Quantum anomalous vortex and Majorana zero mode without external magnetic field

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In topological insulators doped with magnetic ions, spin-orbit coupling and ferromagnetism give rise to the quantum anomalous Hall effect. Here we show that in $s$-wave superconductors with strong spin-orbit coupling, magnetic impurity ions can generate topological vortices in the absence of external magnetic fields. Such vortices, dubbed quantum anomalous vortices, support robust Majorana zero-energy modes when superconductivity is induced in the topological surface states. We demonstrate that the zero-energy bound states observed in Fe(Fe,Se) superconductors are possible realizations of the Majorana zero modes in quantum anomalous vortices produced by the interstitial magnetic Fe. The quantum anomalous vortex matter not only advances fundamental understandings of topological defect excitations of Cooper pairing, but also provides new and advantageous platforms for manipulating Majorana zero modes in quantum computing.

Introduction

Harvesting localized Majorana fermion excitations has thrived in condensed matter and materials physics for both its fundamental value and its potential for fault-tolerant nonabelian quantum computing [1–11]. An important and promising path discovered thus far is to combine spin-orbit coupling (SOC) and Berry phase of the electrons with superconductivity. Localized Majorana zero-energy modes (MZM) have been proposed to arise in the vortex core when the Dirac fermion surface states of a topological insulator are proximity-coupled to an $s$-wave superconductor [2], or when superconductivity is induced in a semiconductor with strong Rashba SOC and time-reversal symmetry breaking Zeeman field [3]. Experimental realizations of these proposals are under active current investigations [12–16]. There exists, however, fundamental challenges that come with using external magnetic field induced vortices. The existence and the stability of the MZM in real materials are not guaranteed due to the low-energy vortex core states [5, 17, 18] as well as disorder and vortex creep. It is difficult, if not impossible, to move the field-induced vortex lines individually on the Abrikosov lattice, which greatly reduces the ability to manipulate the MZM for operations such as braiding. Moreover, the requirement of external field is difficult to be integrated into quantum computation devices and limits their applications.

We propose here a new form of vortex matter - the quantum anomalous vortex matter that can support robust MZM without applying external magnetic field. In conventional spin-singlet $s$-wave superconductors, a time-reversal symmetry breaking magnetic impurity is known to create a vortex-free defect hosting the Yu-Shiba-Rusinov (YSR) bound states [19, 20] inside the superconducting (SC) gap. We find that this folklore changes in a fundamental way in $s$-wave superconductors with strong SOC. In this case, topological defect excitations can be generated by a quantized phase winding of the SC order parameter around the magnetic impurity, all without applying an external magnetic field. The role of the magnetic field is played by the combination of the exchange field and SOC as in the anomalous Hall effect. The emergence of such vortices is thus remarkably analogous to the quantum anomalous Hall effect in topological insulator thin films doped with magnetic ions [22, 23]. Hence the term quantum anomalous vortex (QAV). We demonstrate with theoretical calculations that (i) The QAV nucleates around the magnetic ion by the exchange coupling between the local moment and spin-angular momentum locked SC quasiparticles that lowers its energy compared to the vortex-free YSR state. (ii) When superconductivity is induced in the topological surface states, MZM emerge inside the QAV core, again without applying external magnetic field. (iii) A remarkable property of the QAV is that the Caroli-de Gennes-Matricon (CdGM) vortex core states [24, 25] with nonzero effective angular momenta are expelled into the continuum above the SC gap. A comparison of the vortex profile and core states between the QAV and the field-induced vortex is shown in Fig. 1a. The “gapping” of the core states critically enhances the stability and robustness of the MZM by preventing the mixing with the CdGM states at nonzero energy [3, 17, 18]. At low densities of magnetic ions, a new electronic matter, the QAV matter with surface MZM as depicted in Fig. 1b, would arise in such layered superconductors and provide an unprecedented platform of robust and manipulatable MZM for nonabelian quantum computing.

We find that the QAV matter is pertinent to the Fe-based superconductor Fe(Fe,Se) (FTS), exhibiting spectroscopic properties remarkably consistent with the surprising discovery of robust zero-energy bound states (ZBS) near the excess Fe by STM in the absence of external magnetic fields [26]. Topological surface states (TSS) in FTS [27, 28] have been observed by ARPES recently.
and acquire a SC gap below $T_c$ by the natural coupling to bulk superconductivity in the same crystal [29]. The condition for the applied magnetic field induced vortices to host ZBS is still unclear, with one group reporting its absence and CdGM vortex core states at nonzero energies [30] and another finding the ZBS in about 20% of the vortices [31]. However, the observation of ZBS at all excess Fe sites in zero-field is ubiquitous with measured properties fully consistent with MZM [26].

To study the SC state with a complex inhomogeneous Cooper pairing order parameter, it is convenient to perform the Bogoliubov transformation

$$
\psi_{\uparrow}(r) = \sum_n [u_{n\sigma}(r)\gamma_n^\dagger + v_{n\sigma}(r)\gamma_n],
$$

where $\gamma_n^\dagger$ creates a Bogoliubov quasiparticle, and obtain the Bogoliubov-de Gennes (BdG) equation

$$
\begin{bmatrix}
H & \Delta(r) \\
\Delta^*(r) & -\sigma_y H \sigma_y
\end{bmatrix} \Phi_n(r) = E_n \Phi_n(r),
$$

where $\Delta(r) = g \langle \psi_{\uparrow}(r) \psi_{\uparrow}(r) \rangle$ is the self-consistent pairing potential for an attraction $g$ [41]. We choose $g = 11$meV such that $|\Delta(r)| = |\Delta| = 1.5$meV gives the bulk SC gap far away from the magnetic ion [26, 29]. Diagonalizing the BdG equation yields the energy spectrum $E_n$ and Nambu wavefunctions $\Phi_n(r) = [u_{n\uparrow}(r), u_{n\downarrow}(r), v_{n\uparrow}(r), v_{n\downarrow}(r)]^T$ for both the vortex-free and vortex solutions with $\Delta(r) = \Delta(r) e^{i\nu\theta}$, where the integer $\nu$ is the vorticity.

We have obtained the solutions in the disc geometry for a SC layer with the isolated magnetic ion at its center (Fig. 2b) in polar coordinates $r = (r, \theta)$. See supplemental material for details [41]. The SOC in Eq. (2) reduces to $-\lambda_{so}(r)L_z\sigma_z$ with $L_z = -i\hbar \partial_s$. The wavefunction is factorizable according to

$$
\Phi_{n\mu}(r, \theta) = e^{i\mu\theta}[u_{n\mu+1}(r)e^{i\theta}, u_{n\mu+1}(r)e^{i\theta}, v_{n\mu+1}(r)e^{-i\theta}, v_{n\mu+1}(r)e^{-i\theta}]^T,
$$

where the principal quantum number $n$ is determined by solving the radial $(u, v)$ in the basis of Bessel functions and the angular quantum number $\mu = \ell - \frac{\delta}{2}$ with $\ell$ an integer [24, 25, 41, 42]. We use the coherence length $\xi \approx 2nm$ measured in FTS [43] as the length unit. Setting $\xi \equiv 1$, the disc radius $R = 250$. The SOC and exchange coupling are assumed to decay exponentially $\lambda_{so}(r)$, $J_{ex}(r) \propto e^{-r/r_0}$ with a common decay length $r_0 = 2$ (Fig. 2b) for simplicity and easy comparison.

FIG. 1: Schematic rendering of (a) conventional vortex (top panel) and QAV around magnetic ion (bottom panel), showing energy levels of in-gap CdGM states localized in vortex core. Negative energy states are occupied. (b) Quantum anomalous vortex matter in layered superconductors. Red and blue dots/arrows indicate opposite $c$-axis moment directions of magnetic ions, while arrowed circles vorticity of each QAV. Black lines are continuous flux lines piercing SC layers through magnetic ions. Zero-bias peaks indicate localized MZM from TSS in QAV cores where flux lines enter and leave sample surface.
states are doubly degenerate, carry the half-integer quan-
tistic Friedel-like oscillations [42, 44], and approaches the 
∆(r) is shown in Fig. 2c for the field-induced vortex so-
the self-consistent vortex profile calculated using the full
Consequently, the energy of the CdGM states is lowered
H_{ex} = -m(r)j_z with m(r) = |J_{ex}(r)|M \equiv m_0 e^{-r/r_0}. 
Consequently, the energy of the CdGM states is lowered (raised) by \(-m(r)j_z\) for all positive (negative) \(j_z\). The spatial dependence of \(m(r)\) causes an additional shift by mixing with other states of the same \(j_z\). Fig. 2e shows the self-consistent vortex profile calculated using the full Hamiltonian \(H\). The vortex core sharpens considerably and the Friedel oscillations become more prominent compared to the normal field-induced vortex in Fig. 2c. The eigenstate energies are plotted in Fig. 2f. All but two of the CdGM states \(|j_z, \sigma_z\rangle\) are expelled away from the gap center into the continuum; the remaining two just below the gap edges have \(j_z = 0\). The enhanced binding energy of the occupied CdGM states significantly lowers the vortex state energy. In contrast, the vortex-free (\(\nu = 0\)) state obtained using the same parameters shows a much broader deformation in \(\Delta(r)\) near the magnetic ion (Fig. 2g) and fosters two sets of spin-orbit coupled mid-gap YSR states (Fig. 2h) that must be occupied at

Normal vortex state The self-consistent pairing profile \(\Delta(r)\) is shown in Fig. 2c for the field-induced vortex solution with \(\nu = -1\) in the absence of the magnetic ion. It vanishes at the vortex center, exhibits the characteristic Friedel-like oscillations [42, 44], and approaches the bulk value for \(r \gtrsim 10\). The eigenstate energies are plotted in Fig. 2d, zoomed in to the range \((-\Delta, \Delta)\) to display the in-gap CdGM vortex core states. These bound states are doubly degenerate, carry the half-integer quantum number \(\mu\), and grow with \(\mu\) initially as \(E_\mu \propto \mu z r / r_0\), \(\mu = \pm \frac{1}{2}, \pm \frac{3}{2}, \ldots\) [24, 29]. Owing to the small \(\varepsilon_f\), the onset of the CdGM states is at \(E_{-\frac{1}{2}} \approx 0.38\)meV (Fig. 2d). Define the vortex binding energy as

\[
E_{vb} = E_{vortex} - E_{vortex-free},
\]

where \(E_{vortex}\) and \(E_{vortex-free}\) are the energy of the vortex and vortex-free states respectively. There is an energy cost \((E_{vb} > 0)\) for creating the normal vortex, since the supercurrent-carrying mid-gap CdGM states with \(E_\mu < 0\) are occupied. An external magnetic field must be applied to break the time-reversal symmetry and generate the normal vortex.

Quantum anomalous vortex state Let’s switch on the SOC, \(H_{soc} = -\lambda_{soc}(r)L_z \sigma_z\) with \(\lambda_{soc}(r) = \lambda_0 e^{-r/r_0}\) in Eq. \(2\). It splits off in energy the nonzero angular momentum partial waves with different spin-\(\sigma_z\) projections [41]. Because \(\lambda_{soc}(r)\) is localized around the impurity, the effects on the vortex states are most pronounced for small \(\mu\), i.e. the mid-gap CdGM states. As shown in Fig. 2d by the colored symbols, each doubly-degenerate CdGM state splits into \(|j_z, \pm \frac{1}{2}\rangle\) by an amount controlled by \(\lambda_0\) and the mixing of the states carrying the same quantum number \(j_z = \mu \pm \frac{1}{2}\) due to the inhomogeneous \(\lambda_{soc}(r)\). The negative energy CdGM states are all occupied. The binding energy of the QAV comes from the exchange interaction in Eq. \(3\) under SOC, which is qualitatively different from the proposal of spontaneous vortex lattice in ferromagnetic superconductors [45]. Since magnetic transition metal ions usually have a large momentum, such as the excess Fe moment in LTS [32] pointing along the c-axis due to the magnetic anisotropy induced by SOC, the impurity moment can be treated classically, i.e. \(\mathbf{I}_{imp} = M \hat{z}\). The exchange interaction becomes \(H_{ex} = -m(r)j_z\) with \(m(r) = |J_{ex}(r)|M = m_0 e^{-r/r_0}\). Consequently, the energy of the CdGM states is lowered (raised) by \(-m(r)j_z\) for all positive (negative) \(j_z\). The spatial dependence of \(m(r)\) causes an additional shift by mixing with other states of the same \(j_z\). Fig. 2e shows the self-consistent vortex profile calculated using the full Hamiltonian \(H\). The vortex core sharpens considerably and the Friedel oscillations become more prominent compared to the normal field-induced vortex in Fig. 2c. The eigenstate energies are plotted in Fig. 2f. All but two of the CdGM states \(|j_z, \sigma_z\rangle\) are expelled away from the gap center into the continuum; the remaining two just below the gap edges have \(j_z = 0\). The enhanced binding energy of the occupied CdGM states significantly lowers the vortex state energy. In contrast, the vortex-free (\(\nu = 0\)) state obtained using the same parameters shows a much broader deformation in \(\Delta(r)\) near the magnetic ion (Fig. 2g) and fosters two sets of spin-orbit coupled mid-gap YSR states (Fig. 2h) that must be occupied at
an energy cost. Thus, the energy of the vortex state can be lower than the vortex-free state ($E_{v<0}$). Fig. 2g inset shows the calculated vortex binding energy $E_{vb}$ as a function of $m_0$. A transition between the vortex-free YSR state and the QAV state occurs at a critical $m_0^c$. For $m_0 > m_0^c$, it becomes more energetically favorable for the SC order parameter to develop a quantized phase winding with supercurrents flowing around the magnetic ion. Hence the formation of the QAV. The small $\varepsilon_f$ and superfluid density/stiffness in FTS superconductors uniquely favor the QAV state.

**Majorana zero-energy bound state in QAV** We turn to the emergence of localized MZM when superconductivity is induced in the helical Dirac fermion TSS. In the vicinity of the magnetic ion, the Hamiltonian with primes indicating TSS is given in the spinor basis by,

$$H' = v_D(\sigma \times \mathbf{p}) \cdot \mathbf{z} - \varepsilon_f' + H'_{soc} + H'_{ex},$$

where $v_D = 0.216eV\cdot\AA$ and the Fermi level of the electron doped TSS is $\varepsilon_f' = 4.5meV$ above the Dirac point as shown in Fig. 2a for FTS. The impurity-induced SOC is $H'_{soc} = \lambda'_{soc}(r) L_z \sigma_z$ and $H'_{ex} = -J'_{ex}(r) F_{imp} J_z$ is the exchange coupling between the TSS and the local moment. In general, $\lambda'_{soc}(r)$ and $J'_{ex}(r)$ can be different from those in the bulk states. In the corresponding BdG equation, the induced pairing potential for the TSS is $\Delta'(r) = \Delta_{QAV}(r) e^{i\theta}$, where $\Delta_{QAV}(r)$ is the pairing profile of the QAV shown in Fig. 2e. The obtained vortex energy spectrum for the TSS is plotted in Fig. 3a. The “isolated” bound state at $E = 0$ is precisely the MZM, i.e. the $\mu' = 0$ element of the chiral CdGM states $E_{\mu'} = \mu' \Delta^2 / \varepsilon_f'$, where $\mu' = 0, \pm 1, \pm 2, \cdots$ is now an integer due to the additional Berry phase of the Dirac fermions. Note that all other CdGM states with nonzero $\mu'$ in Fig. 3b obtained without coupling to the magnetic ion are pushed into the continuum above the SC gap by the exchange field via the same mechanism that produced the QAV. The gapping of the nonzero energy CdGM states prevents the level crossing induced topological vortex transition and protects the robustness of the MZM even at higher doping of the TSS.

There are remarkable agreements between the calculated LDOS at the center of the QAV plotted in Fig. 3c and the tunneling conductance measured by STM at the interstitial excess Fe sites reproduced in the inset. Both show the V-dip around $-4.5meV$ corresponding to the Dirac point of the TSS, the absence of coherence peaks at the gap energies $\pm \Delta$, and a spectrum free of mid-gap states other than the zero-bias peak. Note that without coupling to the magnetic ion, the mid-gap vortex core states produce multiple conductance peaks and reduce considerably the spectral weight of the MZM as shown in Fig. 3d. Indeed, the small satellite peak at $\sim 1.44meV$ in Fig. 3c comes from the CdGM states expelled to the continuum by the exchange field. It is tempting to identify a similar satellite in the STM spectrum at $\sim 1.6meV$ with such a resonance. These findings further support that the ZBS observed by STM are MZM in the QAV induced by the excess Fe. Since the QAV has trapped a SC flux quantum, flux-quantization protects the QAV and MZM from external magnetic fields applied along the c-axis, consistent with the insensitivity of the ZBS to fields up to 8 Tesla observed by STM.

**Quantum anomalous vortex matter** Let’s consider a low density of dilute magnetic ions such that the SC transition temperature $T_c$ is reduced but the SC ground state remains stable. For Fe$_{1+y}$Te$_{0.55}$Se$_{0.45}$, this is the case for excess Fe density $y < 0.03$. The theory thus predicts a QAV matter illustrated in Fig. 1b with localized MZM at the ends of the flux lines as they enter or leave the sample’s surface via the magnetic ion. Note that while the vorticity of the QAV is confined to the magnetic ion, the magnetic flux lines must be continuous and pierce through the SC layers only where a magnetic ion resides by the nucleation of a QAV. An immediate consequence is the appearance of QAV with opposite vorticities, i.e. both vortices and anti-vortices accompanied by the flipping of the local magnetic moment direction along the c-axis. This prediction could serve as an experimental test of the theory by spin-polarized STM and/or scanning probe SQUID. Since it is relatively easy to move the impurity atoms on the surface, the QAV matter provides an advantageous platform for studying the statistics and interactions of the MZM by manipulating the impurity ions and accomplishing crucial operations such as braiding in nonabelian quantum computing.
The QAV matter is likely to have been realized in FTS superconductors. A crucial observation of Ref. [26] is that when two interstitial Fe atoms sit close together, a striking simultaneous reduction in the amplitudes of the zero-bias peaks occurs without any observable energy shift. As shown in Fig. 1b, the continuous magnetic flux line now favors the formation of an entangled quantum anomalous vortex-antivortex pair, providing a natural explanation via the annihilation of a pair of MZM. Finally, with increasing excess Fe concentration, the density of the QAV increases, which may provide a novel mechanism for the suppression of bulk superconductivity and the eventual superconductor to metal quantum phase transition.

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