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## Quantum walk with one variable absorbing boundary

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### ABSTRACT

Quantum walks constitute a promising ingredient in the research on quantum algorithms; consequently, exploring different types of quantum walks is of great significance for quantum information and quantum computation. In this study, we investigate the progress of quantum walks with a variable absorbing boundary and provide an analytical solution for the escape probability (the probability of a walker that is not absorbed by the boundary). We simulate the behavior of escape probability under different conditions, including the reflection coefficient, boundary location, and initial state. Moreover, it is also meaningful to extend our research to the situation of continuous-time and high-dimensional quantum walks.

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### 1. Introduction

A random walk describes the stochastic motion of a particle around a discrete space and is widely applied as a statistical tool in areas ranging from physics to computer science and from economics to biology [1]. In a classical version of a random walk with discrete steps, every time a walker arrives at a crossroad, he has to choose the route to take by flipping a coin [with heads (tails) leading to the left (right)]. After several random steps the position of the walker is described by a Gaussian distribution. For the quantum case, we define a two-dimensional Hilbert space, the coin space  $\mathcal{H}_c$ , spanned by  $\{|L\rangle, |R\rangle\}$ , and the walker space  $\mathcal{H}_w$ , an infinite-dimensional Hilbert space which is spanned by  $\{|x\rangle\}$ , with  $x$  supposing all possible integer values. The state of the system is described as a tensor product  $\mathcal{H}_c \otimes \mathcal{H}_w$  and the evolution of the system is given by a sequence of coin-tossing and shift operations. The unitary operator of the evolution is given first by using the unitary coin-flipping operator

$$\hat{H}(\theta) = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix}, \quad (1)$$

and then following it by a conditional shift operation

$$\hat{S} = \sum_x [ |L\rangle \langle L| \otimes |x-1\rangle \langle x| + |R\rangle \langle R| \otimes |x+1\rangle \langle x| ]. \quad (2)$$

The final state after  $t$  steps of evolution is indicated by the expression

$$|\Psi_t\rangle = \left\{ \hat{S} \cdot \left[ \hat{H}(\theta) \otimes \hat{I}_w \right] \right\}^t |\Psi_0\rangle. \quad (3)$$

For different initial coin states, a quantum walk gives different probability distributions of the walker. Moreover, the modulus of a superposition of complex amplitudes, in contrast with the addition of positive weights in a classical manner, leads to the standard deviation of the probability distributions being proportional to  $t$  rather than the square root dependence of the classical random walk. Thus, the quantum walk offers a quadratic gain over its classical counterpart.

Since the seminal paper by Aharonov et al. establishing a quantum analogy to the classical walk, different versions and applications of the original proposal have been widely investigated [2–11]. It has been demonstrated that quantum walks can be used to realize quantum search algorithms and universal quantum computation [12–15]. Furthermore, quantum walks present a versatile approach to model the energy transfer in photosynthetic systems [16, 17], quantum diffusion [18,19], and electrical breakdown [20,21]. Accordingly, quantum walks may pave the way to simulate, control, and understand the dynamics of a variety of physical and biological systems. Meanwhile, experimental implementations of quantum walks have been presented in recent years by using trapped ions [22–24], atoms [25,26], nuclear magnetic resonance systems [27, 28], waveguides [29–34], and photons [35–43]. All these achievements have attracted more attention to quantum walks and are advancing the field toward the ultimate goals of quantum computation.

Recently, the one-dimensional quantum walk with an absorbing, reflecting boundary has been widely analyzed in many papers [44–47]. In 2006, Amanda et al. investigated the two-dimensional

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1 quantum walk in infinite and finite lattices with rectangular and  
2 diamond boundaries [48]. Leong et al. also studied the one-  
3 dimensional quantum walk with a moving absorbing wall [49].  
4 Our research focuses on the situation of a quantum walk with  
5 a variable reflective boundary. We first describe the definition of  
6 this late-model quantum walk and compare it with its classical  
7 counterpart. Next, we provide an analytical solution for the escape  
8 probability in this case. Finally, we discuss the impact of the re-  
9 flection coefficient, the boundary location, and the initial state on  
10 the distribution of quantum walks, and come to a conclusion.

11 **2. Quantum walk with variable reflective boundary**

12 We consider a game that gives a probability  $p$  of winning one  
13 dollar and  $1 - p$  of losing one dollar. If a player has  $n$  dollars  
14 in the beginning, and intends to play until he gains  $N_1$  dollars, what  
15 is the probability that the player will go bankrupt before achiev-  
16 ing his target? This is the well-known gambler's ruin game [50].  
17 The classical walk with an absorbing boundary can be regarded as  
18 a variant of this game, and we can map this game to a classical  
19 walk in which the walker starts at position  $n$  with an absorbing  
20 boundary situated at position  $N$ . For simplicity, we suppose that  
21 the walk starts at position 0 and the boundary is placed initially at  
22 position  $N = 1$ . It is acknowledged that the probability to get  
23 absorbed by the boundary is equal to 1 in the long time limit; that is  
24 to say, the walker will never escape from the absorbing wall in a  
25 classical random walk. However, for the quantum walk, specifically  
26 the Hadamard quantum walk ( $\theta = \frac{\pi}{4}$ ) with an absorbing bound-  
27 ary in position 1 and starting with the initial state  $|R\rangle \otimes |0\rangle$ , has  
28 a probability  $p = 1 - 2/\pi$  to escape from the boundary [44]. More  
29 generally, for different initial states and locations of the bound-  
30 ary the numerical value of the escape probability is nonzero in all  
31 cases.

32 For the sake of calculating the escape probability of a quan-  
33 tum walk with boundary, we use the eigenfunction method that is  
34 mentioned in Ref. [47]. Supposing  $L(n, t)$  stands for the amplitude  
35 of the walker state, which holds coin  $|L\rangle$  and stays at position  $n$  after  
36  $t$  steps and  $R(n, t)$  stands for the amplitude of the walker state  
37 which holds coin  $|R\rangle$  and stays at position  $n$  after  $t$  steps. Based  
38 on the coin-flipping and conditional shift operation discussed in  
39 the previous section, the dynamical equations of the quantum walk  
40 can be written as

41 
$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L(n+1, t-1) \cos \theta + R(n+1, t-1) \sin \theta \\ L(n-1, t-1) \sin \theta - R(n-1, t-1) \cos \theta \end{pmatrix},$$
 (4)

42 and the solutions of Eq. (4) are

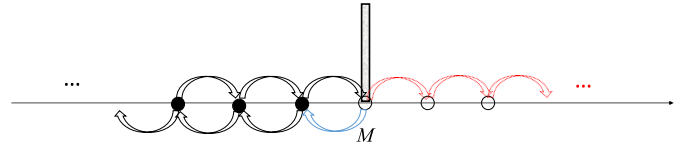
43 
$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} A_k \\ B_k \end{pmatrix} e^{i(kn - \omega_k t)}.$$
 (5)

44 To meet the demands of Eq. (4), we can get the eigenfunctions

45 
$$A_{k\pm} = \frac{1}{\sqrt{2N}} \sqrt{1 \pm \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}}},$$
  
46 
$$B_{k\pm} = \pm \frac{e^{-ik}}{\sqrt{2N}} \sqrt{1 \mp \frac{\cos k}{\sqrt{1/\rho - \sin^2 k}}},$$
 (6)

47 where  $N$  is a coefficient to ensure the probabilities sum to 1 and  $\rho$   
48 is equal to  $\cos^2 \theta$ . The corresponding eigenvalues are  $\lambda_{k\pm} = e^{-i\omega_{k\pm}}$   
49 in which  $\omega_{k+}$  is equal to  $-\sin^{-1}(\sqrt{\rho} \sin k)$ , and it gives the dis-  
50 persion relation  $\omega_{k-} = \pi - \omega_{k+}$  as well.

51 As shown in Fig. 1, a boundary with reflection coefficient  $r$  is  
52 located at position  $M$  in walker space. The walker will be reflected



53 **Fig. 1.** Diagram of quantum walk on the line with one variable absorbing bound-  
54 ary placed at position  $M$ . The walker will either be absorbed by the boundary with  
55 probability  $1 - r^2$  or be reflected with probability  $r^2$ . The solid black arrow rep-  
56 resents the dynamical process without the influence caused by the boundary. The  
57 solid blue arrow shows the reflection when the walker hits the barrier. The dashed  
58 red arrow indicates that the walker is absorbed by the boundary and would never  
59 return. (For interpretation of the references to color in this figure legend, the reader  
60 is referred to the web version of this article.)

61 or absorbed with the probability  $r^2$  or  $1 - r^2$ , respectively. Accord-  
62 ing to the settings, in the next iteration we can get the final state  
63 with the equations:

64 For  $n < M - 1$ :

65 
$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L(n+1, t-1) \cos \theta + R(n+1, t-1) \sin \theta \\ L(n-1, t-1) \sin \theta - R(n-1, t-1) \cos \theta \end{pmatrix},$$
 (7)

66 for  $n \geq M$ :

67 
$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \begin{pmatrix} L(n+1, t-1) \\ kR(n-1, t-1) \end{pmatrix},$$
 (8)

68 in which

69 
$$k = \begin{cases} -\cos \theta & \text{if } n = M, \\ \sqrt{1 - r^2} & \text{if } n = M + 1, \\ 1 & \text{if } n > M + 1. \end{cases}$$
 (9)

70 Finally, for the boundary condition

71 
$$\begin{pmatrix} L(M-1, t) \\ R(M-1, t) \end{pmatrix} = \begin{pmatrix} L(M, t-1) + rR(M, t-1) \\ L(M-2, t-1) \sin \theta - R(M-2, t-1) \cos \theta \end{pmatrix}.$$
 (10)

72 When the walkers go through the barrier they no longer return, so  
73 one must have  $L(M, t) = 0$  at all times  $t$ .

74 The boundary condition shown in Eq. (10) indicates that  
75  $L(M-1, t) = rR(M, t-1)$  should be fulfilled consistently. There-  
76 fore, the walker evolves according to Eq. (4) and satisfies this con-  
77 straint condition. However, the eigenstates of the system discussed  
78 above clearly do not meet the requirements of this condition. The  
79 only case to ensure  $L(M, t)$  vanishes invariably is that the con-  
80 tributions from different  $k$  have the same value of  $\omega$  to interfere  
81 destructively.

82 As mentioned in Ref. [44], in order to write the initial condi-  
83 tion as a superposition of eigenfunctions, the simplest way to do  
84 this is to use the method of images. Therefore, we assume a sys-  
85 tem without a boundary but which has another walker that exists  
86 symmetrically about the boundary position. This imaginary walker  
87 enforces that the whole system meets the opportune boundary  
88 condition and therefore the solutions of the above equations can  
89 be written in the form:

90 
$$\begin{pmatrix} L(n, t) \\ R(n, t) \end{pmatrix} = \sum_{k \in (-\pi/2, \pi/2)} e^{-i\omega_{k\pm} t} \left[ \left\{ C_{k\pm} \begin{pmatrix} A_{k\pm} \\ B_{k\pm} \end{pmatrix} e^{ikn} \right. \right.$$
  
91 
$$+ C_{(\pi-k)\pm} \begin{pmatrix} A_{(\pi-k)\pm} \\ B_{(\pi-k)\pm} \end{pmatrix} e^{i(\pi-k)n} \left. \right\}$$
  
92 
$$+ \left\{ D_{k\pm} \begin{pmatrix} A_{k\pm} \\ B_{k\pm} \end{pmatrix} e^{ik(n-2(M-1))} \right.$$
  
93 
$$+ D_{(\pi-k)\pm} \begin{pmatrix} A_{(\pi-k)\pm} \\ B_{(\pi-k)\pm} \end{pmatrix} e^{i(\pi-k)(n-2(M-1))} \left. \right\} \right].$$
 (11)

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