Impurity-induced bound states in superconductors with topological order

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Abstract

The study of classical spins in topological insulators (Liu and Ma 2009 Phys. Rev. B 80 115216) is generalized to topological superconductors. Based on the characteristic features of the so-called $F$-function, the Bogoliubov–de Gennes Hamiltonian for superconductors is classified to positive, negative, and zero ‘gap’ categories for topologically trivial and nontrivial phases of a topological superconductor as well as a BCS superconductor, respectively. It is found that the $F$-function determines directly the presence or absence of localized excited states, induced by bulk classical spins and nonmagnetic impurities, in the superconducting gap and their persistence with respect to impurity strength. Our results provide an alternative way to identify topologically insulating and superconducting phases in experiments without resorting to the surface properties.

(Some figures may appear in colour only in the online journal)

1. Introduction

Time-reversal (TR) invariant topological insulators (TI) are new state of matter in condensed matter physics, which have a full insulating gap in the bulk, but gapless edge or surface states consisting of an odd number of Dirac fermions [1]. Materials for TR invariant TIs, including HgTe/CdTe quantum wells, Bi$_1$-$\alpha$Sb$_\alpha$, alloys, binary (Bi$_2$Te$_3$, Sb$_2$Te$_3$, Bi$_2$S$_2$Te$_3$) and ternary (TiBiTe$_2$, TiBiS$_2$) compounds, have been confirmed experimentally according to the above characteristic definition, by either transport measurements of the quantized edge conductance $2e^2/h$, or angle-resolved photoemission spectroscopy measurements of the linear dispersion of the surface states as well as its odd numbers [1]. However, all these measurements aim only at the surface properties of the TR invariant TIs. While in a recent work [2] by two of the authors, through examining the localized excited states (LES) in the insulating gap induced by bulk impurities in quantum anomalous Hall (QAH) systems [3], in two-dimensional (2D) HgTe/CdTe quantum spin Hall (QSH) systems [4], as well as in TR invariant 3D strong TIs [5], they point out that distinctive behaviors between topological and conventional insulators exist, which help to distinguish topologically different insulating phases experimentally without resorting to surface features.

Soon after the discovery of TR invariant TIs, the study was generalized to TR invariant and breaking topological superconductors (TSC) [1, 6–16]. This generalization is natural because there is a direct analogy between superconductors and insulators, where the Bogoliubov–de Gennes (BdG) Hamiltonian for the quasiparticles of a superconductor is analogous to the Hamiltonian of a band insulator, with the superconducting gap corresponding to the band gap of the insulator. Instead of Dirac fermions, the gapless surface states of a TR invariant TSC consist of an odd number of Majorana cones, which only have half the degrees of freedom of Dirac fermions. While for TR breaking TSC, the vortex core carries an odd number of Majorana zero modes [1], giving rise to non-Abelian statistics and providing a possible platform for topological quantum computing [17]. Several ways to realize topological superconductivity by making use of the superconducting proximity effect on the 2D surface states of 3D TR invariant TIs [10], or on the 2D TR breaking TIs [11], and on semiconductors with strong Rashba
spin–orbit coupling have been imposed. However, no definitive proofs in experiments have yet been found so far.

Gapped systems can be classified into ten symmetry classes, among which four are the BdG classes for superconductors. Bearing in mind the extreme analogy between the BdG Hamiltonian of a superconductor and that of a band insulator, we show in this work that the BdG Hamiltonian for superconductors can also be assorted in another viewpoint into three categories of positive, negative, and zero ‘gap’ superconductors according to the so-called F-functions. By doping into bulk magnetic (which we treat as classical spins) and nonmagnetic impurities, we show that the characteristic properties of the F-functions determine directly the presence or absence of LES, induced by the impurities, in the superconducting or insulating gap, as well as the persistence of the LES with respect to impurity strength. Based on this observation, a generic method is proposed, by testing the response to classical spins as well as nonmagnetic impurities in the bulk, to differentiate the topologically nontrivial superconducting or insulating phases from the trivial ones in general, and also to distinguish a TSC from a conventional BCS superconductor in particular.

Specifically speaking, using the T-matrix method, it is found that, similarly as in TIs, in TSCs there are always four LES in the superconducting gap for the spin-dependent potential, whereas there are only two such LES for the ordinary potential. Moreover, these LES survive under arbitrary impurity strength. While when the TSC transits into the topologically trivial phase, the LES exist only at small impurity strength but then disappear into bulk bands at strong impurity strength. The classical spins localized in a BCS superconductor have been discussed by Shiba in 1968. In the viewpoint of F-functions, BCS superconductors fall into the critical category between the topologically trivial and nontrivial phases of a TSC. It is shown that two LES appear only for a spin-dependent potential but no such LES exist for ordinary potentials. Moreover, these two LES persistently tend nearer to the band edges at strong impurity strength, which is in a tricky contrast to the trivial phase of a TSC. Therefore, through the observation of the LES in superconducting (band) gap induced by bulk impurities, the potential strength of both spin-dependent and ordinary impurities can be used to tell the topologically nontrivial from the trivial phases of a TSC (TI), whereas nonmagnetic impurities can be used to distinguish a TSC from an ordinary (BCS) superconductor.

The rest of this paper is organized as follows. In section 2, we first briefly review the symmetry classification of the BdG Hamiltonian for superconductors. Through this classification, all categories of the BdG Hamiltonian can be reduced, if the additional particle–hole symmetry (PHS) is imposed, to the model Hamiltonian of either the 2D QSH system, or the 3D strong TI, or half the spin degree of freedom of the above two which breaks the TR symmetry. The responses to classical spins and nonmagnetic impurities of all these correspondences in TIs have been studied in [2], with the only exception being class C superconductors [20]. In section 3, we study the classical spins in superconducting (band) gap induced by bulk impurities serves as an effective criterion to tell the topological superconducting (insulating) phase. This work is finally concluded in section 4.

2. Brief review of symmetry classification of the BdG Hamiltonian for superconductors

In this section, we briefly review the symmetry classification of the BdG Hamiltonian for superconductors. It is concluded that within all topologically nontrivial categories of the four BdG classes in dimension two and three, only class C in dimension two is left unaddressed for a complete discussion.

In a recent pioneering work by Schnyder et al, ten symmetry classes of single-particle Hamiltonians for gapped systems are classified according to the presence or absence of TR symmetry, PHS, as well as sublattice symmetry. Among which, four symmetry classes (named as D, DIII, C, CI) arise in the BdG Hamiltonian for superconductors because of the definitive PHS but the alternative presence of TR symmetry or SU(2) spin rotational symmetry.

A general form of the BdG Hamiltonian for the dynamics of quasiparticles deep inside the superconducting state of a superconductor can be written as

\[ H = \frac{i}{2} \sum_k \left( c_k^\dagger c_k \right) \begin{pmatrix} \varepsilon_k & \Delta_k^\dagger \\ \Delta_k & -\varepsilon_k \end{pmatrix} \begin{pmatrix} c_k \\ c_k^\dagger \end{pmatrix}, \]

where \( c_k \) and \( c_k^\dagger \) can be either column or row vectors, \( \varepsilon_k = k^2/2m - \mu \) is the single-particle energy dispersion, \( \Delta_k = (d_k \cdot \mathbf{i})(\varepsilon_k) \) is the gap parameter with \( \mathbf{i} \) being the electron spin Pauli matrix vector, and \( d_k \) is a 3D vector in spin space as a function of momentum \( k \).

In class D, where neither SU(2) invariance nor TR symmetry is present, there exist topologically nontrivial superconducting phases in both 1D and 2D. A typical example of a BdG Hamiltonian in this class in 2D is the spinless chiral p-wave (\( p \pm ip \)) superconductors, where the gap parameter is explicitly \( \Delta_k = \Delta(k_x - ik_y), \Delta \in \mathbb{R} \). We notice that this BdG Hamiltonian of TR breaking p-wave superconductors is nothing else but the BHZ model of a QSH system with half the spin degree of freedom, or the QAH system studied by Qi et al [3], by dropping the terms proportional to the identity matrix to maintain the generic PHS. In this sense, a TSC can be viewed as a TI with PHS. Classical spins in QSH and QAH systems have been studied in the context of TI [2], where the term which breaks the PHS is shown to be unimportant to the topological properties of the systems under study. Therefore, definitively proofs in experiments have yet been found so far.

4 By classical spins, here and all throughout the paper, we refer to the classical limit of magnetic impurities where no quantum effect of spin-flipping is considered. In this sense, the classical spins can be viewed as a spin-dependent potential, whereas nonmagnetic impurities are treated as ordinary (spin-independent) potentials.

5 TSCs and TIs in one dimension are not included in our discussion.
it is safe to conclude that the $p + ip$ superconductors have nontrivial responses to spin-dependent (ordinary) potentials, where there are always two (one) LES in the superconducting gap in the topologically nontrivial phase, which disappear in the trivial phase.

In class DIII, although full $SU(2)$ invariance is still absent, TR symmetry is restored. The simplest way to regain TR symmetry is to make two copies of the TR breaking system, but with the whole being a TR conjugate pair. In this class, topologically nontrivial superconducting phases exist in all three dimensions. An interesting example in 2D is the equal superposition of two chiral $p$-wave superconductors with opposite chiralities ($p_x + ip_y$ and $p_x - ip_y$ waves), namely the helical $p + ip$ superconductors, where the $d$-vector is explicitly $d_\text{h} = \Delta(-k_x, k_y, 0)$. In the basis of $(c_{r}^\dagger c_{l}) = (c_{k}^\dagger c_{-k}^\dagger)$, we see that the BdG Hamiltonian of the helical $p + ip$ superconductors is completely identical to that of the BHZ model in HgTe/CdTe quantum wells with PHS, where spin up (down) electrons form Cooper pairs. Hence the response of such helical $p + ip$ superconductors is similar to that of the QSH systems, where persistent LES exist in the superconducting gap. In 3D, a member of class DIII is the Balian–Werthamer (BW) state [22] of the B phase of liquid $^3$He described by the $d$-vector $d_\text{h} = \Delta(k_x, k_y, k_z)$. In the same basis as the helical $p + ip$ superconductors, the model Hamiltonian of the BW state is the same as that of a 3D TI, which reduces exactly to the 2D QSH system in the limit $k_z \sim (k_z) \approx 0$. We have also studied the sp–d exchange coupling in 3D TIs [2], where again the LES behave distinctively in topologically nontrivial and trivial phases, which is also valid for the BW state of topological superfluids.

With the presence of full $SU(2)$ invariance, the BdG Hamiltonians fall into the C and CI classes in the absence and presence of TR symmetry. Nontrivial topological phases exist in 2D in class C, while in 3D in class CI. A full focus on the five categories of TR invariant TIs in 3D out of ten symmetry classes have been laid out in the pioneering work by Schnyder et al [7], therefore for a complete discussion the only unaddressed one is the 2D case in class C, which is our main attention in this work. The interesting example in class C in 2D is the TR breaking superconductors with $(d + id)$-pairing [20]. Under the basis $(c_{r}^\dagger c_{l}) = (c_{k}^\dagger c_{-k}^\dagger)$, the gap parameter in $d + id$ superconductors is

$$\Delta_s = \Delta_{d2-\gamma^2} (k_x^2 - k_y^2) - i\Delta_{xy} k_x k_y,$$

where $\Delta_{d2-\gamma^2}$ and $\Delta_{xy}$ are real amplitudes.

In the following, we study the topological properties of the $d + id$ superconductors as well as its response to classical spins and nonmagnetic impurities in bulk using the $T$-matrix method. It is found that the $d + id$ superconductors show the same behavior as that of TIs. Specifically, in the topologically nontrivial phase, there are four LES in the superconducting gap for magnetic impurities and two LES for nonmagnetic impurities at arbitrary impurity strength. These LES then disappear into the bulk bands at large impurity strength as the system transits into the topologically trivial phase. For comparison, no LES appear with nonmagnetic impurities in a BCS superconductor. Therefore, by testing the response to both magnetic and nonmagnetic impurities, not only a topologically nontrivial phase can be distinguished from a trivial one, but also a conventional BCS superconductor can be discriminated from a TSC.

3. Classical spins in $d_{p2-\gamma^2} + id_{xy}$ superconductors

In this section, we study $d + id$ superconductors described by equation (2) as a specific example in class C in parallel to the previous work in [2]. The results are stated in the language of superconductors in particular, which are also valid for insulating systems in general.

The single-particle Hamiltonian of $d + id$ superconductors in momentum space is written as $h(\mathbf{k}) = f_0(\mathbf{k}) \sigma^\alpha \mathbf{f}$, where $\alpha = 1–3$, and in tight-binding model, $f(\mathbf{k}) = (\Delta_{d2-\gamma^2} (\cos k_x - \cos k_y), -\Delta_{xy} \sin k_x \sin k_y, t(4 - \cos k_x - \cos k_y) - \mu)$, with $t$ being the hopping energy. The Hall conductivity of this two-band system at zero temperature when the chemical potential lies inside the band gap is calculated using the standard Kubo formula as [3]

$$\sigma_{xy} = -\frac{1}{8\pi^2} \int_{FBZ} \frac{dk_x dk_y \mathbf{f} \cdot \partial_{k_x} \mathbf{f} \times \partial_{k_y} \mathbf{f}}{E_F - E_{\mathbf{k}}},$$

where $f_0(\mathbf{k}) = f_{0x}(\mathbf{k})/|f(\mathbf{k})|$ is the unit vector along the direction $f_{0x}$ and $f(\mathbf{k}) = \sqrt{f_{0x}(\mathbf{k}) f_{0y}(\mathbf{k})/|f(\mathbf{k})|^2}$. This Hall conductivity is related to the so-called Skyrme number $[3, 24]$ by $\sigma_{xy} = -Q_{sky}/2\pi$, which is an integer, and in $d + id$ superconductors it is shown to be

$$Q_{sky} = \begin{cases} -2\text{sgn}(\Delta_{d2-\gamma^2}/\Delta_{xy}), & 0 < \mu < 8, \\ 0, & \mu < 0 \text{ or } \mu > 8. \end{cases}$$

Therefore the bulk-edge correspondences tell us that there should localize two edge states at each boundary in the topologically nontrivial phase, which is indeed true, as seen in figure 1, where typical energy spectra of $d + id$ superconductors are shown.

To consider the single-particle excitations in the superconducting gap, our starting point is to rewrite the BdG
Hamiltonian of $d + id$ superconductors in Nambu space [18, 23] as

$$H_{\text{BdG}} = \frac{1}{2} \sum_{k} \sum_{k'} A_k^{\dag} \begin{pmatrix} \varepsilon_k & \Delta_k & 0 & 0 \\ \Delta^*_k - \varepsilon_k & -\Delta_k & 0 & 0 \\ 0 & 0 & -\varepsilon_{k'} & 0 \\ 0 & 0 & 0 & -\varepsilon_{k'} \end{pmatrix} A_{k'},$$

where the gap parameter $\Delta_k$ is given in equation (2), and $A_k^{\dag} = \{c_{k+}^\dag, -c_{-k}^\dag, c_{k}^\dag, c_{-k}^\dag\}$. This is because the Green’s function (GF) formulation in Nambu space can be easily generalized to include the paramagnetic impurities as well as the Kondo effect. Also notice that the above BdG Hamiltonian of a $d + id$ superconductor in Nambu space is formally similar to the 2D Luttinger model in the hole bands of a semiconductor. [3]

In the presence of a localized spin or an ordinary potential in bulk, their interactions between conduction electrons are respectively

$$H_{\text{ex}} = \langle J/2 \rangle \sum_{k\varepsilon} c_k^{\dag} S \cdot \sigma c_{\varepsilon}, \quad H' = \langle V/2 \rangle \sum_{k\varepsilon} c_k^{\dag} c_{\varepsilon},$$

where $S = (S_x, S_y, S_z)$ is the vector of a localized spin with modulus $S^2 = S_a S^a$. Again in Nambu space they take the form

$$H_{\text{ex}} = \frac{J}{2} \sum_{kk'} \sum_{\alpha} A_k^{\dag} \begin{pmatrix} S_+ & S_- & 0 & 0 \\ S_- & S_+ & 0 & 0 \\ 0 & 0 & -S_+ & -S_- \\ 0 & 0 & -S_- & -S_+ \end{pmatrix} A_{k'},$$

$$H' = \frac{V}{2} \sum_{kk'} \sum_{\alpha} A_k^{\dag} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} A_{k'},$$

with the diagonal elements

$$F_{\epsilon(h)}(\omega) = \frac{1}{N} \sum_{k} \frac{\omega + (-)^{\epsilon_k}}{\omega^2 - \epsilon_k^2 - |\Delta_k|^2}.$$  

It is interesting to notice that this $F$-function in $d + id$ superconductors is diagonal too, as that in the QSH system in HgTe/CdTe quantum wells with $p$-wave symmetry studied before [2]. This is because the off-diagonal terms are momentum integrations of the gap parameter $\Delta_k$; although $\Delta_k$ has a quadratic dependence on momentum, the integration of the real part cancels exactly since the integrand is symmetric with respect to $k_x$ and $k_y$, while the imaginary part vanishes uniformly as the integrand is an odd function of $k_x$ and $k_y$.

Therefore, the eigenenergies for the LES induced by classical spins and ordinary potentials are obtained by finding the poles of the above $T$-matrix in (10) and (11) respectively for energies in the superconducting gap as

$$(JS/2)F_{\text{id}}(\omega) = \pm 1,$$  

$$(V/2)F_{\text{e}}(\omega) = 1, \quad \text{and} \quad (V/2)F_{\text{h}}(\omega) = -1,$$

which consist of four conditions when the impurity is spin-dependent whereas only two conditions when the impurity is spin-independent.

To see how these conditions are satisfied for general impurity strength $J$ and $V$, we numerically examine the momentum integrations in equation (13) in both topologically nontrivial and trivial phases which are identified in equation (4) by constraining the frequency $\omega$ in the superconducting gap only. Using the tight-binding model where $\varepsilon_k = t(4 - \cos k_x - \cos k_y) - \mu$, $|\Delta_k|^2 = \Delta_0^2(\cos k_x - \cos k_y)^2 + \Delta_0^2\sin^2 k_x \sin^2 k_y$, and replacing $(1/N)\sum_k \rightarrow (1/4\pi^2) \int dk_x dk_y$, several representative $F$-functions are plotted versus frequency for topologically nontrivial phases in figures 2(a)–(d), and for topologically trivial phases in figures 2(e)–(h). A striking difference of the $F$-functions between topologically nontrivial and trivial phases is immediately recognized in these figures. First of all, it is seen that each of the electron band $F$-function $F_{\text{e}}(\omega)$ and the hole band $F$-function $F_{\text{h}}(\omega)$ wind from $-\infty$ to $\infty$ within the entire range of $\omega$ in the superconducting gap, and there is a negative ‘gap’ between $F_{\text{e}}(\omega)$ and $F_{\text{h}}(\omega)$ in topologically nontrivial phase. (See figures 2(a)–(d)). Therefore, all of the four resonant conditions in equation (14) for classical spins can be satisfied at any impurity strength $J S$ (for both $J > 0$ and $J < 0$), and we expect four persistent LES to exist in the superconducting gap. Similarly for the ordinary potential, both of the resonant conditions in equation (15) can also be met with arbitrary $V (>0$ or $<0)$, hence two persistent LES in the superconducting gap are expected when the impurity is spin-independent. While in a sharp contrast, in the topologically trivial phase, both of the electron band $F$-function and the hole band $F$-function terminate at some finite value at one end of number-axis whereas they diverge at the other end, which are separated by a positive ‘gap’. (See figures 2(e)–(h)). Consequently, only one condition in each of $F_{\text{e}}(\omega)$ and $F_{\text{h}}(\omega)$ in equation (14) becomes true at small $JS$, but fails for strong enough impurity strength in the case of
potential is presented. We see that in the topologically figures 3(c)–(f), real space diagonalization with an ordinary is, the deeper the LES are localized in the gap. While in
nontrivial phase (lower panel), and the stronger the gap at arbitrary impurity strength in the topologically superconducting gap for different $\mu$'s. (a)–(d) $F$-functions in the topologically trivial phase. The electron band $F$-function $F_e(\omega)$ is shown as red lines while the hole band $F$-function $F_h(\omega)$ is shown as green lines. Parameters are taken as $\text{sgn}(\Delta,_{2\mu,\nu} \Delta,_{\nu\mu}) = -1$ and all energies are measured in units of $t$.

![Figure 2. $F$-functions versus $\omega$ which lies in the bulk superconducting gap for different $\mu$'s. (a)–(d) $F$-functions in the topologically trivial phase. The electron band $F$-function $F_e(\omega)$ is shown as red lines while the hole band $F$-function $F_h(\omega)$ is shown as green lines. Parameters are taken as $\text{sgn}(\Delta,_{2\mu,\nu} \Delta,_{\nu\mu}) = -1$ and all energies are measured in units of $t$.](image)

classical spins. The case is trickier for ordinary potentials, and depends on the sign of product of $V$ and $\mu$, $\text{sgn}(V\mu)$. Since the electron band $F$-function $F_e(\omega)$ is negative definite and the hole band $F$-function $F_h(\omega)$ is positive definite for $\omega$ in the superconducting gap when $\mu < 0$ (see figures 2(e)–(f)), no LES exist for repulsive interactions but two LES appear for attractive interactions. And in the attractive situation, the two LES finally disappear at large $V$. Vice versa when $\mu > 8$.

As an independent examination of the above statements analyzed solely from the $F$-function behaviors, we have also directly diagonalized the total Hamiltonian $H = H_{BdG} + H_{\text{imp}}(H')$ in real space as a function of impurity strength $|JS|$ ($|V|$) in figure 3. In figures 3(a) and (b), real space diagonalization with spin-dependent potential is shown, where we see that in the topologically trivial phase (up panel) there are indeed two LES winding through the superconducting gap at small $|JS|$, which disappear at strong $|JS|$. Nevertheless, four LES persist in the superconducting gap at arbitrary impurity strength in the topologically nontrivial phase (lower panel), and the stronger the $|JS|$ is, the deeper the LES are localized in the gap. While in figures 3(c)–(f), real space diagonalization with an ordinary potential is presented. We see that in the topologically nontrivial phases for both signs of $V$ (figures 3(d) and (f)), two persistent LES exist in the superconducting gap. And in the topologically trivial phases, no LES appear in the superconducting gap when $V\mu < 0$ (figure 3(c)), but two persistent LES exist at small $|V|$ when $V\mu > 0$ (figure 3(e)). These pictures support perfectly our predictions merely from the $F$-function properties given in figure 2. In addition, we could expand the $\delta$-function of the impurity potential and consider a finite range spin-dependent scattering with $V = V_0|\mathbf{r} - \mathbf{r}_0|^2 + \Gamma^2$.

For comparison, we now discuss the $F$-functions as well as LES induced by classical spins and nonmagnetic impurities in BCS superconductors, which were studied quite early by H. Shiba [18]. In a BCS superconductor, the corresponding $F$-function is analytically obtained as $F_{\text{BCS}}(\omega) = -\pi N_F((\omega/\Delta_0) \pm 1)\sqrt{1 - (\omega/\Delta_0)^2}$, where $\Delta_0$ is the real gap parameter and $N_F$ is the density of states at the Fermi energy in the normal state. This $F$-function $F_{\text{BCS}}(\omega)/(\pi N_F)$ versus energy is plotted in figure 4(a) for $|\omega/\Delta_0| < 1$, where we see that both the electron and hole band $F$-functions diverge at one end while terminating at the same value at the other end. Therefore, in this sense, a BCS superconductor can be viewed as a zero ‘gap’ superconductor compared to the positive ‘gap’ topologically trivial and negative ‘gap’ topologically nontrivial phases of a TSC. For classical spins in a BCS superconductor, there are always two LES in the superconducting gap at energies $\pm \omega_{\text{BCS}} = \pm \Delta_0(1 - (JS\pi N_F/2)^2)/(1 + (JS\pi N_F/2)^2)$, as shown in figure 4(b), where we see that they behave critically between the topologically trivial and nontrivial phases exhibited in figure 3. The two LES in the BCS superconducting gap persistently tend nearer to the band edges as the impurity strength goes to infinity, but never disappear. While in contrast, the two LES of the trivial phase in a TSC go to the band edges with the increase of impurity strength and then disappear into the bulk at some finite value of $|JS|$ or $|V|$. For the ordinary potential in BCS superconductors, it is shown that LES never appear because the corresponding $F$-matrix has no singularities in the superconducting gap.

The response of a TSC to classical spins and nonmagnetic impurities compared with that of a conventional BCS superconductor is summarized in table 1, where those persistent LES which survive at arbitrary impurity strength are numbered in bold. This result provides an effective way to distinguish the topologically trivial and nontrivial phases of a TSC, and also to tell a conventional BCS superconductor from a potential TSC, without resorting to the surface properties. This is the main result of our work.
Figure 3. Real space diagonalization of the total Hamiltonian $H_{\text{BdG}} + H_{\text{ex}}$ in (a)–(b) and $H_{\text{BdG}} + H'$ in (c)–(f) as a function of impurity strength. The bulk states are represented by blue lines and LES in superconducting gap are denoted in red lines. Parameters are taken as $\text{sgn}(1 - \frac{y^2}{2}) = -1$ in all the figures, $\mu = \pm 3$ in topologically nontrivial and trivial phases, and all energies are measured in units of $t$. (a)–(b) Topologically trivial and nontrivial phases for a spin-dependent potential. (c)–(d) Topologically trivial and nontrivial phases with $V > 0$ for an ordinary potential. (e)–(f) Topologically trivial and nontrivial phases with $V < 0$ for an ordinary potential.

Figure 4. (a) $F$-function in BCS superconductors where the electron and hole band $F$-functions terminate at the same value (see the dotted line) and form a zero ‘gap’. (b) Eigenenergies of two LES induced by classical spins versus impurity strength in a BCS superconductor.

Table 1. The number of LES in the superconducting gap induced by classical spins and nonmagnetic impurities in a TSC as well as in a conventional BCS superconductor. The bold numbers indicate that the corresponding LES exist at arbitrary impurity strength.

| $JS/2$ | Trivial-TSC | Nontrivial-TSC | BCS |
|-------|-------------|----------------|-----|
| $V/2$ | 2           | 4              | 2   |
|       | 0, $\text{sgn}(V\mu) < 0$ | 2              | 0   |
|       | 2, $\text{sgn}(V\mu) > 0$ |                |     |

4. Conclusions and discussions

In conclusion, classical spins in generic TIs and TSCs are studied in an earlier [2] and the present work. In particular, an $F$-function is defined in such systems, where the differences of which from electron and hole bands classify the BdG Hamiltonian of superconductors into positive, negative, and zero ‘gap’ categories respectively for the topologically trivial and nontrivial phases of a TSC and a BCS superconductor. The characteristic features of $F$-functions determine directly the presence or absence of LES, induced by bulk classical spins and nonmagnetic impurities, in the superconducting gap as well as their persistence with respect to impurity strength. The responses of TSC and BCS superconductors to bulk classical spins and nonmagnetic impurities are summarized, where it is shown that the potential strength of both spin-dependent and ordinary impurities can be used to tell the topologically nontrivial from the trivial phases of a TSC, whereas nonmagnetic impurities can be used to distinguish a TSC from an BCS superconductor. Our results provide an alternative way to identify topologically insulating and superconducting phases in experiments without resorting to the surface properties.

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