Switching effect of the side chain on quantum walks on triple graphs

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We consider a continuous-time quantum walk on a triple graph and investigate the influence of the side chain on propagation in the main chain. Calculating the interchange of the probabilities between the two parts of the main chain, we find that a switching effect appears if there is an odd number of points in the side chain when concrete conditions between the length of the main chain and the position of the side chain are satisfied. However, such an effect does not occur if there is an even number of points in the side chain. We also suggest two proposals for experiments to demonstrate this effect, which may be employed to design a new type of switching device.

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I. INTRODUCTION

Although the quantum walk was proposed as the quantum mechanical counterpart of the classical random walk [1], it exhibits exotic features and has extensive potential applications in many fields compared with the classical random walk. For example, the quantum walk not only can provide us a simple model for study of coherent quantum control over atoms or photons in physical systems but also offer us an advanced tool for new quantum algorithms [2–4]. So study of the quantum walk has received increasing attention in recent years. In the context of quantum information, continuous-time and discrete-time quantum walks were sequentially proposed [1,5] with the goal of applying them to quantum algorithms. For discrete-time quantum walks, one needs a quantum coin to generate a superposition state for each step, whereas for continuous-time quantum walks, the quantum coin is not needed and the quantum-walk process is realized through continuous tunneling between neighbor sites, which implies that the continuous-time quantum walk can be implemented at some possible lattice sites.

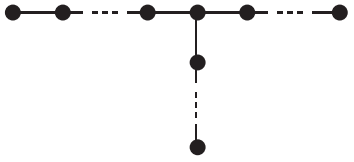
The propagation features of the quantum walk are obviously affected by the graph where the quantum walk is implemented. So far, quantum walks on different graphs, such as hypercube [6–10], cycle [11–13], hypercycle [14], and percolation [15–17] graphs, have been widely investigated. For example, the mixing time and hitting time of quantum walks were studied in Refs. [6–10] where the hitting time of quantum walks in opposite corners in the hypercube graph was shown to be exponentially faster than that of classical random walks. The upper bound of the mixing time of quantum walks on a cycle graph was also estimated in Ref. [12]. Additionally, in some studies [18–21], the quantum walk was used to distinguish the isomorphism of the graph.

Since quantum walks on different graphs can exhibit different characters, studying this not only can simulate some phenomena in conventional systems but also can help us to find more potential applications of the quantum walk. Therefore we consider a continuous-time quantum walk on a triple graph in this paper. We show how the length and the position of the side chain and the length of the main chain influence the propagation properties. Especially, we find that the quantum-walk system can exhibit obviously different propagation properties when the parity of the number of points in the side chain is changed. This parity effect on quantum walks is expected to be used for switching devices. A similar effect was noted in mesoscopic metal rings [22], where there is a circulating current when a magnetic flux crosses the mesoscopic metal ring. Such a circulating current can be influenced by the parity of the number of electrons, which implies that the parity effect can be exhibited in mesoscopic metal microstructures. In a word, comparing quantum walks in one-dimensional lattices, the existence of a side chain can obviously change the propagation properties of quantum walks, therefore it is worthwhile for us to study quantum walks on triple graphs.

This paper is organized as follows. In the next section, we present the model of the system. In Sec. III A, with the help of the Green function we investigate the quantum walk on a triple graph with a side chain of one point and find that the system can exhibit the switching effect via changing the length of the main chain or the position of the side chain when the tunneling strength in the side chain is much greater than that in the main chain. In Secs. III B and III C, we investigate the case of side chains with two points and more points, respectively. We find that when the number of points in the side chain is even, the system cannot exhibit the switching effect no matter what the length of the main chain is, which is in contrast to the case of a side chain with an odd number of points. In the last section (IV), we propose two possible experimental schemes in which to observe or apply the dynamical properties exhibited in the system we consider and give a brief summary.

II. MODELING QUANTUM RANDOM WALKS IN A TRIPLE GRAPH

We consider quantum random walks of a single particle on the following triple-type graph:



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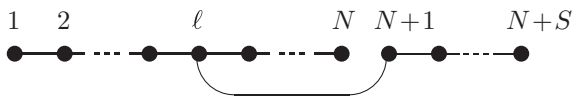
The graph contains a main chain of N points and a side chain of S points where the side chain is connected to a certain point on the main chain. It becomes more convenient for us to label the points in the main chain $1, 2, \ldots, N$, and the points in the side chain $N+1, N+2, \ldots, N+S$. Then the graph can be equivalently plotted as



This is a one-dimensional chain of $N+S$ points with the connection broken between point N and point $N+1$ but with an additional "long-distance" connection between point ℓ and point $N+1$. This implies that ℓ is a special point that divides the main chain into two parts. Then we can model the quantum random walk on the triple-type graph by the Hamiltonian

$$H = \left(-\sum_{j=1}^{N-1} |\, j\rangle\langle j+1\,| - J \sum_{j=N+1}^{N+S-1} |\, j\rangle\langle j+1\,| - J\,|\,\ell\rangle\langle N+1\,| \right) + \text{H.c.}, \tag{1}$$

where $|j\rangle$ denotes the state where a particle occupies the jth site on a one-dimensional lattice and J is the hopping strength in the side chain and that between the side chain and the ℓth point in the main chain. The hopping strength in the main chain is set to unity for simplicity.

We know that the properties of continuous-time quantum walks sensitively depend on the type of graphs on which the quantum walk is implemented. Although the quantum walk in one dimension has been well studied, the addition of a side chain can obviously change the propagation character of quantum walks. Thus our main purpose is to determine how the side chain influences state evolution in the main chain by calculating the interchange of the probabilities between the two parts of the main chain. And we further expect to use the side chain to manipulate the evolution of the probability in the main chain, which may be enlightening for switching devices.

III. GREEN FUNCTION AND DYNAMICAL PROPAGATION FEATURES

Let us start from the main-chain-relevant part of the total Hamiltonian, (1),

$$H_M = -\sum_{j=1}^{N-1} |j\rangle\langle j+1| + \text{H.c.}$$

We know that its eigenvalues and the eigenstates are given by

$$E_m = -2\cos\left(m\frac{\pi}{N+1}\right), \qquad |\psi_m\rangle = \sum_{j=1}^{N}\sqrt{\frac{2}{N+1}}\sin\left(jm\frac{\pi}{N+1}\right)|j\rangle. \tag{2}$$

Here, $m = 1,2,\ldots,N$, and $j = 1,2,\ldots,N$. Then we can obtain the Green function of the main-chain Hamiltonian H_M:

$$g_0(z) = \sum_{m=1}^{N} \frac{|\psi_m\rangle\langle\psi_m|}{z + 2\cos\left(\frac{m\pi}{N+1}\right)}. \tag{3}$$

Note that when the side chain is included, the Green function of our model, (1), can also be obtained. Then with the help of the Green function and numerical calculation, we mainly aim to find out how the side chain influences state evolution in the main chain by calculating the interchange of the probabilities between the two parts of the main chain. Here the points to the left of the connection point ℓ (i.e., points j with $1 \leqslant j < \ell$) constitute the left part, and the other points in the main chain (i.e., points j with $\ell < j \leqslant N$) make up the right part. Taking the two cases of $S = 1$ and $S = 2$ as examples (i.e., there are one or two sites on the side chain, respectively), we find that the propagation features for $S = 1$ and $S = 2$ are completely different even if the other parameters and initial states are the same. Additionally, we also show the influence of the position of the connection point ℓ and the number of points in the main chain on the propagation properties of the system.

A. Side chain with one point

Now we are in a position to consider the case of a side chain with one point (i.e., $S = 1$). In this case, the Green function can be written as

$$G_1 = \frac{|N+1\rangle\langle N+1|}{z} + g_0 + \frac{g_0|\ell\rangle\langle\ell|g_0}{z/J^2 - \langle\ell|g_0|\ell\rangle} + \frac{\langle\ell|g_0|\ell\rangle}{z} \times \frac{|N+1\rangle\langle N+1|}{z/J^2 - \langle\ell|g_0|\ell\rangle} - \frac{1}{J} \times \frac{g_0|\ell\rangle\langle N+1| + |N+1\rangle\langle\ell|g_0}{z/J^2 - \langle\ell|g_0|\ell\rangle}. \tag{4}$$

From the above Green function, one can easily obtain the eigenvalues of Hamiltonian (1) for $S = 1$. We find that the existence of a side chain with one point divides the eigenvalues of the main-chain Hamiltonian H_M into two kinds. Eigenvalues of H_M remain when the corresponding eigenstates satisfy $\langle\ell|\psi_m\rangle = 0$ [i.e., these eigenvalues are also eigenvalues of Hamiltonian (1) for $S = 1$], while the others are shifted and no longer the eigenvalues of Hamiltonian (1) for $S = 1$ due to the existence of the side chain. Except for the remaining eigenvalues of H_M, the other eigenvalues of Hamiltonian (1) for $S = 1$ can be obtained via the roots of the equation $z/J^2 - \langle\ell|g_0|\ell\rangle = 0$.

Let us look at the case of $J \gg 1$, where the above equation can be solved analytically, and the corresponding roots read

$$z = \begin{cases} z_0 + \triangle(z_0), \\ \pm J, \end{cases} \qquad \triangle(z_0) = -\frac{z_0}{J^2\langle\ell|g_0(z_0)^2|\ell\rangle}, \tag{5}$$

where z_0 is determined by $\langle\ell|g_0(z_0)|\ell\rangle = 0$. Substituting Eq. (3) into Eq. (5), we can obtain the value of z_0. Then the

changed energy levels can be written as

$$E_n = -2\cos\left(\frac{n\pi}{\ell}\right), \tag{6}$$

$$E_{n'} = -2\cos\left(\frac{n'\pi}{N+1-\ell}\right), \tag{7}$$

with $n = 1,2,\ldots,\ell-1$ and $n' = 1,2,\ldots,N-\ell$. Here the perturbation term $\Delta(z_0) \sim \frac{1}{J^2}$ is neglected due to the fact that $J \gg 1$. From the above expressions of $E_{n(n')}$, we can find that if $(N+1)$ and ℓ have a greatest common divisor larger than 2, some energy levels of E_n can be degenerate with that of $E_{n'}$, respectively, and the corresponding values of these degeneracy energy levels are just equal to those remaining eigenvalues of H_M. However, if $(N+1)$ and ℓ do not have a greatest common divisor larger than 2, once the side chain with one point is included, none of the eigenvalues of H_M remain and the energy levels of E_n and $E_{n'}$ are not degenerate. The above expression implies that the relation between the position of the connection point and the number of points in the main chain can obviously affect the distribution of the energy levels of the system. So the propagation properties on the triple graph we considered can exhibit essentially different features for different numbers of points in the main chain and positions of the connection point.

In order to investigate the propagation features of a particle on the triple graph, let us observe the time evolution of the probability amplitude. Assuming that the particle is at the j_2th site of the main chain, one can write the probability amplitude $A(j_1,j_2)$ for the particle being at the j_1th site at time t as

$$A(j_1,j_2) = \sum_E \mathrm{Res} G_1(E,j_1,j_2)\exp(-iEt), \tag{8}$$

where $G_1(E,j_1,j_2) = \langle j_1|G_1(E)|j_2\rangle$, with E including all the eigenvalues of Hamiltonian (1) for $S = 1$, and Res stands for the residue of a function. If $j_1 > \ell$ and $j_2 < \ell$, the probability amplitude can be given as

$$p(j_1,j_2) = O\left(\frac{1}{J^2}\right) + \sum_{E\in E_r}\frac{2}{N+1}\sin[j_1\theta(E)] \times \sin[j_2\theta(E)]e^{(-iEt)}[e^{(-i\Delta(E)t)} - 1], \tag{9}$$

where E_r refer to the remaining eigenvalues of H_M [i.e., E_r are the energies given in Eq. (2) whose corresponding eigenstates $|\psi_m\rangle$ satisfy $\langle\ell|\psi_m\rangle = 0$], $\theta(E) = \arccos(-\frac{E}{2})$, and the expression of $\Delta(E)$ is given in Eq. (5). From expression (9), we find that for $J \gg 1$, the value of $p(j_1,j_2)$ is not 0 only when nonzero eigenvalues of H_M remain, i.e., $(N+1)$ and ℓ have a greatest common divisor larger than 2. So the particle can cross the connection point from one part into the other part of the main chain for $(N+1)$ and ℓ having a greatest common divisor larger than 2, while the particle is always in the initial part of the main chain for $(N+1)$ and ℓ not having a greatest common divisor larger than 2, which is confirmed in Fig. 1. Additionally, we can also obtain the probability amplitude of a particle's crossing from the main chain into the side chain,

$$\mathrm{Res}\langle j|G_1(J)|N+1\rangle = -\frac{1}{2}\delta_{j\ell} - \frac{1}{2J}\langle j|H_M|\ell\rangle, \tag{10}$$

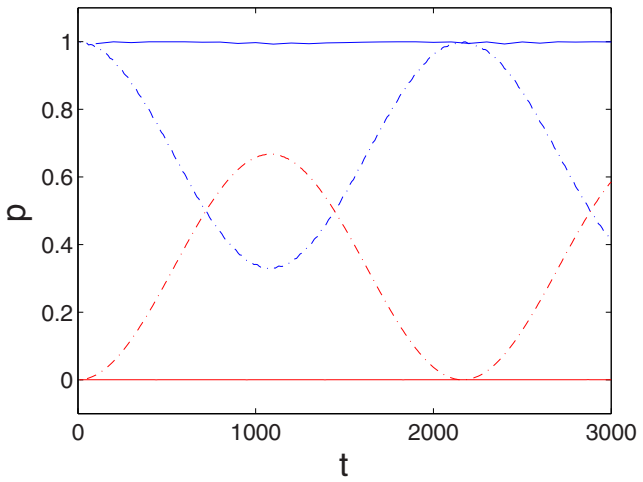


FIG. 1. (Color online) Time evolution of the probabilities for the particle in the two parts of the main chain, respectively, for $S = 1$. Parameters are $J = 10$, $N = 11$, and $\ell = 5$ for solid lines and $\ell = 6$ for dotted lines.

which is 0 as long as the particle is not at the connection point at the initial time.

In Fig. 1, we plot the time evolution of probabilities for particles in the left part and in the right part of the main chain, respectively, for different values of ℓ. Note that in this and the following figures, the time t is in units of the inverse of the hopping strength in the main chain, and the tunneling strength J is in units of the hopping strength in the main chain. At the initial time, the particle is at the third point so that the particle is initially in the left part of the main chain. Since the probability amplitude $A(j_1,j_2)$ for the particle's tunneling between different points is given in Eq. (9), the probability of the particle in the right part of the main chain at time t can be written as $\sum_{\ell<j_1\leqslant N}|A(j_1,3)|^2$, and that in the left part of the main chain as $\sum_{1\leqslant j_1<\ell}|A(j_1,3)|^2$. Note that once the particle is in the left part of the main chain, which concrete points the particle is in does not affect the evolutionary features of the probability distribution in the two parts of the main chain. This is also true for the case of a side chain with more than one point. In Fig. 1, we find that for the particle with $\ell = 6$ ($N+1$ and ℓ having a greatest common divisor larger than 2), the probabilities in the left and right parts of the main chain oscillate quasiperiodically with time. However, the particle always stays in the left part of the main chain and has no probability of crossing the connection point ℓ into the right part of the main chain for $\ell = 5$ ($N+1$ and ℓ not having a greatest common divisor larger than 2), which demonstrates the switching effect of the side chain. Note that, except for the position of the connection point (i.e., the value of ℓ), all the other parameters and the initial states are the same for the two cases.

B. Side chain with two points

For Hamiltonian (1) with $S = 2$, the Green function of the system is written as G_2, whose expression can be given carefully. Then the energy eigenvalues of the system can also be obtained with the help of G_2. For the case of $J \gg 1$, some

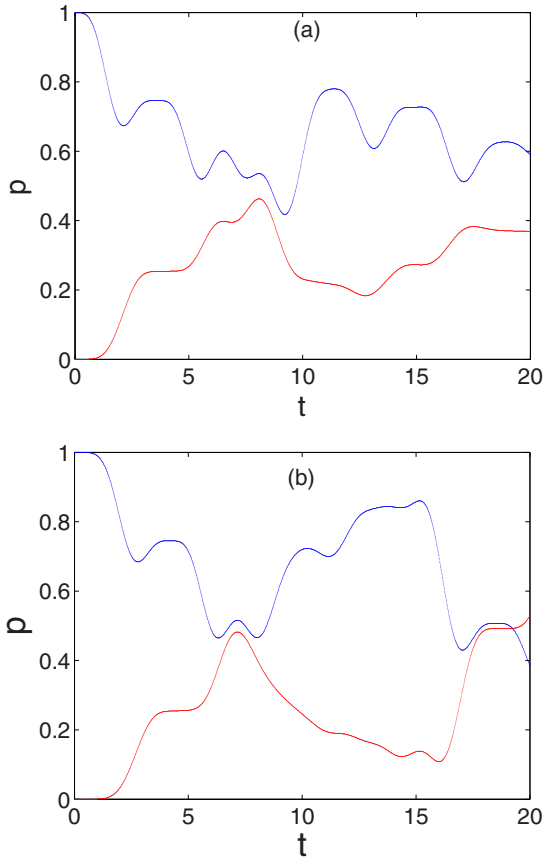


FIG. 2. (Color online) Time evolution of the probabilities for a particle in the two parts of the main chain for $S = 2$. Parameters are $J = 10$, $N = 11$, and (a) $\ell = 5$ and (b) $\ell = 6$.

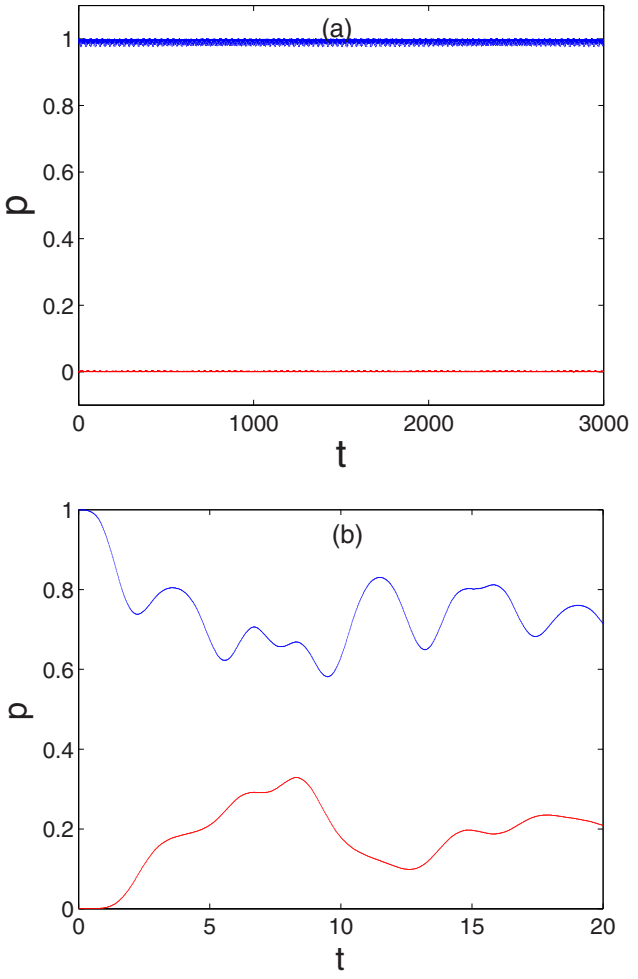


FIG. 3. (Color online) Time evolution of the probabilities for particles in the two parts of the main chain for different values of S. Parameters are $\ell = 5$, $J = 10$, $N = 11$, and (a) $S = 3$ and (b) $S = 4$.

energy levels of H_M also remain if $(N + 1)$ and ℓ have a greatest common divisor larger than 2, and the others are determined via the roots of

$$\frac{1}{z} + \langle \ell | g_0 | \ell \rangle = 0 \tag{11}$$

and are not degenerate regardless whether $(N + 1)$ and ℓ have a greatest common divisor larger than 2. In analogy to the discussion in the above subsection, we can obtain the probability amplitude of a particle crossing from one point to another point in the main chain by calculating the residues of

$$\langle j_1 | G_2 | j_2 \rangle = \langle j_1 | g_0 | j_2 \rangle + \frac{\langle j_1 | g_0 | \ell \rangle \langle \ell | g_0 | j_2 \rangle}{z/J^2 - \left(\frac{1}{z} + \langle \ell | g_0 | \ell \rangle\right)}. \tag{12}$$

Although it is difficult to give the analytical expression of the residues of Eq. (12), we find that the summation of these residues is never 0 for any values of $(N + 1)$ and ℓ because the nonzero energy levels near 0 also exist for a system with a side chain of two points. This implies that the particle can always cross the connection point into the other part of the main chain whether or not $(N + 1)$ and ℓ have a greatest common divisor larger than 2, which is confirmed in Fig. 2.

In Fig. 2, we plot the time evolution of the probability of a particle in the left and right parts of the main chain, respectively. Note that we find that the probabilities of a particle in the left and right parts of the main chain oscillate very rapidly through the numerical calculation. So in order to make Fig. 2 clear, we take a shorter time compared to Fig. 1. At the initial time, the particle is in the left part of the main chain. From this figure, we find that the probabilities of a particle in the two parts of the main chain oscillate with time for both $\ell = 5$ and $\ell = 6$, which is in contrast to the case of a side chain with one point (see Fig. 1). Additionally, the oscillation of the probability is not quasiperiodical like that in Fig. 1 due to the fact that the roots of Eq. (11) are not periodical.

C. Side chain with more points

In the above subsections, we consider the two examples of side chains with one and two points, respectively. Now let us look at the case of a side chain with more than two points. In Fig. 3, we plot the time evolution of the probability distribution in the left and right parts of the main chain, respectively, for different values of S. Here the value of $\ell = 5$, i.e., $N + 1$ and ℓ have no greatest common divisor larger than 2, and the particle is in the left part of the main chain at the initial time. In this figure, we find that the particle cannot cross the connection point into the other part of the main chain for $S = 3$, which

is in contrast to the cases of $S = 4$. Meanwhile, comparing Fig. 3(a) with Fig. 1 and Fig. 3(b) with Fig. 2 (a), respectively, we can see that the system of a side chain with an odd number of points (even number of points) exhibits analogous propagation features. But the features of a system with a side chain of an odd number of points differ significantly from those of a system with a side chain of an even number of points. This feature can be regarded as the parity effect in the quantum walk, which can be explained with the help of the Green function. The parity effect also appears in other physical systems, such as the mesoscopic metal ring [22].

For the system of a side chain with more points, the Green function of the system can be written as

$$G_S = \tilde{g}_0 + g_0 + \frac{g_0|\ell\rangle J^2 \times \langle N+1|\tilde{g}_0|N+1\rangle\langle\ell|g_0}{1 - J^2 \times \langle N+1|\tilde{g}_0|N+1\rangle\langle\ell|g_0|\ell\rangle} + \frac{\tilde{g}_0|N+1\rangle J^2 \times \langle\ell|g_0|\ell\rangle\langle N+1|\tilde{g}_0}{1 - J^2 \times \langle N+1|\tilde{g}_0|N+1\rangle\langle\ell|g_0|\ell\rangle} - \frac{J\tilde{g}_0|N+1\rangle\langle\ell|g_0 + Jg_0|\ell\rangle\langle N+1|\tilde{g}_0}{1 - J^2 \times \langle N+1|\tilde{g}_0|N+1\rangle\langle\ell|g_0|\ell\rangle}, \tag{13}$$

where

$$\tilde{g}_0(z) = \frac{2}{S+1}\sum_{n=1}^{S}\frac{|n\rangle\langle n|}{z + 2J\cos\left(\frac{n\pi}{S+1}\right)}.$$

As in the previous discussion, one can neglect the perturbation term of $\Delta(z_0)$ if $J \gg 1$. Then except for the remaining energy levels of H_M, the other energy levels of the system for a side chain with S points are obtained as

$$\begin{aligned} \langle\ell|g_0(z_0)|\ell\rangle &= 0, \quad S = \text{odd}, \\ \langle\ell|g_0(z_0)|\ell\rangle + \frac{\lambda_S}{z_0} &= 0, \quad S = \text{even}, \end{aligned} \tag{14}$$

where $\lambda_S = \frac{1}{2(S+1)}\sum_{n=1}^{S}\tan^2\frac{n\pi}{S+1}$. We find that if the number of points in the side chain is odd, the energy levels of the system are the same as in the case of $S = 1$, which is discussed in Sec. III A. This implies that the distributions of the energy levels for the cases of side chains with an odd number of points are the same. Then the propagation features of a particle on the triple graph for a side chain with an odd number of points are analogous. So all systems with side chains with an odd number of points exhibit the switching effect when the number of points in the main chain and the position of the side chain satisfy concrete conditions. Additionally, for the case of S being even, the distribution of the energy levels resembles the case of $S = 2$ discussed in Sec. III B due to the fact that the second Eq. (14) is of the same kind except for the difference in the coefficient λ_S. So the propagation features of particles on triple graphs for a side chain with an even number of points resemble each other and never exhibit the switching effect, which is shown in Figs. 2(a) and 3(b). According to the above discussion, we find that whether the particle can cross through the connection points into the other part of the main chain can be significantly influenced by the parity of the number of points in the side chain, which differs from the case studied in Ref. [23]. In that reference, the quantum walk in a chain of points with an attached NAND tree was studied, where the transmission coefficient is determined by the evaluation results of the NAND tree. Additionally, the transmission coefficient can only be 0 or 1. In the system we considered, we show that the probability of a particle in one part of the main chain can oscillate with time for a side chain with even points.

IV. EXPERIMENT PROPOSAL AND CONCLUSION

Since the quantum-walk system we consider can exhibit the above novel features, we expect that it can be observed in experiments and even be designed as a switching device. Then we propose the following possible experimental proposals. First, we expect to realize such a quantum-walk system in solid systems. Assume that there is a one-dimensional lattice system and a particle with spin can tunnel between nearest sites. If one applies an external magnetic field B to the lattice system, the spin will be polarized in the direction of the magnetic field when the temperature is low enough. In this case, the spin degree of the particle is frozen, and thus the Hamiltonian describing this system amounts to that of a quantum walk in a one-dimensional lattice without a side chain. Meanwhile, if one applies another magnetic field whose value and direction are equal and opposite to those of B, respectively, to site ℓ, the total magnetic field at site ℓ is 0. Then once the particle tunnels to site ℓ, the spin degree of the particle will be released so that there is a probability of the particle spin's flipping into the other direction at site ℓ. Assuming that the particle is an electron with spin 1/2, one can easily find that the Hamiltonian of this solid system is essentially equal to Eq. (1) with $S = 1$. So it is possible to realize in this system a quantum walk on a triple graph with a side chain of one point. Naturally, for a particle with spin larger than 1/2, such a system can also be used to realize a quantum walk on a triple graph with a side chain of more points. Note that in the conventional solid system it is difficult to simulate a quantum walk on a triple graph with a side chain of more points because the spin of the particle in the conventional solid system is usually equal to 1/2 and it is difficult to reach larger values. However, cold-atom systems trapped in a magnetic lattice can make up for this defect due to the fact that the spin of the particle can vary more for different alkali and alkali earth metals.

The aforementioned quantum-walk system is also expected to be realized in artificial systems. For example, N qubits are coupled by a single-mode resonant cavity, and the interaction Hamiltonian is given in Ref. [24]. If at the initial time, one of the qubits is applied into a microwave pulse that is resonant with the transition between two levels of the qubit, the initial state of the N-qubit system is $\prod_{k\neq j}|\mathrm{g}\rangle_k|\mathrm{e}\rangle_j|0\rangle_c$. Such an initial state means that the jth qubit is in its exited state $|\mathrm{e}\rangle$, the others are in the ground state $|\mathrm{g}\rangle$, respectively, and the cavity mode is initially in the vacuum state $|0\rangle_c$. For convenience, the initial state of the system can be written as $|\mathrm{e}\rangle_j|0\rangle_c$. In second-order perturbation and taking the state $\prod_k|\mathrm{g}\rangle_k|1\rangle_c$ as the medium state, the effective Hamiltonian is just Eq. (1) without the side chain, and the Fock basis corresponding to the system can be simply denoted as a single-particle state $|j\rangle$ ($j = 1,2,\ldots,N$). Additionally, one can set up other S qubits coupled by another single-mode resonant cavity as the side chain and, meanwhile, couple the first qubit of the side chain with the ℓth qubit of the above N qubits. In this case, the system can simulate

the quantum walk on the triple graph we considered. Note that the coupling strength J can be tuned due to the device parameters and/or the placement of the qubits in the cavity can be changed. So the coupled-qubit system may be more powerful for realizing the quantum walk on the triple graph we considered.

In this paper, we have investigated the quantum random walk on a triple-type graph and shown the effect of the side chain on the propagation features of the main chain. We found that if the tunneling strength in the side chain is much greater than that in the main chain, the system can exhibit the switching effect in the case of a side chain with an odd number of points when the number of points in the main chain and the position of the side chain satisfy concrete conditions. However, for the case of a side chain with an even number of points, the particle can always pass through the connection point into the other part of the main chain no matter where the connection point between the main chain and the side chain is located. So the quantum walk on a triple-type graph with a side chain with an even number of points cannot exhibit the switching effect, which is in contrast to the case of a side chain with an odd number of points. Such propagation properties were explained with the help of the Green function. We also suggest two proposals for experiments to demonstrate this effect, which are expected to be enlightening for the design of a new type of switching device.

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