The fate and heir of Majorana zero modes in a quantum wire array

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Experimental signatures of Majorana zero modes in a single superconducting quantum wire with spin-orbit coupling have been reported as zero bias peaks in the tunneling spectroscopy. We study whether these zero modes can exist in an array of coupled wires, and if not, what their remnant could be. The bulk exhibits topologically distinct gapped phases and an intervening gapless phase. Even though the bulk pairing structure is topological, the interaction between Majorana zero modes and superfluid phases leads to spontaneous time-reversal symmetry breaking. Consequently, edge supercurrent loops emerge and edge Majorana fermions are in general gapped out except when the number of chains is odd, in which case one Majorana fermion survives.

Introduction

Majorana fermions are intriguing objects because they are their own antiparticles. In condensed matter physics, Majorana fermions arise not as elementary particles, but rather as superpositions of electrons and holes forming the zero mode states in topological superconducting states. Majorana fermions were first proposed to exist in vortex cores and on boundaries of the p-wave Cooper pairing systems. More recently, they were also predicted in conventional superconductors in the presence of strong spin-orbit (SO) coupling and the Zeeman field. In cold atom physics, SO coupling has been realized by using atom-laser coupling. This progress offers an opportunity to realize and manipulate Majorana fermions in a highly controllable manner, which has attracted a great deal of attention both theoretically and experimentally.

Experimental signatures of Majorana zero modes have been reported as zero bias peaks in the tunneling spectroscopy of a single quantum wire with strong SO coupling which is either coupled with an s-wave superconductor through the proximity effect, or, is superconducting by itself. A further study of an array of quantum wires is natural, in particular for the purpose of studying interaction effects among edge Majorana zero modes. Topological states in an array of parallel wires in magnetic fields in the fractional quantum Hall regime have been studied recently. Without imposing self-consistency, flat bands of Majorana zero modes have been found for the uniform pairing as well as the Fulde-Ferrell-Larkin-Ovchinnikov pairing, because under time-reversal (TR) symmetry these Majorana zero modes do not couple.

However, the band flatness of the edge Majorana zero modes is unstable due to interaction effects. Li and two of the authors proposed the mechanism of spontaneous TR symmetry breaking for the gap opening in the edge Majorana flat bands. Even in the simplest case of spinless fermions without any other interaction channels, the coupling between Majorana zero modes and the pairing phase spontaneously generates staggered circulating currents near the edge such that Majorana modes can couple to each other to open the gap due to the breaking of TR symmetry. Similar results are also obtained recently in Refs. 26 and 47. The mechanism of gap opening based on spontaneous TR symmetry breaking also occurs in the helical edge modes of the 2D topological insulators under strong repulsive interactions which leads to edge magnetism.

Main results

In this article, we investigate a coupled array of s-wave superconducting chains with intra-chain SO coupling and external Zeeman field. We consider both the proximity-induced superconductivity and the intrinsic one. For the proximity-induced case, the array is placed on top of a bulk superconductor, the phase coherence induces a nearly uniform pairing distribution in the quantum chains, \( \Delta_r = \Delta \). The bulk band structure exhibits several topologically distinct gapped phases intervened by a gapless phase. In the gapless phase, edge Majorana zero modes interpolate between nodes in the bulk energy spectrum. In the topological gapped phase, they extend into a flat band across the entire edge Brillouin zone. On the other hand, if either the phase coherence of the bulk superconductor is weak, or the superconductivity is intrinsic, such as in the case of Pb nanowires or cold atom systems near Feshbach resonance, then \( \Delta_r \) has to be solved self-consistently. We find that when the bulk is in the topological gapped phase, the phase distribution of pairing order parameters is inhomogenous along the edge exhibiting TR symmetry breaking. It induces edge currents and gaps out the edge Majorana zero modes except when the chain number is odd, in which case one Majorana zero mode survives. If the bulk is in the gapless phase, in general TR breaking is observed but not always, because Majorana modes associated with opposite winding numbers can coexist on the same edge which can be coupled by TR invariant perturbations.

Model of quantum wire array

Consider an array of SO coupled chains with the proximity effect induced s-wave pairing along the \( x \)-direction, which are juxtaposed along the \( y \) direction. The band Hamiltonian is

\[
H_0 = - \sum_{r,\sigma} t \left( c_{r,\sigma}^\dagger c_{r+\hat{x},\sigma} + h.c. \right) - \mu c_{r,\sigma}^\dagger c_{r,\sigma} - \sum_r \lambda \left( c_{r+\hat{x},\sigma}^\dagger c_{r,\sigma} - c_{r,\sigma}^\dagger c_{r+\hat{x},\sigma} \right) + h.c. - \sum_{r,\sigma} t_\perp \left( c_{r,\sigma}^\dagger c_{r+\hat{y},\sigma} + h.c. \right),
\]
where \( \Delta_r \) is the pairing order parameter on site \( r \), and \( B \) is the external Zeeman field.

**Uniform pairing** Let us first consider a uniform pairing \( \Delta_r = \Delta \) which can be chosen as real without loss of generality. Under periodic boundary conditions in both \( x \) and \( y \)-directions, the Hamiltonian Eqs. 1 and 2 can be written in momentum space, \( H = H_{\text{band}} + H_{\text{ex}} = \sum_k \psi_k \psi_k^\dagger \), where \( \psi_k = [c_{r\uparrow}, c_{r\downarrow}]^t \), and

\[
h_k = T_k \tau_3 + \Lambda_k \sigma_3 - B \sigma_1 \tau_3 + \Delta \tau_2 , \tag{3}
\]

with \( T_k = -2t \cos k_x - 2t_\perp \cos k_y - \mu + \Lambda_k = 2 \lambda \sin k_y \). The two sets of Pauli matrices \( \sigma_i \) and \( \tau_i \) \((i = 1, 2, 3)\) act in the spin and particle-hole spaces, respectively. The energy spectrum of Eq. 3 is

\[
E_k^2 = T_k^2 + \Lambda_k^2 + B^2 + \Delta^2 \pm 2 \sqrt{T_k^2 \Lambda_k^2 + T_k^2 B^2 + B^2 \Delta^2} , \tag{4}
\]

Although \( h_{k_x,k_y} \) does not carry 2D topological indices, nevertheless, we consider the 1D index of \( h_{k_x,k_y} \) at each fixed value \( k_y \). It is invariant under both particle-hole (\( \Xi \)) and TR (\( \Theta \)) symmetries: define \( \Xi = \tau_1 \) and \( \Theta = \sigma_1 \tau_5 \), then \( \Xi h_{k_x,k_y} \Xi^{-1} = -\Theta h_{k_x,k_y} \Theta^{-1} = -h_{-k_x,-k_y}^* \). Here both transformations satisfy \( T^2 = \Xi^2 = 1 \) rather than \(-1\). These two symmetries can be combined into a chiral symmetry defined as \( C = \Xi \Theta \), which gives \( Ch_{k_x,k_y} C^{-1} = -h_{-k_x,-k_y} \). These symmetries put \( h_{k_x,k_y} \) at fixed \( k_y \) in the BDI class as pointed out in Ref. [39], which is characterized by a \( k_y \)-dependent 1D topological index denoted as \( W_{k_y} \). A unitary transformation is performed as \( U = e^{i(\pi/4)\sigma_1} u e^{-i(\pi/4)\tau_1} \) where \( u = \frac{1}{2} (\sigma_0 + \sigma_3) + \frac{i}{2} \tau_3 (\sigma_0 - \sigma_3) \).

It transforms \( h_k \) into an off-diagonal form

\[
U^{-1} h_k U = \begin{bmatrix} A_k & \Lambda_k^* \\ \Lambda_k & 0 \end{bmatrix} , \tag{5}
\]

where \( A_k = \Delta \sigma_1 - i(T_k \sigma_0 + \Lambda_k \Lambda_1 + 2B \tau_3) \). \( W(k_y) \) is defined as the winding number of \( A_k \) in the complex plane as \( \kappa_x \) sweeps a \( 2\pi \) cycle, viz., Ref. [39, 50]

\[
W_{k_y} = -\frac{i}{2\pi} \int_{k_0}^{2\pi} \frac{dz(k)}{z(k)} = \frac{1}{2} \left[ \text{sgn}(M_+) - \text{sgn}(M_-) \right] \text{sgn}(\lambda \Delta) , \tag{6}
\]

where \( z(k) = \det A_k / |\det A_k| \); \( \det A_k = B^2 - T_k^2 - (\Delta - i\Lambda_k)^2 \); \( M_+(k_y) = \det A_{k_y=0,k_y} \), and \( M_-(k_y) = \det A_{k_y=\pi,k_y} \). \( W_{k_y} \) is \( \pm 1 \) requires the condition of \( M_+(k_y) M_-(k_y) < 0 \), and then \( h(k_y) \) is topologically nontrivial. \( W_{k_y} \) changes discretely if a gap closing state appears on the line of \( k_y \) such that \( M_+(k_y) = 0 \), or, \( M_-(k_y) = 0 \). The momenta of these states \((k_x,k_y)\) satisfy that \( k_x = 0 \) or \( \pi \), and another condition \( T_k^2 + \Delta^2 - B^2 = 0 \) which determines \( k_y \).

Based on \( W_{k_y} \)’s behavior over the range of \([-\pi, \pi]\), we plot the bulk phase diagram for the 2D Hamiltonian Eqs. 1 and 2 in the parameter plane \( \mu-B \) shown in Fig. 1(a).
The gapped phases are characterized by $k_y$-independent values of $W$: two phases with $W = \pm 1$ are weak topological pairing states, and the other two with $W = 0$ are trivial pairing states. For the gapless phase, a momentum averaged topological number is defined as

$$ r = \int \frac{dk_y}{2\pi} W(k_y). $$

The values of $W_{k_y}$ v.s. $\mu$ and $k_y$ are depicted in Fig. 1(b) along the line cuts $L_1 \sim L_5$ in Fig. 1(a). Usually, $W_{k_y}$ only changes the value by 1 at one step as varying $k_y$, but along line $L_3$, $W_{k_y}$ can directly change between 1 and -1 without passing 0, which means two Dirac points $(0, k_y)$ and $(\pi, k_y)$ appear at the same value of $k_y$.

Next we discuss edge spectra in the above different phases. The open boundary condition is applied along the $x$-direction. In the topological trivial phase shown in Fig. 2(a), the zero energy edge modes are absent, while they appear and run across the entire 1D edge Brillouin zone in the gapped weak topological pairing phase shown in Fig. 2(b). In the gapless phase, flat Majorana edge modes appear in the regimes with $W(k_y) = \pm 1$ and terminate at the gap closing points. These flat Majorana edge modes are lower dimensional Majorana analogues of Fermi arcs in 3D Weyl semi-metals\cite{3D Weyl semi-metals}. This analogy goes further as in both cases: the gapless phase intervenes topologically distinct gapped phases.

The flat edge Majorana modes in the gapless phase can behave differently. In Fig. 2(b), all the edge flat Majorana modes are associated with the same value of $W_{k_y}$. In this case, these Majorana modes on the same edge are robust at the zero energy if TR symmetry is preserved, which means that they do not couple. Nevertheless, TR symmetry may be spontaneously broken to gap out these zero modes\cite{TR symmetry breaking}. On the other hand, for states inside the white dashed diamond in Fig. 1(a), edge Majorana modes appear with both possibilities of $W_{k_y} = \pm 1$. In particular, in the case of $\mu = 0$, the relation $W(k_y) = -W(k_y + \pi)$ holds for edge Majorana modes as shown in Fig. 2(d). Majorana modes with opposite winding numbers on the same edge can couple to each other even without TR breaking, and thus are not topologically stable. $r$ represents the net density of states of zero modes in the edge Brillouin zone which are stable under TR-conserved perturbations.

**Self-consistent solution** We now impose self-consistency on the pairing order parameter $\Delta_r$, which is necessary for the case of intrinsic pairings. The pairing interaction is modeled as $H_\Delta = -g \sum_{\alpha} n_{\alpha \uparrow} n_{\alpha \downarrow}$, and the self-consistent equation is $\Delta_r = -g \langle G | \gamma_{\alpha \downarrow} c_{\alpha \uparrow} | G \rangle$, where $\langle G | ... | G \rangle$ means the ground state average. We have verified numerically that $\Delta_r$ is nearly uniform inside the bulk. Thus the bulk shares a similar phase diagram to the case of uniform pairing (cf. Fig. 1), except that the values of $\Delta$ should be self-consistently determined.

Nevertheless, near edges $\Delta_r$ varies spatially in the self-consistent solutions. If the bulk is in the topological gapped phase, the edge Majorana zero modes can couple with each other by breaking TR symmetry spontaneously as shown in Ref. [25]. Because of the band flatness, this effect is non-perturbative. This will gap out the zero Majorana modes and lower the edge energy. The system converges to an inhomogeneous distribution of $\text{arg} [\Delta_r]$. 

![FIG. 2. Edge spectra with the open and periodical boundary conditions along the x and y-directions, respectively. (a), (b), (c), and (d) correspond to points I, II, III, and IV marked in Fig. 1(a), respectively. (a) gapped trivial phase; (b) gapless phase with edge modes associated with the same winding number; (c) gapped weak topological phase; (d) gapless phase with edge modes associated with opposite winding numbers. Parameters used are the same as those in Fig. 1(a).](image)

![FIG. 3. Self-consistent solutions for $\Delta_r$ (a) and supercurrent $J_{rr'}$ (b). Parameter values are $L_x = 120, L_y = 8, B = 1.25, t = 1, t_z = 0.5, \mu = -2, \lambda = 2, g = 5$. Open and periodical boundary conditions are used along the x-direction (vertical) and y-direction (horizontal), respectively. Only the first 10 sites from the upper edge are plotted. The distributions of $\Delta_r$ and $J_{rr'}$ are reflection symmetric with respect to the center line of the system. (a) Direction and length of each arrow represent the phase and amplitude of $\Delta_r$ on site $r$. Its distribution is nearly uniform in the bulk but exhibits spatial variations near the edge. (b) Each arrow represents $J_{rr'}$ on bond $rr'$, which is prominent near the edge but vanishes in the bulk.](image)
near the edges as shown in Fig. 3 (a), even if this costs energy by disturbing the Cooper pairing. This edge inhomogeneity in the pairing phase leads to an emergent current pattern as depicted in Fig. 3 (b).

A natural question is under what conditions TR symmetry is spontaneously broken near edges. We have carried out extensive numerical studies and results of $\mu = -2$ are plotted in Fig. 4 (a) and (b). TR symmetry is always broken in the topological gapped phase such that Majorana edge fermions are pushed to midgap energies, while TR symmetry remains unbroken in the trivial gapped phase. The latter is easy to understand because there are no Majorana fermions to begin with. If the bulk is in the gapless phase (shaded area in Fig. 4), the situation is more complicated. TR symmetry breaking solutions are found in most part of the gapless phase. In this regime, $|r| < 1$ and thus the number of stable Majorana modes on one edge is less than the number of chains $L_y$. These modes are associated with the same value of $W_k$, and thus TR symmetry breaking is needed to gap out these edge modes. There exists a small region inside the gapless phase in which TR symmetry is unbroken in Fig. 4 (a), which is largely due to the finite value of $L_y$. We have tested that as increasing $L_y$ the TR breaking regime is extended, and thus we expect that it will cover the entire gapless phase in the thermodynamic limit. On the other hand, for the case of the gapless phase with $\mu = 0$ in which $r = 0$ for even values of $L_y$, our calculations show that all the Majorana modes are gapped out without developing currents. Instead a bond-wave order appears at the wavevector of $k_y = \pi$ along the edge, which is consistent with the fact that TR invariant perturbations can destroy Majorana zero energy modes at $r = 0$. In general, we expect that TR symmetry is spontaneously broken in the case of $r \neq 0$ in the thermodynamic limit.

However, not all Majorana edge modes have to be gapped out in the topological gapped phase. As shown in Fig. 4 (b), for the case of $L_y = 8$, all the edge modes become gapped due to TR symmetry breaking, whereas for $L_y = 7$, one Majorana mode survives at zero energy. The reason is that breaking TR brings the system from class BDI to class D, and the latter is characterized by a $\mathbb{Z}_2$ index. Physically it is because (in the infinite chain length limit) only the Majorana modes on the same edge can be paired and gapped out, thus beginning with $L_y$ Majorana fermions per edge, for odd $L_y$, one of them will always remain unpaired. In short, if TR is spontaneously broken, only $L_y \mod 2$ Majorana fermion per edge will persist at zero energy.

**Summary and discussion** We have studied quantum wire arrays with SO coupling and s-wave superconductivity in an external Zeeman field. The relation between edge Majorana zero modes and the bulk band structure is investigated in both topologically nontrivial gapped phase and the gapless phase. The coupling between Majorana modes and superfluid phases leads to spontaneous TR symmetry breaking. Our results have several experimental bearings. For proximity effect induced superconductivity, the number of edge Majorana fermions in the gapless phase can be tuned by the Zeeman field from zero all the way up to the number of chains. This could be detected as a prominent change in the height of zero bias peaks in tunneling spectroscopy experiments. For the intrinsic superconductivity, edge supercurrent loops resulting from spontaneous TR breaking will induce small magnetic moments, which can be detected using magnetically sensitive experiments such as nuclear magnetic resonance or neutron scattering. The fluctuation in the number of persisting Majorana mode between 1 and 0, in the TR-broken topological gapped phase, may also show up in tunneling spectroscopy.
We thank Yi Li for early collaborations, Hui Hu and D. P. Arovas for helpful discussions, and D. P. Arovas for comments after reading a draft of this paper. DW and CW are supported by the NSF DMR-1105945 and AFOSR FA9550-11-1-0067 (YIP). ZSH is supported by NSF through grant DMR-1007028. CW acknowledges the support from the NSF of China under Grant No. 11328403.

Note added Upon the completion of this work, we became aware of the nice paper on a similar topic, and after this work is posted, we noticed another related work.

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