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Two-Dimensional Topological Superconductors with Spin-Orbit Coupling and Zeeman Term

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Abstract

Topological superconductors have attracted much attention for their potential applications in realizing topological quantum computing. In this paper, we show a system with 8 × 8 Bogoliubov-de Gennes Hamiltonian. The system has particle-hole symmetry. By adding a Zeeman term to the model, we discuss this system from two situations. In the first case of breaking the inversion symmetry while preserving the mirror symmetry, it is obtained from the topological phase diagram of the system that it is a topological superconductor. In another case where the mirror symmetry is broken while preserving the inversion symmetry, the system has two nodes connected by a flat band of zero-energy Andreev edge states and the topological number is non-zero $W(q_{\parallel}=0)\neq 0$. It can be concluded that the system is a topological nodal superconductor.

Keywords

Topological Superconductors, Zeeman Term, Flat Band

1. Introduction

Topological superconductors have attracted a lot of attention in the past few years, characterized by having gap in the bulk and topologically protected gapless edge states composed of Majorana fermions [1]-[9]. Interest in topological superconductors is closely related to the exotic Majorana fermions, which are self-Hermitian particles and have potential applications in quantum computing [6] [7] [10] [11] [12] [13] [14]. Edge states generated from *p*-wave superconductors can prevent decoherence topologically [11] [15] [16]. Fu and Kane proposed that topological insulators proximitized by s-wave superconductors that could lead to Majorana zero modes at vortices [17]. Although two-dimensional and three-dimensional topological insulators have been recently discovered [18] [19], finding suitable topological insulators for these experiments remains a challenge. Adding Zeeman field to semiconductors with Rashba spin orbit coupling and inducing *s*-wave pairing through proximity effect is another method to obtain chiral *p*-wave superconductors [20] [21] [22] [23] [24]. Majorana zero modes have been reported iron-based superconductors [25], which indicates that there is topological superconductivity in iron-based superconductors. One of the motivations for this paper is that iron-based superconductors have a property that can withstand large in-plane magnetic fields [26] [27].

The remainder of this paper is organized as follows. In Section 2, we describe our efficient model 8 × 8 Bogoliubov-de Gennes Hamiltonian and perform a symmetry analysis on it. Results and discussion are given in Section 3. In Section 3.1, under the transformation *U*, when $\Delta_s = 0$, the transformed Hamiltonian is block diagonalized, and each block is still particle-hole symmetric. Adding a Zeeman term to the original Hamiltonian, when the breaks the inversion symmetry while preserving the mirror symmetry, we plot a topological phase diagram about $\Delta_t - c$ plane. We can see from this topological phase diagram that the system is a topological superconductor. In Section 3.2, adding a Zeeman term to the original Hamiltonian, when breaking the mirror symmetry while preserving the inversion symmetry, we plot the band structures of the lattice model and the density of states distribution under the same parameters. From the band structure, it can be seen that the two nodes are connected by a flat band of zero-energy Andreev edge states. The topological number is non-zero $W(q_{\|} = 0) = 1$. Therefore, the system in this case is a topological nodal superconductor. A brief summary is given in Section 4.

2. Model

Under the Nambu basis, the electron operator $\Psi_N = \left(\psi_{1\uparrow\boldsymbol{q}}, \psi_{1\downarrow\boldsymbol{q}}, \psi_{2\uparrow\boldsymbol{q}}, \psi_{2\downarrow\boldsymbol{q}}, \psi^{\dagger}_{1\uparrow-\boldsymbol{q}}, \psi^{\dagger}_{1\downarrow-\boldsymbol{q}}, \psi^{\dagger}_{2\uparrow-\boldsymbol{q}}, \psi^{\dagger}_{2\downarrow-\boldsymbol{q}}\right)^{\mathrm{T}}$, where 1 and 2 denote the top and bottom surface states and $\uparrow$ and $\downarrow$ represent spin-up and spin-down states, respectively. In momentum space, this system is described by an 8 × 8 Bogoliubov-de Gennes Hamiltonian $H = \frac{1}{2}\sum_{\boldsymbol{q}} \Psi^{\dagger}_N h(\boldsymbol{q}) \Psi_N$, with

$$h(\boldsymbol{q}) = \begin{pmatrix} \lambda-\mu & q_x - iq_y & t & 0 & 0 & -\Delta & 0 & \Delta_s+\Delta_t \\ q_x+iq_y & -\lambda-\mu & 0 & t & \Delta & 0 & -\Delta_s+\Delta_t & 0 \\ t & 0 & \lambda-\mu & -q_x+iq_y & 0 & \Delta_s-\Delta_t & 0 & \Delta \\ 0 & t & -q_x-iq_y & -\lambda-\mu & -\Delta_s-\Delta_t & 0 & -\Delta & 0 \\ 0 & \Delta & 0 & -\Delta_s-\Delta_t & -\lambda+\mu & q_x+iq_y & -t & 0 \\ -\Delta & 0 & \Delta_s-\Delta_t & 0 & q_x-iq_y & \lambda+\mu & 0 & -t \\ 0 & -\Delta_s+\Delta_t & 0 & -\Delta & -t & 0 & -\lambda+\mu & -q_x-iq_y \\ \Delta_s+\Delta_t & 0 & \Delta & 0 & 0 & -t & -q_x+iq_y & \lambda+\mu \end{pmatrix} \quad (1)$$

where v_F is the Fermi velocity to be set to unity, $\boldsymbol{q} = (q_x, q_y)$, where σ_i, χ_i

and $\tau_i\left(i=x,y,z\right)$ are Pauli matrices acting on the spin, surface and particle-hole space, respectively. t describes the tunneling effect between the top and bottom surface states, its specific form is $t\to t_0+t_1\left(2-\cos\left(q_x\right)-\cos\left(q_y\right)\right)$. μ is the chemical potential. Δ is the spin singlet intra-surface pairing strength. Δ_s is the spin triplet pairing strength and Δ_t is the spin triplet pairing strength. λ is the Zeeman term. The matrix form of the Hamiltonian (1) has a special symmetry, which is the particle-hole symmetry, $\mathcal{C}h(\boldsymbol{q})\mathcal{C}^{-1}=-h(-\boldsymbol{q})$ with $\mathcal{C}=\sigma_0\chi_0\tau_x\mathcal{K}$, where $\mathcal{K}$ is the complex conjugation operator. For the Hamiltonian (1) has inversion symmetry $\mathcal{P}h(\boldsymbol{q})\mathcal{P}^{-1}=h(-\boldsymbol{q})$ with $\mathcal{P}_{\Delta_s=0}\equiv\mathcal{P}=\sigma_0\chi_x\tau_z$. When we choose the Zeeman term $\lambda=0$, the Hamiltonian (1) is time-reversal invariant. We define a time-reversal operator $\mathcal{T}_{\Delta_t=0}\equiv\mathcal{T}=i\sigma_y\chi_0\tau_0\mathcal{K}$ that satisfies $\mathcal{T}h(\boldsymbol{q})\mathcal{T}^{-1}=h^*(-\boldsymbol{q})$. The Hamiltonian (1) also has mirror symmetry $\mathcal{M}_{\Delta_s=0}\equiv\mathcal{M}=-i\sigma_z\chi_x\tau_0$, with $\mathcal{M}h(\boldsymbol{q})\mathcal{M}^{-1}=h(\boldsymbol{q})$, this is mirror symmetry about the xy plane.

3. Results and Discussion

3.1. Breaking Inversion $\mathcal{P}$ While Preserving Mirror $\mathcal{M}$

We have $U\mathcal{M}U^{-1}=diag\left(-i,-i,-i,-i,i,i,i,i\right)$, with the transformation matrix

$$U=\frac{1}{\sqrt{2}}\begin{pmatrix}0&0&0&0&1&0&1&0\\0&1&0&-1&0&0&0&0\\1&0&1&0&0&0&0&0\\0&0&0&0&0&1&0&-1\\1&0&-1&0&0&0&0&0\\0&0&0&0&0&1&0&1\\0&0&0&0&1&0&-1&0\\0&1&0&1&0&0&0&0\end{pmatrix}. \tag{2}$$

We can transform the model Hamiltonian (1) into the following, then

$$Uh(\boldsymbol{q})U^{-1}=\begin{pmatrix}-t-\lambda+\mu&\Delta+\Delta_t&0&q_x+iq_y&0&0&0&-\Delta_s\\\Delta+\Delta_t&-t-\lambda-\mu&q_x+iq_y&0&0&0&\Delta_s&0\\0&q_x-iq_y&t+\lambda-\mu&-\Delta-\Delta_t&0&\Delta_s&0&0\\q_x-iq_y&0&-\Delta-\Delta_t&t+\lambda+\mu&-\Delta_s&0&0&0\\0&0&0&-\Delta_s&-t+\lambda-\mu&-\Delta+\Delta_t&0&q_x-iq_y\\0&0&\Delta_s&0&-\Delta+\Delta_t&-t+\lambda+\mu&q_x-iq_y&0\\0&\Delta_s&0&0&0&q_x+iq_y&t-\lambda+\mu&\Delta-\Delta_t\\-\Delta_s&0&0&0&q_x+iq_y&0&\Delta-\Delta_t&t-\lambda-\mu\end{pmatrix}, \tag{3}$$

with the basis

$$U\Psi_N=\frac{1}{\sqrt{2}}\left(\psi^\dagger_{1\uparrow-\boldsymbol{q}}+\psi^\dagger_{2\uparrow-\boldsymbol{q}},\psi_{1\downarrow\boldsymbol{q}}-\psi_{2\downarrow\boldsymbol{q}},\psi_{1\uparrow\boldsymbol{q}}+\psi_{2\uparrow\boldsymbol{q}},\psi^\dagger_{1\downarrow-\boldsymbol{q}}-\psi^\dagger_{2\downarrow-\boldsymbol{q}},\psi_{1\uparrow\boldsymbol{q}}-\psi_{2\uparrow\boldsymbol{q}},\psi^\dagger_{1\downarrow-\boldsymbol{q}}+\psi^\dagger_{2\downarrow-\boldsymbol{q}},\psi^\dagger_{1\uparrow-\boldsymbol{q}}-\psi^\dagger_{2\uparrow-\boldsymbol{q}},\psi_{1\downarrow\boldsymbol{q}}+\psi_{2\downarrow\boldsymbol{q}}\right)^{\mathrm{T}}.$$

When $\Delta_s=0$, we can turn the above Hamiltonian into block diagonal $h_1\oplus h_2$ with

$$h_1(\boldsymbol{q})=\begin{pmatrix} -t-\lambda+\mu & \Delta+\Delta_t & 0 & q_x+iq_y \\ \Delta+\Delta_t & -t-\lambda-\mu & q_x+iq_y & 0 \\ 0 & q_x-iq_y & t+\lambda-\mu & -\Delta-\Delta_t \\ q_x-iq_y & 0 & -\Delta-\Delta_t & t+\lambda+\mu \end{pmatrix}, \tag{4}$$

$$h_2(\boldsymbol{q})=\begin{pmatrix} -t+\lambda-\mu & -\Delta+\Delta_t & 0 & q_x-iq_y \\ -\Delta+\Delta_t & -t+\lambda+\mu & q_x-iq_y & 0 \\ 0 & q_x+iq_y & t-\lambda+\mu & \Delta-\Delta_t \\ q_x+iq_y & 0 & \Delta-\Delta_t & t-\lambda-\mu \end{pmatrix}. \tag{5}$$

The terms that break inversion while preserving mirror is $\sigma_x\chi_z$, adding a term $c\sigma_x\chi_z\tau_z$ with a constant c to the original Hamiltonian (1),

$$h(c)=\begin{pmatrix} \lambda-\mu & q_x-iq_y+c & t & 0 & 0 & -\Delta & 0 & \Delta_s+\Delta_t \\ q_x+iq_y+c & -\lambda-\mu & 0 & t & \Delta & 0 & -\Delta_s+\Delta_t & 0 \\ t & 0 & \lambda-\mu & -q_x+iq_y-c & 0 & \Delta_s-\Delta_t & 0 & \Delta \\ 0 & t & -q_x-iq_y-c & -\lambda-\mu & -\Delta_s-\Delta_t & 0 & -\Delta & 0 \\ 0 & \Delta & 0 & -\Delta_s-\Delta_t & -\lambda+\mu & q_x+iq_y-c & -t & 0 \\ -\Delta & 0 & \Delta_s-\Delta_t & 0 & q_x-iq_y-c & \lambda+\mu & 0 & -t \\ 0 & -\Delta_s+\Delta_t & 0 & -\Delta & -t & 0 & -\lambda+\mu & -q_x-iq_y+c \\ \Delta_s+\Delta_t & 0 & \Delta & 0 & 0 & -t & -q_x+iq_y+c & \lambda+\mu \end{pmatrix},$$

then

$$Uh(c)U^{-1}=\begin{pmatrix} -t-\lambda+\mu & \Delta+\Delta_t & 0 & -c+q_x+iq_y & 0 & 0 & 0 & -\Delta_s \\ \Delta+\Delta_t & -t-\lambda-\mu & c+q_x+iq_y & 0 & 0 & 0 & \Delta_s & 0 \\ 0 & c+q_x-iq_y & t+\lambda-\mu & -\Delta-\Delta_t & 0 & \Delta_s & 0 & 0 \\ -c+q_x-iq_y & 0 & -\Delta-\Delta_t & t+\lambda+\mu & -\Delta_s & 0 & 0 & 0 \\ 0 & 0 & 0 & -\Delta_s & -t+\lambda-\mu & -\Delta+\Delta_t & 0 & c+q_x-iq_y \\ 0 & 0 & \Delta_s & 0 & -\Delta+\Delta_t & -t+\lambda+\mu & -c+q_x-iq_y & 0 \\ 0 & \Delta_s & 0 & 0 & 0 & -c+q_x+iq_y & t-\lambda+\mu & \Delta-\Delta_t \\ -\Delta_s & 0 & 0 & 0 & c+q_x+iq_y & 0 & \Delta-\Delta_t & t-\lambda-\mu \end{pmatrix}. \tag{6}$$

For $\Delta_s=0$, the transformed Hamiltonian is block diagonalized, and each block is still particle-hole symmetric with $\tilde{\mathcal{C}}_-=\sigma_0\Gamma_x\mathcal{K}$. The physical meaning of the c term is that, on the untransformed basis,

$$\begin{aligned} &\sum_{\boldsymbol{q}}\Psi_N^\dagger\left(c\sigma_x\chi_z\tau_z\right)\Psi_N \\ &=\sum_{\boldsymbol{q}}c\left(\psi_{1\uparrow\boldsymbol{q}}^\dagger\psi_{1\downarrow\boldsymbol{q}}+\psi_{1\downarrow\boldsymbol{q}}^\dagger\psi_{1\uparrow\boldsymbol{q}}-\psi_{2\uparrow\boldsymbol{q}}^\dagger\psi_{2\downarrow\boldsymbol{q}}-\psi_{2\downarrow\boldsymbol{q}}^\dagger\psi_{2\uparrow\boldsymbol{q}}+h.c.\right), \end{aligned} \tag{7}$$

which, in the real space, is an on-site x-Zeeman term but in opposite directions in the two layers, namely the staggered x-Zeeman term. Make the following substitution for the basis $U\Psi_N=\left(\Psi_1,\Psi_2\right)^{\mathrm{T}}$, where $\Psi_1=\left(a_\uparrow,a_\downarrow,a_\uparrow^\dagger,a_\downarrow^\dagger\right)^{\mathrm{T}}$ and $\Psi_2=\left(b_\uparrow,b_\downarrow,b_\uparrow^\dagger,b_\downarrow^\dagger\right)^{\mathrm{T}}$. While for the transformed Hamiltonian, this term for h_1 reads

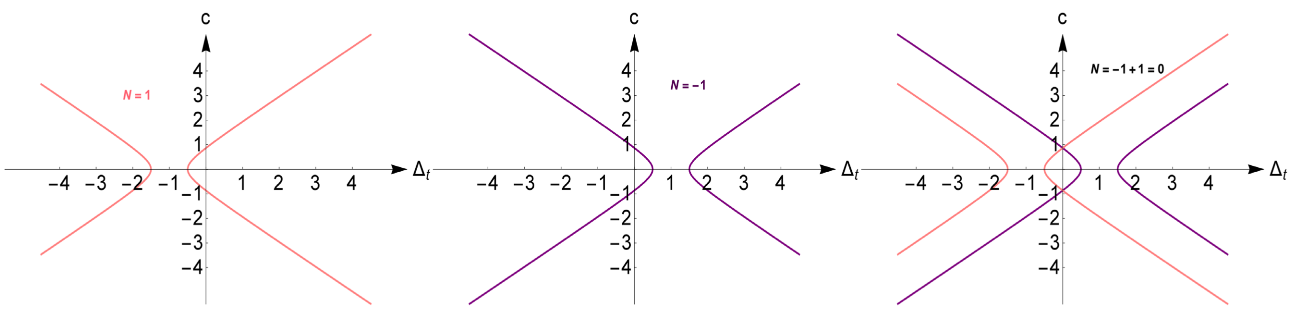
$$\sum_{q} c\left(a_{\uparrow q} a_{\downarrow -q} + a_{\downarrow q} a_{\uparrow -q} + h.c.\right), \tag{8}$$

which is a spin-singlet *s*-wave pairing. In the presence of both spin-singlet *s*-wave pairing and spin-triplet *p*-wave pairing, the inversion is no longer a conserved quantity. The result for h_2 is similar, one only needs to substitute $c \to -c$ and $a \to b$. We show the Topological phase diagram in the $\Delta_t - c$ plane in **Figure 1** and **Figure 2**. As can be seen in **Figure 1(c)** in the middle-up and -down regime, the Chern number is a nontrivial zero, then it can also be written as $(N=1) \oplus (N=-1)$, while in the centered middle regime, Chern number is a trivial zero. As show in **Figure 2(c)** in the middle regime, the Chern number is a nontrivial zero, namely $(N=1) \oplus (N=-1)$.

When an x-Zeeman term $c\sigma_x \chi_z \tau_z$ is added to the model Hamiltonian (1), x-Zeeman term breaks inversion symmetry while protecting mirror symmetry. And it can be known from **Figure 1** and **Figure 2** that this system is a topological superconductor at this time. Next, we discuss the case of adding a Zeeman term that preserves inversion symmetry while breaking mirror symmetry.

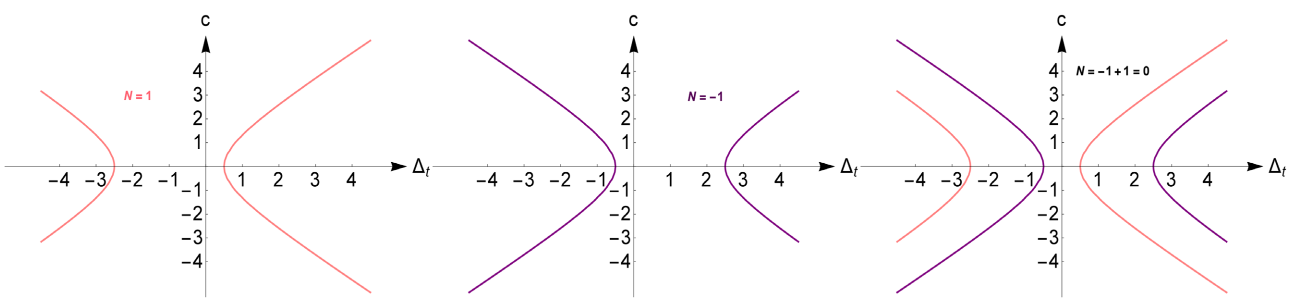
3.2. Breaking Mirror $\mathcal{M}$ While Preserving Inversion $\mathcal{P}$

The terms that break mirror while preserve inversion is $\sigma_x \chi_x$. Adding the x-Zeeman term $\lambda_x \sigma_x \chi_x \tau_z$ to the original Hamiltonian,



(a) (b) (c)

Figure 1. (color online) Topological phase diagrams of (a) h_1, (b) h_2, (c) h in $\Delta_t - c$ plane with $\lambda = 0$, $\mu = 0$, $\Delta = 1$, $\Delta_s = 0$ and $t = 0.5$.



(a) (b) (c)

Figure 2. (color online) Topological phase diagrams of (a) h_1, (b) h_2 (c) h in $\Delta_t - c$ plane with $\lambda = 0$, $\mu = 0$, $\Delta = 1$, $\Delta_s = 0$ and $t = 1.5$.

$$h_{\lambda_x}(\boldsymbol{q})=\begin{pmatrix} \lambda-\mu & q_x-iq_y & t & \lambda_x & 0 & -\Delta & 0 & \Delta_s+\Delta_t \\ q_x+iq_y & -\lambda-\mu & \lambda_x & t & \Delta & 0 & -\Delta_s+\Delta_t & 0 \\ t & \lambda_x & \lambda-\mu & -q_x+iq_y & 0 & \Delta_s-\Delta_t & 0 & \Delta \\ \lambda_x & t & -q_x-iq_y & -\lambda-\mu & -\Delta_s-\Delta_t & 0 & -\Delta & 0 \\ 0 & \Delta & 0 & -\Delta_s-\Delta_t & -\lambda+\mu & q_x+iq_y & -t & -\lambda_x \\ -\Delta & 0 & \Delta_s-\Delta_t & 0 & q_x-iq_y & \lambda+\mu & -\lambda_x & -t \\ 0 & -\Delta_s+\Delta_t & 0 & -\Delta & -t & -\lambda_x & -\lambda+\mu & -q_x-iq_y \\ \Delta_s+\Delta_t & 0 & \Delta & 0 & -\lambda_x & -t & -q_x+iq_y & \lambda+\mu \end{pmatrix}.$$

under the transformation U,

$$Uh_{\lambda_x}(\boldsymbol{q})U^{-1}=\begin{pmatrix} -t-\lambda+\mu & \Delta+\Delta_t & 0 & q_x+iq_y & 0 & -\lambda_x & 0 & -\Delta_s \\ \Delta+\Delta_t & -t-\lambda-\mu & q_x+iq_y & 0 & -\lambda_x & 0 & \Delta_s & 0 \\ 0 & q_x-iq_y & t+\lambda-\mu & -\Delta-\Delta_t & 0 & \Delta_s & 0 & \lambda_x \\ q_x-iq_y & 0 & -\Delta-\Delta_t & t+\lambda+\mu & -\Delta_s & 0 & \lambda_x & 0 \\ 0 & -\lambda_x & 0 & -\Delta_s & -t+\lambda-\mu & -\Delta+\Delta_t & 0 & q_x-iq_y \\ -\lambda_x & 0 & \Delta_s & 0 & -\Delta+\Delta_t & -t+\lambda+\mu & q_x-iq_y & 0 \\ 0 & \Delta_s & 0 & \lambda_x & 0 & q_x+iq_y & t-\lambda+\mu & \Delta-\Delta_t \\ -\Delta_s & 0 & \lambda_x & 0 & q_x+iq_y & 0 & \Delta-\Delta_t & t-\lambda-\mu \end{pmatrix}, \quad (9)$$

which is not block diagonalized for $\Delta_s=0$. Although the addition of the x-Zeeman term $\lambda_x\sigma_x\chi_x\tau_z$ to the Hamiltonian (1) breaks the time-reversal symmetry of the system, Hamiltonian respects an effective time-reversal symmetry $\mathcal{T}_1 h_{\lambda_x}(\boldsymbol{q})\mathcal{T}_1^{-1}=h_{\lambda_x}^*(-\boldsymbol{q})$, where $\mathcal{T}_1=\sigma_x\chi_x\tau_0\mathcal{K}$. Combining time-reversal symmetry and particle-hole symmetry yields the chiral symmetry $\mathcal{S}h_{\lambda_x}(\boldsymbol{q})\mathcal{S}^{-1}=-h_{\lambda_x}(\boldsymbol{q})$, with $\mathcal{S}=\mathcal{C}\mathcal{T}_1=\sigma_x\chi_x\tau_x$. As a result, Hamiltonian belongs to the class BDI [1]. For a superconducting system with chiral symmetry, an explicit expression of the topological number is given by [28],

$$W(q_{\parallel})=\frac{1}{2\pi}Im\left(\int \mathrm{d}q_{\perp}\partial_{q\perp}\ln\left(\det\hat{Q}(\boldsymbol{q})\right)\right), \quad (10)$$

with $q_{\parallel}$ denotes the momentum with periodic boundary condition and $q_{\perp}$ the one with open boundary condition in the numerics. For the parameters chosen in **Figure 3**, namely, $\lambda=\Delta_s=0$, $\mu=0.9$, $t=t_0=0.5$, $t_1=1$, $\Delta=0.35$, $\Delta_t=0$ and $\lambda_x=0.8$, then $W(q_{\parallel}=0)=1$ and $W(q_{\parallel}=\pi)=0$, which is consistent with **Figure 3(a)**. In **Figure 3(a)**, we plot the band structures of the lattice model. From **Figure 3(a)**, the two nodes are connected by a flat band of zero-energy Andreev edge states. **Figure 3(b)** shows the wave function distribution for the flat band of the zero-energy Andreev edge states. Therefore, when breaking the mirror symmetry while preserving the inversion symmetry, the system is a topological nodal superconductor.

4. Conclusion

In summary, we show a system with 8 × 8 Bogoliubov-de Gennes Hamiltonian and add a Zeeman term to the system. Under the transformation U, the system is still particle-hole symmetry. When breaking the inversion symmetry while

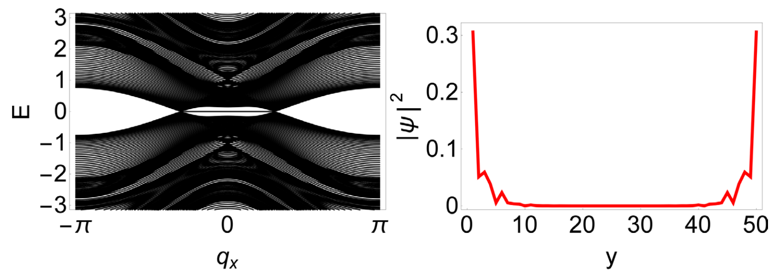


Figure 3. (color online) The band structures of h with 50-sites along the y-direction with $\lambda = \Delta_s = 0$, $\mu = 0.9$, $t = t_0 = 0.5$, $t_1 = 1$, $\Delta = 0.35$, $\Delta_t = 0$ and $\lambda_x = 0.8$, We also plot the spacial distributions of lowest positive energy states at $q_x = 0.5$ in the right-hand side accordingly.

preserving the mirror symmetry, according to the topological phase diagram of the system in the $\Delta_t - c$ plane in **Figure 1** and **Figure 2**, the system is a topological superconductor. When breaking the mirror symmetry while preserving the inversion symmetry, the system has chiral symmetry. The two nodes are connected by a flat band of zero-energy Andreev edge states (**Figure 3(a)**) and the topological number is non-zero $W(q_{\parallel} = 0) = 1$. Therefore, the system is a topological nodal superconductor.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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