Tunable cooperating and competing vortex topologies in [100] iron-based superconducting nanowire

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We study the vortex Majorana physics in the iron-based superconducting when the magnetic filed is along [100] direction. While the vortex phase along [001] direction has been widely studied, our theory establishes a new Majorana vortex phase transition paradigm for multiple bands superconducting system which is unique for the [100]-vortex. According to the symmetry of the system, the vortex states can be classified by the eigenvalues of the $C_{2x} = \pm 1$. We find that for the vortex states carried by Dirac band, the C_{4z} symmetry breaking term can determine the topological phase transition to happen in which C_{2x} sectors while this mechanism is absent for [001] vortex. More importantly, this paradigm can enhance the topological vortex regime when considering the interplay between the Dirac and topological insulator bands. Meanwhile, either TI or Dirac bands carrying the vortex states always have full gap which is helpful to reduce the in-gap trivial states. As a result, we propose that the iron-based superconducting nanowire along [100] direction is a promising platform to realize Majorana zero modes with potential advantages in controllability.

Introduction– Majorana zero modes (MZMs) have attracted many theoretical and experimental interests in view of their non-Abelian statistical properties and their great potential to achieve fault-tolerant quantum computation[1–8]. Recent studies have revealed that iron-based superconducting materials simultaneously possess superconductivity and topological energy band structure and can therefore support MZM in the presence of vortices with no need to fabricate complex heterostructures. This offers a great advantage for the experimental realization and detection of MZM. For example, clear zero-bias conductivity peaks[9–13] and integer quantized Carolic states [14, 15] have been observed in a variety of iron-based superconducting materials [9, 14, 16–18]. However, the multi-bands near the Fermi level may complicate the vortex Majorana physics. So far, all the study of the vortex Majorana physics in iron-based superconductors focus on the magnetic field along [001] direction. In this case, while the multi-band effects enrich the topological phase diagrams, such as the coexistence of the MZM and nodal vortex, it also narrows the regime for the existence of locally single MZMs with fully gapped bulk bands. Meanwhile, the implementing Majorana vortex state in the iron-based superconducting nanowire is a crucial step toward braiding MZMs in iron-based superconducting system. To the best of our knowledge, so far the grown iron-based superconducting nanowire is along [100] direction.

In this work, we study the vortex Majorana physics with the magnetic field along [100] direction. We show that the superconducting band is always fully gapped for $k_x \neq 0$ or π. Therefore, the topological regime is fully determined by the physics at $k_x = 0$ given the electronic band inversion is at $k = (0, 0, \pi)$. When the chemical potential is around the bulk Dirac point, we find a hidden symmetry which leads to the superconducting bands grouped as two degenerate sectors when the electronic Hamiltonian respects C_{4z} rotational symmetry. The states in these two sectors have opposite C_{2x} eigenvalues $\pm i$. As a result, the gap close, if any, must be even times, which leads to a double vortex nodal states when the chemical potential near the Dirac point. The C_{4z} symmetry breaking term will gap the system while only one sector becomes topological non-trivial vortex state. Surprisingly, the sign of the C_4 breaking term determines which sector becomes topologically non-trivial due to the anti-commutation relation between the hidden symmetry and the C_{2x} operators. When the chemical potential is around the bulk TI band gap, the topological vortex phase transition is always at $C_{2x} = -1$ sector. We find that when the two topological vortex phase transitions happen in the different sectors and the Dirac band and TI band are close, the overlap between the two topological regimes is trivialized from the MZMs coupling as it is for the vortex state along the [001] direction. More importantly, when the two topological vortex phase transition happen in the same C_{2x} sector, the two topological regime is fused to one larger topological regime without trivialization which is absent for the vortex physics along [001] direction and is thus a new paradigm of the Majorana vortex phase transition due to the multi-bands effect. Moreover, it shows the great advantage of studying Majorana vortex physics along [100] direction. At last, we discuss the experimental implementation and control the Majorana vortex phase transition along [100] direction. The work is organized as follows. In Sec II, we provide the system Hamiltonian and its symmetry analysis. In Sec III, we study the vortex phase transition along [001] direction. In Sec IV, we give a brief discussion of the experimental realization and conclusion.

System- Focusing on the topological bands around $\Gamma - Z$, we adopt the BdG Hamiltonian as

$$H_{\mathrm{S}} = \begin{pmatrix} H_{\mathrm{e}}(\boldsymbol{r}) - \mu & \hat{\Delta}(\boldsymbol{r}) \\ \hat{\Delta}^{\dagger}(\boldsymbol{r}) & -H_{\mathrm{e}}^{*}(\boldsymbol{r}) + \mu \end{pmatrix} , \tag{1}$$

with μ the chemical potential and $\hat{\Delta}(\boldsymbol{r})$ the superconducting gap function. To capture the multi-band features of iron-based superconductor, we consider $H_{\mathrm{e}}(\boldsymbol{r})$ in the six-bands basis $(|z\uparrow\rangle, |z\downarrow\rangle, |-i(x+iy)z\downarrow\rangle, |-i(x-iy)z\uparrow\rangle, |-i(x+iy)z\uparrow\rangle, |i(x-iy)z\downarrow\rangle)$, which in momentum space takes the form

$$H_{\rm e}(k)=H_{\rm e}^{0}(k)+H_{\rm e}^{\prime}(k), \tag{2}$$

with

$$H_0(\mathbf{k})=\epsilon(\mathbf{k})+\begin{pmatrix} M(\mathbf{k}) & T_1(\mathbf{k}) & T_2(\mathbf{k}) \\ T_1^{\dagger}(\mathbf{k}) & -M(\mathbf{k}) & T_3(\mathbf{k}) \\ T_2^{\dagger}(\mathbf{k}) & T_3^{\dagger}(\mathbf{k}) & -M(\mathbf{k})+\lambda \end{pmatrix}, \tag{3}$$

where

$$\begin{aligned}
\epsilon(\mathbf{k}) =& C+2D(2-\cos k_x+\cos k_y)+2D_3(1-\cos k_z),\\
M(\mathbf{k}) =& M_0+2B(2-\cos k_x+\cos k_y)+2B_3(1-\cos k_z),\\
T_1(\mathbf{k}) =& A(\hat{s}_x\sin k_x+\hat{s}_y\sin k_y)+A_3\hat{s}_z\sin k_z,\\
T_2(\mathbf{k}) =& A(\hat{s}_z\sin k_x+i\sin k_y)+A_3^{\prime}\hat{s}_x\sin k_z(\cos k_x-\cos k_y),\\
T_3(\mathbf{k}) =& i[\alpha\hat{s}_x\sin k_x\sin k_y-\beta\hat{s}_y(\cos k_x-\cos k_y)],\\
H_e^{\prime}(\boldsymbol{k}) =& A_3^{\prime}\hat{s}_x\sin k_z.
\end{aligned} \tag{4}$$

Note that the Hamiltonian $H_0(k)$ describes the band structures of the iron-based superconductors around $\Gamma-Z$ and has D_{4h} group symmetry. There is a Dirac point in the $\Gamma-Z$ line due to the C_{4z} rotational symmetry. The $H^{\prime}(k)$ is finite when breaking the C_{4z} symmetry appropriately, and the DSM band becomes a strong TI band while the system now has D_{2h} group symmetry. For studying the vortex along (100), we take the periodic boundary condition in this direction and open the boundary in the other two directions, giving $H_{\rm S}(k_x,y,z)$ which has C_{2x} rotational symmetry. Therefore, the system can be block diagonalized as $H_{\rm S}=\sum_{k_x}\left[H_{\rm S}^{+}(k_x)\bigoplus H_{\rm S}^{-}(k_x)\right]$ with $C_{2x}=\pm1$ respectively. As the Hamiltonian terms with $\sin k_x\neq0$ break local particle-hole symmetry, the sectors of $H_{\rm S}(k_x\neq0,\pi)$ are always gapped. Meanwhile, the vortex system can be considered as quasi-1D, which belongs to class D of the Altland-Zirnbauer classification []. Therefore the vortex topology is fully characterized by the $\mathbb{Z}_2$ topological invariant [19]

$$\nu=\operatorname{sgn}\left\{\frac{\operatorname{Pf}[\mathcal{H}_{\rm Mj}^{+}(k_x=0)]\operatorname{Pf}[\mathcal{H}_{\rm Mj}^{-}(k_x=0)]}{\operatorname{Pf}[\mathcal{H}_{\rm Mj}^{+}(k_x=\pi)]\operatorname{Pf}[\mathcal{H}_{\rm Mj}^{-}(k_x=\pi)]}\right\}, \tag{5}$$

where $\mathcal{H}_{\rm Mj}(k_x=0,\pi)$ is the Hamiltonian $H_{\rm s}(k_x=0,\pi)$ written in the Majorana basis. As we can change the sign of the topological invariant only when the gap of $H_{\rm s}(k_x=0,\pi)$ is closed and reopened, it is convenient to show the topological phase transition through the spectrum evolution with varying the system parameters in each sector. In the large λ-limit with finite $A_3^{\prime}$, the system can be considered as two independent superconducting topological insulators which correspond to the two topological phase transitions (TPTs) separated in the energy axis shown in Fig. **??**. When the chemical potential is near the lower TI gap, there exists band close and reopening, which indicates the Kitaev vortex phase transition. This is similar to the case of vortex along [001] because the band structure is topologically equivalent in an arbitrary direction for the strong TI. When the chemical potential is around the Dirac semi-metal phase with $A_3^{\prime}=0$, the system is gapless, and the eigenenergies are double degenerate, which is consistent to the previous study with C_4 symmetry. When $A_3^{\prime}\neq0$, the system is generally fully gapped and undergoes the vortex phase transition. Remarkably, the phase transition happens in $C_{2x}=1$ and $C_{2x}=-1$ for $A_3^{\prime}>0$ and $A_3^{\prime}<0$ respectively. This is very different from the vortex phase transition along [001], which always happens in the $C_{2z}=-1$ section. Meanwhile, as λ is much larger than the TI gap, the phase transitions around the lower and higher TI band gaps are well separated and has no fundamental difference for $A_3^{\prime}>0$ and $A_3^{\prime}<0$. However, when decreasing $\lambda<A_3$, close to the SOC strength in LiFeAs, the different sign of $A_3^{\prime}$ gives two different vortex phase transitions. When the two vortex phase transitions happen in different C_{2x} sectors, their phase diagram has an overlap at which the system has two pairs of MZMs. This is topologically equivalent to the TPT with the magnetic field along the (001) direction []. Remarkably when the two vortex phase transition happens in the same C_{2x} section for small SOC strength λ, they merge into one vortex phase transition which covers both the TI and Dirac semi-metal non-trivial regime. To show this more clearly, we plot the phase diagram for these two cases in Fig. For the former case, with decreasing λ, the overlap of the two vortex phase transitions narrows the topological non-trivial regime that also happens for the vortex along [001] direction. For the latter, decreasing λ induces the fuse of the two vortex phase transitions into one, which enlarges the topological non-trivial regime. This means the multi-band of iron-based superconductor with smaller SOC can be beneficial rather than detrimental to the Kitaev vortex phase transition with the vortex along [100] direction.

To better understand the $A_3^{\prime}$-induced topological phase transition in the weak SOC regime, we consider the continuous model of the Hamiltonian (Eq. ()) in the momentum space as [20**?**]

$$\mathcal{H}_k^{\rm BdG}=\begin{pmatrix} H(k)-\mu & i\frac{\Delta_0(\hat{r})}{\xi}(\partial_{k_x}-i\partial_{k_y}) \\ i\frac{\Delta_0(\hat{r})}{\xi}(\partial_{k_x}+i\partial_{k_y}) & \mu-H_k \end{pmatrix} \tag{6}$$

In the block, the electronic Hamiltonian takes

$$H_k=\begin{pmatrix} M(k) & -i(A_1k_y-iA_3k_z) & -i(A_1k_y-iA_3k_z) \\ i(A_1k_y-iA_3k_z) & -M(k) & 0 \\ i(A_1k_y-iA_3k_z) & 0 & -M(k)+\delta \end{pmatrix}.($$

in the zero SOC limit ($\lambda=0$) with $|A_3^{\prime}|=A_3=A$ for simplicity. It has the same eigenvalues $E_1=-M(k)$ and $E_{2(3)}=+(-)\sqrt{M^2(k)+2A^2k^2}$ for both $A_3^{\prime}=\pm A_3$ and the corresponding wave function

$$\psi_1^{\pm} = (0, e^{i(1\pm1)\theta}, -e^{i(1\pm1)\theta})^{\mathrm{T}},$$
$$\psi_{i=2,3} = (\frac{e^{i\theta}\,(M(k)+E_i)}{Ak}, e^{i(1\pm1)\theta}, e^{i(1\pm1)\theta})^{\mathrm{T}}. \quad (8)$$

The electronic band is gapless and looks like a classical TI band ($E_2(k)$, $E_3(k)$) plus a normal parabolic band ($E_0(k)$) across the TI band gap. When the chemical potential is in side the TI band gap, there is only parabolic band at the Fermi surface. When projecting the system to the Fermi surface, it gives U(1) Berry connection. The integral $\oint_{FS} \boldsymbol{A}\cdot d\boldsymbol{l} = 0, 2\pi$ for $\psi_0^{\pm}$ cannot support any zero energy state [21]. When the chemical potential reach the TI band, say conduction band for example, the gauge potentials are very different for $\psi^{\pm}$. For $A_3' = -A_3$, although there are two bands around the Fermi surface, the state ψ_0^- contribute nothing to the Berry connection because it is totally $\boldsymbol{k}$-independent. In this case, the vortex phase transition through varying μ performs similar with the classical superconducting TI [16, 20]. For $A_3' = A_3$, the Berry connection is non-Abelian and takes

$$\mathcal{A} = \frac{1}{\sqrt{k}} \quad (9)$$

Note that our system has rotational symmetry with the angular momentum J_z =???, we can make the unitary transformation

$$U = \frac{1}{\sqrt{k}}\left(\right), \quad (10)$$

we obtain the 4×4 Jackiw-Rebbi model like Hamiltonian with non-Abelian gauge potential. When the eigenvalues of the non-Abelian gauge potential is equal to $\pm1/2$, we have two zero modes at the same chemical potential μ_c whose angular momenta differ by 1. Therefore, these two zero modes belong to $C_{2x} = \pm1$ respectively. When varying $|A_3'| \neq A_3 \neq A_1$ or $\delta \neq 0$, it is hard to get the analytical result. However these variations do not break the C_{2x} symmetry and therefore should not affect the existence of the zero energy states. In Fig. **??**, we plot the gratitude of the most close to zero eigenenergy with varying A_3' and μ with fixed $\lambda = A_3/2$. It clearly shows the evolution of the phase transition point from 4 to 2. For the former case, with decreasing λ, the overlap of the two vortex phase transitions narrows the topological nontrivial regime (Fig. **??**) that also happens for the vortex along [001] direction. For the latter, decreasing λ induce the fuse of the two vortex phase transition which enlarge the topological non-trivial regime (Fig. **??**). This means the smaller SOC such as LiFeAs can be beneficial rather than detrimental to the Kitaev vortex phase transition with the vortex along [100] direction if we can control the sign of A_3' when breaking C_{4z} symmetry.

Through the Slater–Koster tight-binding method calculation, we obtain that $A_3' = V_x \cos k_x - V_y \cos k_y$ with V_x and V_y the interlayer coupling between p_z and $d_{z(x\pm iy)}$ orbitals through SOC $l_z s_z$ as shown in Fig. **??**. Assuming the coupling is constant, say $V_x > 0$, we have $a_x \lessgtr a_y$ to give $A_3' \gtrless 0$. Therefore, we can breaking the C_{4z} rotational symmetry by applying an tensile strain in x-direction or compressive strain in y-direction to get a pair of MZMs in the low SOC iron-based superconductors such as LiFeAs.

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