(0, 0, 1) = \frac{1}{2\pi} \int_0^{2\pi} |R(\theta)|^2 \, d\theta = \frac{1}{2\pi} \int_0^{2\pi} |r(e^{i\theta})|^2 \, d\theta \approx 0.6693.
\]

The analytical absorbing probabilities are matched with the simulation results, as shown in Fig. 1. We can see that the absorbing probabilities converge toward their limiting values very quickly. The fast convergence indicates that the remaining probability amplitudes spread rapidly to the right and never go back.
3.2 Arbitrary boundary

The reason that the generating functions $l(z)$, $s(z)$ and $r(z)$ are important in analyzing absorbing probability for arbitrary boundary is as follows. Suppose now that the boundary is located at $-M$ for some $M \geq 1$ and the walker’s initial state is $|0, R\rangle$. Consider a generating function defined similarly to $r(z)$, except for the boundary at position $-M$ rather than 1. Then this generating function is simply $r(z)(l(z))^{M-1}$, which follows from the fact that to reach the boundary $-M$ from original position 0, the walker has to move left $M$ times effectively. For each move after the first, the coin state is always $|L\rangle$. The first move is with coin state $|R\rangle$. The process is depicted in Fig. 2. Likewise, the generating functions corresponding to staring in states $|0, L\rangle$ and $|0, S\rangle$ are simply $(l(z))^M$ and $s(z)(l(z))^{M-1}$. Then from the discussions in the previous section we know how to calculate the absorbing probabilities for these simple cases:

\[
\begin{align*}
P_{-M,0,\infty}(1, 0, 0) &= \frac{1}{2\pi} \int_{0}^{2\pi} |L(\theta)|^{2M} \, d\theta, \\
P_{-M,0,\infty}(0, 1, 0) &= \frac{1}{2\pi} \int_{0}^{2\pi} |S(\theta)|^2 |L(\theta)|^{2M-2} \, d\theta, \\
P_{-M,0,\infty}(0, 0, 1) &= \frac{1}{2\pi} \int_{0}^{2\pi} |R(\theta)|^2 |L(\theta)|^{2M-2} \, d\theta.
\end{align*}
\]

Figure 3 illustrates the relation between the absorbing probabilities (on y-axis) and the boundary $M$ (on x-axis). We can see that the absorbing probability $P_{-M,0,\infty}(0, 0, 1)$ undergoes an extreme fast decay when the boundary is moved from $-1$ to $-2$, and then rapidly reaches its limiting value as the $M$ becomes large. This rather strange phenomenon is emerged due to the oscillating localization effect in Grover walks. It has been proved that Grover walks on an infinite line will result in localization when the system is initialized to state $|0, R\rangle$. The localization probability is 0.202 at the origin (position 0) [30] and is exponentially decaying with the distance from the origin [23]. However, localization is also shown at position $-1$ in this special case, which violates the exponentially decaying conclusion stated in [23], and has not been studied to the best of my knowledge. The localization probability at $-1$ is approximate to 0.202 by simulation, as shown in Fig. 4. From Fig. 4 we can infer that the probabilities of finding the walker at position $-1$ and 0 are sum to constant 0.404, while the two probabilities are oscillating around 0.202. These two probabilities will finally both be 0.202 when the walker evolves for long enough time. By analyzing the
Fig. 3 (Color online) Theoretical absorbing probabilities $P_{-M,0,\infty}(1,0,0)$, $P_{-M,0,\infty}(0,1,0)$ and $P_{-M,0,\infty}(0,0,1)$ evolving with the absorbing boundary in Grover walks with one boundary.

Fig. 4 (Color online) Oscillating localization effect in Grover walks. The probabilities at position $-1$ and $0$ are oscillating around the theoretical localization probability 0.202. The sum of these two probabilities is a constant 0.404.

numerical data, we also find that the probabilities at the left of $-1$ decay exponentially with the distance from $-1$, while the probabilities at the right of 0 decay exponentially with the distance from 0. This is a new two-peak localization phenomenon. We
conjecture that it is the oscillating effect that results in the two-peak localization—a fair part of the system state is oscillating between position $-1$ and $0$, and never leave that region. When a boundary is located at $-1$, the amplitudes that should have been oscillating between $-1$ and $0$ are absorbed by that boundary, resulting in the disappearance of localization. When a boundary is located at $-2$, some of the amplitudes are oscillating between position $-1$ and $0$, resulting in the amplitudes absorbed by the boundary $-2$ are much less than in the former case. The two-peak oscillation now revives at $-1$ and $0$. From this point of view, we figure out the reason for the extreme fast decay of $P_{-M,0,\infty}(0,0,1)$. We have only considered the cases where the boundaries were located to the left of the walker so far. The symmetric cases (where the boundaries are to the right of the walker) are easy to analyze as the Grover operator is permutation symmetric. A Grover walk with some initial state $(\alpha, \beta, \gamma)$ and a boundary $M \geq 0$ is equivalent to a Grover walk with some initial state $(\gamma, \beta, \alpha)$ and a boundary $-M$ in the sense that they have the symmetric probability distribution and the same absorbing probability. Let $P_{\infty,0,M}(\alpha, \beta, \gamma)$ denote the absorbing probability where the boundary is positioned at $M \geq 0$. Its relationship to $P_{-M,0,\infty}(\alpha, \beta, \gamma)$ is stated in the following proposition.

**Proposition 2** In Grover walks with one boundary, the absorbing probability satisfies

$$P_{\infty,0,M}(\alpha, \beta, \gamma) = P_{-M,0,\infty}(\gamma, \beta, \alpha),$$

where $M \geq 0$ is a boundary, and $(\alpha, \beta, \gamma)$ are amplitudes corresponding to $|L\rangle$, $|S\rangle$, $|R\rangle$ coin components.

4 Two boundaries

We study Grover walks with two boundaries in the following way. First, we fix the left boundary at $-1$ and move the right boundary $N$ relatively to observe how the left absorbing probability changes with $N$. To simplify the analysis, we consider three simple cases: (1) The initial state is $|0, L\rangle$; (2) the initial state is $|0, S\rangle$; and (3) the initial state is $|0, R\rangle$. The left boundary is fixed at $-1$ for above cases. The left absorbing probabilities $P_{-1,0,N}(1,0,0)$, $P_{-1,0,N}(0,1,0)$ and $P_{-1,0,N}(0,0,1)$ are studied both numerically and analytically. Recall that these notations are defined in Sect. 2.3. Then, arbitrary left boundary $-M$ and arbitrary right boundary $N$ are investigated. We make use of the generating functions defined in the former case to express the absorbing probabilities studied in this one. We will show that the sum of the left and right absorbing probabilities is less than 1 for almost arbitrary left and right boundaries $-M$, $N$, which is strikingly different from that of Hadamard walks and random walks with boundaries. This is due to the localization effect uniquely in Grover walks. Some of the system state is trapped near the origin and cannot be absorbed by either boundary, resulting in the sum $<1$. 

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4.1 Generating functions

Three special initial cases are considered: The initial state is $|0, L\rangle$, $|0, S\rangle$ and $|0, R\rangle$, respectively, and the left boundary is always fixed at $-1$. We define three functions $l(N, z)$, $s(N, z)$, $r(N, z)$ for these cases as

\begin{align}
I(N, z) &= \sum_{t=1}^{\infty} \langle -1, L | U \left( \prod_{n_o}^{N} \prod_{n_o}^{-1} U \right)^{t-1} | 0, L \rangle z^t, \\
S(N, z) &= \sum_{t=1}^{\infty} \langle -1, L | U \left( \prod_{n_o}^{N} \prod_{n_o}^{-1} U \right)^{t-1} | 0, S \rangle z^t, \\
R(N, z) &= \sum_{t=1}^{\infty} \langle -1, L | U \left( \prod_{n_o}^{N} \prod_{n_o}^{-1} U \right)^{t-1} | 0, R \rangle z^t.
\end{align}

Some explanations on the left generating function $l(N, z)$:

- The initial state is $|0, L\rangle$.
- The left boundary is fixed at $-1$.
- The right boundary is at $N \geq 1$.
- $\langle -1, L | U \left( \prod_{n_o}^{N} \prod_{n_o}^{-1} U \right)^{t-1} | 0, L \rangle$ is the (non-normalized) probability amplitude that the quantum walker first hits the left boundary $-1$ before hitting the right boundary $N$ after walking $t$ steps.
- We encode all probability amplitudes that will result in the left absorption into the coefficients of $z^t$ in $l(N, z)$.

Other two generating functions $s(N, z)$, $r(N, z)$ have the same explanations as $l(N, z)$ except that the latter two have initial states $|0, S\rangle$, $|0, R\rangle$, respectively.

Let’s define $L(N, \theta) = l(N, e^{i\theta})$, $S(N, \theta) = s(N, e^{i\theta})$ and $R(N, \theta) = r(N, e^{i\theta})$. Based on the reasoning techniques described in Sect. 3.1, we can calculate the absorbing probabilities for above three cases by the following equations

\begin{align}
P_{-1,0,N}(1, 0, 0) &= \sum_{t=1}^{\infty} \frac{1}{2\pi} \int_{0}^{2\pi} |L(N, \theta)|^2 d\theta, \\
P_{-1,0,N}(0, 1, 0) &= \sum_{t=1}^{\infty} \frac{1}{2\pi} \int_{0}^{2\pi} |S(N, \theta)|^2 d\theta, \\
P_{-1,0,N}(0, 0, 1) &= \sum_{t=1}^{\infty} \frac{1}{2\pi} \int_{0}^{2\pi} |R(N, \theta)|^2 d\theta,
\end{align}

where $\langle z^t \rangle l(N, z)$ is the coefficient of $z^t$ in $l(N, z)$, and similarly for $\langle z^t \rangle s(N, z)$, $\langle z^t \rangle r(N, z)$.

In Grover walks with two boundaries, the generating functions defined in Eqs. 13, 14 and 15 can be solved. For details on the solving procedure, the readers can refer to “Appendix 2” section. We only summarize the results here. Let $l(0, z) = s(0, z) =$
By combining Eqs. 16–21, we can calculate the left absorbing probabilities.

Grover walks on a line with absorbing boundaries.

The left absorbing probabilities $P_{-1,0,N}(0,0,1)$ to be constant, we find the solutions to these equations, as stated in Theorem 3.

**Theorem 3** The generating functions $l(N, z)$, $s(N, z)$ and $r(N, z)$ defined in Grover walks with two boundaries satisfy the following recurrences

\[
l(N, z) = \frac{-z + z^2}{3 + z - (2z + 2z^2) \cdot r(N - 1, z)}, \tag{19}
\]

\[
s(N, z) = \frac{2z - 2z^2 \cdot r(N - 1, z)}{3 + z - (2z + 2z^2) \cdot r(N - 1, z)}, \tag{20}
\]

\[
r(N, z) = \frac{2z + 2z^2 - (z^2 + 3z^3) \cdot r(N - 1, z)}{3 + z - (2z + 2z^2) \cdot r(N - 1, z)}, \tag{21}
\]

for arbitrary $N \geq 1$, with initial conditions $l(0, z) = s(0, z) = r(0, z) = 0$.

By combining Eqs. 16–21, we can calculate the left absorbing probabilities $P_{-1,0,0}(1,0,0)$, $P_{-1,0,N}(0,1,0)$ and $P_{-1,0,N}(0,0,1)$ for arbitrary right boundary $N \geq 0$. As an example, we calculate these values for 10 different right boundaries.

The results are shown in Fig. 5. We can see that the left absorbing probability reaches to its limiting value rapidly when the right boundary is shifting.

We derive a closed recurrence for $P_{-1,0,N}(0,0,1)$, as stated in Theorem 4. The theorem perfectly matches with the simulation data. We prove its correctness in “Appendix 3” section. Solving the recurrence, we get the left absorbing probability when the right boundary is infinitely far to the right: $\lim_{N \to \infty} P_{-1,0,N}(0,0,1) = 1/\sqrt{2}$.

**Theorem 4** The left absorbing probabilities $P_{-1,0,N}(0,0,1)$ obey the following recurrence.

\[
P_{-1,0,0}(0,0,1) = 0,
\]

\[
P_{-1,0,N+1}(0,0,1) = \frac{2 + 3 P_{-1,0,N}(0,0,1)}{3 + 4 P_{-1,0,N}(0,0,1)}, \quad N \geq 1.
\]

**4.2 Arbitrary boundaries**

Suppose now the left boundary is at $-M$ ($M \geq 1$), and the right boundary is at $N$ ($N \geq 1$). Let’s define generating functions $l(-M, N, z)$, $s(-M, N, z)$ and $r(-M, N, z)$.
Fig. 5 (Color online) Theoretical left absorbing probabilities \(P_{-1,0,N}(1,0,0)\), \(P_{-1,0,N}(0,1,0)\) and \(P_{-1,0,N}(0,0,1)\) evolving with the right absorbing boundary in Grover walks with two boundaries. The left absorbing boundary is at \(-1\).

Similarly to \(l(N, z)\), \(s(N, z)\) and \(r(N, z)\). We now show that \(r(-M, N, z)\) can be represented by \(l(N, z)\) and \(r(N, z)\). For a walker with initial state \(|0, R\rangle\), if it wishes to be absorbed by the left boundary \(-M\) rather than the right boundary \(N\), it must reach positions \(-1, -2, \cdots, -M\) sequentially without being trapped by the right. That is, the walker has to move left \(M\) times effectively. For the first move from 0 to \(-1\) with coin state \(|R\rangle\), \(r(N, z)\) counts the paths. For an intermediate move from \(-k\) to \(-(k+1)\) with coin state \(|L\rangle\), \(l(N+k, z)\) counts the paths. Then we have \(r(-M, N, z) = r(N, z) \prod_{k=1}^{M-1} l(N+k, z)\). Likewise, \(l(-M, N, z) = l(N, z) \prod_{k=1}^{M-1} l(N+k, z)\) and \(s(-M, N, z) = s(N, z) \prod_{k=1}^{M-1} l(N+k, z)\). As \(l(N, z)\), \(s(N, z)\) and \(r(N, z)\) can be calculated by the recurrences stated in Theorem 3, \(l(-M, N, z)\), \(s(-M, N, z)\) and \(r(-M, N, z)\) are solvable. With \(l(-M, N, z)\), \(s(-M, N, z)\) and \(r(-M, N, z)\) in hand, we can calculate the left absorbing probabilities for arbitrary left and right boundaries by the following formulas.

\[
P_{-M,0,N}(1,0,0) = \sum_{t=1}^{\infty} \left\| z^t \right\|^2 l(-M, N, z)^2 \right\| = \frac{1}{2\pi} \int_0^{2\pi} l(N, \theta) \prod_{k=1}^{M-1} l(N+k, \theta) d\theta, \tag{22}
\]

\[
P_{-M,0,N}(0,1,0) = \sum_{t=1}^{\infty} \left\| z^t \right\|^2 s(-M, N, z)^2
\]
Grover walks on a line with absorbing boundaries

\[ P_{-M,0,N}(0,0,1) = \sum_{t=1}^{\infty} \|z^t\|^2 r(-M, N, z) \]

\[ = \frac{1}{2\pi} \int_{0}^{2\pi} \left| s(N, \theta) \prod_{k=1}^{M-1} l(N + k, \theta) \right|^2 d\theta, \quad (23) \]

\[ = \frac{1}{2\pi} \int_{0}^{2\pi} \left| r(N, \theta) \prod_{k=1}^{M-1} l(N + k, \theta) \right|^2 d\theta. \quad (24) \]

Up to now, we have only discussed how to estimate the left absorbing probability \( P_{-M,0,N}(\alpha, \beta, \gamma) \). How to calculate the right absorbing probability \( Q_{-M,0,N}(\alpha, \beta, \gamma) \)?

As the Grover operator is permutation symmetric, a Grover walk with some initial state \((\alpha, \beta, \gamma)\), a left boundary \(-M\) and a right boundary \(N\) is equivalent to a Grover walk with some initial state \((\gamma, \beta, \alpha)\), a left boundary \(-N\) and a right boundary \(M\) in the sense that they have the symmetric probability distributions and the symmetric left/right absorbing probabilities. The relationship between the left and right absorbing probabilities is stated in Proposition 5.

**Proposition 5** In Grover walks with two boundaries, the left and right absorbing probabilities satisfy

\[ Q_{-M,0,N}(\alpha, \beta, \gamma) = P_{-N,0,M}(\gamma, \beta, \alpha), \]

where \( M \geq 1, N \geq 1 \) are boundaries, and \((\alpha, \beta, \gamma)\) are amplitudes corresponding to \( |L\), \(|S\) \(|R\) coin components.

Now we analyze how localization affects the absorbing probabilities in Grover walks with two boundaries. To simplify the analysis, we only consider a special case that the system is initialized to \(|0, R\rangle\). The methods can be applied to more complicated cases smoothly. Let’s define \( l(-M, N) = P_{-M,0,N}(0,0,1)\), \( r(-M, N) = Q_{-M,0,N}(0,0,1)\), \( l(-M, N) \) and \( r(-M, N) \) are the absorbing probabilities that the walker starts from state \(|0, R\rangle\) and is absorbed by the left and the right. We also define \( s(-M, N) \) to be the sum of two absorbing probabilities: \( s(-M, N) = l(-M, N) + r(-M, N)\). Table 1 shows the values of \( l(-2, N), r(-2, N) \) and \( s(-2, N) \) for different right boundaries \( N \) (\( N \) varies from 1 to 6).

From Table 1, we observe that \( s(-2, N) \) is \(<1\), which is in sharp contrast to the Hadamard walk case. In Hadamard walks with two boundaries, it is stated that

\[ \forall M, N \geq 1, \quad s(-M, N) = 1, \quad (5, \text{PROPOSITION 9}), \]

which indicates that the Hadamard walker is absorbed by either the left or the right boundary after walking enough steps. However, this equation doesn’t hold in Grover walks with two boundaries. Due to the localization effect, there is some probability that the walker is trapped around origin. Let \( o(-M, N) \) be the localization probabilities when two boundaries are presented, then we have a similar equation for Grover walks with two boundaries
Table 1  Left and right absorbing probabilities when the left boundary is at $-2$ and the right boundary varies from 1 to 6

| $-M$ | $N$ | $l(-M, N)$ | $r(-M, N)$ | $s(-M, N)$ | $p(N)$ | $\ln(p(N))$ |
|------|-----|------------|------------|------------|--------|-------------|
| $-2$ | 1   | 0.15294117671 | 0.447058823529 | 0.600000000000 | 0.004040404040 | $-5.5114$ |
| $-2$ | 2   | 0.1616161616 | 0.434343434343 | 0.595959595960 | 0.000000000000 | $-10.0964$ |
| $-2$ | 3   | 0.161910656810 | 0.434007710537 | 0.595183673470 | 0.000000000000 | $-14.6812$ |
| $-2$ | 4   | 0.161919722633 | 0.433998223971 | 0.595179466040 | 0.000000000000 | $-19.2666$ |
| $-2$ | 5   | 0.161919993553 | 0.433997948759 | 0.595179423120 | 0.000000000000 | $-25.2096$ |
| $-2$ | 6   | 0.161920001578 | 0.433997940723 | 0.59517942301 | 0.000000000000 | $-25.2096$ |

These probabilities are calculated by Eqs. 22–24, with 12 digits reserved. $s(-M, N)$ is the sum of $l(-M, N)$ and $r(-M, N)$. $p(N) = s(-2, N) - s(-2, N + 1)$ is the localization probability at position $N$. The values of $\ln(p(N))$ decrease linearly with $N$.

$$\forall M, N \geq 1, \quad s(-M, N) + o(-M, N) = 1.$$ 

when the gap between the left and right boundaries becomes larger (i.e., $M + N$ becomes larger), more localization probabilities are introduced, as these bounded positions can reserve more probability amplitudes. Thus, the bigger the gap, the larger $o(-M, N)$ and the smaller $s(-M, N)$.

The localization probabilities decay exponentially in Grover walks, as stated in [18,30]. This phenomenon is also observed in Grover walk with two boundaries. Now let’s dig deeper on the data given in Table 1. For arbitrary $N \geq 1$, we define $p(N) = s(-2, N) - s(-2, N + 1)$. Actually, $p(N)$ is the localization probability at position $N$ when the left boundary is at $-2$ and the right boundary is at $N + 1$. In order to show that $p(N)$ suffers exponentially decay, we calculate the natural logarithm of $p(N)$. The values of $p(N)$ and $\ln(p(N))$ are presented in Table 1, and $\ln(p(N))$ is visualized in Fig. 6. From Fig. 6, we can see that the log-scale values of $p(N)$ decrease linearly with $N$, which indicates the exponential decay of localization probabilities in Grover walk with two boundaries.

5 Conclusion

We analyze in detail the dynamics of Grover walks on a line with one and two absorbing boundaries in this paper. Both cases illustrate interesting differences between Grover walks and Hadamard walks with boundaries.

In the one boundary case, we begin with three special initial states and define generating functions for these simple cases. These generating functions have closed form solutions. Then, we use the solutions to calculate the absorbing probability for arbitrary boundary. The oscillating localization phenomenon is observed and numerically studied in Grover walks with one boundary. It offers a nice explanation for the extreme fast decrease of the absorbing probabilities when the boundary is moved from $-1$ to $-2$.

We study the two boundaries in almost the same way as what we did in the former case. Generating functions are defined for three special initial states. We then derive recurrence solutions to these generating functions. These solutions are used to solve
Grover walks on a line with absorbing boundaries

Fig. 6 Natural logarithm of localization probabilities $p(N)$ in Grover walks with two boundaries. The left boundary is at $-2$, and the right boundary is at $N + 1$. $\ln(p(N))$ decreases linearly with $N$, indicating that $p(N)$ decays exponentially.

more complicated cases. The absorbing probabilities (both the left and right absorbing probability) for arbitrary left and right boundary can be calculated to arbitrary accuracy by recursively applying these solutions. When the left boundary is at $-2$, the quantum walk leads to localization. We show that the localization probabilities decay exponentially.

Many questions are still left unsolved. We cannot calculate the absorbing probability when the boundary approaches infinity in the one boundary case. In the two boundaries case, we are unable to analytically calculate the left and right absorbing probabilities with arbitrary coin states. A further detailed study on these questions will appear in our forth-coming paper.

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Appendix 1: Recurrences for generating functions of one boundary

In Grover walk with one boundary, the left generating function $l(z)$ in Eq. 4 can be rewrote by $l(z)$, $s(z)$ and $r(z)$. The derivation is as follows. It must be pointed out the derivation is capable of solving three-state quantum walks with arbitrary coin operators, not limited to the Grover operator.
\[ l(z) = \sum_{t=1}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-1} |0, L) z^t \]
\[ = (-1, L|U|0, L) z + \sum_{t=2}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-2} \Pi^{-1}_{no} U|0, L) z^t \]
\[ = \frac{1}{3} z + \frac{2}{3} \sum_{t=2}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-2} |0, S) z^{t-1} \]
\[ + \frac{2}{3} z \sum_{t=2}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-2} |1, R) z^{t-1} \]
\[ = \frac{1}{3} z + \frac{2}{3} \sum_{t=1}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-1} |0, S) z^t \]
\[ + \frac{2}{3} z \sum_{t=1}^{\infty} (-1, L|U \left( \Pi^{-1}_{no} U \right)^{t-1} |1, R) z^t \]
\[ = -\frac{1}{3} z + \frac{2}{3} z \cdot s(z) + \frac{2}{3} z \cdot l(z) r(z). \]

By similar arguments, we get three recurrences for these generating functions:

\[ l(z) = -\frac{1}{3} z + \frac{2}{3} \cdot s(z) + \frac{2}{3} z \cdot l(z) r(z), \]
\[ s(z) = \frac{2}{3} z - \frac{1}{3} z \cdot s(z) + \frac{2}{3} z \cdot l(z) r(z), \]
\[ r(z) = \frac{2}{3} z + \frac{2}{3} z \cdot s(z) - \frac{1}{3} z \cdot l(z) r(z). \]

Solving these equations and discarding the solutions that don’t have Taylor expansions, we get the desired answers

\[ l(z) = \frac{-3 - 4z - 3z^2 + (1 + z) \Delta}{2z}, \]
\[ s(z) = \frac{-3 - z + \Delta}{2z}, \]
\[ r(z) = \frac{3 + 2z + 3z^2 + (z - 1) \Delta}{4z}, \]

where \(\Delta = \sqrt{9 + 6z + 9z^2}.\)

**Appendix 2: Recurrences for generating functions of two boundaries**

As in the case of one boundary, the left generating function \(l(N, z)\) defined by Eq. 13 in Grover walk with two boundaries can also be represented by \(l(N, z), s(N, z)\) and
$r(\cdot, z)$. The derivation is as follows.

$$l(N, z) = \sum_{t=1}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-1} \mid 0, L \rangle z^t$$

$$= \langle -1, L \mid 0, L \rangle z + \sum_{t=2}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-2} \left( \prod_{no}^N \prod_{no}^{-1} U \right) \mid 0, L \rangle z^t.$$

And for any $N \geq 2$, we have

$$\langle -1, L \mid 0, L \rangle = \langle -1, L \mid \left( \frac{1}{3} \mid -1, L \rangle + \frac{2}{3} \mid 0, S \rangle + \frac{2}{3} \mid 1, R \rangle \right) = -\frac{1}{3},$$

$$\prod_{no}^N \prod_{no}^{-1} U \mid 0, L \rangle = \frac{2}{3} \mid 0, S \rangle + \frac{2}{3} \mid 1, R \rangle.$$

Then

$$l(N, z) = \langle -1, L \mid 0, L \rangle z + \sum_{t=2}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-2} \left( \prod_{no}^N \prod_{no}^{-1} U \right) \mid 0, L \rangle z^t$$

$$= -\frac{1}{3} z + \sum_{t=2}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-2} \left( \frac{2}{3} \mid 0, S \rangle + \frac{2}{3} \mid 1, R \rangle \right) \rangle z^t$$

$$= -\frac{1}{3} z + \frac{2}{3} z \sum_{t=2}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-2} \mid 0, S \rangle z^{t-1}$$

$$+ \frac{2}{3} z \sum_{t=2}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-2} \mid 1, R \rangle z^{t-1}$$

$$= -\frac{1}{3} z + \frac{2}{3} z \sum_{t=1}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-1} \mid 0, S \rangle z^t$$

$$+ \frac{2}{3} z \sum_{t=1}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-1} \mid 1, R \rangle z^t.$$

Let’s take a closer look at the last two terms. We have

$$\sum_{t=1}^{\infty} \langle -1, L \mid U \left( \prod_{no}^N \prod_{no}^{-1} U \right)^{t-1} \mid 0, S \rangle z^t = s(N, z)$$

by definition. For a walker with initial state $\mid 1, R \rangle$, if it wants to exit from the left boundary $-1$, it must first reach 0. The generating function for reaching 0 from state $\mid 1, R \rangle$ is $r(N - 1, z)$, while the generating function for reaching $-1$ from state $\mid 0, L \rangle$ is $l(N, z)$. In a word, we can derive
Conjecture 11 in [5]. For the remainder of this section, let Thus, this proof of Theorem 4 closely follows the argument laid out in [27] for the proof of Appendix 3: Proof of Theorem 4

Prior to proving Theorem 4, we provide a few preliminary results:

Proposition 6 For $|w|, |z| < 1$, we have $|f(w, z)| < 1$ where $f(w, z) = \frac{2z(z+1)-z^2(1+3z)}{z(z+3)-2z(z+1)w}$. Proof Let us rewrite $f(w, z)$ as $f(w, z) = z^3 \frac{b(z)}{b(\frac{1}{z}) \cdot a(z) - w}$, where $a(z) = \frac{2z(z+1)}{z^2(1+3z)}$ and $b(z) = z^2(1+3z)$. Notice that for fixed $z$, the function $g_z(w) = f(w, z)$ is a linear fractional transformation. These transformations map circles to circles. In particular,
for $|z| = 1$ we have $g_z(w) = e^{i\theta} \frac{c-w}{1-cw}$. Since $|z| = 1 \Rightarrow a(z) \leq 1$, it follows that $|z| = 1, |w| \leq 1 \Rightarrow |f(w, z)| \leq 1$. Now consider the function $h_w(z) = f(w, z)$ for fixed $w$. For $|w| \leq 1$, $w \neq 1, h_w(z)$ is analytic in the unit disk, the result follows from the maximum modulus principle and an appeal to continuity for the case $w = 1$. □

Corollary 7 For all $n \in \mathbb{N}$, the function $r_n(z)$ is analytic in $|z| < 1$.

Proposition 8 For all $n \in N$, we may write $r_n(z) = \frac{p(z)}{q(z)}$ where $\deg(p) = \deg(q) + 1$.

Proof Clearly $r_1(z)$ satisfies this condition. Let $r_{n+1}(z) = \frac{p'(z)}{q'(z)}$ and suppose $r_n(z) = \frac{p(z)}{q(z)}$ where $\deg(q) = d$ and $\deg(p) = \deg(q) + 1$. Then $p'(z) = 2z(z+1)q(z) - z^2(1+3z)p(z)$ and $q'(z) = (z+3)q(z) - 2z(z+1)p(z)$. This implies $\deg(p') = d+4$ and $\deg(q') = d+3$. □

Proposition 9 The functions $r_n(z)$ have the following closed form:

$$r_n(z) = \frac{2z(z+1)R_n(z)}{R_{n+1}(z) + z^2 (1+3z)R_n(z)}$$

where $R_n(z) = \lambda^n_+(z) - \lambda^n_-(z)$ and $\lambda_{\pm} = \frac{1}{2} \left( 3 + z - (z^2 + 3z^3) \pm \sqrt{(3+z+z^2+3z^3)^2 - 4(2z+2z^2)^2} \right)$.

Proof If we let $r_n(z) = \frac{p_n(z)}{q_n(z)}$ (not to be confused with the absorption probability $p_n$), then we have the relation:

$$\frac{p_{n+1}(z)}{q_{n+1}(z)} = \frac{2z(z+1)q_n(z) - z^2 (1+3z)p_n(z)}{(z+3)q_n(z) - 2z(z+1)p_n(z)}.$$ 

As such, if we let $v_n(z) = \begin{bmatrix} p_n(z) \\ q_n(z) \end{bmatrix}$, we have that $v_n(z) = (M(z))^n v_0(z)$ where $v_0 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$ and $M(z) = \begin{bmatrix} -z^2(1+3z) & 2z(z+1) \\ -2z(z+1) & z+3 \end{bmatrix}$. We compute $M^n$ using an eigenvalue expansion:

$$M^n v_0 = \frac{1}{d} \begin{bmatrix} 2z(z+1) & 2z(z+1) \\ \lambda_+ + z^2 (1+3z) & \lambda_- + z^2 (1+3z) \end{bmatrix} \begin{bmatrix} \lambda_+^n & 0 \\ \lambda_-^n & \lambda_+^n \end{bmatrix} = \frac{1}{d} \begin{bmatrix} 2z(z+1) & 2z(z+1) \\ \lambda_+ + z^2 (1+3z) & \lambda_- + z^2 (1+3z) \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \frac{1}{d} \begin{bmatrix} 2z(z+1) & 2z(z+1) \\ \lambda_+ + z^2 (1+3z) & \lambda_- + z^2 (1+3z) \end{bmatrix} \begin{bmatrix} -2z(z+1) \lambda_+^n \\ 2z(z+1) \lambda_-^n \end{bmatrix} = \frac{1}{d} \begin{bmatrix} 4z^2(z+1)^2 (\lambda_-^n - \lambda_+^n) \\ 2z(z+1)(\lambda_-^{n+1} - \lambda_+^{n+1}) + 2z^3(1+3z)(z+1)(\lambda_-^n - \lambda_+^n) \end{bmatrix}.$$
Here, $d$ is the determinant of this eigenvector matrix and $\lambda_{\pm}(z)$ are the eigenvalues of $M$. We may compute $\lambda_{\pm}$ to be as they are above. If we let $R_n(z) = \lambda_+^n(z) - \lambda_-^n(z)$ and take the quotient of the two entries of $M^n v_0$, our closed form expression for $r_n(z)$ results.

It is worthwhile to note that though the closed form expression of $r_n$ involves square roots, it is still a rational function by its recursive form.

**Proposition 10** We have the relation: $\frac{1}{z} r_n(z) r_n \left( \frac{1}{z} \right) = \frac{2}{3 z^2 - 2 z + 3} \left[ r_n(z) + r_n \left( \frac{1}{z} \right) \right]$.

**Proof** First, let us compute $r_n \left( \frac{1}{z} \right)$. Note that $\lambda_{\pm} \left( \frac{1}{z} \right) = -\frac{1}{z^2} \lambda_{\mp}(z)$. From this it follows that $R_n \left( \frac{1}{z} \right) = - \left( -\frac{1}{z^3} \right)^n R_n(z)$. Using this substitution we find $r_n \left( \frac{1}{z} \right) = \frac{2 z (z + 1) R_n(z)}{(z+3) R_n(z) - R_{n+1}(z)}$. Now consider the expression from the proposition:

$$I_n(z) := \frac{1}{z} r_n(z) r_n \left( \frac{1}{z} \right) = \frac{4 z(z+1)^2 R_n^2}{(R_{n+1} + z^2(1+3z)R_n)((z+3)R_n - R_{n+1})}.$$

Let us assume the following partial fractions expansion:

$$I_n(z) = \frac{a(z)}{R_{n+1} + z^2(1+3z)R_n} + \frac{b(z)}{(z+3)R_n - R_{n+1}}.$$

This allows us to write:

$$[b(z) - a(z)] R_{n+1}(z) + \left[ (z+3)a(z) + z^2(1+3z)b(z) \right] R_n(z) = 4z(z+1)^2 R_n(z)^2.$$

This equation holds if the following system has satisfied:

$$b(z) - a(z) = 0, \text{ and } (z+3)a(z) + z^2(1+3z)b(z)] R_n(z) = 4z(z+1)^2 R_n(z)^2.$$

These equations imply $a(z) = b(z) = \frac{R_n(z)}{3 z^2 - 2 z + 3}$. Plugging this back into $I_n(z)$ gives us the desired relation.

**Proposition 11** For all $n \in \mathbb{N}$, $r_n(\omega)$ is purely imaginary where $\omega = \frac{1}{3} + \frac{2 \sqrt{2} \imath}{3} i$.

**Proof** This is immediately apparent by plugging $\omega$ into the recursion relation:

$$r_{n+1}(\omega) = \frac{2 \sqrt{2} \imath - 3 r_n(\omega)}{3 - 2 \sqrt{2} \imath r_n(\omega)}.$$

We are now ready to state the proof of Theorem 4.

**Proof** From [31], we note the following representation governing the Hadamard product of two functions $f$ and $g$ (with radius of convergence $R$ and $R'$, respectively):

$$(f \odot g)(z) = \frac{1}{2 \pi \imath} \int_C \frac{1}{w} f(w) g \left( \frac{z}{w} \right) dw.$$
Here, $C$ is a contour for which $|w| < R$ and $|\frac{z}{w}| < R'$. Clearly, we have $p_n = (r_n \odot r_n)(1)$, so we may write:

$$p_n = \frac{1}{2\pi i} \int_{|z|=1} \frac{1}{z} r_n(z) r_n \left( \frac{1}{z} \right) dz.$$  

By Corollary 7, if $z_0$ is a pole of $r_n(z)$, then it follows that $|z_0| > 1$. Similarly, if $z_0$ is a pole of $r_n \left( \frac{1}{z} \right)$, then $|z_0| < 1$. Thus, for every $n \in \mathbb{N}$ there exists an $\epsilon > 0$ such that:

$$p_n = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{1}{z} r_n(z) r_n \left( \frac{1}{z} \right) dz.$$  

We substitute our relation from Proposition 10:

$$p_n = \frac{1}{\pi i} \int_{|z|=1+\epsilon} \frac{r_n(z)}{3z^2 - 2z + 3} dz + \frac{1}{\pi i} \int_{|z|=1+\epsilon} \frac{r_n \left( \frac{1}{z} \right)}{3z^2 - 2z + 3} dz.$$  

Let $\omega = \frac{1}{3} + \frac{2\sqrt{2}}{3} i$ and $\bar{\omega}$ be roots of the equation $3z^2 - 2z + 3 = 0$, and note that $|\omega| = |\bar{\omega}| = 1$. The right integrand has all poles within the contour and is a rational function with representation $\frac{p(z)}{q(z)}$ where $\deg(q) = \deg(p) + 3$ by Proposition 8. A result from complex analysis tells us that for a rational function $\frac{p(z)}{q(z)}$ with $\deg(q') > \deg(p') + 1$, the sum of the residues vanishes. As such, we are left with

$$p_n = \frac{1}{\pi i} \int_{|z|=1+\epsilon} \frac{r_n(z)}{3z^2 - 2z + 3} dz.$$  

The only poles enclosed by the contour are $\omega$ and $\bar{\omega}$. By Cauchy’s integral formula, we thus have:

$$p_n = \frac{i}{2\sqrt{2}} (r_n(\bar{\omega}) - r_n(\omega)).$$  

By Proposition 11, $r_n(\omega)$ is purely imaginary. Moreover, since $r_n$ is a rational function with real coefficients, we have $r_n(\bar{z}) = r_n(z)$. This implies the following simplification:

$$p_n = -\frac{i}{\sqrt{2}} r_n(\omega).$$  

We can now readily prove the recurrence:

$$p_{n+1} = -\frac{i}{\sqrt{2}} r_{n+1}(\omega)$$

$$= -\frac{i}{\sqrt{2}} \left( \frac{2\omega (\omega + 1) - \omega^2 (1 + 3\omega) r_n(\omega)}{(\omega + 3) - 2\omega (\omega + 1) r_n(\omega)} \right)$$

$$= -\frac{i}{\sqrt{2}} \left( \frac{-8 + 20\sqrt{2} i}{9} + \frac{10 + 2\sqrt{2} i}{3} \cdot \frac{r_n(\omega)}{(10 + 2\sqrt{2} i) + \frac{8 - 20\sqrt{2} i}{9}} \right)$$
\[
\begin{align*}
&= -i \sqrt{\frac{2}{3}} \left( \frac{2\sqrt{\frac{2}{3}} i + r_n(\omega)}{1 - 2\sqrt{\frac{2}{3}} i r_n(\omega)} \right) \\
&= -i \sqrt{\frac{2}{3}} \left( \frac{2\sqrt{\frac{2}{3}} i + i \sqrt{\frac{2}{3}} p_n}{1 + \frac{4}{3} p_n} \right) \\
&= \frac{2 + 3 p_n}{3 + 4 p_n}.
\end{align*}
\]

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