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One-dimensional quantum walk with a moving boundary

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Quantum walks are interesting models with potential applications to quantum algorithms and physical processes such as photosynthesis. In this paper, we study two models of one-dimensional quantum walks, namely, quantum walks with a moving absorbing wall and quantum walks with one stationary and one moving absorbing wall. For the former, we calculate numerically the survival probability, the rate of change of average position, and the rate of change of standard deviation of the particle's position in the long time limit for different wall velocities. Moreover, we also study the asymptotic behavior and the dependence of the survival probability on the initial particle's state. While for the latter, we compute the absorption probability of the right stationary wall for different velocities and initial positions of the left wall boundary. The results for these two models are compared with those obtained for the classical model. The difference between the results obtained for the quantum and classical models can be attributed to the difference in the probability distributions.

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I. INTRODUCTION

Analysis of random walks form the basis for the description of many physical processes such as diffusion processes (e.g., Brownian motion or energy transfer in biomolecules for photosynthesis) [1], percolation theory in condensed matter physics, [2] and even the prediction of prices in the stock market.

The ubiquitous application of classical random walks in numerous physical phenomena has motivated a search for a quantum analog, which has proven to be useful as a primitive for quantum algorithms and computing. Indeed, a quantum walk can be viewed as a multipath interference phenomena. Moreover, there have been some recent preliminary proofs that quantum walks could be responsible for the transmission of the excitation energy to reaction centers in photosynthetic complexes such as Fenna-Matthews-Olson (FMO) bacteriochlorophyll complex [3]. Experimental demonstration of quantum walks has been shown for nuclear magnetic resonance systems [4,5], optical systems [6–9], waveguide lattices [10], ion traps [11,12], and even trapped neutral ions in an optical lattice [13]. For a gentle introduction to the basics of quantum walks, please refer to [14].

In Ref. [15], the authors investigated the distribution of the time spent by a classical random walker to the right of a boundary moving with constant velocity v. In this paper, we look at the possibility of analyzing the situation of a quantum walk with a moving boundary. For a one-dimensional quantum walk with a stationary absorbing boundary, it has been shown [16] that the escape probability is slightly greater than 1/3, unlike the case of a classical random walk, in which the escape probability is zero.

II. ONE-DIMENSIONAL CLASSICAL AND QUANTUM WALKS ON AN INFINITE LINE

In this section, we briefly review some of the known results for classical and quantum walks. For a one-dimensional classical random walk, one starts at the origin and moves to the right or left with probability p and $1-p$, respectively. It is well known from the central limit theorem that in the long time limit or as $t \to \infty$, the probability distribution function for the position is given by the Gaussian probability distribution

$$p(x) = \frac{e^{-(x-\mu)^2/2\sigma}}{\sqrt{2\pi}\sigma} \tag{1}$$

with mean position at $\mu = (2p-1)t\ell$ and variance $(\sigma^2) = 4tp(1-p)\ell^2$ where ℓ is the step length.

For the quantum version, one could consider a particle starting with an extra degree of freedom, namely the coin state. The coin state is spanned by two basis states: $|R\rangle$ and $|L\rangle$, which indicate that the particle will move one unit, for the next step, to the right and to the left, respectively. The first step in the quantum walk is a unitary operation U acting on the coin state that corresponds to the coin toss in the classical setting. In this paper we will only consider the Hadamard coin operator, denoted by H, which acts on the coin state as follows:

$$\begin{aligned} H: |L\rangle &\mapsto \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle), \\ H: |R\rangle &\mapsto \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle). \end{aligned} \tag{2}$$

The Hadamard coin flip is then followed by the translation operation. The conditional translation of the system is described by the unitary translation operator

$$T = |R\rangle\langle R| \otimes \sum_i |i+1\rangle\langle i| + |L\rangle\langle L| \otimes \sum_i |i-1\rangle\langle i|, \tag{3}$$

where the index i runs over all integers. Subsequently, the Hadamard followed by the translation operator repeatedly act upon the particle state. At time $t = 0$, the particle is described by an initial state, $|\psi_0\rangle \in \mathcal{H}_C \otimes \mathcal{H}_P$, where $\mathcal{H}_C$ is the Hilbert space of the coin space and $\mathcal{H}_P$ is the Hilbert space of the position space. After t steps, the state of the system is given by

$$|\psi_t\rangle = (W)^t|\psi_0\rangle, \tag{4}$$

where $W = T \cdot (H \otimes I)$ is the walk operator.

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TABLE I. The values of $\frac{\langle x\rangle}{t}$ and $\frac{\sigma(x)}{t}$ for Hadamard walk with different initial coin states $|\varphi\rangle$.

$\lvert\varphi\rangle$	$\frac{\langle x\rangle}{t}$	$\frac{\sigma(x)}{t}$
$(1/\sqrt{2},i/\sqrt{2})^{\mathrm{T}}$	0	$\sqrt{\frac{2-\sqrt{2}}{2}}=0.54119$
$(0,e^{i\theta})^{\mathrm{T}}$	$\frac{2-\sqrt{2}}{2}=0.29289$	$\sqrt{\frac{\sqrt{2}-1}{2}}=0.45508$
$(e^{i\theta},0)^{\mathrm{T}}$	$\frac{\sqrt{2}-2}{2}=-0.29289$	$\sqrt{\frac{\sqrt{2}-1}{2}}=0.45508$
$(1/\sqrt{2},1/\sqrt{2})^{\mathrm{T}}$	$\frac{\sqrt{2}-2}{2}=-0.29289$	$\sqrt{\frac{\sqrt{2}-1}{2}}=0.45508$

The probability distribution and average position of the particle after t steps depend on the initial state of the particle. A limit theorem for the particle's position x has been derived in Ref. [17] where it is shown that as $t\to\infty$, $X=\frac{x}{t}\to Y$, where Y is the limiting random variable. For the initial state $|\varphi\rangle\otimes|0\rangle=(\alpha|L\rangle+\beta|R\rangle)\otimes|0\rangle$ and unitary coin operator

$$U=\begin{pmatrix} a & b\\ c & d\end{pmatrix},$$

the probability distribution for the particle's position has been shown in Ref. [17] to be

$$f(X)=\frac{\sqrt{1-|a|^2}}{\pi(1-X^2)\sqrt{|a|^2-X^2}}\times\left[1-\left(|\alpha|^2-|\beta|^2+\frac{a\alpha\overline{b\beta}+\overline{a\alpha}b\beta}{|a|^2}\right)X\right] \tag{5}$$

for $X\in(-|a|,|a|)$ and $f(X)=0$ for $|X|\geqslant|a|$ with the average and variance given by

$$\langle Y\rangle=-\left(|\alpha|^2-|\beta|^2+\frac{a\alpha\overline{b\beta}+\overline{a\alpha}b\beta}{|a|^2}\right)\times(1-\sqrt{1-|a|^2}) \tag{6}$$

and

$$\langle Y^2\rangle=1-\sqrt{1-|a|^2}. \tag{7}$$

The rates of change of the average position $\frac{\langle x\rangle}{t}$ and standard deviation $\frac{\sigma(x)}{t}$ for different initial coin states $|\varphi\rangle$ are given in Table I.

III. ONE-DIMENSIONAL RANDOM WALK WITH A STATIONARY ABSORBING BOUNDARY

The classical random walk with a stationary absorbing boundary can be regarded as a variant of the gambler's ruin problem. The gambler's ruin problem can be described as follows: A player begins with n dollars but each time he plays the game, he either wins a dollar with probability p or loses the same amount with a probability $1-p$. The player wishes to attain a goal of N dollars in which case he stops playing. The problem is to determine the probability that he owes the banker an infinite amount of money (and therefore is broke). This problem can be mapped to a classical random walk with the particle initially located at position n and a stationary absorbing wall placed at position N. In this paper, we consider the particle to be initially located at $n=0$ and the absorbing boundary to be placed at position $N=1$. The particle has a probability p of moving to the right and $1-p$ of moving to the left. Each step of the walk is independent of the previous steps. For this model, one can show that the escape probability of the particle (i.e., the probability that the particle will never be absorbed by the absorbing wall for $t\to\infty$), is given by

$$P^{\mathrm{esc}}=\begin{cases}\frac{1-2p}{1-p}, & \text{for}\quad p<1/2,\\ 0, & \text{for}\quad 1/2\leqslant p\leqslant 1.\end{cases} \tag{8}$$

In this paper, we only consider the symmetric classical random walk with equal probability of moving to the left and to the right. As shown in Eq. (8), for a symmetric classical random walk, $P^{\mathrm{esc}}=0$.

Quantum walks with a stationary absorbing boundary have been discussed at length in Ref. [16]. In this model, the walk operator W followed by the projective measurements are repeatedly applied on the particle's state until the particle is absorbed by the wall. The projective measurements are given by the operators $\Pi^N_{\mathrm{yes}}=I\otimes\sum_{j\geqslant N}|j\rangle\langle j|$ and $\Pi^N_{\mathrm{no}}=I-\Pi^N_{\mathrm{yes}}$, which correspond to asking the question of whether the particle has reached location N. If the particle's state is $|\Psi\rangle$, then the answer is yes with probability $||\Pi^N_{\mathrm{yes}}|\Psi\rangle||^2$ and no with probability $||\Pi^N_{\mathrm{no}}|\Psi\rangle||^2$ where after the measurement the state becomes respectively $\Pi^N_{\mathrm{yes}}|\Psi\rangle$ and $\Pi^N_{\mathrm{no}}|\Psi\rangle$ (renormalized).

For the case where the initial state of the particle is $|R,0\rangle$ and the boundary is placed at position 1; after the first walk the state will evolve to $\frac{1}{\sqrt{2}}|L,-1\rangle-\frac{1}{\sqrt{2}}|R,1\rangle$. The measurement at this step then yields an answer yes with a probability

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

and an answer no with another half of the probability after which the state collapses to $|R,1\rangle$ and $|L,-1\rangle$, respectively. If the answer is yes then the walk is stopped, otherwise the walk followed by the measurement operators are continuously applied until a yes answer is obtained. The absorption probability, which is the probability that a yes answer is obtained, is given by

$$P^{\mathrm{abs}}_{|R\rangle}(t)=\sum_{t'=1}^{t}\left|\langle R,1|W\left(\Pi^1_{\mathrm{no}}W\right)^{t'-1}|R,0\rangle\right|^2, \tag{9}$$

where $W=T\cdot(H\otimes I)$. In contrast to the symmetric classical random walk, the Hadamard quantum walk with a stationary absorbing boundary has a nonzero escape probability. For the Hadamard walk, the escape probability P^{esc} is $1-\frac{2}{\pi}\approx 0.36338$ [16,18].

IV. ONE-DIMENSIONAL RANDOM WALK WITH A MOVING ABSORBING BOUNDARY

In this section, we consider a quantum and a classical one-dimensional random walk starting at the origin with a moving absorbing semi-infinite wall. The wall extends infinitely to the right with its boundary initially located at position $N=1$. In this model as the particle walks with unit step, the wall moves with constant step length $|v|$. The wall step length is measured in the unit of the spacing between two nearest-neighbor points on a line, namely,

(i) $|v| < 1$ if the wall step length is smaller than the lattice spacing,

(ii) $|v| = 1$ if the wall step length is the same as the lattice spacing, and

(iii) $|v| > 1$ if the wall step length is larger than the lattice spacing.

The wall velocity v is taken to be positive if the wall moves to the right and negative if the wall moves to the left. Clearly if the wall moves away from the particle with a velocity $v \geqslant 1$ per unit time, the particle is never going to encounter the wall, so that the escape probability is always unity. On the other hand, if the wall moves toward the particle with a velocity $v \leqslant -1$, in the long time limit, the particle will definitely be absorbed by the wall. Hence, the nontrivial case is when $-1 < v < 1$.

For quantum walks, the particle absorption process is represented by projective measurements. The position of the wall boundary at time t is given by $N_t = 1 + vt$. Since the wall moves, the projective measurements applied in this model vary with time. The projective measurements are given as follows:

$$\Pi_{\text{yes}}^{\lceil N_t \rceil} = I \otimes \sum_{j \geqslant \lceil N_t \rceil} |j\rangle\langle j|, \qquad \Pi_{\text{no}}^{\lceil N_t \rceil} = I - \Pi_{\text{yes}}^{\lceil N_t \rceil}, \tag{10}$$

where $\lceil x \rceil$ is ceiling(x), a function that gives an integer not smaller than x. The projective operators $\Pi_{\text{yes}}^{\lceil N_t \rceil}$ and $\Pi_{\text{no}}^{\lceil N_t \rceil}$ correspond to asking the question of whether the particle hits the moving absorbing wall whose boundary is at location N_t at time t. For this model, the absorption probability of the wall for any arbitrary initial coin state $|\varphi\rangle$ can be written as

$$P_{|\varphi\rangle}^{\text{abs}}(t) = \sum_{i=1}^{\lceil |N_t - 1| \rceil} \sum_{t' = \lfloor \frac{i-1}{|v|} \rfloor + 1}^{\lfloor \frac{i}{|v|} \rfloor} \sum_{j \geqslant 2 + i\,\text{sgn}(v) - \lceil H(v) \rceil} \times |\langle R, j | \Lambda_i(t') | \varphi, 0 \rangle|^2 \lceil H(t - t') \rceil, \tag{11}$$

where $\lfloor x \rfloor$ is floor(x), a function that gives an integer not larger than x. The operator $\Lambda_i(t')$ in Eq. (11) is given as follows

$$\Lambda_i(t') = \left(\Pi_{\text{no}}^{2 + i\,\text{sgn}(v) - \lceil H(v) \rceil} W\right)^{t' - \lfloor \frac{i-1}{|v|} \rfloor - 1} \times \prod_{k=1}^{i-1} \left(\Pi_{\text{no}}^{2 + k\,\text{sgn}(v) - \lceil H(v) \rceil} W\right)^{\lfloor \frac{k}{|v|} \rfloor - \lfloor \frac{k-1}{|v|} \rfloor},$$

where W is the walk operator given by $W = T \cdot (H \otimes I)$, $H(v)$ is the Heaviside step function, which is defined as

$$H(v) = \begin{cases} 0 & \text{if} \quad v < 0, \\ 1/2 & \text{if} \quad v = 0, \\ 1 & \text{if} \quad v > 0, \end{cases} \tag{12}$$

and sgn(v) is the signum function, which is defined as follows:

$$\text{sgn}(v) = \begin{cases} -1 & \text{if} \quad v < 0, \\ 0 & \text{if} \quad v = 0, \\ 1 & \text{if} \quad v > 0. \end{cases} \tag{13}$$

The survival probability is simply given by

$$P_{|\varphi\rangle}^{\text{surv}}(t) = 1 - P_{|\varphi\rangle}^{\text{abs}}(t). \tag{14}$$

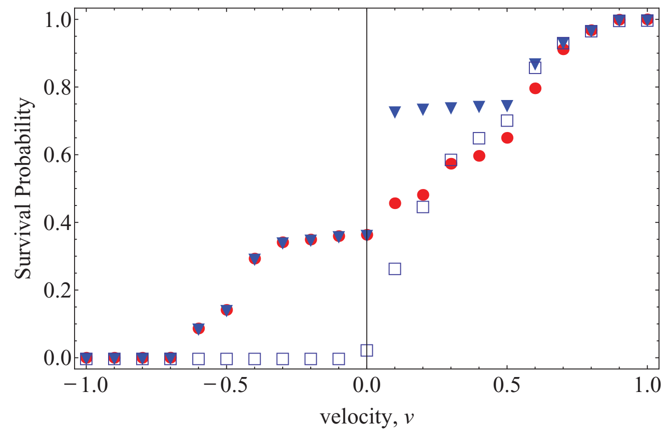


FIG. 1. (Color online) Survival probability of a particle undergoing classical random walks (open squares) and quantum walks with initial coin state $|R\rangle$ (red dots) and $|L\rangle$ (blue down triangles) as a function of the velocity of the wall. Positive velocity corresponds to the situation in which the absorbing wall moves away from the particle, and negative velocity to the situation in which the wall moves toward the particle. The results are obtained from running the simulation for 1000 time steps.

Similar to the classical case, for the quantum version when the wall moves with a velocity $v \geqslant 1$ or $v \leqslant -1$, the escape probability is unity and zero, respectively. However for $v = 0$, which corresponds to the case of a stationary absorbing boundary, it has been shown in Ref. [16,18] that the escape probability is $1 - 2/\pi = 0.36338$, in contrast with the classical case where the escape probability is zero. To study the survival probability for different wall velocities v, we carry out numerical simulations of the quantum and classical model for 1000 time steps. Figure 1 shows the survival probability of a particle undergoing classical random walks (open squares) and quantum walks with initial coin state $|R\rangle$ (red dots) and $|L\rangle$ (blue down triangles) as a function of the wall velocity v.

Note that for $v \leqslant 0$, the survival probability values for quantum walks with initial coin state $|L\rangle$ and $|R\rangle$ are the same. This result can be deduced from looking at how the state evolves. If the initial state is $|R,0\rangle$, the state will become $\frac{1}{\sqrt{2}}(|L,-1\rangle - |R,1\rangle)$ after the first walk. For wall velocity $-1 \leqslant v \leqslant 0$, the state $|R,1\rangle$ always gets absorbed by the wall at the first measurement. Hence after the first walk, the no projective measurement collapses the state into $|L,-1\rangle$ with a probability of $\frac{1}{2}$. The same thing happens for the initial state $|L,0\rangle$. The subsequent walks will then begin from the same state $|L,-1\rangle$. Hence, the survival probability values for both cases are the same. In general, if the initial coin state is $|\varphi\rangle = \cos\theta|L\rangle + e^{i\phi}\sin\theta|R\rangle$, after the first walk, the state will evolve to $\frac{1}{\sqrt{2}}(\cos\theta + e^{i\phi}\sin\theta)|L,-1\rangle + \frac{1}{\sqrt{2}}(\cos\theta - e^{i\phi}\sin\theta)|R,1\rangle$. Subsequently, the no projective measurement collapses the state to $|L,-1\rangle$ with probability $\frac{1}{2}|\cos\theta + e^{i\phi}\sin\theta|^2$. So for $v \leqslant 0$, the survival probability for an arbitrary initial coin state $|\varphi\rangle$, $P_{|\varphi\rangle}^{\text{surv}}(t)|_{v\leqslant 0}$, is related to the survival probability for initial coin state $|R\rangle$, $P_{|R\rangle}^{\text{surv}}(t)|_{v\leqslant 0}$, by the following equation:

$$P^{\text{surv}}_{|\varphi\rangle}(t)\big|_{v\leqslant 0} = \frac{1/2|\cos\theta + e^{i\phi}\sin\theta|^2}{1/2} P^{\text{surv}}_{|R\rangle}(t)\big|_{v\leqslant 0} = |\cos\theta + e^{i\phi}\sin\theta|^2 P^{\text{surv}}_{|R\rangle}(t)\big|_{v\leqslant 0}, \quad (15)$$

where $|\varphi\rangle = \cos\theta|L\rangle + e^{i\phi}\sin\theta|R\rangle$. For $v \leqslant 0$, the maximum survival probability is obtained for initial coin state $\frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)$ while the minimum is obtained for initial coin state $\frac{1}{\sqrt{2}}(|L\rangle - |R\rangle)$.

Figure 1 shows that there exists a value of wall velocity above which the survival probability of the classical random walks is higher than that of the quantum walks with initial coin state $|R\rangle$. This value has been numerically determined from the data as $v \approx 0.22$. It is also observed numerically that the crossover between the quantum survival probability with initial coin state $|L\rangle$ and its classical counterpart happens at $v \approx 0.67$.

To calculate the survival probability for quantum walks with an absorbing boundary moving with velocity $-1 < v < 1$, one can also consider the dynamics of the walks from the wall's reference frame. In this frame, the wall is stationary and the particle performs biased quantum walks with right-step length $1 - v$ and left-step length $1 + v$. If the values of $1 + v$ and $1 - v$ are rational numbers, we can multiply these two values by a common rescaling factor κ to make them become integer numbers. After the rescaling, the left-step and the right-step length will become l and r respectively, where $l,r \in \mathbb{Z}^+$ and the initial position of the wall will rescaled to κ. The walks can then be viewed as biased quantum walks on a rescaled lattice in the presence of a stationary absorbing boundary. Looking at the walks from this perspective, we can write the absorption probability as

$$P^{\text{abs}}_{|R\rangle}(t) = \sum_{t'=1}^{t}\sum_{i=0}^{r-1} \left|\langle R,\kappa + i|W_s\left(\Pi^{\kappa}_{\text{no}}W_s\right)^{t'-1}|R,0\rangle\right|^2 \quad (16)$$

where $W_s = T_s \cdot (H \otimes I)$ and

$$T_s = |R\rangle\langle R| \otimes \sum_i |i + r\rangle\langle i| + |L\rangle\langle L| \otimes \sum_i |i - l\rangle\langle i|.$$

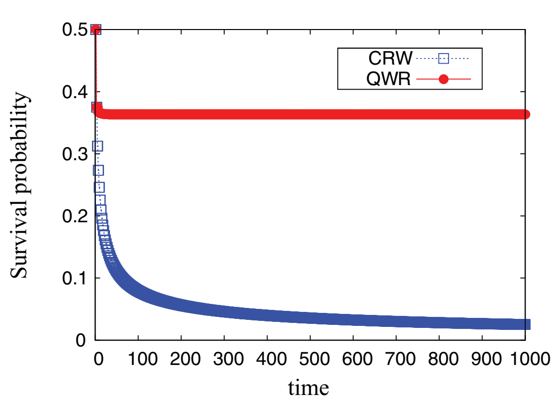


FIG. 2. (Color online) The survival probability versus time plots for classical random walks (CRW) and quantum walks with initial coin state $|R\rangle$ (QWR) in the presence of stationary absorbing wall ($v = 0$) placed at position 1. The particle is initially placed at position 0.

From the absorption probability, we can then calculate the survival probability by simply subtracting the absorption probability from unity.

From the simulation, we observe that the asymptotic behavior of the survival probability for the quantum walks differs from that for the classical random walks. As can be seen from Fig. 2, the survival probability for classical random walks decays as $1/\sqrt{t}$ in the long time limit while the survival probability for quantum walks reaches the asymptotic value faster than its classical counterpart. This is due to the fact that the quantum walk behaves as two moving wave packets, one moving to the right and the other one moving to the left. The right-moving wave packet moves ballistically toward the wall. As soon as it is absorbed by the wall, the survival probability reaches its asymptotic value as the left-moving wave packet always moves away from the wall hence it will never be absorbed by the wall. On the other hand for the classical walk, the particle spreads diffusely, which explains the slower rate of convergence of the classical survival probability compared to its quantum counterpart.

For each time step, the probability distribution for the particle's position changes and hence the average position of the particle also varies with time. From the simulation results, we calculate the rate of change of average position of the particle in the long time limit. The average position of the particle $\langle x\rangle$ is calculated as follows. The probability distribution for the position is continuously renormalized to unity at each time step to take into account those probabilities that have been absorbed by the wall. The average position at each time step is then calculated from this renormalized probability. From the values of the average position obtained, we compute the rate of change of average position of the particle. Figure 3 displays the graph of the rate of change of the particle's average position $\frac{\langle x\rangle}{t}$ in the long time limit versus the wall velocity v.

As shown in Fig. 3 for the classical case, the value of $\frac{\langle x\rangle}{t}$, in the long time limit, does not change for $v > 0$ and it is equal to the wall velocity v for $v < 0$. The reason for the above observation can be argued as follows. For $v > 0$, where the wall moves away from the particle, the long time limit probability distribution for the particle's position can be approximated as a truncated Gaussian distribution where

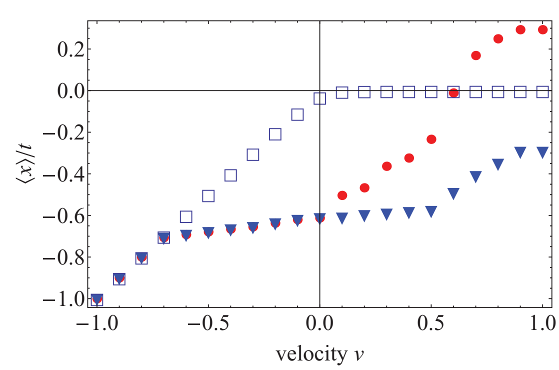


FIG. 3. (Color online) The rate of change of the particle's average position as a function of the velocity of the wall v for classical (open squares) and quantum walks with initial coin state $|R\rangle$ (red dots) and $|L\rangle$ (blue down triangles).

the truncation happens at the tail of the distribution. In the long time limit, the probability that the particle is absorbed by the wall at each time step is small compared to the survival probability, hence the truncated Gaussian distribution does not change with time when the remaining probabilities are renormalized. As a result, the average position of the particle also remains unchanged with time.

On the other hand, for $v < 0$, which corresponds to the case where the wall moves toward the particle, at each time step the probability that the particle is absorbed by the wall is no longer small compared to the survival probability. However, from the simulation result, it is observed that the renormalized probability distribution can still be approximated by a truncated Gaussian distribution, where the truncation occurs at the position of the wall $N_t = 1 + vt$.

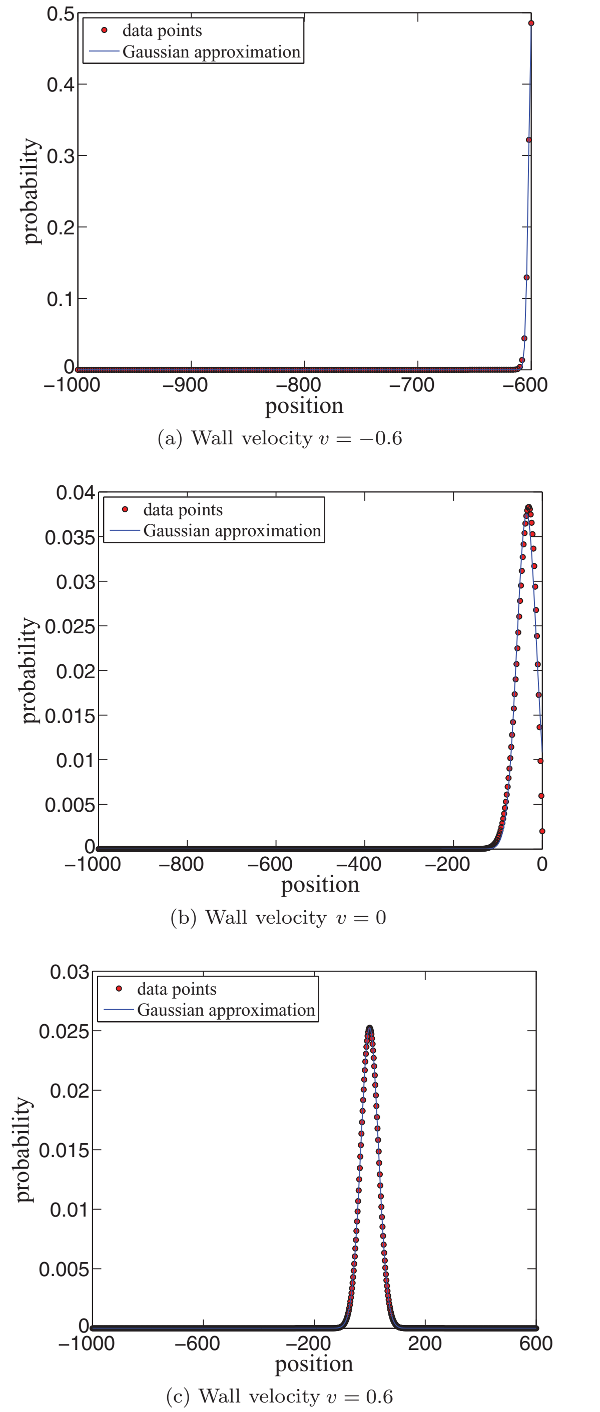
Figure 4 shows the probability distributions for several values of v. From the figure, we can see that the probability distributions for a classical random walk with a moving absorbing wall are well approximated by the Gaussian distributions. For $v < 0$, it is also observed from the simulation that the peak of each Gaussian distribution drifts with a velocity equal to the wall velocity v. So, the peak position of the Gaussian distribution at time t can be expressed as $\mu(v) = vt + \alpha(v)$, where $\alpha(v)$ is a constant whose value depends on the wall velocity. To a good approximation, the renormalized probability distribution can be approximated by

$$f(x) = \frac{1}{Z}\frac{1}{\sigma(v)\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu(v)}{\sigma(v)}\right)^2\right] \tag{17}$$

where $Z = \int_{-\infty}^{1+vt} \frac{1}{\sigma(v)\sqrt{2\pi}} \exp[-\frac{1}{2}(\frac{x-\mu(v)}{\sigma(v)})^2]dx$. For $v < 0$, the average position for the classical random walk is then given by

$$\begin{aligned}
\langle x\rangle &= \int_{-\infty}^{1+vt} x f(x) dx \\
&= \int_{-\infty}^{1+vt} \frac{1}{Z}\frac{1}{\sigma(v)\sqrt{2\pi}} x \exp\left[-\frac{1}{2}\left(\frac{x-\mu(v)}{\sigma(v)}\right)^2\right] dx \\
&\approx \mu(v) - \frac{1}{Z}\frac{\sigma(v)}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{1+vt-\mu(v)}{\sigma(v)}\right)^2\right] \\
\frac{\langle x\rangle}{t} &= v + \frac{\alpha(v)}{t} - \frac{1}{Zt}\frac{\sigma(v)}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}\left(\frac{1+vt-\mu(v)}{\sigma(v)}\right)^2\right] \\
&\xrightarrow{t\to\infty} v.
\end{aligned} \tag{18}$$

So, in the long time limit, for $v < 0$ the rate of change of the particle's average position is equal to the wall velocity v. This agrees with the numerical simulation results plotted in Fig. 3. For $v > 0$, the rate of change of the average position goes asymptotically (with t) to zero since the peak of the Gaussian distribution remains stationary at position 0. Moreover, it can also be seen from Fig. 3 that the value of $\frac{\langle x\rangle}{t}$ for classical and quantum walks are the same for $v \leqslant -0.7$. There is a bifurcation between the classical and quantum graphs at $v \approx -0.7$. This can be attributed to the reason that for $-1 \leqslant v \leqslant -0.7$, the probability distributions induced by these two types of walks can be approximated by a truncated Gaussian distribution, which can be verified from the



(a) Wall velocity $v = -0.6$

(b) Wall velocity $v = 0$

(c) Wall velocity $v = 0.6$

FIG. 4. (Color online) The probability distribution of the particle's position for classical random walks with a moving absorbing boundary after 1000 time steps. The wall moves with a velocity v and is initially placed at position 1.

simulation. Outside this velocity range, the average position for the quantum and classical walks changes with different rate.

For quantum walks with wall velocity $v \leqslant 0$, the rate of change of the particle's average position is the same for all initial coin states. The reason is that regardless of the initial coin state, the surviving state after the first measurement is always $|L,-1\rangle$. Hence, the subsequent evolutions after the first measurement will give rise to the same renormalized probability distribution for all initial coin states.

For the quantum case, it is also observed that the value of $\frac{\langle x\rangle}{t}$ is about -0.612 when $v=0$, but it is different for different initial coin states for $v>0$. For the initial coin state $|R\rangle$, $\frac{\langle x\rangle}{t}$ is zero when $v\approx 0.6$ and asymptotically approaches 0.2929 when v increases to 1. It is likely that the value for $\frac{\langle x\rangle}{t}$ is zero at $v=0.612$. This is because the particle is drifting with an average speed of 0.612 away from the wall when it is not moving, so when the wall is moving at 0.612, the speed of the particle will be nearly zero, the relative speed being the same. For the initial coin state $|L\rangle$, $\frac{\langle x\rangle}{t}$ is always negative because the left wave packet, having a higher peak than the right wave packet, always moves to the left. The value of $\frac{\langle x\rangle}{t}$ for coin state $|L\rangle$ asymptotically approaches -0.2929 when v increases to 1.

For $v\geqslant 1$, there are effectively no boundaries and for a quantum walk with initial coin state $|R\rangle$, the probability density function $f_R(X)$, Eq. (5) [17,18] with $\alpha=0$ and $\beta=1$ and Hadamard coin operator, is given by

$$f_R(X)=\frac{1}{\pi(1-X)\sqrt{1-2X^2}}, \tag{19}$$

for $-1/\sqrt{2}\leqslant X\leqslant 1/\sqrt{2}$, giving an asymptotic rate of change of average position as $\frac{2-\sqrt{2}}{2}\approx 0.2929$ (Table I). For the initial coin state $|L\rangle$, the probability density function $f_L(X)$ for $-1/\sqrt{2}\leqslant X\leqslant 1/\sqrt{2}$ is

$$f_L(X)=\frac{1-X}{\pi(1-X^2)\sqrt{1-2X^2}}, \tag{20}$$

giving an asymptotic value of $\frac{\langle x\rangle}{t}$ for $v\geqslant 1$ as $\frac{-2+\sqrt{2}}{2}\approx -0.2929$ (Table I).

Figure 5 shows the rate of change of standard deviation versus the wall velocity v for quantum walks with initial coin state $|L\rangle$ and $|R\rangle$. For both cases, the value of $\frac{\sigma(x)}{t}$ is $\sqrt{(\sqrt{2}-1)/2}\approx 0.4551$ for $v\geqslant 1$. For $0<v<1$, the value of $\frac{\sigma(x)}{t}$ is greater for coin state $|R\rangle$ because in this velocity range, the probability distribution for coin state $|R\rangle$ is more

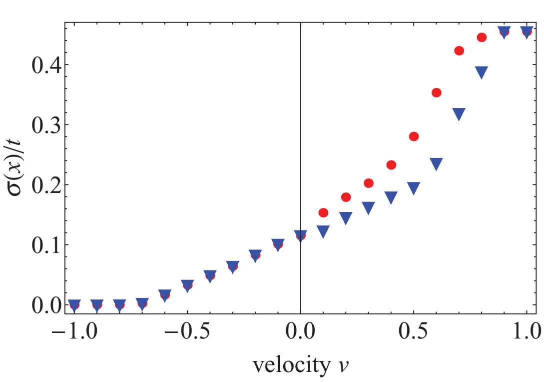


FIG. 5. (Color online) The rate of change of the standard deviation of the particle's position for quantum walks with initial coin state $|R\rangle$ (red dots) and $|L\rangle$ (blue down triangles) as a function of the velocity of the wall v. The graph approaches the value of $\sqrt{(\sqrt{2}-1)/2}$ as v increases to 1. For the classical case, the rate of change of the standard deviation is proportional to $1/\sqrt{t}$ which goes to zero as $t\to\infty$.

spread out, which can be verified from the numerical results. In contrast to the quantum case, the rate of change of standard deviation for a classical random walk follows $\frac{1}{\sqrt{t}}$ behavior, so that the value approaches zero as $t\to\infty$.

V. ONE-DIMENSIONAL RANDOM WALK WITH A MOVING ABSORBING LEFT BOUNDARY AND A STATIONARY ABSORBING RIGHT BOUNDARY

In this section, we consider classical and quantum walks on a line with one stationary and one moving absorbing semi-infinite wall. The stationary wall has its boundary placed at position $N=1$ and extends infinitely to the right, while the moving absorbing wall extends infinitely to the left with its boundary initially placed at position $-M$, where $-M\in\mathbb{Z}^-$. The particle is initially located at the origin. As the particle walks, the left wall moves with a constant velocity v_M (measured in the unit of lattice spacing). The velocity v_M is positive if the wall moves to the right and negative if it moves to the left. So at time t, the position of the left wall is $M_t=-M+v_Mt$ and the particle's position x is constrained in the region where $\lceil M_t\rceil\leqslant x\leqslant 0$.

For the quantum case, the projective measurements are given as follows

$$\Pi^1_{\rm yes}=I\otimes\sum_{j\geqslant 1}|j\rangle\langle j|,$$
$$\Pi^{\lfloor M_t\rfloor}_{\rm yes}=I\otimes\sum_{i\leqslant\lfloor M_t\rfloor}|i\rangle\langle i|,\quad\text{and}$$
$$\Pi^{(1,\lfloor M_t\rfloor)}_{\rm no}=I-\Pi^1_{\rm yes}-\Pi^{\lfloor M_t\rfloor}_{\rm yes},$$

where $\lfloor x\rfloor$ is floor (x), a function that gives an integer not larger than x. The projective operator $\Pi^1_{\rm yes}$ corresponds to asking the question of whether the particle hits the right stationary absorbing wall at position 1. Similarly, the projective operator $\Pi^{\lfloor M_t\rfloor}_{\rm yes}$ corresponds to asking the question of whether the particle hits the left-moving absorbing wall whose boundary is at location M_t at time t. The third projective measurement $\Pi^{(1,\lfloor M_t\rfloor)}_{\rm no}$ gives an answer no to the question "Does the particle hit either of the absorbing walls?".

For this model, we are interested in finding out the probability that the particle is absorbed by the right stationary wall $P^{\rm abs}(t)$ in the long time limit. The absorption probability of the right wall for an arbitrary initial coin state $|\varphi\rangle$ can be written as

$$P^{\rm abs}_{|\varphi\rangle}(t)=\sum_{i=1}^{\lceil|M_t+M|\rceil}\ \sum_{t'=\lfloor\frac{i-1}{|v_M|}\rfloor+1}^{\lfloor\frac{i}{|v_M|}\rfloor}\times\sum_{j\geqslant 1}|\langle R,j|\Lambda_i(t')|\varphi,0\rangle|^2\lceil H(t-t')\rceil. \tag{21}$$

The operator $\Lambda_i(t')$ in Eq. (21) is given by

$$\Lambda_i(t')=\left(\Pi_{\rm no}^{(1,-1+i\,{\rm sgn}(v_M)-\lfloor H(v_M)\rfloor)}W\right)^{t'-\lfloor\frac{i-1}{|v_M|}\rfloor-1}\times\prod_{k=1}^{i-1}\left(\Pi_{\rm no}^{(1,-1+k\,{\rm sgn}(v_M)-\lfloor H(v_M)\rfloor)}W\right)^{\lfloor\frac{k}{|v_M|}\rfloor-\lfloor\frac{k-1}{|v_M|}\rfloor},$$

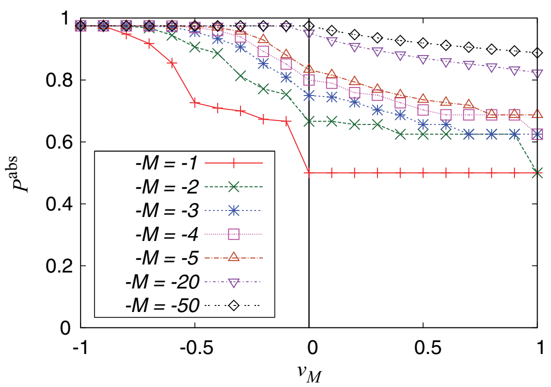


FIG. 6. (Color online) The absorption probability of the right wall versus left wall velocity v_M plots for two-boundaries classical random walks with the left wall having different initial position $-M$ and the right stationary wall placed at position 1. The results are obtained from running the simulation for 1000 time steps.

where W is the walk operator given by $W = T \cdot (H \otimes I)$, $H(v)$ and $\mathrm{sgn}(v)$ are the Heaviside step function and signum function defined in Eqs. (12) and (13), respectively.

To obtain the absorption probability of the right wall $P^{\mathrm{abs}}(t)$ for different velocity v_M and initial position of the left wall $-M$, we run the simulation for 1000 time steps. The simulation results obtained for the classical and quantum case are shown in Figs. 6 and 7, respectively.

For the quantum case, we consider the initial coin state $|R\rangle$. The simulation results obtained for $v_M = 0$, which corresponds to two stationary absorbing boundaries case, are exactly the same as the analytical results given in Ref. [19]. From the simulation results, a comparison is made between the absorption probability for the two walls case and that for the one stationary absorbing wall case. This comparison reveals that the presence of the left wall at position $-M \leqslant -2$, moving with a velocity $-1 < v \leqslant 0$, increases the value of the absorption probability of the right stationary wall beyond the absorption probability value of $2/\pi = 0.6366$ for the one stationary boundary case. This is due to the reason that the presence of the left wall disturbs the interference pattern of the particle's state in such a way that it increases the absorption probability of the right wall. For the case where $v_M = 0$, one can show that, by using the method given in [19], the absorption probability of the right wall follows the conjecture given in [18], where

$$P^{\mathrm{abs}}_{|R\rangle} = \frac{1}{\sqrt{2}} \times \frac{(3+2\sqrt{2})^M - 1}{(3+2\sqrt{2})^M + 1}, \quad \text{for} \quad M \geqslant 0. \tag{22}$$

For the model considered here, the absorption probability is the same for the initial coin state $|R\rangle$ and $|L\rangle$. This fact can be deduced from looking at the evolution of the particle's state. Following the same reasoning given for the one stationary boundary case, we can obtain the absorption probability for an arbitrary initial coin state $|\varphi\rangle$ from the absorption probability for the initial coin state $|R\rangle$ as follows. After the first walk, the initial state $|R,0\rangle$ will evolve to $\frac{1}{\sqrt{2}}(|L,-1\rangle - |R,1\rangle)$. The state $|R,1\rangle$ is then absorbed with probability 1/2 and the state $|L,-1\rangle$ is measured with another half of the probability. For the initial state $|\varphi\rangle \otimes |0\rangle$, after the first walk, the state will evolve to $\frac{1}{\sqrt{2}}(\cos\theta + e^{i\phi}\sin\theta)|L,-1\rangle + (\cos\theta - e^{i\phi}\sin\theta)|R,1\rangle)$. The $|R,1\rangle$ state is then absorbed by the right wall with probability $\frac{1}{2}|(\cos\theta - e^{i\phi}\sin\theta)|^2$. Subsequently, the evolution will begin from the state $|L,-1\rangle$ with probability amplitude $(\cos\theta + e^{i\phi}\sin\theta)$. Thus, for the first measurement, the absorption probability for initial coin state $|\varphi\rangle$ is the same as the absorption probability for coin state $|R\rangle$ multiplied by $|\cos\theta - e^{i\phi}\sin\theta|^2$. After the first measurement, the probability absorbed at each time step for initial coin state $|\varphi\rangle$ is then equal to the probability absorbed for the initial coin state $|R\rangle$ multiplied by $|\cos\theta + e^{i\phi}\sin\theta|^2$. Therefore, the absorption probability for an arbitrary coin state $|\varphi\rangle$ can be written as

$$\begin{aligned} P^{\mathrm{abs}}_{|\varphi\rangle}(t=t') &= |\cos\theta - e^{i\phi}\sin\theta|^2 P^{\mathrm{abs}}_{|R\rangle}(t=1) + |\cos\theta \\ &\quad + e^{i\phi}\sin\theta|^2\left[P^{\mathrm{abs}}_{|R\rangle}(t=t') - P^{\mathrm{abs}}_{|R\rangle}(t=1)\right] \\ &= (|\cos\theta - e^{i\phi}\sin\theta|^2 - |\cos\theta + e^{i\phi}\sin\theta|^2)\tfrac{1}{2} \\ &\quad + |\cos\theta + e^{i\phi}\sin\theta|^2 P^{\mathrm{abs}}_{|R\rangle}(t=t') \\ &= -2\cos\theta\sin\theta\cos\phi + |\cos\theta \\ &\quad + e^{i\phi}\sin\theta|^2 P^{\mathrm{abs}}_{|R\rangle}(t=t'), \end{aligned} \tag{23}$$

where $P^{\mathrm{abs}}_{|\varphi\rangle}(t=t')$ and $P^{\mathrm{abs}}_{|R\rangle}(t=t')$ are the absorption probability of the right wall at time t' for arbitrary initial coin state $|\varphi\rangle$ and $|R\rangle$, respectively. In the third line of Eq. (23), we have used the fact that $P^{\mathrm{abs}}_{|R\rangle}(t=1) = \frac{1}{2}$.

Now, let us compare the results between the quantum and the classical case. As shown in Fig. 7, for quantum walks the absorption probability of the right wall has only a weak dependence on the initial position of the left wall. The reason is that regardless of the initial position of the left wall, only the right-moving wave packet is absorbed by the right wall while the left-moving wave packet always moves away from the right wall. On the other hand, for classical random walks the absorption probability of the right wall depends strongly on the left wall's initial position, as can be seen from Fig. 6. This is because for the classical case the particle moves randomly to the left or to the right, which gives rise to a

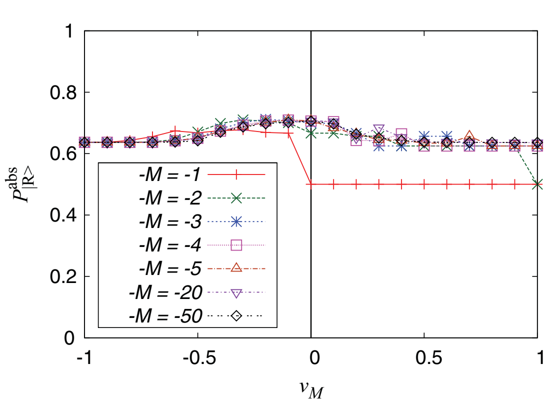


FIG. 7. (Color online) The absorption probability of the right wall versus left wall velocity v_M plots for two-boundaries quantum walks with the left wall having different initial position $-M$ and the right stationary wall placed at position 1. The results are obtained from running the simulation of quantum walks with initial coin state $|R\rangle$ for 1000 time steps.

probability distribution that broadens with time but has a peak remaining stationary at the initial position of the particle. If the left wall's position is closer to the initial position of the particle, the particle has a higher chance to be absorbed by the left wall, hence the absorption probability of the right wall decreases.

VI. CONCLUSION

We have discussed one-dimensional classical and quantum walks in the presence of a moving absorbing wall. These two types of walks differ in the probability distribution, survival probability, and the rate of change of average and standard deviation of the particle's position. For the case of the discrete classical random walk with a moving absorbing boundary initially placed at position $N = 1$, the survival probability vanishes for $v \leqslant 0$ while the survival probability for its quantum counterpart only goes to zero when the wall moves toward the particle with a velocity $v \leqslant -0.7$. Furthermore, as the wall velocity v increases to 1, there is a crossover between the survival probability for the classical and quantum case. The value of the wall velocity v at which this crossover happens is dependent on the initial coin state of the quantum walks. For initial coin state $|R\rangle$, this happens at $v \approx 0.22$ while for initial coin state $|L\rangle$, it happens at $v \approx 0.67$.

Moreover, we have also shown that for $v \leqslant 0$, the survival probability for quantum walks with an arbitrary initial coin state $|\varphi\rangle$ can be related by a simple expression to the survival probability for initial coin state $|R\rangle$. In terms of its asymptotic behavior, the survival probability for the classical case decays as $1/\sqrt{t}$ while that for the quantum case approaches its asymptotic value faster than this rate.

Besides the survival probability, we have also studied the rate of change of the average position for quantum and classical random walks with a moving absorbing boundary. For wall velocity $-1 \leqslant v < 0$, the rate of change of the average position for the classical random walks is equal to the wall velocity v while for $v > 0$, the average position of the particle does not move at all. For quantum walks, the value of $\frac{\langle x\rangle}{t}$ depends on the initial coin state for $v > 0$. The values for the classical and quantum walks are identical for $v < -0.7$. The difference between quantum and classical walks is also reflected in the standard deviation of the position. For quantum walks, the standard deviation is proportional to t, while for classical walk, it is proportional to $\sqrt{t}$.

For the case of quantum walks with one stationary and one moving absorbing boundary, we have shown that the absorption probability for an arbitrary initial coin state $|\varphi\rangle$ is related to that for initial coin state $|R\rangle$ in a simple way. For the trivial case where the velocity of the left wall is zero, we reproduce the analytical result obtained in the literature. Furthermore, it is also observed that the presence of the left wall at position $-M \leqslant -2$ moving with velocity $-1 \leqslant v \leqslant 0$ increases the absorption probability of the right stationary wall, which is placed at position $N = 1$, beyond the absorption probability value for the one stationary boundary case.

To end the discussion, here we suggest a few possible directions for future research. One natural extension of the study of random walks on a line is the study of the walk on a general graph and higher dimension, which may reveal other interesting features of the quantum walk dynamics. Moreover, it is also interesting to extend the study to the case of continuous-time quantum walks. The results obtained from these studies may help us to understand more about the differences between the quantum and classical case.

Classical random walks with moving absorbing boundary are widely used to model a variety of phenomena such as the deposition, coalescence, diffusion capture process, etc. [20]. Therefore, we expect the quantum walks with moving absorbing boundary to play a significant role in simulating various physical phenomena at quantum level. Future study on this subject may reveal more of the power of quantum walks as a modeling tool for physical phenomena.

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[1] R. J. Sension, Nature (London) **446**, 740 (2007).

[2] J. Rudnick and G. Gaspari, Science **237**, 384 (1987).

[3] G. S. Engel *et al.*, Nature (London) **446**, 782 (2007); see also: H. Lee, Y. C. Cheng, and G. R. Fleming, Science **316**, 1462 (2007); T. R. Calhoun *et al.*, J. Phys. Chem. B **113**, 16291 (2009); D. Beljonne, C. Curutchet, G. D. Scholes, and R. J. Silbey, *ibid.* **113**, 6583 (2009); M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik, J. Chem. Phys. **129**, 174106 (2008); M. B. Plenio and S. F. Huelga, New J. Phys. **10**, 113019 (2008).

[4] J. Du, H. Li, X. Xu, M. Shi, J. Wu, X. Zhou, and R. Han, Phys. Rev. A **67**, 042316 (2003).

[5] C. A. Ryan, M. Laforest, J. C. Boileau, and R. Laflamme, Phys. Rev. A **72**, 062317 (2005).

[6] B. Do *et al.*, J. Opt. Soc. Am. B **22**, 499 (2005).

[7] A. Schreiber, K. N. Cassemiro, V. Potoček, A. Gábris, P. J. Mosley, E. Andersson, I. Jex, and Ch. Silberhorn, Phys. Rev. Lett. **104**, 050502 (2010).

[8] M. A. Broome, A. Fedrizzi, B. P. Lanyon, I. Kassal, A. Aspuru-Guzik, and A. G. White, Phys. Rev. Lett. **104**, 153602 (2010).

[9] A. Peruzzo *et al.*, Science **329**, 1500 (2010).

[10] H. B. Perets, Y. Lahini, F. Pozzi, M. Sorel, R. Morandotti, and Y. Silberberg, Phys. Rev. Lett. **100**, 170506 (2008).

[11] H. Schmitz, R. Matjeschk, C. Schneider, J. Glueckert, M. Enderlein, T. Huber, and T. Schaetz, Phys. Rev. Lett. **103**, 090504 (2009).

[12] F. Zähringer, G. Kirchmair, R. Gerritsma, E. Solano, R. Blatt, and C. F. Roos, Phys. Rev. Lett. **104**, 100503 (2010).

[13] M. Karski *et al.*, Science **325**, 174 (2009).
[14] J. Kempe, Contemp. Phys. **44**, 307 (2003).
[15] C. Godreche and J. M. Luck, J. Phys. A: Math Gen. **34**, 7153 (2001).
[16] E. Bach, S. Coppersmith, M. P. Goldschen, R. Joynt, and J. Watrous, J. Comput. Syst. Sci. **69**, 562 (2004).
[17] N. Konno, Quant. Info. Proc. **1**, 345 (2002); Quantum Inf. Comput. **2**, 578 (2002).
[18] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, in *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, (ACM, New York, 2001), pp. 37–49.
[19] N. Konno, T. Namiki, T. Soshi, and A. Sudbury, J. Phys. A: Math. Gen. **36**, 241 (2003).
[20] Sidney Redner, *A Guide to First-Passage Processes* (Cambridge University Press, Cambridge, 2001).