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Emerging edge states in the monolayer FeSe superconductor with the spin-orbital coupling

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Topological superconductors have attracted tremendous attentions in the field of the condensed matter physics, partially due to the realization of Majorana zero modes at their surfaces or vortex cores, which has potential application in the topological quantum computation [1]. Theoretically, the early proposed candidate platforms include the chiral $p + ip$ superconductors and the artificially created heterostructures including a superconductor and a spin-orbital coupled material. Experimentally, signatures of Majorana zero modes have indeed been observed in various heterostructures. However, the proximity induced superconducting pairing magnitude is generally rather small. And it is challenging to make use of the complicated heterostructures for further detections or applications. Recently, it was predicted theoretically and indicated experimentally that the topological superconductors and Majorana zero modes may be realized in many families of iron based superconductors [2]. This provides exciting opportunities to realize the intrinsic nontrivial topology and high-T_c superconductivity in one material.

The high-T_c superconductivity in iron-based materials has been studied intensively since their discovery in 2008. Generally in the normal state, the Fermi surface includes two hole pockets around the $\Gamma = (0, 0)$ point and two electron pockets around the $M = (\pi, \pi)$ point [3]. The density of states near the Fermi level is mainly contributed by the $3d$ orbitals of the iron ions. Thus a five-orbital model considering all of the Fe $3d$ orbitals was proposed and describes well the properties of the iron-based superconductor. On the other hand, a minimal two-orbital model was also proposed. This minimal model reproduces qualitatively correct the normal state Fermi surface and can describe most of the low energy physics of iron based superconductors. However, both models cannot describe directly the nontrivial topology of iron-based superconductors. Actually, the topological properties for the iron-based superconductors depend strongly on the materials. Theoretically, the topologically nature for both three-dimensional and two-dimensional $FeSe_{1-x}Te_x$ materials have been discussed sufficiently and well understood. For the $FeSe_{1-x}Te_x$ system, the $5p$ orbital of Te ions are more expended and have stronger spin-orbital interaction than $4p$ orbitals of Se ions. The hybrids between the p and d orbitals are important for the nontrivial topology. Therefore, an effective model describing both the superconductivity and the topological properties of the $FeSe_{1-x}Te_x$ compound may be rather complicate.

For the monolayer FeSe material, the p orbitals of the Se ions are far away from the Fermi level. Therefore, the minimal model describing the FeSe compound should be much simpler that describes the $FeSe_{1-x}Te_x$ compound. Moreover, the monolayer FeSe superconductor has several unique features compared with other iron-based superconductors, namely, the superconducting transition temperature T_c is rather high. And in the normal state, only electron pockets around the M point exist. The hole pockets around the Γ point is absent, different from most of other iron-based superconductors. A topological phase in the normal state emerges through considering an intrinsic spin-orbital coupling [4], while in the superconducting state, it was indicated theoretically that the nontrivial topology only appear for the odd parity pairing [5]. For the usual $s_{\pm}$ pairing, the system is topologically trivial. On the other hand, experimentally, signatures of Majorana zero modes were also revealed in the monolayer FeSe compound. Therefore, actually it is still not clear whether the superconducting monolayer FeSe

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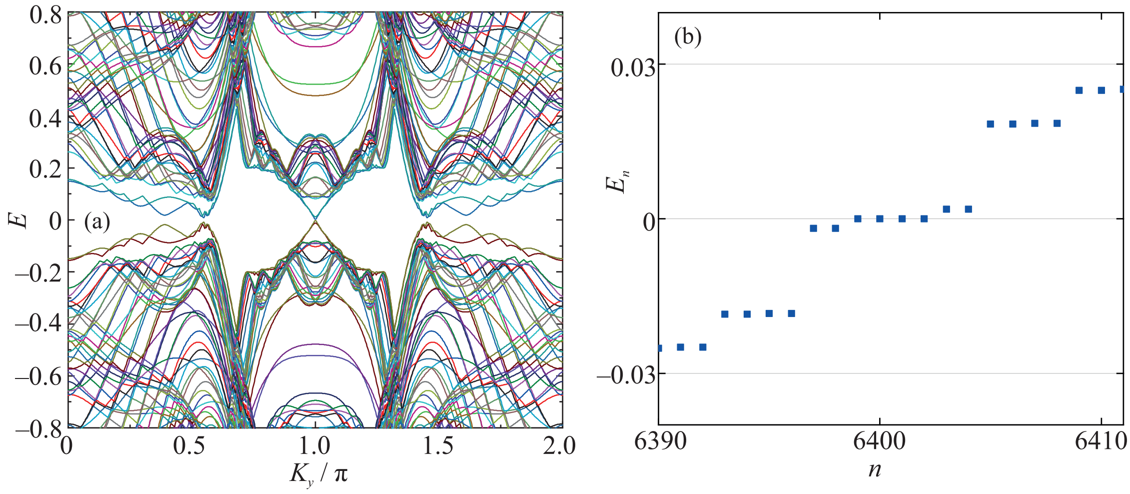

Fig. 1. (Color online) (a) – The energy bands as a function of the momentum k_y with the spin-orbital interaction with considering the open boundary condition along the x-direction. (b) – The low energy eigenvalues of the Hamiltonian with two vortices

material is topologically trivial. Now it is rather necessary to explore this issue theoretically and construct a minimal model to describe both the high-T_c superconductivity and the possible Majorana excitations of the monolayer FeSe material.

Starting from a two-orbital model which can describe qualitatively the superconducting properties of the monolayer FeSe superconductor [6], we propose that the edge states and the zero modes in the vortex core can emerge when an additional spin-orbital coupling term is considered. Our main results are indicated in Fig. 1. As is seen in Fig. 1a, when the open boundary condition is considered, the edge states indeed emerge. The low energy eigenvalues of the Hamiltonian in the presence of the two vortices are presented in Fig. 1b. As is seen, four zero energy eigenvalues exist. This can explain qualitatively the experimental signatures of the Majorana zero modes in this material. However, based on the calculation of the topological invariant and the Wilson loop technique, our results indicate that this system is still a topologically trivial system. We provide a possible explanation for the emergence of the zero modes in the monolayer FeSe material. However, the edge states and zero modes disappear when the normal state hole-like Fermi pockets appear upon changing the chemical potential. Therefore, the observations of the edge states and Majorana zero modes in other iron-based superconductors cannot be simply explained merely through adding an additional spin-orbital interaction into the original Hamiltonian.

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