Quantum walks in the commensurate off-diagonal Aubry-André-Harper model

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Due to the topological nature of the Aubry-André-Harper (AAH) model, interesting edge states have been found existing in one-dimensional periodic and quasiperiodic lattices. In this article, we investigate continuous-time quantum walks of identical particles initially located on either edge of commensurate AAH lattices in detail. It is shown that the quantum walker is delocalized among the whole lattice until the strength of periodic modulation is strong enough. The inverse participation ratios (IPRs) for all of the eigenstates are calculated. It is found that the localization properties of the quantum walker is mainly determined by the IPRs of the topologically protected edge states. More interestingly, the edge states are shown to have an evident "*repulsion*" effect on quantum walkers initiated from the lattice sites inside the bulk. Furthermore, we examine the role of nearest-neighbor interaction on the quantum walks of two identical fermions. Clear enhancement of the *repulsion* effect by strong interaction has been shown.

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I. INTRODUCTION

Quantum walks, the quantum analog of classical random walks, describe the random dynamics of quantum particles on a discrete lattice [1,2], which is inherently governed by the time-dependent wave function of the system. Compared to the classical random walks, dramatically different behavior is shown in quantum walks due to the coherent superposition and interference of the wave function. For example, it is well known now that a quantum walker can propagate linearly with respect to the expansion time, which is much faster than its classical counterpart. This may be exploited in the designing of more efficient quantum search algorithms for quantum computation [2–6]. Having witnessed the huge success of classical random walks, people believe that quantum walks may have widespread applications in quantum algorithms [2,3], quantum computing [5], quantum information [7], quantum simulation [8], quantum biology [9], and so on. Motivated by this promising prospect, more and more research activities on quantum walks have been undertaken by both experimentalists and theorists. Actually, quantum walks have been experimentally implemented in a variety of quantum systems [10], such as optical resonators [11], nuclear magnetic resonance [12], trapped ions [13], trapped cold neutral atoms [14,15], single photons in bulk [16], fiber optics [17], and coupled waveguide arrays [18,19]. On the theoretical side, quantum walks have been proposed to investigate topological phases [20], and fundamental effects of quantum statistics [21,22], interactions [22–25], disorders [26–28], defects [29,30], and hopping modulations [25,30–32] on quantum walks have been intensively investigated.

In this article, we investigate the quantum walks of one and two identical fermions on a one-dimensional optical lattice with periodically modulated hoppings, which is described by the commensurate off-diagonal Aubry-André-Harper (AAH) model. The original version of AAH model [33,34] which contains an incommensurate potential was initially introduced to study the localization phenomena in one dimension. Compared to the one-dimensional Anderson localization model [35], the AAH model features the appearance of a nontrivial localization transition which is more interesting from the perspective of the physics of the disorder-induced metal-insulator transition. Afterwards, the original AAH model has been generalized to a variety of versions adapting to different physical problems. For instance, an AAH model with pure off-diagonal couplings has been used to investigate topological adiabatic pumping [31,36,37]. And it has been shown that the AAH model with on-site and/or off-diagonal modulation is topologically equivalent to Fibonacci lattices of the same quasiperiodicity [38,39]. Topologically protected edge states have been found both in incommensurate [31] and commensurate [40–42] AAH models.

Here in this work, we first look at the quantum walks of identical particles initially located at either boundary of a period-2 commensurate off-diagonal AAH lattice with topologically protected edge states to investigate the effect of periodic hopping modulations. It is found that the quantum walker is delocalized among the whole lattice until the strength of the modulation on the hopping term is strong enough. However, for the topological phase with the phase factor ϕ of the hopping modulations varying outside the interval $(-\pi/2,\pi/2)$, the quantum walker is always delocalized. It is shown that this phenomena is attributed to the topological properties of the commensurate off-diagonal AAH model. We calculate the inverse participation ratios (IPRs) for all of

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the eigenstates and find that the localization of the quantum walker is mainly determined by the IPRs of the topologically protected edge states. Second, we examine the quantum walks of identical particles initially setting out from lattice sites in the bulk. It turns out that a quantum walker initially located on any lattice site in the bulk may expand ballistically as usual and no evidence of localization shows as the strength of the hopping modulation varies. However, an interesting and subtle phenomenon emerges when we look at either boundary of the lattice. It seems that the topologically protected edge state has an interesting *repulsion* effect which make the lattice boundary unreachable for a quantum walker setting out from bulk sites. Third, we investigate quantum walks of two identical fermions with nearest-neighbor interaction and find that strong interactions enhance the interesting *repulsion* effect of the edge states. Brief discussions on the experimental realization of these effects and their potential applications in the future's quantum information techniques are given therein.

The paper is organized as follows. In Sec. II, we introduce the commensurate off-diagonal AAH model. Nearest-neighbor interaction is also considered. We construct the Hilbert space for quantum walkers and briefly show the method we use to describe the time evolution of the density distribution of quantum walkers. Single-particle quantum walks in the commensurate off-diagonal AAH model are shown in Sec. III. Time evolution of the density distributions and IPRs of all the eigenstates are calculated. Detailed analysis corresponding to the dynamical properties is addressed therein. In Sec. IV, we turn to investigate quantum walks of two identical fermions with nearest-neighbor interactions. Finally, a brief summary is given in Sec. V.

II. MODEL AND METHOD

We investigate the continuous-time quantum walks of one and two identical fermions on a one-dimensional lattice with periodically modulated hoppings. The dynamics of such a system is governed by the so-called commensurate off-diagonal AAH model. Additionally, nearest-neighbor interaction between particles is also considered. Therefore, the Hamiltonian of this system reads

$$H = -\sum_i J_i \hat{c}_{i+1}^\dagger \hat{c}_i + V \sum_i \hat{n}_i \hat{n}_{i+1}, \tag{1}$$

with

$$J_i = t + \lambda_{od} \cos(2\pi i/T + \phi), \tag{2}$$

where $\hat{c}_i^\dagger$ ($\hat{c}_i$) is the creation (annihilation) operator of fermions, and $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ denotes the particle number of fermions on site i. The hopping amplitude t is set to be the unit of energy ($t = 1$). All other parameters are scaled by t in the following numerical and analytical investigations. λ_{od} describes the strength of the cosine off-diagonal modulation, T is the periodicity of the modulation, ϕ is a phase factor, and V is the strength of the nearest-neighbor interaction between particles. Since in this paper the AAH lattice we considered is commensurate, T is set to be an integer. Specifically, our analysis and discussions in the following are mainly based on the period-2 case, i.e., $T = 2$, as shown in Fig. 1. And the lattices we studied in this paper are all finite.

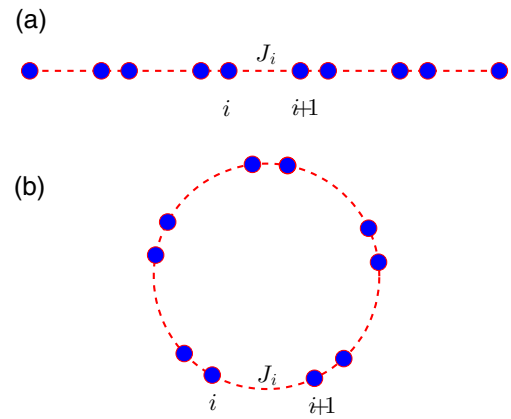

FIG. 1. Sketch of a one-dimensional period-2 off-diagonal AAH lattice under different boundary conditions. (a) Open boundary condition. (b) Periodic boundary condition.

To investigate the dynamics of quantum walkers initially located on well defined sites of the commensurate off-diagonal one-dimensional AAH lattice of length L, we resort to numerical techniques to solve the time-dependent Schrödinger equation exactly. Since $[N,H] = 0$, the total particle number $N = \sum_i \hat{n}_i$ is conserved, and the system will evolve in the Hilbert space with a fixed particle number. For single-particle quantum walks, the Hilbert space involved is simply spanned by basis $B^{(1)} = \{|i\rangle = c_i^\dagger|\mathbf{0}\rangle, 1 \leqslant i \leqslant L\}$, where $|\mathbf{0}\rangle$ denotes the vacuum state. With this basis, it is easy to construct the single-particle Hamiltonian matrix $H^{(1)}$. In units of $\hbar = 1$, the time evolution of an arbitrary single-particle state $|\psi^{(1)}(t)\rangle$ obeys the time-dependent Schrödinger equation,

$$i\frac{d}{dt}|\psi^{(1)}(t)\rangle = H^{(1)}|\psi^{(1)}(t)\rangle, \tag{3}$$

with $|\psi^{(1)}(t)\rangle = \sum_i a_i(t)|i\rangle$. Similarly, for quantum walks of two identical fermions, the Hilbert space is spanned by the basis $B^{(2)} = \{|ij\rangle = c_i^\dagger c_j^\dagger|\mathbf{0}\rangle, 1 \leqslant i < j \leqslant L\}$. And the the time evolution of an arbitrary two-particle state $|\psi^{(2)}(t)\rangle$ obeys

$$i\frac{d}{dt}|\psi^{(2)}(t)\rangle = H^{(2)}|\psi^{(2)}(t)\rangle, \tag{4}$$

where $|\psi^{(2)}(t)\rangle = \sum_{i<j} a_{ij}(t)|ij\rangle$.

By solving the time-dependent equation (3) or (4) numerically, the wave function $|\psi^1(t)\rangle$ or $|\psi^2(t)\rangle$ which governs the dynamics of quantum walkers on the AAH lattice is obtained. Therefore, the time-dependent density distribution of quantum walkers is given by

$$\langle n_i^{(s)}(t)\rangle = \langle\psi^{(s)}(t)|\hat{c}_i^\dagger \hat{c}_i|\psi^{(s)}(t)\rangle, \tag{5}$$

with $s = 1$ or 2 corresponding to a single-particle or two-particle quantum walk.

III. SINGLE-PARTICLE QUANTUM WALKS

First, we investigate continuous-time quantum walks of single particles initially located on either boundary of an

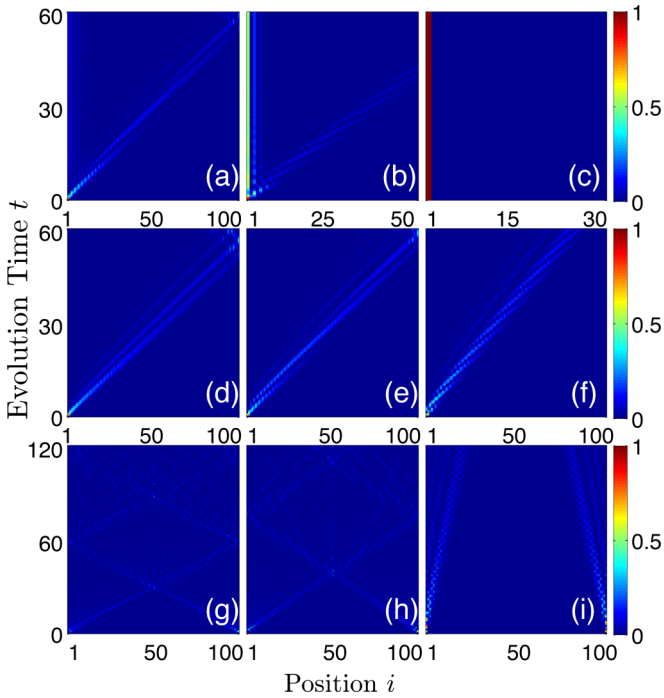

FIG. 2. Single-particle quantum walks on a one-dimensional period-2 off-diagonal AAH lattice with $L = 100$. The quantum walker is initially positioned on the left boundary site. (a)–(c) $\phi = 0$, open boundary condition. (d)–(f) $\phi = 0.6\pi$, open boundary condition. (g)–(i) $\phi = 0$, periodic boundary condition. The first column is corresponding to $\lambda_{od} = 0.1$, the second to $\lambda_{od} = 0.3$, and the third to $\lambda_{od} = 0.9$.

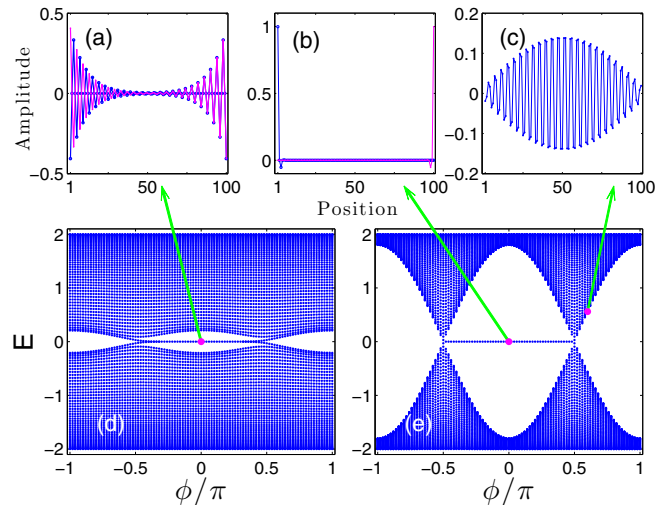

FIG. 3. Upper panel shows the edge states of the one-dimensional period-2 off-diagonal AAH lattice with $L = 100$ under the open boundary condition. The lower panel is the energy spectrum plotted as a function of ϕ. (a),(d) $\lambda_{od} = 0.1$. (b),(c),(e) $\lambda_{od} = 0.9$.

off-diagonal AAH lattice with $T = 2$. The corresponding results are shown in Fig. 2. The length of the one-dimensional AAH lattice is $L = 100$. Figures 2(a)–2(f) are for the AAH lattice with the open boundary condition, while Figs. 2(g)–2(i) are under the periodic boundary condition. In Figs. 2(a)–2(c) and 2(g)–2(i), the value of the off-diagonal modulation phase is $\phi = 0$, and in Figs. 2(d)–2(f), the phase ϕ is chosen to be 0.6π.

It is found that the quantum walker is well localized on the boundary site of the AAH lattice for sufficiently strong off-diagonal modulation; see Fig. 2(c) with $\lambda_{od} = 0.9$. In order to observe the localization phenomenon more clearly, only 30 sites are shown. This interesting localization phenomenon [31] is attributed to the appearance of topologically protected edge states [41] in the energy spectrum of AAH lattices. As shown in Fig. 3(e), a pair of edge states indeed appear in the energy spectrum of the AAH model with $\lambda_{od} = 0.9$. The probability amplitude distribution of corresponding eigenstates are shown in Fig. 3(b).

As we have seen in Fig. 3(e), the interesting edge states only occur in the regime with $-\pi/2 < \phi < \pi/2$. This is actually determined by the topological properties of the commensurate off-diagonal AAH model, which could be characterized by the Zak phase [43–45], i.e., the one-dimensional Berry phase across the Brillouin zone. The Zak phase is explicitly defined as

$$\gamma = i \int_{BZ} dk \langle \Phi(k) | \frac{d}{dk} | \Phi(k) \rangle, \tag{6}$$

where $\Phi(k)$ is the eigenstate of the occupied Bloch band. In Fig. 4, we have calculated the Zak phase of the commensurate off-diagonal AAH model. It is shown that this model has a nontrivial Zak phase of $\gamma = \pi$ in the regime $\phi \in (-\pi/2, \pi/2)$. And it turns out that the Zak phase is insensitive to the strength of the off-diagonal modulations. Therefore, for weak off-diagonal modulations, edge states also appear in the energy spectrum under open boundary condition according to the bulk-edge correspondence, as is shown in Fig. 3(d).

However, the quantum walker is not well localized until the off-diagonal modulation is strong enough; see Figs. 2(a)–2(c). To quantify the localization property of the quantum walker, we compute the IPR for all of the eigenstates of the off-diagonal AAH model with $T = 2$ and $\phi = 0$. For an eigenstate φ_n, which is spanned as $\varphi_n = \sum_i u_i^n |i\rangle$ in the

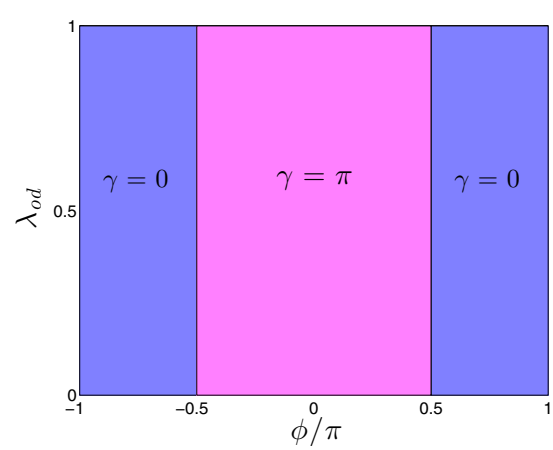

FIG. 4. Phase diagram of the one-dimensional period-2 off-diagonal AAH model. γ is the Zak phase plotted as a function of the phase ϕ and the strength λ_{od} of the off-diagonal modulations.

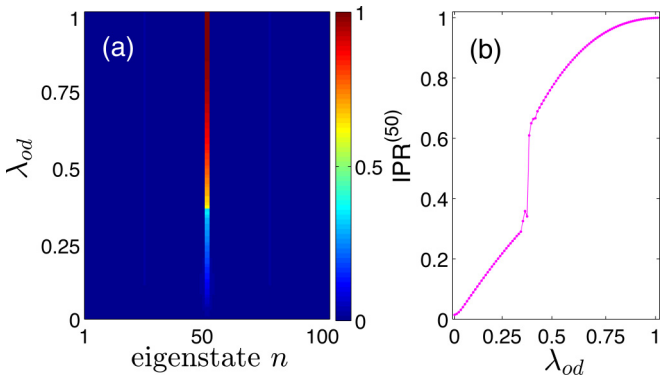

FIG. 5. (a) Inverse participation ratio of all eigenstates plotted as a function of the strength of the off-diagonal modulations λ_{od} for the one-dimensional period-2 off-diagonal AAH model under the open boundary condition with $\phi = 0$ and $L = 100$. (b) Inverse participation ratio of the edge state as a function of λ_{od}.

single-particle Hilbert space $B^{(1)}$, the IPR [46] is defined as

$$\mathrm{IPR}^{(n)} = \frac{\sum_i |u_i^n|^4}{\left(\sum_i |u_i^n|^2\right)^2}. \tag{7}$$

In Fig. 5(a), we show the IPRs for all of the eigenstates. It turns out that the localization property of the quantum walker is mainly determined by the IPRs of the edge states since all of the rest of eigenstates are delocalized. In Fig. 5(b), the IPR of one of the edge states is shown. It is found that for $\phi = 0$ and $T = 2$, the IPR of the edge state increases as the off-diagonal modulation grows stronger.

For comparison, we also show in Figs. 2(d)–2(f) the dynamics of the quantum walker in a commensurate off-diagonal AAH lattice with $\phi = 0.6\pi$ where the model has a trivial Zak phase, i.e., $\gamma = 0$ and thus there is no edge state in the system's spectrum. It is found that the quantum walker is well delocalized as the strength of the off-diagonal modulation grows from $\lambda_{od} = 0.1$ to $\lambda_{od} = 0.9$. The variation of the off-diagonal modulation only slightly affects the expansion speed of the quantum walker. In Figs. 2(g)–2(i), the dynamics of the quantum walker in a commensurate off-diagonal AAH lattice under the periodic boundary condition is shown. The quantum walker shows no localization phenomenon since no edge state exists in the off-diagonal AAH lattice with the periodic boundary condition even for the phase of $\phi = 0$.

Second, we investigate the dynamics of the quantum walker initially located on the lattice sites inside the bulk. As is shown in Figs. 6(a)–6(c), for the open boundary condition and phase $\phi = 0$, the quantum walker initiated from the center site expands ballistically and no localization phenomenon is shown as the strength of the off-diagonal modulation grows from $\lambda_{od} = 0.1$ to $\lambda_{od} = 0.9$. However, close and careful observation reveals an intriguing effect of the topologically protected edge state. If we focus on the two boundary sites of the lattice in Figs. 6(a)–6(c), we will find that as the strength of the off-diagonal modulation increases, the distribution of the quantum walker on the boundary sites decreases gradually and finally disappears. This may be seen as a *repulsion* effect of the edge states, and its strength is determined by the localization

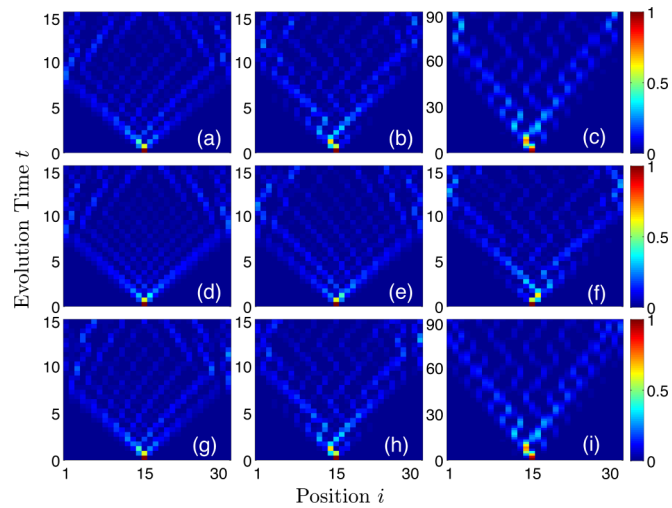

FIG. 6. Single-particle quantum walks on a one-dimensional period-2 off-diagonal AAH lattice with $L = 30$. The quantum walker is initially positioned on the center site 15. (a)–(c) $\phi = 0$, open boundary condition. (d)–(f) $\phi = 0.6\pi$, open boundary condition. (g)–(i) $\phi = 0$, periodic boundary condition. The first column is corresponding to $\lambda_{od} = 0.1$, the second to $\lambda_{od} = 0.3$, and the third to $\lambda_{od} = 0.9$.

properties of the edge states. To be much clearer, we show the time-dependent distribution $n_1(t)$ of the quantum walker on left edge of the lattice for a long time period. It is evident that for strong off-diagonal modulation $\lambda_{od} = 0.9$, the quantum walker is repelled from reaching the boundary site as the distribution on site 1 remains zero all the time; see Fig. 7(a). Here in Figs. 6 and 7, the lattice size is chosen to be $L = 30$ for clarity.

Conversely, for the open boundary condition with phase $\phi = 0.6\pi$ and the periodic boundary condition with $\phi = 0$ when there is no edge state in the spectrum of the off-diagonal

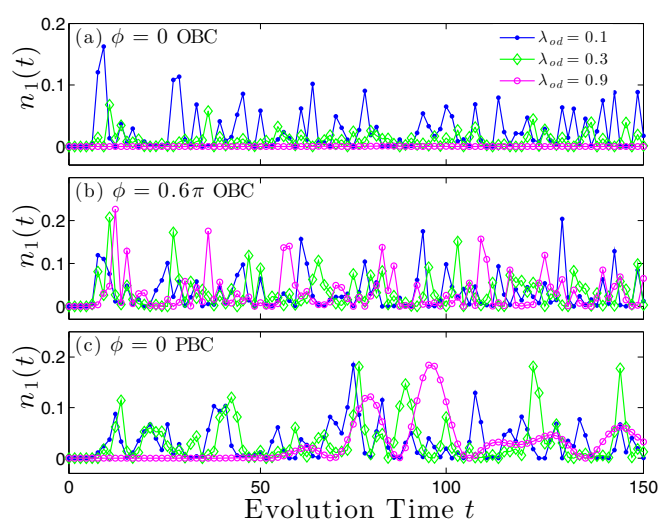

FIG. 7. The time-dependent distribution of the quantum walker on the left boundary site for a relatively long time. The quantum walker is initially positioned on the center site 15. (a) $\phi = 0$, open boundary condition. (b) $\phi = 0.6\pi$, open boundary condition. (c) $\phi = 0$, periodic boundary condition.

AAH model, the quantum walker could reach the boundary sites easily; see Figs. 6(d)–6(i) and Figs. 7(b) and 7(c). The increasing of the off-diagonal modulation only affects the expansion speed of the quantum walker.

In a word, we have shown that the existence of topologically protected edge states in a period-2 off-diagonal AAH model have an interesting *trapping* effect on the quantum walker initiated from the boundary sites of the lattice making the quantum walker localized and also an intriguing *repulsion* effect on the quantum walker set out from lattice sites inside the bulk prohibiting the quantum walker from reaching the boundary sites. These two interesting effects should be observable with existing experimental platforms, for example, an array of coupled photonic waveguides written in bulk glass using femtosecond laser microfabrication technology as used in [31,47]. And they may have potential applications in the designing of micro-architectures for quantum information and quantum computing. Imagine that two optical signals: one is injected into the photonic waveguide at the boundary, and the other is injected into a photonic waveguide in bulk. By modulating λ_{od} or phase ϕ, these two signals could be made to meet each other or transmit separately.

IV. TWO-PARTICLE QUANTUM WALKS

In this section, we turn to investigate the continuous-time quantum walks of two identical fermionic particles on the commensurate off-diagonal AAH lattice with $T = 2$. As is shown in Eq. (1), the nearest-neighbor interaction between the two identical fermionic particles is considered. We mainly focus on the effect of nearest-neighbor interaction on the dynamics of the two quantum walkers setting out from different initial states. Both in Figs. 8 and 9, the open boundary condition is adopted, the phase is set to $\phi = 0$, and the strength of the off-diagonal modulation is set to be $\lambda_{od} = 0.9$ when the *trapping* and the *repulsion* effects of the topologically protected edge states come into force on the dynamics of the quantum walkers. For clear visibility, the length of the AAH lattice is set to be $L = 30$.

At first, we consider the case that one quantum walker is initially located on an edge site of the AAH lattice and the other one is positioned on a site inside the bulk of the lattice. In Fig. 8, the initial state is chosen to be $|1,15\rangle$. According to the discussions on single-particle quantum walks, we can infer that if no interaction is considered ($V = 0$), the quantum walker on the edge site will be localized and the other quantum walker initiated from the center site will expand inside the bulk. They will propagate separately. This is exactly the picture shown in Fig. 8(a). In Fig. 8(b), the nearest-neighbor interaction is set to $V = 1$. It is found that the nearest-neighbor interaction dramatically enhances the *repulsion* effect of the topologically protected edge states existing in the spectrum of the commensurate off-diagonal AAH model. Thiagonal AAH model. The region that can be reached by the quantum walker initiated from inside the bulk is evidently compressed.

Then we investigate the quantum walks of two identical fermionic particles initially located on the left-most two lattice sites of the off-diagonal AAH lattice, i.e., the initial state is prepared as $|1,2\rangle$. Similarly as in Fig. 8(a), when the

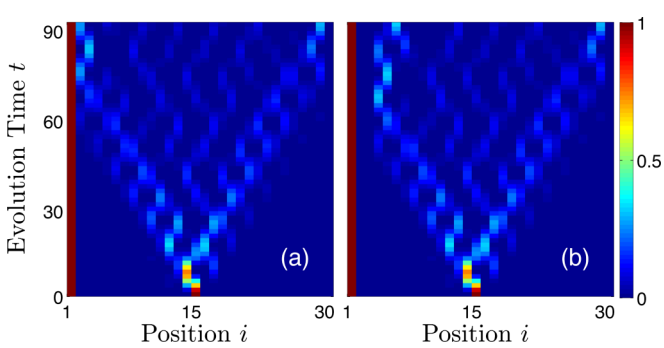

FIG. 8. Quantum walks of two identical fermionic particles with nearest-neighbor interaction on a one-dimensional period-2 off-diagonal AAH lattice with $L = 30$ under the open boundary condition. The phase $\phi = 0$ and $\lambda_{od} = 0.9$. One quantum walker is initially positioned on the left boundary site, and the other is located on the center site 15. (a) $V = 0$. (b) $V = 1$.

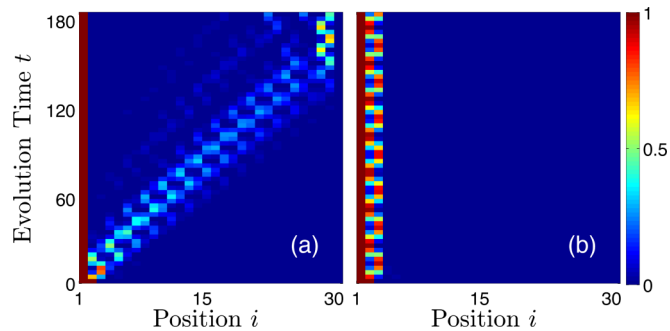

FIG. 9. Quantum walks of two identical fermionic particles with nearest-neighbor interaction on a one-dimensional period-2 off-diagonal AAH lattice with $L = 30$ under the open boundary condition. The phase $\phi = 0$ and $\lambda_{od} = 0.9$. The initial state is prepared on $|1,2\rangle$. (a) $V = 0$. (b) $V = 1$.

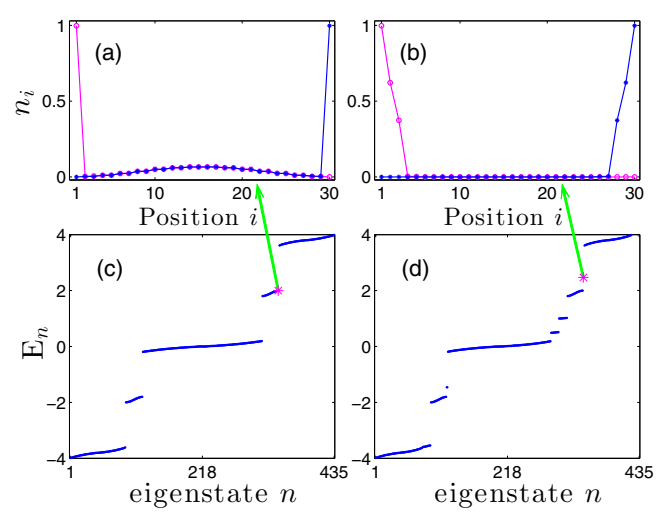

FIG. 10. (a),(b) Density distributions of eigenstates corresponding to the eigenenergies in (c) and (d) denoted by star symbols. (c),(d) Eigenenergies in ascending order for a period-2 off-diagonal AAH lattice with $\lambda_{od} = 0.9$, $\phi = 0$, and $L = 30$ under the open boundary condition. The nearest-neighbor interaction is (c) $V = 0$; (d) $V = 1$.

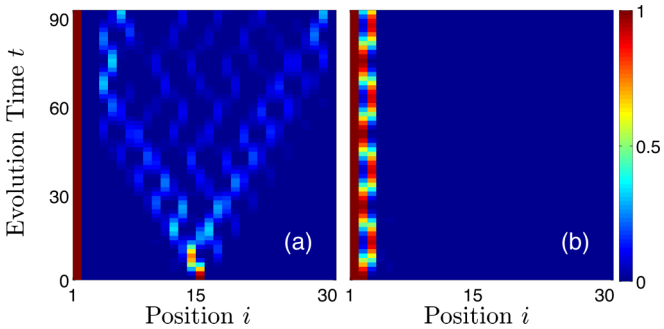

FIG. 11. Quantum walks of two identical fermionic particles with attractive nearest-neighbor interaction on a one-dimensional period-2 off-diagonal AAH lattice with $L = 30$ under the open boundary condition. The phase $\phi = 0$, $\lambda_{od} = 0.9$, and $V = -1$. (a) The initial state is prepared on $|1,15\rangle$. (b) The initial state is prepared on $|1,2\rangle$.

strength of the nearest-neighbor interaction V is zero, the two quantum walkers transmit on the edge and inside the bulk, respectively; see Fig. 9(a). However, in Fig. 9(b) we show that the quantum walker on the second site can be firmly *pinned* by the quantum walker on the boundary site when the nearest-neighbor interaction is set to $V = 1$. This is another interesting phenomenon that may have potential applications in microarchitecture designing.

These intriguing behaviors of quantum walkers are intimately related to the band structure and the eigenstates of the commensurate off-diagonal AAH model. In Fig. 10(c), we show the eigenenergies in ascending order for the off-diagonal AAH lattice with $\lambda_{od} = 0.9$, $V = 0$, $\phi = 0$, and $L = 30$ under the open boundary condition. The density distributions of two typical eigenstates which contribute to the corresponding dynamical behavior of quantum walks in Figs. 8(a) and 9(a) are shown in Fig. 10(a). The feature of these eigenstates is that half of the density of the quantum walker dwells on the single boundary site and the other half of the density distributes among the rest of lattice sites. The parameters in Fig. 10(d) is the same as in Fig. 10(c) except the nearest-neighbor interaction $V = 1$. Compared to Fig. 10(c) with $V = 0$, eigenstates with density distributions like those shown Fig. 10(b) are singled out by the nearest-neighbor interaction. A small energy gap appears; see Fig. 10(c). As shown in Fig. 10(b), almost all of the quantum walkers are distributed among a small region surrounding the lattice boundary. These eigenstates contribute to the intriguing *pinning* effect demonstrated in Fig. 9(b). Actually, this phenomenon essentially resulted from the combination of topologically protected edge states and the well-known repulsively bound-pair [48] mechanism.

Furthermore, we investigate the case with attractive nearest-neighbor interaction, i.e., $V < 0$. Interestingly, the *repulsion* effect of the topologically protected edge states is also clearly enhanced even under attractive interaction; see Fig. 11(a). For two quantum walkers initially located on the two left-most sites, the *pinning* effect is also shown under attractive nearest-neighbor interaction just as expected.

V. CONCLUSIONS

In summary, we have investigated the single-particle and two-particle continuous-time quantum walks on a one-dimensional commensurate off-diagonal AAH lattice. Especially, the effect of the topological property of the commensurate off-diagonal AAH model on the dynamics of the quantum walks has been addressed. In the parameter region where the model has a nontrivial Berry phase, edge states will emerge in the spectrum of an off-diagonal AAH lattice under the open boundary condition. The quantum walker initiated from the boundary site of the AAH lattice will be localized when the IPRs of the edge states are large, which can be modulated by the strength of the off-diagonal modulation. When the quantum walker initially set out from a lattice site inside the bulk, it will encounter an intriguing *repulsion* effect of the topologically protected edge states. For quantum walks of two identical fermions, it is found that the nearest-neighbor interaction could dramatically enhance the *repulsion* effect of these edge states. Also, an interesting *pinning* effect is revealed in the quantum walks of two identical fermions initially positioned on the two left-most sites. These effects may be observed experimentally in a one-dimensional array of photonic waveguides [31,47], double-well potentials [49–51], optical lattices [52,53], or semiconductor structures [54,55]. And they may have prosperous applications in the designing of microarchitectures for quantum information and quantum computing.

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