Topological phase transitions driven by next-nearest-neighbor hopping in noncentrosymmetric cold Fermi gases*

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We investigate the topological phase marked by the Thouless–Kohmoto–Nightingale–Nijs (TKNN) number and the phase transitions driven by the next nearest neighbor (NNN) hopping in noncentrosymmetric cold Fermi gases, both spin-singlet pairing and spin-triplet pairing are considered. There exists a critical t'_c for the NNN hopping, at which the quantum phase transition occurs, and the system changes from an Abelian (non-Abelian) phase to a non-Abelian (Abelian) one. By numerically diagonalizing the Hamiltonian in the real space, the energy spectra with edge states for different topological phases and the Majorana zero modes are discussed. Although the spin-triplet pairing does not contribute to the gap closing and the phase diagram, it induces gapless states in the presence of a magnetic field, and the TKNN number in this region is still zero.

Keywords: topological phase transition, Fermi gases, Majorana fermion

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1. Introduction

Topological phases and topological phase transitions are two of the most active research areas in physics.[1–5] These topological states, which have a full gap in the bulk and topologically protected gapless states on the boundary,[6–9] are usually characterized by some global topological quantum numbers, such as the Thouless–Kohmoto–Nightingale–Nijs (TKNN) number.[10] The topological order supports the existence of chiral Majorana edge modes, and the vortices with Majorana fermion modes are neither fermions nor bosons but non-Abelian anyons, which obey the non-Abelian statistics.[11–13] Majorana fermion could be exploited as a decoherence qubit and has attracted much attention for its remarkable application in fault-tolerant topological quantum computation.[14–16] Sato *et al.* have pointed out that an s-wave superconductor with Rashba spin–orbit coupling (SOC) could have a non-Abelian topological phase,[11] where a large Zeeman magnetic field is essentially needed. It was also reported that a spin-triplet superconductor with broken time-reversal symmetry possesses a zero-energy Majorana mode, and hence can realize a non-Abelian topological phase in the presence of Rashba SOC.[17,18]

Two-dimensional (2D) ultra-cold Fermi gases can be utilized to simulate many other systems due to their controllability and operability.[19–24] Recently, the experimental realization of SOC in ultra-cold atoms was reported.[25–29] This opens a completely new avenue for exploring many-body physics in the presence of SOC. The simplest way to realize the SOC in ultra-cold Fermi gases is based on the p-wave superfluid of degenerate Fermi gases by means of the p-wave Feshbach resonance.[22] This method is a direct way to realize the simulation, but the very short lifetimes of the p-wave pairs and molecules are a top challenge. Zhang *et al.* suggested that an artificially generated SOC could create an effective $p_x + ip_y$ topological superfluid from an s-wave interaction.[25,30,31]

In most realized square optical lattices, the next nearest neighbor (NNN) hopping (along the diagonal) t' is much smaller than the nearest neighbor (NN) hopping t and it is instructive to set $t' = 0$. Recently, several experimental and theoretical explorations showed that by shaking the optical lattice, the ratio t'/t can be varied in a very large range. It was reported that a periodic shaking with amplitude V_0 and frequency ω can lead to a renormalization of the NN hopping, which becomes multiplied by a Bessel function, $t_{\rm eff} = tJ_0(V_0/\hbar\omega)$. On the other hand, the NNN hopping can also be renormalized by a Bessel function with a different argument. These would lead to a full range of possible values for the ratio $t'_{\rm eff}/t_{\rm eff}$.[32–34] In this paper, we study how the NNN hopping affects the quantum topological phase and the quantum phase transitions in a 2D system, where an isotropic square optical lattice is used to trap the cold Fermi gases.

The organization of this paper is as follows. In Section 2, we give our model and the condition of gap closing. Then the topological phase marked by the TKNN number $I_{\rm TKNN}$ and the quantum phase transitions driven by the NNN hopping are discussed in detail. In Section 3, we investigate the properties

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of the energy spectrum with edge states to prove the bulk–boundary correspondence and the Majorana zero modes. The final section is a summary.

2. Topological phase and phase transitions

The cold Fermi gases with Rashba SOC on an isotropic 2D square optical lattice can be realized by adjusting the intensities of the lasers.[25,26] Both spin-singlet component $\Delta_{\rm s}$ and spin-triplet component $\Delta_{\rm p}$ are considered for the parity mixing of Cooper pairs in our model. With the NNN hopping, the Hamiltonian in real space can written as[17]

$$\begin{aligned} H \;=\; & -t\sum_i (a^\dagger_{i,\uparrow}a_{i+\hat{x},\uparrow}+a^\dagger_{i,\downarrow}a_{i+\hat{x},\downarrow}+a^\dagger_{i,\uparrow}a_{i+\hat{y},\uparrow}+a^\dagger_{i,\downarrow}a_{i+\hat{y},\downarrow}) \\ & -t'\sum_i (a^\dagger_{i,\uparrow}a_{i+\hat{x},i+\hat{y},\uparrow}+a^\dagger_{i,\downarrow}a_{i+\hat{x},i+\hat{y},\downarrow}) \\ & +v_{\rm R}\sum_i [(a^\dagger_{i,\uparrow}a_{i+\hat{x},\downarrow}-a^\dagger_{i,\downarrow}a_{i+\hat{x},\uparrow}) \\ & -{\rm i}(a^\dagger_{i,\uparrow}a_{i+\hat{y},\downarrow}+a^\dagger_{i,\downarrow}a_{i+\hat{y},\uparrow})] \\ & -\Delta_{\rm p}\sum_i (a^\dagger_{i,\uparrow}a^\dagger_{i+\hat{x},\uparrow}+a^\dagger_{i,\downarrow}a^\dagger_{i+\hat{x},\downarrow}-{\rm i}a^\dagger_{i,\uparrow}a^\dagger_{i+\hat{y},\uparrow}+{\rm i}a^\dagger_{i,\downarrow}a^\dagger_{i+\hat{y},\downarrow}) \\ & +\Delta_{\rm s}\sum_i (a^\dagger_{i,\uparrow}a^\dagger_{i,\downarrow}-a^\dagger_{i,\downarrow}a^\dagger_{i,\uparrow}) \\ & +\sum_i [(-\mu-H_z)a^\dagger_{i,\uparrow}a_{i,\uparrow}+(-\mu+H_z)a^\dagger_{i,\downarrow}a_{i,\downarrow}]+{\rm H.C.} \quad (1) \end{aligned}$$

Here the first term is the NN hopping with $a^\dagger_{i,\uparrow}$ ($a^\dagger_{i,\downarrow}$) being the creation operator on site i and t being the hopping strength, where the distance between the nearest neighbors has been set as the unit of length. The second term describes the NNN hopping with the hopping strength t'. In this paper, we adjust t' within the range $[0,1]$. The third term stands for the Rashba SOC. The fourth and the fifth terms describe the spin-triplet pairing with the order parameter $\Delta_{\rm p}$ and the spin-singlet pairing with the order parameter $\Delta_{\rm s}$, respectively. Both terms are the interaction between the electron and the hole. The last term includes the chemical potential μ and the magnetic field H_z. For simplicity, we only consider a negative chemical potential and a positive magnetic field in this paper, i.e., $\mu<0$ and $H_z>0$.

To explore the gapless condition, we will work in the momentum space. After the Fourier transformation and by choosing the Nambu spinor basis $\boldsymbol{\Psi}^\dagger_k=[c^\dagger_{k,\uparrow},c^\dagger_{k,\downarrow},c_{-k,\uparrow},c_{-k,\downarrow}]$, Hamiltonian (1) can be written as $H(k)=\frac{1}{2}\sum_k \boldsymbol{\Psi}^\dagger_k \boldsymbol{M}_k \boldsymbol{\Psi}_k$, where $\boldsymbol{M}_k$ is a 4×4 matrix which preserves the particle–hole symmetry

$$\boldsymbol{M}_k=\begin{pmatrix} \varepsilon_{k,\uparrow} & 2v_{\rm R}J_1 & -2\Delta_{\rm p}J_1 & \Delta_{\rm s} \\ 2v_{\rm R}J_2 & \varepsilon_{k,\downarrow} & -\Delta_{\rm s} & 2\Delta_{\rm p}J_2 \\ -2\Delta_{\rm p}J_2 & -\Delta_{\rm s} & -\varepsilon_{k,\uparrow} & 2v_{\rm R}J_2 \\ \Delta_{\rm s} & 2\Delta_{\rm p}J_1 & 2v_{\rm R}J_1 & -\varepsilon_{k,\downarrow} \end{pmatrix}. \quad (2)$$

Here $J_1=\sin k_y+{\rm i}\sin k_x$, $J_2=\sin k_y-{\rm i}\sin k_x$, and $\varepsilon_{k,\uparrow}$ and $\varepsilon_{k,\downarrow}$ stand for the kinetic energy

$$\begin{aligned} \varepsilon_{k,\uparrow} &= -\mu-2t\cos k_x-2t\cos k_y-4t'\cos k_x\cos k_y-H_z, \\ \varepsilon_{k,\downarrow} &= -\mu-2t\cos k_y-2t\cos k_x-4t'\cos k_x\cos k_y+H_z. \end{aligned}$$

Diagonalizing matrix $\boldsymbol{M}_k$ and defining $\delta\varepsilon_k=\varepsilon_{k,\uparrow}-\varepsilon_{k,\downarrow}$, we can obtain the band structure

$$E^\lambda_{k,\pm}=\lambda\sqrt{\varepsilon^2_{k,\uparrow}+\varepsilon^2_{k,\downarrow}+8J_1J_2(v^2_{\rm R}+\Delta^2_{\rm p})+2\Delta^2\pm E_0}, \quad (3)$$

where $\lambda=\pm 1$ correspond to the electrons (conduction band) and holes (valence band), and

$$E_0=\sqrt{(\varepsilon_{k,\uparrow}+\varepsilon_{k,\downarrow})^2[(\delta\varepsilon_k)^2+16J_1J_2v^2_{\rm R}]+4[(\delta\varepsilon_k)^2+16J_1J_2\Delta^2_{\rm p}]\Delta^2+64(\varepsilon_{k,\uparrow}+\varepsilon_{k,\downarrow})J_1J_2v_{\rm R}\Delta_{\rm p}\Delta_{\rm s}}.$$

The gap of the system closes only when $\varepsilon^2_{k,\uparrow}+\varepsilon^2_{k,\downarrow}+8J_1J_2(v^2_{\rm R}+\Delta^2_{\rm p})+2\Delta^2-E_0=0$. In the presence of the magnetic field, when the spin-triplet pairing $\Delta_{\rm p}$ is stronger than the spin-singlet pairing $\Delta_{\rm s}$, the gap closing occurs only under the conditions of $\varepsilon_{k,\uparrow}\varepsilon_{k,\downarrow}+\Delta^2_{\rm s}=0$ and $J_1J_2=0$. Since J_1J_2 is zero at $k=(0,0),(0,\pi),(\pi,0),(\pi,\pi)$, substituting these values into the former condition, we obtain four equations. As the equation at point $(0,\pi)$ is the same as that at $(\pi,0)$, we finally have three different conditions

$$\begin{aligned} (4t+\mu+4t')^2 &= H^2_z-\Delta^2_{\rm s}, \\ (-\mu+4t')^2 &= H^2_z-\Delta^2_{\rm s}, \\ (4t-\mu-4t')^2 &= H^2_z-\Delta^2_{\rm s}. \end{aligned} \quad (4)$$

In the above conditions, $H_z>\Delta_{\rm s}$ is required. When one of these conditions is satisfied, the energy gap closes. It is noticed that all the conditions do not depend on the Rashba SOC and the spin-triplet pairing. Since the gap closing only happens at $k=(0,0),(0,\pi),(\pi,0),(\pi,\pi)$ where both Rashba SOC $v_{\rm R}(\sin k_y\pm{\rm i}\sin k_x)$ and the spin-triplet pairing $\Delta_{\rm p}(\sin k_y\pm{\rm i}\sin k_x)$ are zero. The spin-triplet pairing could bring an obvious effect on the edge states, which we will discuss later.

For our 2D time-reversal-symmetry-broken system, TKNN number $I_{\rm TKNN}$ is an important topological number, which plays a central role in topological nature.[10] To obtain the TKNN number, we shall begin with the Schrödinger equation

$$H(k)|\phi_n(k)\rangle=E_n(k)|\phi_n(k)\rangle,$$

where $|\phi_n(k)\rangle$ is the normalized wave function of the n-th

band. In terms of the gauge field

$$A_i(k) = \sum_{E_n<0} \langle \phi_n(k) | \partial_i \phi_n(k) \rangle, \tag{5}$$

the Berry connection can be written as $F_{12}(k) = \varepsilon^{ij}\partial_i A_j(k) = \partial_x A_y(k) - \partial_y A_x(k)$. Then, we have

$$I_{\mathrm{TKNN}} = \frac{1}{2\pi \mathrm{i}} \int \mathrm{d}k_x \mathrm{d}k_y F_{12}(k). \tag{6}$$

Here, the derivative ∂_i stands for $\partial/\partial k_i$ with $i = x, y$ and the integral is around the first Brillouin zone. It is noticed that the sum in Eq. (5) is restricted to the occupied bands.

Generally, a nonzero TKNN number allows both non-Abelian topological order which is characterized by the non-Abelian statistics and Abelian topological order without non-Abelian statistics. If the TKNN number is odd, the system is in a non-Abelian topological phase and there exists an odd number of Majorana zero modes in a vortex, which implies that the vortex is a non-Abelain anyon.[11,12] If the TKNN number is even, the system is in an Abelian topological phase and there is no non-Abelain anyon. If the TKNN number is zero, the system will be in a topological trivial phase.

Figure 1 shows the topological phase diagram, where the number in each region is the TKNN number, and the unit of energy is set as t. The red horizontal line in each panel labels Δ_{s}, and the magnetic field must be larger than Δ_{s}. The parameters used here are $\Delta_{\mathrm{s}} = 0.6$, $\Delta_{\mathrm{p}} = 0.8$, and $v_{\mathrm{R}} = 0.5$. Figure 1(a), which is for the case of $t' = 0.3$, shows there are four regions that are topologically distinct. The gap between two boundaries can defined as the height of the topological phase, which is shown in Figs. 1(a) and 1(c), where $\delta = \Delta H_z = |H_{z2} - H_{z3}|$, and H_{z2} and H_{z3} are calculated from the second and the third equations in Eq. (4). For a given μ, δ will be adjusted only by t', and there exists a critical t'_{c} which makes $\delta = 0$ (in our calculation, $t' = 0.5$). In this case, the last two equations in Eq. (4) give the same condition for gap closing, there will be only two different gap closing conditions (Fig. 1(b)), the gap labeled by δ in panel (a) disappears. When $t' > t'_{\mathrm{c}}$, the gap between these two boundaries reopens and the quantum phase transition occurs, so the system changes into another topological quantum phase (Fig. 1(c)). Figure 1(d) shows δ as a function of t', where we have set $\mu = -0.5$. When $t' < t'_{\mathrm{c}}$, the zone described by δ is in a topological Abelian phase marked by $I_{\mathrm{TKNN}} = 2$. As t' increases, the space of this phase is compressed. When $t' = t'_{\mathrm{c}}$, this Abelian phase disappears. Then when $t' > t'_{\mathrm{c}}$, the gap reopens and the system enters into a topological non-Abelian phase marked by $I_{\mathrm{TKNN}} = -1$.

3. Edge states and Majorana fermion

The system is periodic at the y direction and has two open boundaries at $i_x = 0$ and $i_x = 100$. By numerically diagonalizing Hamiltonian (1) in real space, the excitation spectrum E as a function of k_y can be obtained.

Figure 2 shows the energy spectrum with edge states of 2D cold Fermi gases, both spin-singlet pairing and spin-triplet

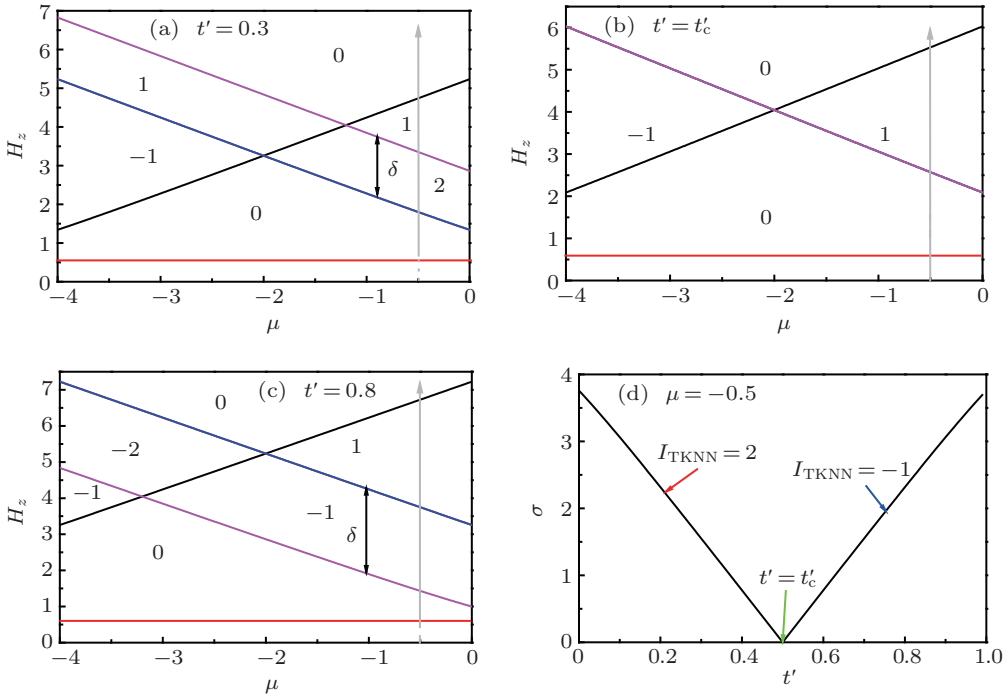


Fig. 1. (color online) (a)–(c) Topological phase diagram and TKNN numbers in different regions. The unit of energy is set as t, the other parameters used here are $v_{\mathrm{R}} = 0.5$, $\Delta_{\mathrm{s}} = 0.6$, and $\Delta_{\mathrm{p}} = 0.8$. (d) The height of the topological quantum phase δ versus t', where $\mu = -0.5$.

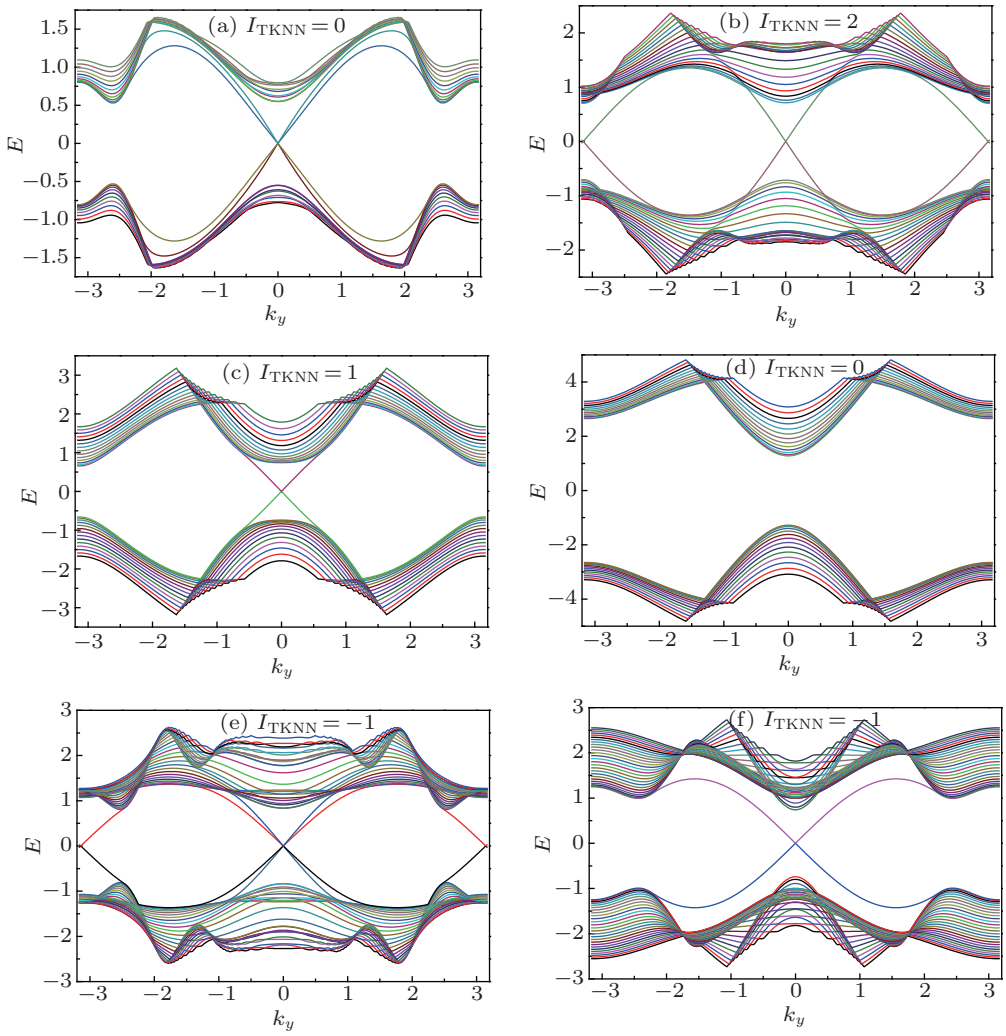


Fig. 2. (color online) The energy spectrum with edge states of 2D cold Fermi gases, both spin-singlet and spin-triplet pairings are considered. The system is periodic at the y direction and has two open edges at $i_x = 0$ and $i_x = 100$. The unit of energy is set as t. The parameters are $v_{\rm R} = 0.5$, $\Delta_{\rm s} = 0.6$, $\Delta_{\rm p} = 0.8$; (a) $\mu = -0.5$, $H_z = 1$, $t' = 0.3$; (b) $\mu = -0.5$, $H_z = 2.5$, $t' = 0.3$; (c) $\mu = -0.5$, $H_z = 4$, $t' = 0.3$; (d) $\mu = -0.5$, $H_z = 6$, $t' = 0.3$; (e) $\mu = -0.5$, $H_z = 2.5$, $t' = 0.8$; (f) $\mu = -3$, $H_z = 3$, $t' = 0.3$.

pairing are considered. Generally, a topologically nontrivial bulk guarantees the existence of topologically stable gapless edge states on the boundaries. For the 2D cold Fermi gases with a magnetic field breaking the time-reversal symmetry while having the particle–hole symmetry, the gapless edge states are chiral Majorana fermion modes. The parameters used here are $\Delta_{\rm s} = 0.6$, $\Delta_{\rm p} = 0.8$, and $v_{\rm R} = 0.5$. In Fig. 1(a), we show that as the magnetic field increases, the system will go through four quantum phases sequentially (see the gray line, where $\mu = -0.5$). Their spectra are correspondingly shown in Figs. 2(a)–2(d). When $t' = 0.8$, the phase in Fig. 2(b) changes to that in Fig. 2(e), corresponding to the phase transition in Fig. 1(d). Figure 2(f) is for the case of $t' = 0.3$, $\mu = -3$, and $H_z = 3$ with the TKNN number $I_{\rm TKNN} = -1$.

It is noteworthy that although figures 2(c), 2(e), and 2(f) are all for the non-Abelian topological phase with an odd TKNN number, the numbers of Majorana zero modes in the figures are quite different. There is only one Majorana zero mode in Figs. 2(c) and 2(f), while there are three Majorana zero modes in Fig. 2(e). Normally, a zero TKNN number corresponds to a topological trivial phase, which indicates that there exists no gapless state, such as the case in Fig. 2(d). However, there are two gapless states in Fig. 2(a). This is a bit surprising because the magnetic field breaks the time-reversal symmetry and the TKNN number is still zero in this region. This is not the first time a gapless state has been found in a region marked by $I_{\rm TKNN} = 0$, similar results can be found in Ref. [12]. In Fig. 2(b), when the TKNN number is even, there are an even number of gapless states in the spectrum and the system is in an Abelian phase.

In Eq. (4), we show that the spin-triplet pairing $\Delta_{\rm p}$ does not contribute to the gap closing and the phase diagram. Under the condition of $t' = 0.3$, the phase diagram for $\Delta_{\rm p} = 0$ is the same as that shown in Fig. 1(a), where we have set $\Delta_{\rm p} = 0.8$. In Fig. 3, we illustrate the energy spectrum with edge states of the 2D Fermi gases with pure spin-singlet pairing. The parameters used here are $\Delta_{\rm s} = 0.6$, $\Delta_{\rm p} = 0$, and $v_{\rm R} = 0.5$. For comparison with Figs. 2(a)–2(d), four spectra under the condition of

$\mu = -0.5$ are given correspondingly in Figs. 3(a)–3(d). There is an obvious difference between Figs. 3(a) and 2(a), both are all for the trivial quantum phase marked by $I_{\rm TKNN} = 0$, but there are no gapless states when the spin-triplet pairing is absent in Fig. 3(a). The spin-triplet pairing does not contribute to the gapless condition, but it can induce gapless states in a topological trivial system.

When the TKNN number is odd (even), an odd (even) number of Majorana zero modes always exists in the spectrum. When the TKNN number is zero, Majorana zero modes do (not) exist when both spin-singlet and spin-triplet pairings are considered (when only the spin-singlet pairing is considered) in the presence of both Rashba SOC and a magnetic field. When we focus on the non-Abelian topological phase and the non-Abelian anyon, the index $(-1)^{I_{\rm TKNN}}$ is of particular interest, since it gives a hallmark of the non-Abelian topological phase, i.e., when $(-1)^{I_{\rm TKNN}} = -1$, it indicates that the phase is a non-Abelian topological one and there is an odd number of Majorana zero modes in a vortex, which implies that the vortex is a non-Abelian anyon.

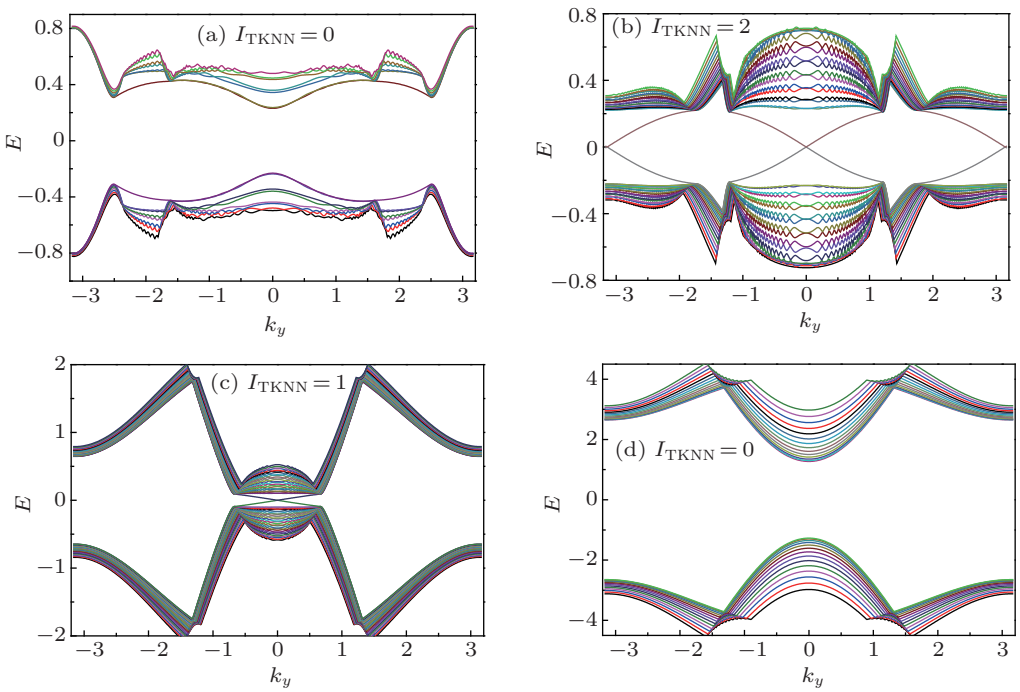


Fig. 3. (color online) The energy spectrum with the edges of 2D Fermi gases with pure spin-singlet pairing. The unit of energy is set as t. The parameters are $t' = 0.3$, $v_{\rm R} = 0.5$, $\mu = -0.5$, $\Delta_{\rm s} = 0.6$, $\Delta_{\rm p} = 0$; (a) $H_z = 1$; (b) $H_z = 2.5$; (c) $H_z = 4$; (d) $H_z = 6$.

4. Conclusion

For the spin-singlet pairing and spin-triplet pairing cold Fermi gases on an isotropic 2D square optical lattice, considering both the NNN hopping and the Rashba SOC, we investigate the gapless condition and the phase diagram in detail. By using TKNN number $I_{\rm TKNN}$ as an index of the quantum phase, we study the topological nature and the quantum phase transitions controlled by the NNN hopping in this 2D cold Fermi gas. There exists a critical $t'_{\rm c}$ for the NNN hopping, at which the quantum topological phase transition occurs, and the system changes from an Abelian (non-Abelian) phase to a non-Abelian (Abelian) one. In addition, the spin-triplet pairing has no contribution to the gapless condition and the phase diagram, but it could induce gapless states in the presence of a weak magnetic field, and the TKNN number is still zero in this region. Last, for a system which is periodic at the y direction and has two open boundaries at the x direction, we numerically calculate the excitation spectra, and discuss the Majorana zero modes. The index $(-1)^{I_{\rm TKNN}} = -1$ indicates that the system is in a non-Abelian topological phase and an odd number of Majorana zero modes exist in a vortex, which implies that the vortex is a non-Abelian anyon.

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