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Topological Superconducting Transition Characterized by a Modified Real-Space-Pfaffian Method and Mobility Edges in a One-Dimensional Quasiperiodic Lattice

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Abstract: A modified real-space-Pfaffian method is applied to characterize the topological superconducting transition of a one-dimensional p -wave superconductor with quasiperiodic potentials. We found that the Majorana zero-energy mode exists in the topological non-trivial phase, and its spatial distribution is localized at ends of the system, whereas in the topological trivial phase, there is no Majorana zero mode. Furthermore, we numerically found that due to the competition between the localized quasi-disorder and the extended p -wave pairing, there are mobility edges in the energy spectra. Our theoretical work enriches the research on the quasiperiodic p -wave superconducting models.

Keywords: Majorana zero mode; topological phase transition; modified Pfaffian method; mobility edge



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1. Introduction

The Majorana fermion is a kind of particular particle, whose antiparticle is itself [1–3]. During the last decade, the signatures of its presence have been found in many condensed matter systems, such as the semiconductor nanowires with strong spin–orbital couplings [4–8], ultracold atoms [9–12], magnetic atom chains [13–16], and the heterojunctions of normal superconductors and topological insulators [17–24]. Because of its application prospect in topological quantum computation [25,26], the Majorana fermion has attracted extensive research interest [27–33].

The Majorana fermion has been theoretically proven to exist in topological superconductors with p -wave pairings, which appears in Majorana zero mode (MZM) and is located at both ends of the system, protected by the topology [34]. As we all know, disorder gives rise to the localization phenomenon [35], which results in the destruction of the topological non-trivial phases in topological superconductors [36–43]. Cai et al. [44] discussed the influence of the quasi-disorder, namely the quasiperiodic disorder on the MZM. They found that, with the increase of the disorder potential, the system undergoes a transition from the topological non-trivial phase to the Anderson localized phase, that is the MZM keeps robust only to the weak disorder. Moreover, such a transition can be characterized by the quench dynamics [45] and the Kibble–Zurek mechanism [46]. Wang et al. [47] investigated in detail the delocalization properties of the topological phase where the MZM exists and revealed a new critical region.

We know that the presence and absence of the above-mentioned MZM can also be characterized by the Pfaffian [34]. With the Pfaffian method, we are capable of obtaining the topological phase diagram of the superconducting models, of either the homogeneous potential [34], the integer-periodic potential [48], or even the quasiperiodic potential [44]. We notice that the localized quasi-disorder will lead to a wider topological phase boundary compared to the extended superconducting pairings in the p -wave superconducting models [34,44]. However, there remain open questions on how the MZM responds to the

competition between the extended p -wave pairing and the localized quasi-disorder and whether a mobility edge exists in a p -wave pairing system. Recently, a slowly varying incommensurate potential has been shown to induce a mobility edge in a topological superconducting model [49]. Nevertheless, beyond a slowly varying configuration, it is of practical interest to propose a more realistic and experimentally accessible potential, such as the quasi-periodic potential, which has been realized in cold atom experiments [50,51]. In addition, the superconducting pairings are within the reach of cold atomic systems by employing atomic internal states and the laser-assisted state-sensitive tunnelings [52–55] and Zeeman field modulated spin–orbital-coupled Fermi atomic gas [9,56]. Previous theoretical research has revealed that the homogeneous potential makes wave functions extended, while the quasi-disorder brings about the Anderson localization [44,47,57]. However, whether there exist mobility edges when both two types of potentials coexist is still elusive. In this paper, we considered a special case in which the potential consists of a homogeneous part and a quasi-disordered one in a p -wave superconducting model and made an attempt to reveal the topological properties and mobility edges to which this potential leads.

The rest of this paper is organized as follows. In Section 2, we introduce the Hamiltonian of a p -wave superconducting model with a generalized potential. In Section 3, we first introduce the modified real-space-Pfaffian method, and then, we discuss the topological properties and the mobility edges of the system. We give a brief summary in Section 4.

2. Model and Hamiltonian

Real quantum systems are more or less affected by disorder. In this paper, we studied a one-dimensional p -wave superconductor with quasiperiodic disordered on-site potentials, which is described by the following tight-binding Hamiltonian:

$$\hat{H} = \sum_{n=1}^{L-1} \left(-t \hat{c}_n^\dagger \hat{c}_{n+1} + \Delta \hat{c}_{n+1}^\dagger \hat{c}_n^\dagger + h.c. \right) + \sum_{n=1}^L V_n \hat{c}_n^\dagger \hat{c}_n \quad (1)$$

where $\hat{c}_n$ ($\hat{c}_n^\dagger$) denotes the fermion annihilation (creation) operator and L is the size of the system with n being the site index. The nearest-neighbor tunneling strength t and the nearest-superconducting pairing parameter Δ are real constants. $t = 1$ is set as the unit of energy. The quasiperiodic on-site potential V_n is:

$$V_n = \frac{V}{1 - b \cos(2\pi\alpha n)}, \quad (2)$$

where V is the potential strength, $b \in (0, 1)$ is the modulation parameter, and $\alpha = (\sqrt{5} - 1)/2$ is the incommensurate modulation frequency. When $b = 0$, the model goes back to the Kitaev model [34], where $V = 2t$ is the phase transition point, namely the topological boundary of the topological non-trivial phase ($V < 2t$) and the topological trivial one ($V > 2t$). The potential can be understood as the superposition of a homogeneous potential and incommensurate potentials with different frequencies:

$$\begin{aligned} V_n &= \frac{V}{\tanh \beta} \cdot \frac{\sinh \beta}{\cosh \beta - \cos(2\pi\alpha n)} = \frac{V}{\tanh \beta} \sum_{r=-\infty}^{\infty} e^{-\beta|r|} e^{ir(2\pi\alpha n)} \\ &= \frac{V}{\tanh \beta} \left[1 + 2 \sum_{r=1}^{\infty} e^{-\beta r} \cos[r(2\pi\alpha n)] \right], \end{aligned} \quad (3)$$

where $\cosh \beta = 1/b$ is the constraint condition. The parameter b controls the number of summation terms. When b is small, V_n can be truncated to the summation with finite terms. As discussed before, the homogeneous potential manifests the topological boundary of the p -wave superconductor located at $V = 2t$, whereas Cai et al. [44] and Wang et al. [47] showed that the considered quasi-periodicity broadens the topological boundary. For our model, it is unknown how the fate of the topological boundary changes when both two types of potentials coexist. In addition, we know that the homogeneous potentials keep the wave functions extended, while the incommensurate potentials lead to the Anderson

localization [44,47,57]. Whether there exist mobility edges is still elusive when both types of potentials coexist. In the next section, we investigate these two aspects.

In the particle–hole picture, the Hamiltonian is diagonalized. In order to obtain the full-energy spectrum, we shall introduce the Bogoliubov–de Gennes (BdG) transformation:

$$\hat{\xi}_j^\dagger = \sum_{n=1}^L [u_{j,n} \hat{c}_n^\dagger + v_{j,n} \hat{c}_n], \quad (4)$$

where j ranges from one to L and the components $u_{j,n}$ and $v_{j,n}$ are real numbers. Thus, the Hamiltonian in Equation (1) is diagonalized as:

$$\hat{H} = \sum_{j=1}^L E_j (\hat{\xi}_j^\dagger \hat{\xi}_j - \frac{1}{2}), \quad (5)$$

where E_j is the eigenenergy, which can be determined by the following BdG equations:

$$\begin{cases} -t(u_{n-1} + u_{n+1}) + \Delta(v_{n-1} - v_{n+1}) + V_n u_n = E_j u_n, \\ t(v_{n-1} + v_{n+1}) + \Delta(u_{n+1} - u_{n-1}) - V_n v_n = E_j v_n. \end{cases} \quad (6)$$

Furthermore, we represent the wave function as the following form:

$$|\psi_j\rangle = (u_{j,1}, v_{j,1}, u_{j,2}, v_{j,2}, \dots, u_{j,L}, v_{j,L})^T, \quad (7)$$

then according to the BdG equations, we have the following BdG matrix:

$$\mathcal{H} = \begin{pmatrix} A_1 & B & 0 & \cdots & \cdots & \cdots & C \\ B^\dagger & A_2 & B & 0 & \cdots & \cdots & 0 \\ 0 & B^\dagger & A_3 & B & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & B^\dagger & A_{L-2} & B & 0 \\ 0 & \cdots & \cdots & 0 & B^\dagger & A_{L-1} & B \\ C^\dagger & \cdots & \cdots & \cdots & 0 & B^\dagger & A_L \end{pmatrix}, \quad (8)$$

where $A_j = \begin{pmatrix} V_j & 0 \\ 0 & -V_j \end{pmatrix}$ and $B = \begin{pmatrix} -t & -\Delta \\ \Delta & t \end{pmatrix}$; C is a null matrix when considering the open boundary condition (OBC) and $C = \begin{pmatrix} -t & \Delta \\ -\Delta & t \end{pmatrix}$ for the periodic boundary condition [47]. Intuitively, $\mathcal{H}$ is a $2L \times 2L$ matrix. By using the Schmidt orthogonal decomposition method to diagonalize the BdG matrix, we can acquire the full-energy spectrum E_j and the associated wave functions $|\psi_j\rangle$ directly. These strategies are favorable for studying the topological properties, such as the MZM and energy gap, as well as the mobility edges. These investigations are presented in the following section.

3. Results

The topological property of the system is directly characterized by a topological invariant. According to Kitaev's work, the Hamiltonian in Equation (1) can be expanded in terms of Majorana operators as:

$$\hat{H} = \frac{i}{4} \sum_{\ell,m} h_{\ell m} \lambda_\ell \lambda_m, \quad (9)$$

where $h_{\ell m}$ is real antisymmetric matrix, satisfying:

$$h_{\ell m}^* = h_{\ell m} = -h_{m\ell}, \quad (10)$$

and λ_ℓ is the Majorana operator with $\{\lambda_\ell, \lambda_m\} = 2\delta_{\ell m}$, which is defined as:

$$\begin{aligned}\lambda_{2n-1} &\equiv \hat{c}_{2n-1}^\dagger + \hat{c}_{2n-1} = \lambda_n^A, \\ \lambda_{2n} &\equiv i(\hat{c}_{2n}^\dagger - \hat{c}_{2n}) = \lambda_n^B.\end{aligned}\quad (11)$$

Accordingly, under the PBC, the represented Hamiltonian is:

$$\begin{aligned}\hat{H} = \frac{i}{4} &\left[\sum_{n=1}^{L-1} (\Delta - t) \lambda_n^A \lambda_{n+1}^B + (\Delta + t) \lambda_n^B \lambda_{n+1}^A \right. \\ &\left. + \sum_{n=1}^L V_n \lambda_n^A \lambda_n^B + (\Delta - t) \lambda_L^A \lambda_1^B - (t + \Delta) \lambda_1^A \lambda_L^B - h.c. \right].\end{aligned}\quad (12)$$

For an antisymmetric matrix, its Pfaffian is defined as:

$$\text{Pf}(h) = \frac{1}{2^L L!} \sum_{\tau \in S_{2L}} \text{sgn}(\tau) h_{\tau(1), \tau(2)} \cdots h_{\tau(2L-1), \tau(2L)}, \quad (13)$$

where S_{2L} denotes a series of permutations on these $2L$ elements with $\text{sgn}(\tau)$ being the sign of permutation. With the Pfaffian of the system, then the topological invariant M can be defined as [34,44]:

$$M = \text{sgn}(\text{Pf}(h)). \quad (14)$$

Although we know that we can calculate the Pfaffian to obtain the topological invariant of the p -wave superconducting system, for the quasiperiodic case, it is difficult to deal with the perturbation group operation directly. Therefore, we present a modified real-space-Pfaffian method to conveniently calculate the topological invariant. This method requires us to make a Schur decomposition [58] on the real anti-symmetric matrix h :

$$h = UDU^T, \quad (15)$$

where U is a unitary matrix and D is an anti-symmetric tridiagonal matrix. Thus, the Pfaffian of h is redefined as:

$$\text{Pf}(h) = \text{Det}(U) \text{Pf}(D), \quad (16)$$

$\text{Det}(U)$ is the determinant of the unitary matrix U . In practice, we can use Equations (14) and (16) to obtain the topological phase diagram, for the reason that $\text{Det}(U)$ and $\text{Pf}(D)$ are numerically available (see the details in Appendix A).

We calculate the Pfaffian by the modified real-space-Pfaffian method and naturally obtain the topological phase diagram of the system, which is presented in Figure 1. The diagram shows that $M = -1$ corresponds to the topological non-trivial phase, whereas $M = 1$ corresponds to the topological trivial phase and the blue dashed line denotes the numerically obtained phase boundary. We know that when $b = 0$, our model goes back to the Kitaev model, whose transition is located at $V = 2t$ [34]. We notice that when b is taken at a small value, the phase transition is almost the same as that of the Kitaev model. This implies that the MZM is robust against the disordered perturbations. When b increases, the phase boundary bends in the direction of the decreasing V . This phenomenon is the direct result of the enhanced disorder effect, which compresses the topological non-trivial region. That is to say that we can not only realize the topological phase transition by adjusting the potential strength V , but also manipulate the phase transition by controlling the strength of the disorder, which is determined by the parameter b in our system.

In topological systems, the topological phase transition is accompanied by the gap closing and reopening. Figure 2 plots the energy gap Δ_g as a function of the potential strength V with various b . The Δ_g is defined as the difference of the $(L+1)$ -th energy level and the L -th energy level under the periodic boundary condition, i.e. $\Delta_g = E_{L+1} - E_L$. It is readily seen that when the topological phase transition happens, the gap undergoes closing and reopening. Different from the quasiperiodic case [44,47], there appears a wider gap when the system is in the topological trivial phase. This phenomenon occurs because the uniform potential energy has more impact on the energy gap than that of quasi-periodic

disordered perturbations [34,44]. Moreover, when b is small, the gap closing point is almost at $V = 2t$. As b increases, the gap closing point moves towards the direction of the decreasing V . This feature is in accord with the topological boundary in Figure 1.

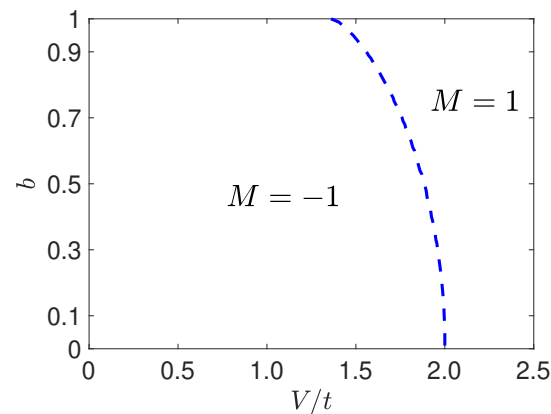


Figure 1. (Color online) b - V/t topological phase diagram for systems with $\alpha = (\sqrt{5} - 1)/2$, $\Delta = 0.5t$. $M = -1$ corresponds to the topological non-trivial phase, and $M = 1$ corresponds to the topological trivial phase. The blue dashed line denotes the phase boundary.

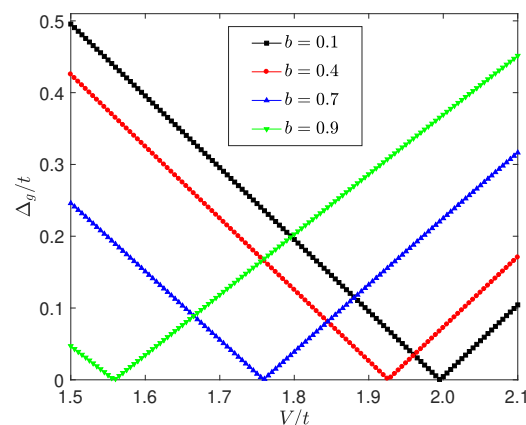


Figure 2. (Color online) The energy gap Δ_g versus V with various b . Other involved parameters are $\alpha = (\sqrt{5} - 1)/2$, $\Delta = 0.5t$, and $L = 1000$.

The topological non-trivial phase implies the presence of the MZMs. Figure 3a shows the excitation energy spectrum as a function of the potential strength V under the open boundary condition. The spectrum reflects that the MZMs are only located in the topological non-trivial phase. To see the distributions of zero energy states, we rewrite the BdG operators as:

$$\eta_j^\dagger = \frac{1}{2} \sum_{n=1}^L [\Phi_{j,n} \lambda_n^A - i \Psi_{j,n} \lambda_n^B], \quad (17)$$

where $\Phi_{j,n} = (u_{j,n} + v_{j,n})$ and $\Psi_{j,n} = (u_{j,n} - v_{j,n})$.

Figure 3b,c respectively plots the spatial distributions Φ and Ψ for the lowest excitation state with $V = 1.5$. Figure 3d,e is the distributions for the lowest excitation state with $V = 2t$. When $V = 1.5t$, we know that the system is in the topological non-trivial phase, so the lowest excitation state is the Majorana zero energy state. As the figures show, the distributions of the corresponding Φ and Ψ are located at the ends of the system, reflecting the bulk boundary correspondence. The contrary consequence is that when $V = 2t$, the system is in the topological trivial phase and the corresponding Φ and Ψ distribute in the bulk of the system. This is interpreted as the system being in the topological trivial phase, and the lowest excitation state is no longer the Majorana edge state, but the bulk state.

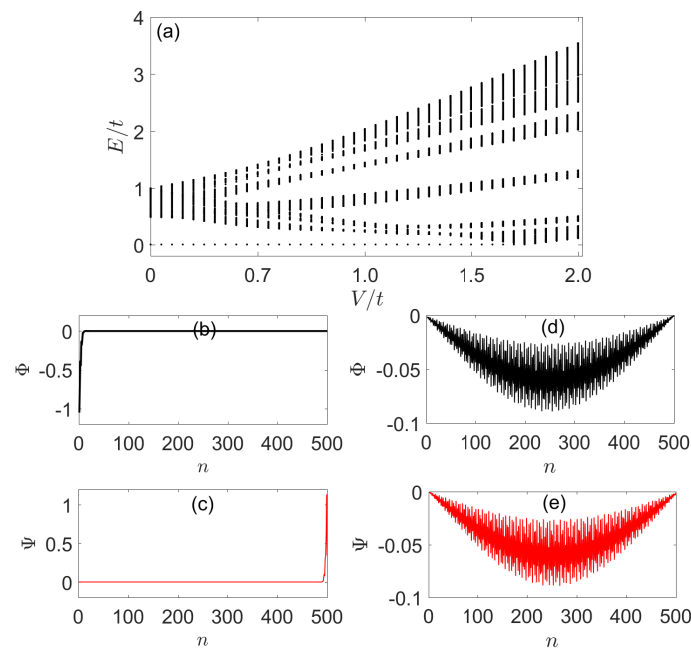


Figure 3. (Color online) (a) Excitation energy spectrum of the system under the open boundary condition. (b–e) are respectively the spatial distributions of Φ and Ψ for the lowest excitation state with $V = 1.5t$ ($V = 2t$). Other involved parameters are $L = 500$, $b = 0.7$, $\alpha = (\sqrt{5} - 1)/2$, and $\Delta = 0.5t$.

We note that in the topological trivial phase, the spatial distributions of Φ and Ψ for the lowest excitation state are no longer localized in the bulk, but expand throughout the whole system, presenting an extended state. We are aware that such a phenomenon in this quasiperiodic superconducting system has relevance for the mobility edge instead of the Anderson localization [44,47]. The localization–delocalization property can be characterized by the inverse participation ratio (IPR). For a given normalized wave function, the associated IPR is defined as [59,60]:

$$\text{IPR}_j = \sum_{n=1}^L \left(|u_{j,n}|^4 + |v_{j,n}|^4 \right). \quad (18)$$

It is well known that for an extended wave function, the IPR scales as L^{-1} , and it approaches one for a localized wave function. We considered $b = 0.7$ as an example to verify the above surmise and made an attempt to qualitatively analyze the influence of the superconducting pairing parameter Δ on the mobility edge. By taking four different Δ , we plot the excitation spectra and IPR as a function of V under the PBC, which are shown in Figure 4a–d, respectively. According to the numerical results, the distinction between the extended states and the localized states can be readily seen from the IPR (the color bar shows this). The transition boundary in energy is just the mobility edge. When Δ is small, the low-energy excitation states are extended states, while those states with higher energy are localized. When Δ becomes larger, the mobility edge moves towards the high-energy region. Moreover, we notice that when the quasiperiodic potential strength V is small, all the excitation states are extended. Moreover, the extended region becomes larger when Δ increases. In other words, the superconducting pairing is robust against the weak disorder and makes the system more extended. From Figure 4a, we also notice that when $V = 2t$, the IPR of the lowest excitation state approaches zero, signaling the extended state. The result answers why the Φ and Ψ in Figure 3d,e distribute throughout the whole system.

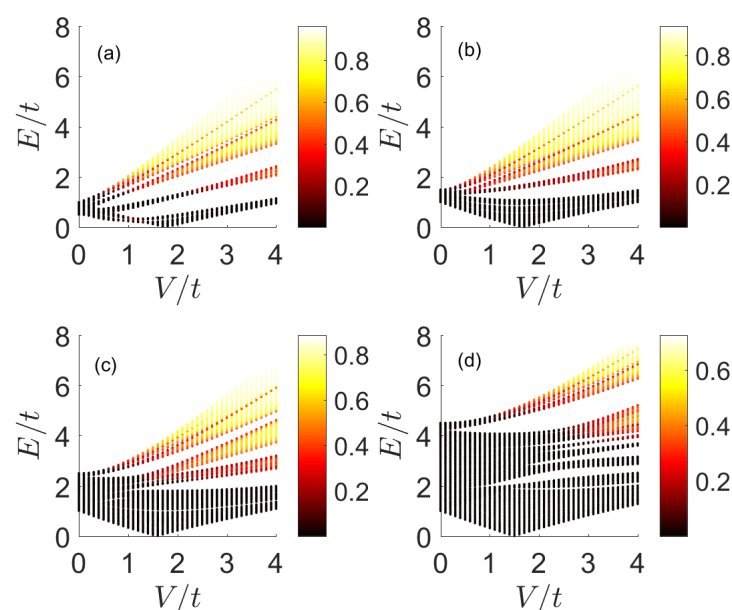


Figure 4. (Color online) The excitation spectrum and IPR as a function of V with $\Delta = 0.5t$ in (a), $\Delta = 1.5t$ in (b), $\Delta = 2.5t$ in (c), and $\Delta = 4.5t$ in (d). Other involved parameters are $b = 0.7$, $\alpha = (\sqrt{5} - 1)/2$, and $L = 500$.

4. Summary

Herein, a quasiperiodic p -wave superconducting model with the coexistence of the homogeneous potential and quasiperiodic potential was investigated. A modified real-space-Pfaffian method was applied to calculate the topological invariants of this system. We demonstrated that the topological phases are protected by the gap. However, compared to the purely quasiperiodic case, the gap in the topological nontrivial is wider. We argued that this phenomenon occurs because the homogeneous potential has more impact on the gap. Besides, we uncovered that there are mobility edges in the p -wave superconducting model. We argued that the mobility edge originates from the competition between the extended p -wave pairing and the localized quasi-disorder. Furthermore, we discussed the influence of the superconducting pairing parameter on the mobility edge. From the analysis, we arrived at the qualitative fact that superconducting pairings tend to make the system extended and stronger pairings move the mobility edge towards the high-energy region. In general, our theoretical work, i.e., the modified real-space Pfaffian method, overcomes the technical problem of using the Pfaffian method to solve the topological invariants of a general p -wave superconductor and makes up for the limitation of the original Pfaffian. Moreover, the uncovered mobility edges promote a further understanding of the quasiperiodic p -wave superconductors.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Modified Real-Space-Pfaffian Method

As mentioned in the main text, we can perform a Schur decomposition [58] on a general anti-symmetric matrix h , i.e., $h = UDU^T$. After this operation, we obtain a $2L \times 2L$ anti-symmetric tridiagonal matrix D , which has the following configuration:

$$D = \begin{pmatrix} 0 & a_1 & & & & \\ -a_1 & 0 & b_1 & & & \\ & -b_1 & 0 & a_2 & & \\ & & -a_2 & \ddots & \ddots & \\ & & & \ddots & 0 & b_{L-1} \\ O & & & & -b_{L-1} & 0 & a_L \\ & & & & & -a_L & 0 \end{pmatrix}. \quad (\text{A1})$$

According to the original definition of the Pfaffian (Equation (13)), we can easily obtain the Pfaffian of the matrix D , which is given as:

$$\text{Pf}(D) = \prod_{i=1}^L a_i. \quad (\text{A2})$$

Therefore, to obtain the Pfaffian of a general anti-symmetric matrix h , a standard strategy is that we first calculate the unitary matrix U and the target matrix D by the Schur decomposition, then obtain the Pfaffian of D by Equation (A2), and finally, obtain the Pfaffian of h by Equation (16). We name the Pfaffian method after the Schur decomposition as the modified real-space-Pfaffian method. In the following, we show how this method is effectively applied to obtain the topological phase diagram of p -wave superconducting models.

Test on the Kitaev model ($V_n = V$) [34]: We considered $t = 1$, $\alpha = (\sqrt{5} - 1)/2$, $\Delta = 0.5t$, and $L = 5$ in all our tests. $V = 1.5t$ and $V = 2.5t$ were two chosen parameters. We know that the topological boundary is located at $V_c = 2t$. Therefore, $V = 1.5t$ corresponds to the topological non-trivial phase and gives $M = -1$; $V = 2.5t$ corresponds to the topological non-trivial phase and gives $M = 1$; taking $V = 1.5t$ and other parameters into h and performing the Schur decomposition, we have $\text{Det}(U) = 1$ and $\text{Pf}(D) = -8.4688$. According to Equation (16), we obtain the topological invariant $M = \text{sgn}(\text{Pf}(h)) = -1$. Next, we take $V = 2.5t$ and other parameters into h . After performing the Schur decomposition, we have $\text{Det}(U) = -1$ and $\text{Pf}(D) = -3.8469$. According to Equation (16), we obtain $M = 1$. If leaving the V changing while other parameters invariable, by means of this method, we can obtain the topological phase diagram of the Kitaev model, as shown in Figure A1.

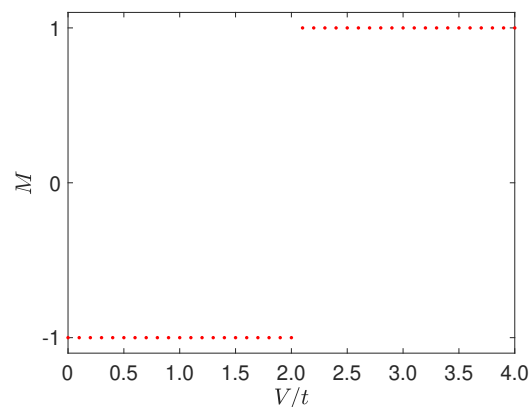


Figure A1. (Color online) M - V/t topological phase diagram of the Kitaev model.

Test on the quasiperiodic p -wave superconducting model [44,47]: This model requires $V_n = V \cos(2\pi\alpha n)$, and its topological boundary is located at $V_c = 2t + 2\Delta$. Without loss of generality, we take $\Delta = 0.5t$; thus, the topological boundary is $V_c = 3t$. $V = 2.8t$

and $V = 3.2t$ are two chosen parameters, corresponding to the topological non-trivial phase ($M = -1$) and topological trivial phase ($M = 1$), respectively. We first tested the case with $V = 2.8t$. After performing the Schur decomposition, we obtain $\text{Det}(U) = -1$ and $\text{Pf}(D) = 1.6637$. Therefore, the topological invariant is $M = \text{sgn}(\text{Det}(U)\text{Pf}(D)) = -1$. Next, we take $V = 3.2t$ and other parameters into h . After performing the Schur decomposition, we obtain $\text{Det}(U) = -1$ and $\text{Pf}(D) = -3.9369$, so the topological invariant is $M = \text{sgn}(\text{Det}(U)\text{Pf}(D)) = 1$. If we change the V continuously and keep other parameters invariable, then we can obtain the topological phase diagram, as shown in Figure A2.

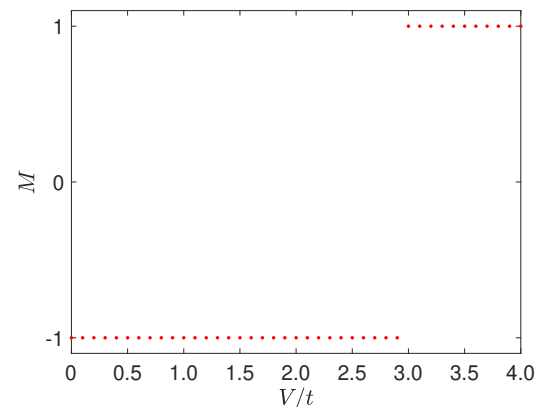


Figure A2. (Color online) M - V/t topological phase diagram of the quasiperiodic p -wave superconducting model.

Test on our model (see Equation (1)): The potential is presented in Equation (2). We considered $b = 0.95$ in our test. According to the topological phase diagram in Figure 1, we know the numerical topological boundary is located at about $V_c = 1.5t$. $V = 1.2t$ and $V = 1.7t$ are two chosen parameters, corresponding to the topological non-trivial phase and topological trivial phase, respectively. We first tested the case with $V = 1.2t$. After performing the Schur decomposition, we have $\text{Det}(U) = -1$ and $\text{Pf}(D) = 9.1651$. Therefore, the topological invariant is $M = \text{sgn}(\text{Det}(U)\text{Pf}(D)) = -1$. Next, we tested the case with $V = 1.7t$. In the same way, we performed the Schur decomposition, then we obtain $\text{Det}(U) = -1$ and $\text{Pf}(D) = -6.9383$. Therefore, in this case, the topological invariant is $M = \text{sgn}(\text{Det}(U)\text{Pf}(D)) = 1$. If we change V continuously and leave other parameters invariable, then we can obtain the topological phase diagram, as shown in Figure A3.

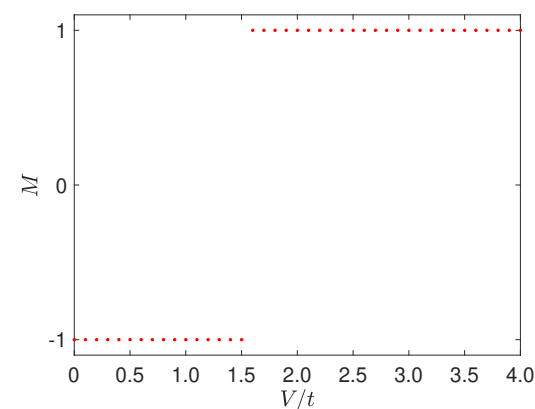


Figure A3. (Color online) M - V/t topological phase diagram of our model.

From the above tests, it is readily seen that this modified real-space-Pfaffian method is very convenient and accurate to numerically obtain the topological phase diagram of the p -wave superconducting model.

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