Localization and recurrence of a quantum walk in a periodic potential on a line*

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We present a numerical study of a model of quantum walk in a periodic potential on a line. We take the simple view that different potentials have different affects on the way in which the coin state of the walker is changed. For simplicity and definiteness, we assume that the walker's coin state is unaffected at sites without the potential, and rotated in an unbiased way according to the Hadamard matrix at sites with the potential. This is the simplest and most natural model of a quantum walk in a periodic potential with two coins. Six generic cases of such quantum walks are studied numerically. It is found that, of the six cases, four cases display significant localization effect where the walker is confined in the neighborhood of the origin for a sufficiently long time. Associated with such a localization effect is the recurrence of the probability of the walker returning to the neighborhood of the origin.

Keywords: quantum walk, periodic potential, localization, recurrence

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1. Introduction

Quantum walks are the quantum analogues of the classical random walks (for review, see Refs. [1] and [2]). They were originally proposed with the aim of finding quantum algorithms that are faster than the classical ones for the same problem. There are two distinct types of quantum walks, namely, discrete time quantum walks with a quantum coin on the line[3–7] or on the graphs,[8,9] and continuous time quantum walks.[10,11] Some new quantum algorithms that are based on quantum walks have been proposed. For instance, a quantum search algorithm based on the discrete time quantum walk architecture was shown to gain an algorithmic speedup over the classical algorithms,[12] and a continuous time quantum walk was shown to be able to find its way across a special type of graph exponentially faster than any classical algorithms.[13]

The reason that quantum walks can escalate many classical algorithms lies in the fact that, in general, quantum walks diffuse faster than their classical counterparts. For a process that gives a symmetric distribution of the walker's positions, the tendency of diffusion can be measured by the standard deviation of the position $\sigma(t)$ as a function of the time (step) t. For the classical random walk , one has $\sigma(t) \propto \sqrt{t}$, while for an unbiased quantum walk on a line with a Hadamard coin (so-called Hadamard walk), one has $\sigma(t) \propto t$. Analytical results for quantum walk limit distributions have since been established.[14–16]

On the other hand, in Ref. [17], it was shown that a quantum random walk in a one-dimensional chain using several types of biased quantum coins, arranged in aperiodic sequences following the Fibonacci prescription, can lead to subballistic wave-function spreading. In Ref. [18], a model with multiple internal coin states was shown to exhibit localization of the walker at the origin. In Refs. [19] and [20], it was shown that, for a class of inhomogeneous quantum walks with multiple coins periodically arranged in position, which is a generalization of the model introduced in Ref. [21], there could be localization at the origin with certain choices of the parameters defining the model. Furthermore, they have shown through numerical studies that the eigenvalue spectrum of such inhomogeneous walks could exhibit a fractal structure similar to that of the Hofstadter butterfly. Konno has presented and proved a theorem on the return probability for a type of space-inhomogeneous walks.[22] Localization was also observed in a quantum walk with two coins operating at different time.[23] Later, it was found that changing a phase (i.e., imposing discontinuity) at a point in a discrete quantum walk results in certain localization effect.[24] In Ref. [25], the differences in limit distributions between the classical random walks and a few models of quantum walks were presented. For a recent review on these issues, see for example, Ref. [26].

The above studies indicate that suitable modifications of the position and/or coin space could lead to a rich variety of possible wave function evolutions of the quantum walker.

In this work, we would like to study if the localization of a quantum walker could occur in a periodic potential; that is, if the coins are arranged periodically in space. It turns out that

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this is possible in the model that we present here.

To the best of our knowledge, a model of quantum walk in a periodic potential on a line was first considered in Ref. [27]. There it was assumed that at sites without potential the walker walks as the normal (coined) Hadamard walk, while when there is a potential the walker walks according to the scattering quantum walks introduced in Ref. [28]. A localization phenomenon was not reported in that work.

It has been shown recently that the scattering walk is equivalent to the coined walk.[29] Thus, it is not necessary to invoke two different approaches to describe the quantum walk in a periodic potential. Here, we shall adopt the discrete coined quantum walks at positions throughout the line. We take the natural assumption that the presence of the potential only affects the way in which the coin is flipped. Hence, we assume that there are two different coins: one for positions without potential, and the other for positions with a potential. We find that for certain potentials and initial states, localization and recurrence of the walkers around the origin are possible.

The rest of this paper is arranged as follows. In Section 2, we define the model of quantum walk in a periodic potential on a line. Six generic cases of such quantum walks are then discussed with numerical results in Section 3. Section 4 provides the conclusion for this paper.

2. The model

The discrete-time or coined quantum walk on a line is defined as follows.[1,3,8] The total Hilbert space is given by $\mathcal{H} \equiv \mathcal{H}_{\rm P} \otimes \mathcal{H}_{\rm C}$, where $\mathcal{H}_{\rm P}$ is spanned by the orthonormal vectors $\{|x\rangle, x = 0, \pm 1, \pm 2, \ldots\}$ representing the positions of the walker, and $\mathcal{H}_{\rm C}$ is a two-dimensional coin space spanned by two orthonormal vectors $|0\rangle$ and $|1\rangle$. The dynamics of the walk are controlled by a coin flip operator C, which modifies the coin state of the walker, and a conditional shift operator S that shifts the walker's position according to the latest state of the coin. Thus, the evaluation operator for one step of walk is $U = S \cdot (C \otimes I)$. If the initial state of the walker and the coin is $|\psi_0\rangle$, then after t steps, the state of the system is $|\psi(t)\rangle = U^t |\psi_0\rangle$. In the original discrete quantum walk proposed in Refs. [3] and [4], the coin operator C is taken to be the Hadamard matrix

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \tag{1}$$

and the position displacement operator is given by

$$\begin{aligned} S = & |0\rangle\langle 0| \otimes \sum_x |x+1\rangle\langle x| \\ & + |1\rangle\langle 1| \otimes \sum_x |x-1\rangle\langle x|. \end{aligned} \tag{2}$$

It is known that the initial state of the walker and the coin given by

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + \mathrm{i}|1\rangle) |0\rangle \tag{3}$$

gives rise to an outgoing symmetric probability distribution of the position when a single Hadamard coin is used. On the other hand, the state

$$|\psi_0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle) |0\rangle \tag{4}$$

leads to an asymmetric distribution.

To define a model of quantum walk in a periodic potential on a line, we take the simple view that different potentials affect the change of the coin state of the walker differently. Thus, we suppose that the coin state is changed by a coin operator C_0 when there is no potential, and by $C_{\rm p}$ when the field is present. The position displacement operator at each position is

$$S_x = |0\rangle\langle 0| \otimes |x+1\rangle\langle x| + |1\rangle\langle 1| \otimes |x-1\rangle\langle x|. \tag{5}$$

Together the evolution operator is

$$\begin{aligned} U = & \sum_{x \text{ without potential}} S_x (C_0 \otimes I) \\ & + \sum_{x \text{ at potential}} S_x \left(C_{\rm p} \otimes I\right). \end{aligned} \tag{6}$$

The most general two-dimensional unitary coin operator is given by

$$C = \begin{pmatrix} \sqrt{\rho} & \sqrt{1-\rho}\, \mathrm{e}^{\mathrm{i}\theta} \\ \sqrt{1-\rho}\, \mathrm{e}^{\mathrm{i}\phi} & -\sqrt{\rho}\, \mathrm{e}^{\mathrm{i}(\theta+\phi)} \end{pmatrix}, \tag{7}$$

where $0 \le \theta, \phi \le \pi$ are arbitrary angles, and $0 \le \rho \le 1$. By choosing the parameters ρ, θ, and ϕ, one can assign different coin operators C_0 and $C_{\rm p}$ to design a quantum walk model in a periodic potential on a line.

The state of the walker after t steps is

$$|\psi(t)\rangle = U^t |\psi_0\rangle = \sum_{x=-\infty}^{\infty} \left[A_x(t)|0\rangle + B_x(t)|1\rangle\right] |x\rangle, \tag{8}$$

where $|\psi_0\rangle$ is the initial state, and

$$\sum_x |A_x(t)|^2 + |B_x(t)|^2 = 1. \tag{9}$$

At time t, the probability that the walker is to be found at position $|x\rangle$ is

$$p(x,t) = |A_x(t)|^2 + |B_x(t)|^2. \tag{10}$$

3. Numerical results

In this work, for simplicity and definiteness, we choose $C_0 = I$ and $C_{\rm p} = H$. These two choices correspond, respectively, to $\{\rho = 1, \theta + \phi = \pi\}$ and $\{\rho = 1/2, \theta = \phi = 0\}$ in Eq. (7). This means that the walker's coin state is unaffected at sites without the potential, and rotated in an unbiased way

according to the Hadamard matrix at sites with the potential. This is the simplest and most natural model of a quantum walk in a periodic potential with two coins.

We are interested in symmetric walks such that $\langle x(t)\rangle = 0$. So the main physical quantity to characterize the quantum walk is the standard deviation $\sigma(t) = \sqrt{\langle x(t)^2\rangle}$. Since we have in mind the possibility of localization of the walker at the origin, we shall also consider the probability $P_0(t)$ of the walker at the origin $x = 0$ as a function of the step t.

Below we shall consider six generic cases of quantum walk in a periodic potential on a line with a period N. For simplicity, we shall adopt the notation $[C_1 : q,\ C_2 : (N-q)]$ to denote the situation in which the coin operator C_1 is to be used in the first q positions and the coin operator C_2 is used in the remaining $N-q$ positions. The origin $x = 0$ is always assumed to be at the middle point of the first q positions (in this work q is always taken to be odd). The six cases are

case IA : $[H:1,\ I:N-1]$,	(use coin H at $x \equiv 0 \pmod N$ and I elsewhere),	$N = 2,3,4,\ldots$;
case IB : $[I:1,\ H:N-1]$,	(use coin I at $x \equiv 0 \pmod N$ and H elsewhere),	$N = 2,3,4,\ldots$;
case IIA : $[H:N-1,\ I:1]$,	(use coin I at $x \equiv N/2 \pmod N$ and H elsewhere),	$N = 2,4,6,\ldots$;
case IIB : $[I:N-1,\ H:1]$,	(use coin H at $x \equiv N/2 \pmod N$ and I elsewhere),	$N = 2,4,6,\ldots$;
case IIIA : $[H:q,\ I:q]$,	(use coin H at $x < (q+1)/2 \pmod{2q}$ and I elsewhere),	$q = 3,5,7,\ldots$;
case IIIB : $[I:q,\ H:q]$,	(use coin I at $x < (q+1)/2 \pmod{2q}$ and H elsewhere),	$q = 3,5,7,\ldots$.

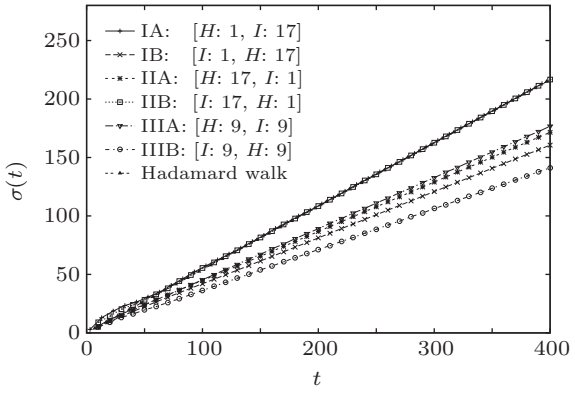


Fig. 1. The standard deviation $\sigma(t)$ versus the number of steps t. Note that $\sigma(t)$ for quantum walks of cases IA and IIB overlap with that for the Hadamard walk at large t. For the other cases, the slopes of $\sigma(t)$ are smaller. This means that the diffusions in cases other than IA and IIB are slower, with case IIIB being the slowest.

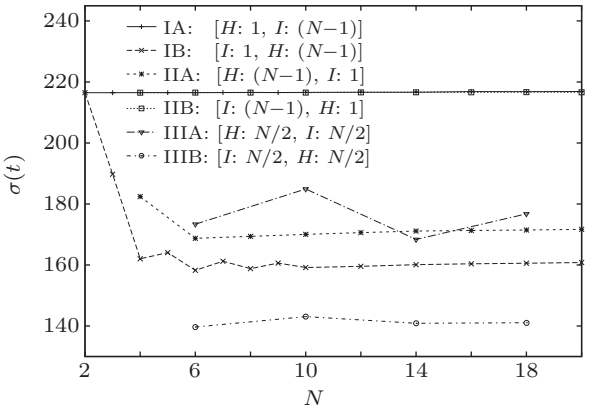


Fig. 2. The standard deviation $\sigma(t)$ at a fixed step $t = 400$ for different periods N. For cases IB and IIA, there exists a critical value of the period N at which the value of $\sigma(t)$ drops by a significant amount.

In Fig. 1, we show the standard deviation $\sigma(t)$ versus the number of steps t. It is seen that, as in the standard unbiased Hadamard quantum walk, $\sigma(t)$ is generally asymptotically linear in t; that is, $\sigma(t) \propto t$. It is also noted that $\sigma(t)$ for cases IA and IIB overlap with that of the standard Hadamard walk at large t. The other cases have smaller slopes, with that for case IIIB being the smallest. This means that the diffusion in cases other than IA and IIB is slower than that of the standard Hadamard walk.

That such is the case can be further seen from the values of $\sigma(t)$ at a fixed step (say, $t = 400$) for different periods N, as depicted in Fig. 2. Furthermore, for cases IB and IIA, there exists a critical value of the period N at which $\sigma(t)$ drops by a significant amount. To further understand the decrease in $\sigma(t)$, we consider each case in detail below.

3.1. Cases IA and IB

In these cases, either the identity coin or the Hadamard coin is used at position $|x\rangle$ such that $x \equiv 0 \pmod N$.

For case IA, the walker encounters the potential field only at positions $|x\rangle$ where x is a multiple of the period N. It is found that two peaks symmetric with respect to the origin just move away from the origin, as in the case of the Hadamard walk. Figure 3 shows the probability $P(x,t)$ at $t = 400$. In Fig. 4, we

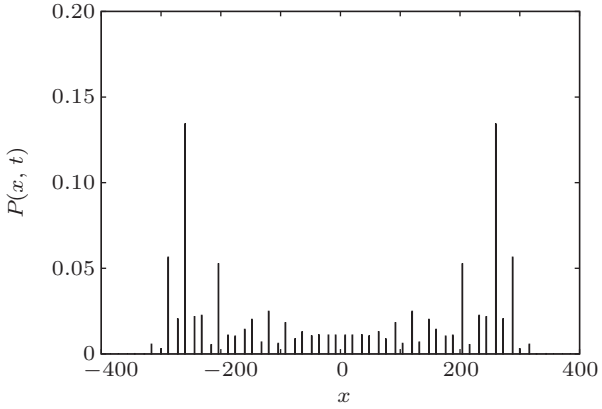


Fig. 3. Probability $P(x,t)$ of the quantum walk of case IA ($[H:1,\ I:13]$) with period $N = 14$ at $t = 400$. Note that the probabilities at positions with odd x are zero. There is no localization.

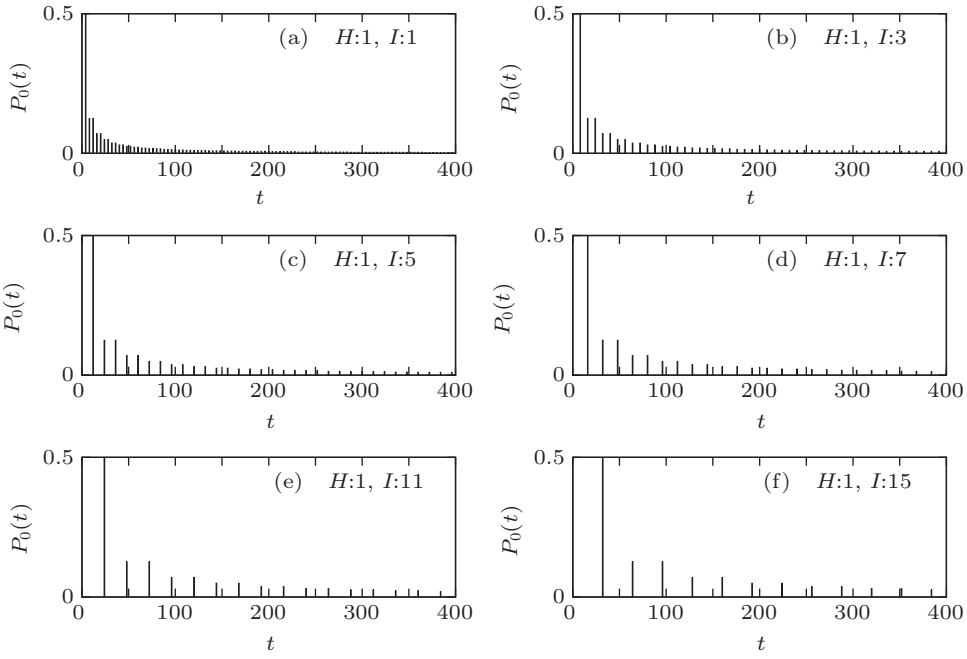


Fig. 4. Probability $P_0(t)$ at the origin of the quantum walk of case IA. The number of steps is taken up to 400. Note that the probability at the origin must be zero when the step t is odd. This is the same for all the other cases considered in this work. There is no localization as $P_0(t)$ dies away at large steps.

show the probability $P_0(t)$ of the walker appearing at the origin $x = 0$. It is seen that the probability just dies out gradually.

Case IB is the dual of the previous case: positions with and without the potential are exchanged. For $N \leq 3$, the system diffuses in a similar pattern as the ordinary quantum walk with a single Hadamard coin: two symmetric peaks moving away from the origin. For $N > 3$, there appears a high probability with which the walker is in the neighborhood of the origin $x = 0$: a localization of the walker is possible. Figure 5 shows the situations for four different periods N. Figure 6 shows the probability $P_0(t)$ with which the walker returns to the origin. For $N = 2$, the probability is small as t increases. While for $N = 4$, we see slight recurrent increase in $P_0(t)$ as a function of t: the recurrence of the walker at the origin appears. The tendency becomes stronger as N increases.

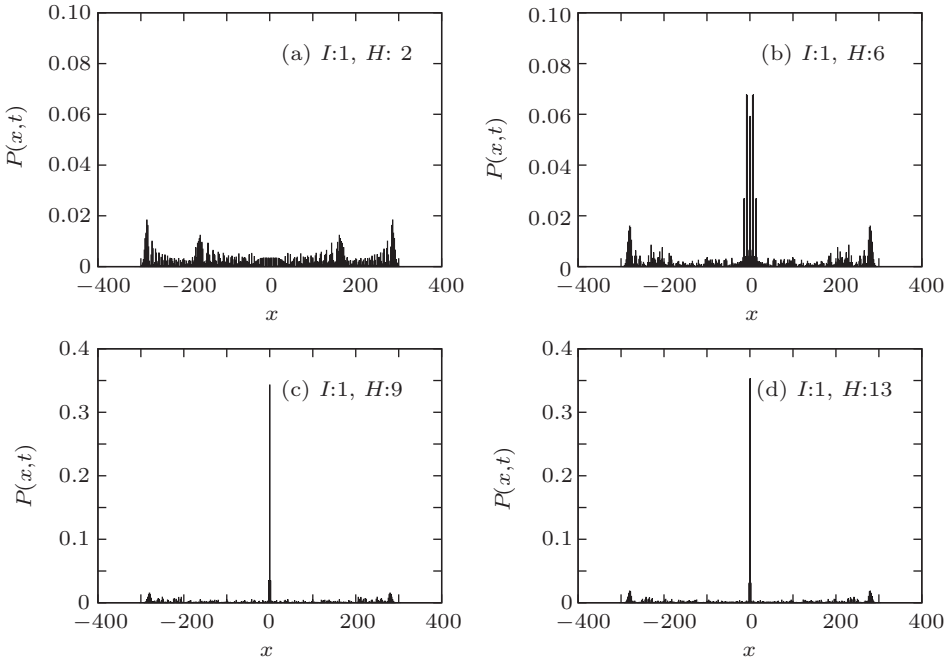


Fig. 5. (color online) Probability $P(x,t)$ of the quantum walk of case IB ($[I : 1,\ H : N-1]$) with period $N = 3, 7, 10, 14$ at $t = 400$. Localization at the origin occurs for $N > 3$.

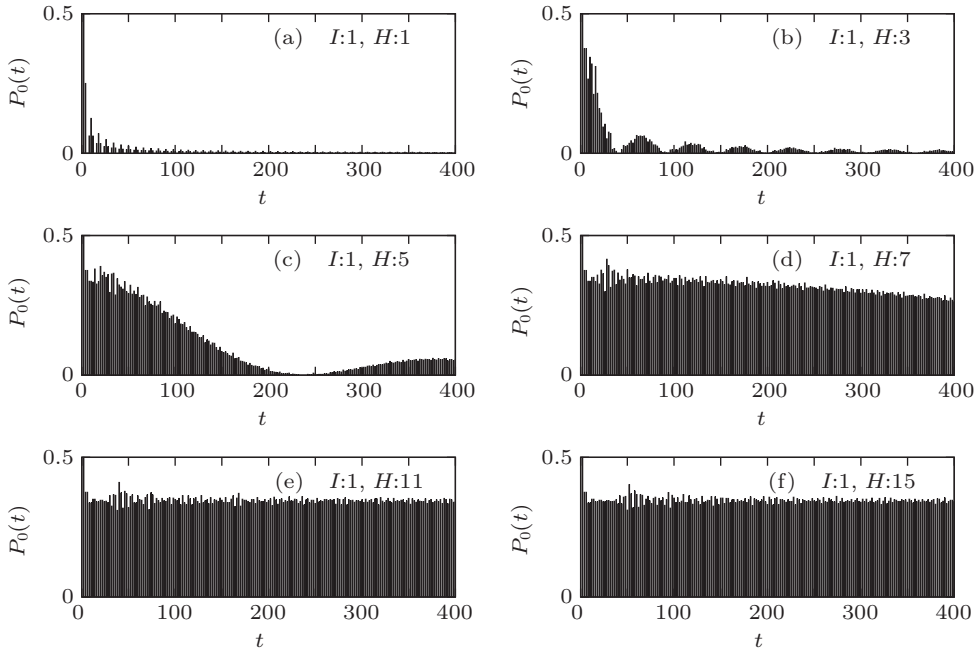


Fig. 6. Probability $P_0(t)$ at the origin of the quantum walk of case IB. The number of steps is taken up to 400. Recurrence of probability at the origin occurs for $N > 3$. The number of steps for recurrence becomes larger as N increases, indicating a stronger localization effect.

3.2. Cases IIA and IIB

In cases IA and IB, the origin is the only point at which the force field is different from the other $(N-1)$ points in a single period N. The cases considered here represent shifted situations: the origin is at the center of the $(N-1)$ points with the same force field. This requires N to be even.

In case IIA, the walker begins its walk at the middle of the potential, and encounters no field at positions x where $x \equiv N/2 \pmod{N}$. For $N \leq 5$, the probability distribution is symmetric with two major peaks moving away from the origin. As N increases, the rate of diffusion becomes smaller. When $N > 5$, a localization near the origin appears. Figure 7 shows the situation for $N = 14$. Recurrence with a high probability at the origin also appears, as depicted in Fig. 8.

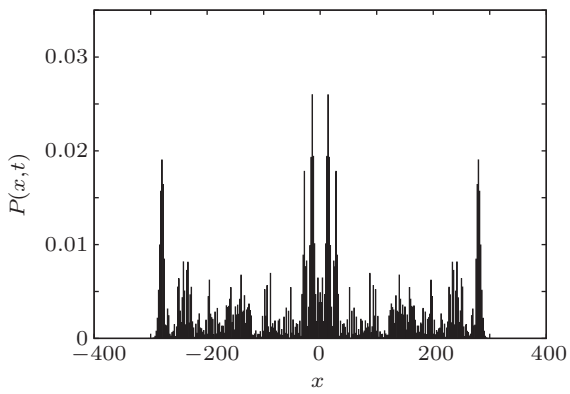


Fig. 7. Probability $P(x,t)$ of the quantum walk of case IIA ($[H: 13, I: 1]$) with period $N = 14$ at $t = 400$. Localization at the origin occurs for $N > 5$.

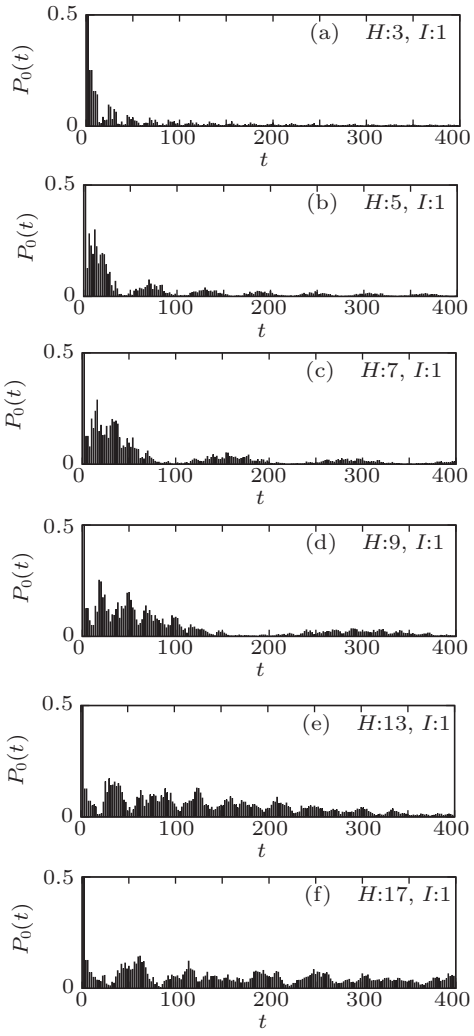


Fig. 8. Probability $P_0(t)$ at the origin of the quantum walk of case IIA. The number of steps is taken up to 400. Significant recurrence occurs for $N > 5$.

Case IIB is the dual of case IIA: the walker begins its walk at the middle of no potential region, and encounters the field at positions x where $x \equiv N/2 \pmod N$. From Figs. 9 and 10, it is seen that there is no localization and recurrence.

3.3. Cases IIIA and IIIB

These cases correspond to periodic potentials (period $N = 2q$) where locations with and without the potential have equal length q. In case IIIA, the walker begins its walk at the middle of the potential, while in case IIIB, the walker begins its walk at the middle of the zero potential region.

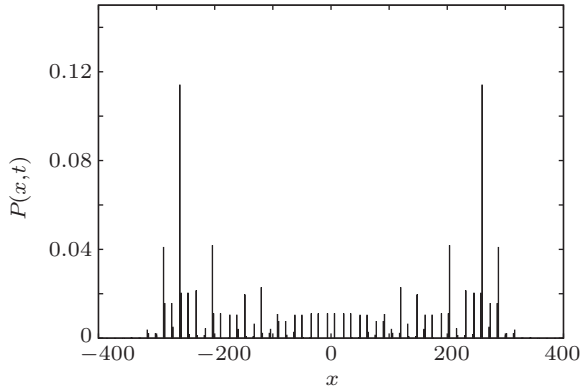


Fig. 9. Probability $P(x,t)$ of the quantum walk of case IIB ([I : 13, H : 1]) with period $N = 14$ at $t = 400$. There is no localization.

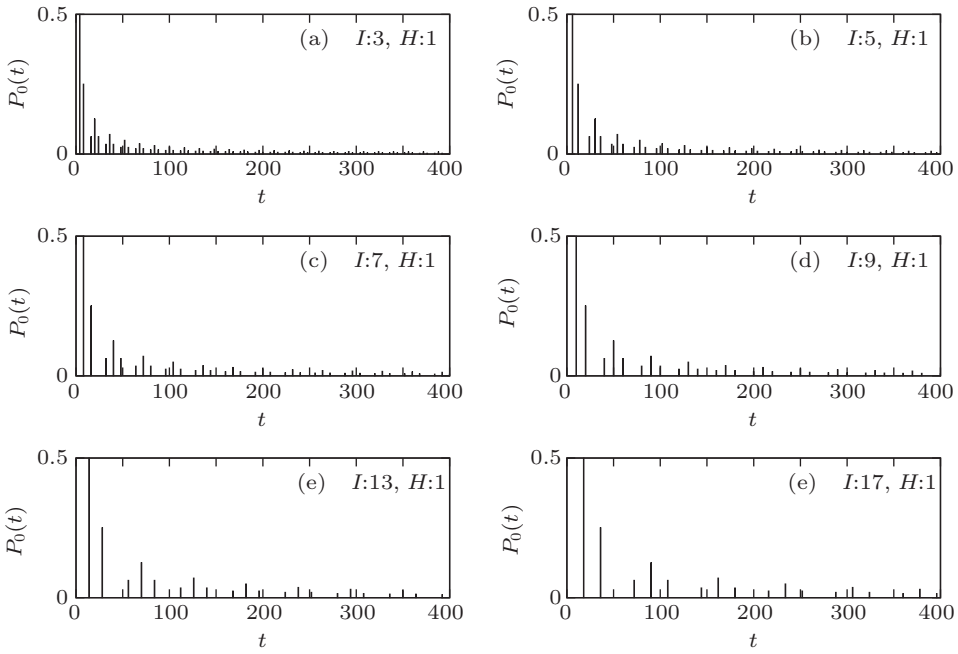


Fig. 10. Probability $P_0(t)$ at the origin of the quantum walk of case IIB. The number of steps is taken up to 400. There is no recurrence.

For case IIIA, the localization effect is not as strong as that in the previous cases. The localization occurs only for $q > 13$. Figures 11 and 12 show some representative situations.

Localization and recurrence occur more significantly for case IIIB. In fact, the localization occurs already for $q > 3$. Figures 13 and 14 show the results very clearly. In fact, of the six cases considered in this work, case IIIB shows the strongest localization and recurrence. Thus, the tendency of diffusion is much slower in this case than that in other cases. This is also reflected in the fact, as depicted in Fig. 1, that the standard deviation $\sigma(t)$ of this case has the smallest slope than that of the other cases.

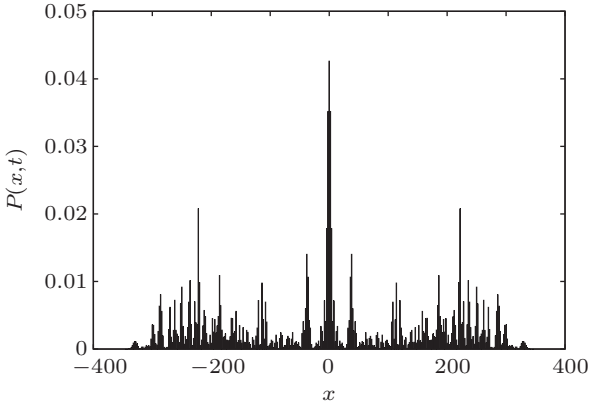


Fig. 11. Probability $P(x,t)$ of the quantum walk of case IIIA ([H : 19, I : 19]) with period $N = 14$ at $t = 400$. Localization at the origin occurs for $q = N/2 > 13$.

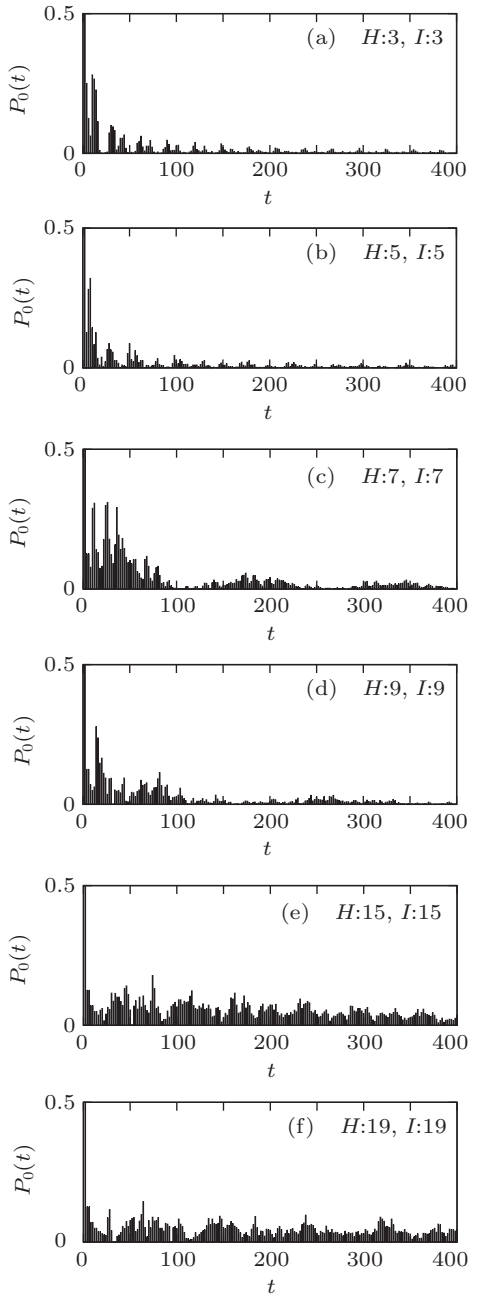


Fig. 12. Probability $P_0(t)$ at the origin of the quantum walk of case IIIA. The number of steps is taken up to 400. Significant recurrence occurs for $q > 13$.

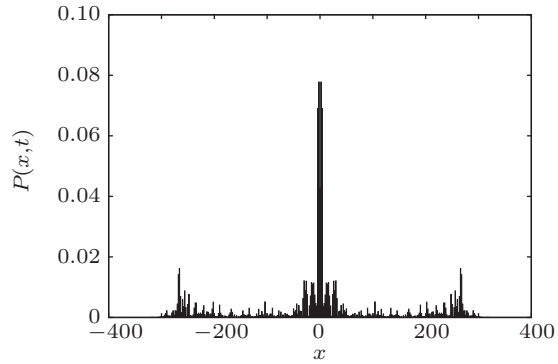


Fig. 13. Probability $P(x,t)$ of the quantum walk of case IIIB ($[I:7,\ H:7]$) with period $N = 14$ at $t = 400$. Localization at the origin occurs for $q = N/2 > 3$.

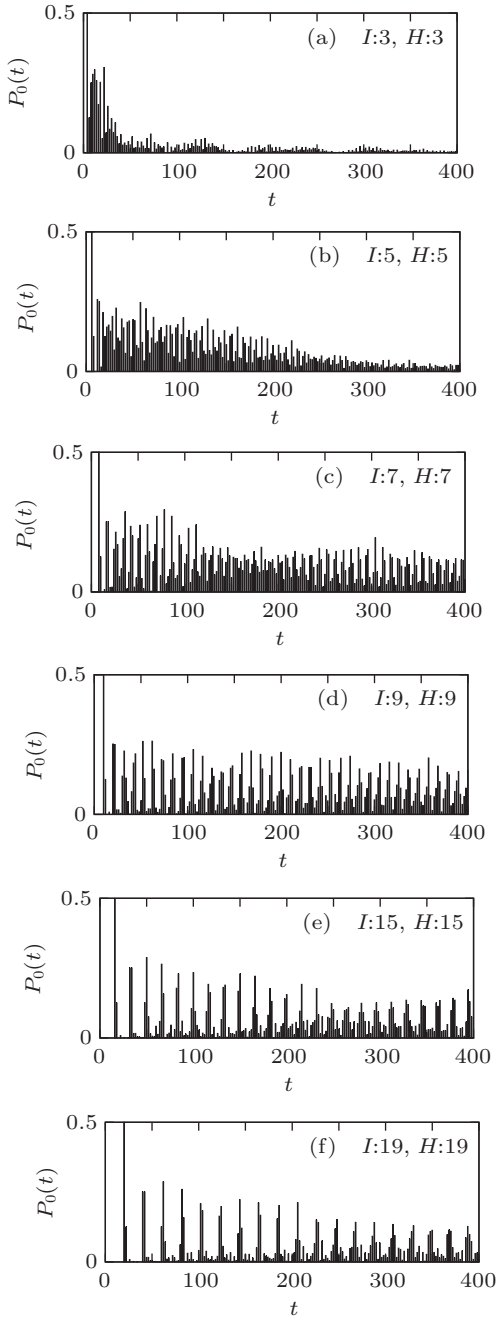


Fig. 14. Probability $P_0(t)$ at the origin of the quantum walk of case IIIB. The number of steps is taken up to 400. Significant recurrence occurs for $q > 3$.

4. Discussion and conclusion

We have presented the model of a quantum walk in a periodic potential on a line by taking the simple view that different potentials affect differently the change of the coin state of the walker. For simplicity and definiteness, we assumed that the walker's coin state is unaffected at sites without the potential, and rotated in an unbiased way according to the Hadamard matrix at sites with the potential. This is the simplest and most natural model of a quantum walk in a periodic potential with two coins.

Six generic cases of such quantum walks were studied numerically. It was found that of the six cases, two cases, cases

IA and IIB, behave similarly as the original Hadamard walk where only a Hadamard coin is used throughout the walk on the line. They show the same standard deviation at large step numbers. On the other hand, in the other four cases, a localization effect is possible, where the walker could be confined in the neighborhood of the origin for sufficiently long time. Associated with such a localization effect is the recurrence of the probability of the walker returning to the neighborhood of the origin.

A notable difference between cases IA and IIB, and the other four cases is the number of the positions with the potential, or the points where the Hadamard coin is used within a single period of the potential: it is smaller than the number of points without the potential (or points using the identity coin). In the other four cases, localization and recurrence only occur when the number of points with the Hadamard coin is sufficiently larger than that using the identity coin. This implies the existence of critical values of period N for these cases.

Furthermore, it was also observed that localization and recurrence are more stronger in cases IIIB and IB, as shown in Figs. 1 and 2. In these two cases, the walker starts at the center of the valley (with the identity coin) of the potential.

To summarize, in the model of quantum walk in a periodic potential proposed in this work, localization and recurrence are stronger if the walker begins its walk in the middle of the valley (with the identity coin) of the periodic potential with a larger portion of potential (with the Hadamard coin).

As a first attempt to study localization and recurrence phenomena of quantum walks in periodic potentials, we have so far relied on a numerical method. We hope to study this problem with an analytic approach in the near future. It is also interesting to study the behaviors of the quantum walk with other choices of coin operators C_0 and C_p. The generalization of the present work to higher-dimensional cases is straightforward. It would be nice if the quantum walks on a periodic potential considered here could be experimentally implemented, for example, in an optical lattice.

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