Impurity and vortex-core states in superconducting spin-helical Dirac fermions

Hiroki Isobe
Massachusetts Institute of Technology
Acknowledgment

Liang Fu

Michał Papaj

HI, M. Papaj, and L. Fu (to appear)
2D topological surface states in proximity to s-wave superconductivity will host Majorana zero modes.

- We look into impurity bound states and vortex core states in detail.
- Is there a way to distinguish Majorana zero modes from another zero energy localized modes?

Results:
- Impurity bound states can also be zero-energy localized modes.
- However, they are different in: spatial distribution, spin configuration...
Search for Majorana zero modes

• Majorana condition $\gamma_0 = \gamma_0^\dagger$
• Localized at an $hc/2e$ vortex in a $p + ip$ superconductor
• It necessarily lies at zero energy in superconductors.

• Non-Abelian statistics and application to quantum computation

Search for Majorana zero modes

However, a Majorana zero mode is not the only one localized midgap modes in superconductors.

Midgap states includes:

• Vortex-core states (Caroli-de Gennes-Matricon, 1964)
  • Include Majorana zero modes

• Impurity bound states (Yu, 1965; Shiba, 1968; Rusinov, 1969)

• Kondo impurity resonance, etc.
Midgap states in superconductors

For conventional $s$-wave superconductors:

$$\mathcal{H}_0 = \sum_{\mathbf{k}\alpha} \varepsilon_{\mathbf{k}} c_{\mathbf{k},\alpha}^\dagger c_{\mathbf{k}\alpha} + \Delta_0 \sum_{\mathbf{k}} \left\{ c_{\mathbf{k}\uparrow}^\dagger c_{-\mathbf{k}\downarrow} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right\}$$

• Impurity bound states – Yu-Shiba-Rusinov states

$$H_{ex} = \frac{1}{2N} \sum_{\mathbf{k},\mathbf{k}',\alpha\beta} J(\mathbf{k} - \mathbf{k}') c_{\mathbf{k},\alpha}^\dagger \sigma_{\alpha\beta} \cdot S c_{\mathbf{k}',\beta}$$

$$\varepsilon_0 = \frac{E_0}{\Delta_0} = \frac{1 - (JS\pi N_0/2)^2}{1 + (JS\pi N_0/2)^2}$$


• Vortex-core states – Caroli-de Gennes-Matricon states

$$\hat{\psi} = \exp \left( i \mathbf{k}_F z \cos \alpha \right) \exp \left( i \mu \theta \right) \hat{f}(r)$$

$$\int_0^\infty \frac{\Delta(r) e^{-2K(r)} dr}{r}$$

$$\varepsilon_{\mu\alpha} = q v_F \sin \alpha = \mu (k_F \sin \alpha)^{-1} \int_0^\infty e^{-2K(r)} dr$$

$$\mu \Delta \propto 2/E_F$$

Realization of topological superconductivity

Majorana zero modes in 2D superconductors:

• Intrinsic \((p+ip)\)-superconductor
  \(\text{Sr}_2\text{RuO}_4\)

• 3D Topological insulator surface states + s-wave SC
  • Proximity effect
  • Intrinsic realization
  \(\text{Cu}_x\text{Bi}_2\text{Se}_3, \text{Sn}_{1-x}\text{In}_x\text{Te}, \text{FeTe}_{1-x}\text{Se}_x\)

• 2D electron gas with Rashba + s-wave SC + Zeeman

See reviews, e.g., Alicea (2012), Sato and Ando (2017)
Suppose that an $s$-wave superconductor is deposited on the surface. Because of the proximity effect, Cooper pairs can tunnel into the surface states. This can be described by adding $V = \Delta \psi_1^\dagger \psi_1^\dagger + \text{H.c.}$ to $H_0$, where $\Delta = \Delta_0 e^{i\phi}$ depends on the phase $\phi$ of the superconductor and the nature of the interface [17]. The states of the surface can then be described by $H = \Psi^\dagger \hat{\mathcal{H}} \Psi / 2$, where in the Nambu notation $\Psi = ((\psi_1, \psi_0), (\psi_0^\dagger, -\psi_1^\dagger))^T$ and

$$\hat{\mathcal{H}} = -i\nu \tau^z \sigma \cdot \nabla - \mu \tau^z + \Delta_0(\tau^x \cos \phi + \tau^y \sin \phi).$$

(2)

$\tau$ are Pauli matrices that mix the $\psi$ and $\psi^\dagger$ blocks of $\Psi$. Time reversal invariance follows from $[\Theta, \mathcal{H}] = 0$, where $\Theta = i\sigma^y K$ and $K$ is complex conjugation. Particle hole symmetry is expressed by $\Xi = \sigma^y \tau^y K$, which satisfies $\{\Xi, \hat{\mathcal{H}}\} = 0$. When $\Delta$ is spatially homogeneous, the excitation spectrum is $E_k = \pm \sqrt{(\pm \nu |k| - \mu)^2 + \Delta_0^2}$. For $\mu \gg \Delta_0$, the low energy spectrum resembles that of a spinless $p_x + ip_y$ superconductor. This analogy can be made precise by defining $c_k = (\psi_{\downarrow k} + e^{i\theta_k} \psi_{\uparrow k})/\sqrt{2}$ for $k = k_0(\cos \theta_k, \sin \theta_k)$ and $u k_0 \sim \mu$. The projected Hamiltonian is then $\sum_k (\nu |k| - \mu)c_k^\dagger c_k + (\Delta e^{i\theta_k} c_k^\dagger c_{-k}^\dagger + \text{H.c.})/2$. Though this is formally equivalent to a spinless $p_x + ip_y$ superconductor, there is an important difference: $\mathcal{H}$ respects time reversal symmetry, while the $p_x + ip_y$ superconductor does not.

FeSe$_{1-x}$Te$_x$: Normal state

DFT calculations
- Band inversion along $\Gamma - Z$ line
- Topological “metal”
- Single Dirac cone on 001 surface

FeSe$_{1-x}$Te$_x$: Superconducting state

DFT calculations

- Energy spectrum along a vortex line (like a Majorana chain)
- Self-doping by excess Fe atoms Fe$_{1+y}$Se$_{0.5}$Te$_{0.5}$ (TSC: 0.03<y<0.06)

FeSe$_{1-x}$Te$_x$: ARPES

FeTe$_{0.55}$Se$_{0.45}$ ($T_c=14.5$K)

- Spin-helical surface Dirac cone

FeSe$_{1-x}$Te$_x$: ARPES

FeTe$_{0.55}$Se$_{0.45}$ ($T_c = 14.5$ K)

- *s*-wave superconducting gap on the surface

**FeSe$_{1-x}$Te$_x$: STM/S (impurity)**

**Pristine Fe(Te,Se) ($T_c=14.5$K)**

At an interstitial iron impurity (excess iron atom)

Highest $T_c$ without IFIs

FeSe$_{1-x}$Te$_x$: STM/S (impurity)

Possibilities for midgap states:

• Majorana zero modes

• Impurity bound states (magnetic or non-magnetic)
  • Pair of spectral peaks, symmetric around zero energy
  • Zeeman split under magnetic field

• Kondo resonance
  • Not at zero energy
  • Zeeman split

• $d$-wave pairing state with an impurity at unitary limit
  • Four-fold pattern in real space

FeSe$_{1-x}$Te$_x$: STM/S (vortex)

FeTe$_{0.55}$Se$_{0.45}$ ($T=0.55$K, $T_c=14.5$K)

- Vortex lattice under magnetic field along the c-axis (4T)

D. Wang et al., arXiv:1706.06074.
Model

• Spin-helical Dirac fermion + $s$-wave superconductivity (2D)

\[ \hat{H}_0 = \Psi^\dagger H_0 \Psi / 2 \]

\[ H_0(r) = -i v \tau^z \mathbf{\sigma} \cdot \nabla - \mu \tau^z + \Delta_0 (\tau^x \cos \phi - \tau^y \sin \phi) \]

\[ \Psi(r) = (\psi_\uparrow, \psi_\downarrow; \psi_\downarrow^\dagger, -\psi_\uparrow^\dagger)^T \]

• Coherence length \( \xi = v / \Delta_0 \)

• Symmetry
  • Time reversal \( \Theta = i \sigma^y K \) \quad [\Theta, H] = 0
  • Particle-hole \( \Xi = \sigma^y \tau^y K \) \quad \{\Xi, H\} = 0
Vortex core states

Apply magnetic field \( B_{c1} < B < B_{c2} \) \( l_B \gg \xi \) \( l_B = \sqrt{\hbar c/eB} \)

Quantized vortex \( \Delta(r) = |\Delta(r)|e^{i\ell\theta} \) \( (\ell: \text{vorticity}) \)

- Around the vortex core, the wave function acquires the phase \( 2\pi \nu + \pi (l - 1) \mod 2\pi \) \( (\nu: \text{angular momentum}) \)
  \[ 2\pi \nu + \pi l \text{ for a conventional } s\text{-wave superconductor} \]

Majorana zero mode \( (l = 1, \nu = 0) \)
\[
\chi(r) = \exp \left( -\int_0^r |\Delta(r')|dr'/\nu \right) \begin{pmatrix} J_0(k_Fr) \\ ie^{i\theta} J_1(k_Fr) \\ e^{-i\theta} J_1(k_Fr) \\ ie^0 J_0(k_Fr) \end{pmatrix}
\]

References:
Vortex core states

Apply magnetic field $B_{c1} < B < B_{c2}$  

$l_B \gg \xi$  

$l_B = \sqrt{\hbar c/eB}$

Quantized vortex  

$\Delta(r) = |\Delta(r)| e^{i l \theta}$  

$l$: vorticity

• Around the vortex core, the wave function acquires the phase

$2\pi \nu + \pi (l - 1)$  

$\nu$: angular momentum

[ $2\pi \nu + \pi l$ for a conventional s-wave superconductor]

Majorana zero mode ($l = 1, \nu = 0$)

$$
\chi(r) = \exp \left( - \int_0^r |\Delta(r')| dr' / \nu \right) \begin{pmatrix}
J_0(k_F r) \\
\frac{i e^{i \theta}}{\nu} J_1(k_F r) \\
e^{-i \theta} J_1(k_F r) \\
i J_0(k_F r)
\end{pmatrix}
$$

References:


Vortex core states

Midgap states at a vortex: $\Delta(r) = |\Delta(r)| e^{i\theta}$
Impurity bound state

Impurity potential \( H_{\text{imp}} = V \delta(r) = (U \tau^Z \sigma^0 - J \tau^0 \mathbf{S} \cdot \mathbf{\sigma}) \delta(r) \)

- \( U \): scalar potential
- \( S \): classical spin \( S \to \infty \) and \( J S \to \text{finite} \).

Bound state energy: pole of T-matrix \( T = H_{\text{imp}} + H_{\text{imp}} G_0 T \)

\[
\det[1 - H_{\text{imp}} G_0(E)] = 0 \quad (-\Delta_0 < E < \Delta_0)
\]

Equivalently, from the Bogoliubov-de Gennes equation

\[
(H_0 + H_{\text{imp}}) \chi(r) = E \chi(r)
\]

\[
[1 - G_0(E) H_{\text{imp}}] \chi(r) = 0
\]

\[
G_0(E) = (E - H_0)^{-1} \quad \chi = (u_\uparrow, u_\downarrow; v_\downarrow, -v_\uparrow)^T
\]

Is there a zero energy state?
Magnetic impurity

Impurity potential \( H_{\text{imp}} = V \delta(\mathbf{r}) = (U \tau^z \sigma^0 - J \tau^0 \mathbf{S} \cdot \mathbf{\sigma}) \delta(\mathbf{r}) \)

- \( U = 0, JS \neq 0 \)

Energy spectrum of midgap states

- Pairs of states at any \( JS \)
- Accidental crossing at a certain \( JS \)

Energy spectrum at large \( \mu \)

\[
E_{\pm} = \pm \Delta_0 \left[ 1 - \left( \pi \rho_0 JS / 2 \right)^2 \right] / \left[ 1 + \left( \pi \rho_0 JS / 2 \right)^2 \right]
\]

- Same form as one for conventional \( s \)-wave superconductors
Magnetic + scalar impurity

Impurity potential \( H_{\text{imp}} = V \delta(r) = (U \tau^z \sigma^0 - J \tau^0 \mathbf{S} \cdot \mathbf{\sigma}) \delta(r) \)

Assume only the spin-up level is on resonance: \( U = JS(= g) \).

• Zero energy states exist in the strong coupling limit.

(There also exist pair states with negative energy.)
Magnetic + scalar impurity

Impurity potential \( H_{\text{imp}} = V \delta(r) = (U \tau^z \sigma^0 - J \tau^0 S \cdot \sigma) \delta(r) \)

Assume only the spin-up level is on resonance: \( U = JS(= g) \).

- **Zero energy states** exist in the strong coupling limit.

Large \( \mu \)

\[ E_{\pm} = \pm \Delta_0 \frac{1}{\sqrt{1 + (\pi \rho_0 g)^2}} \]

(There also exist pair states with negative energy.)
Magnetic + scalar impurity

Impurity potential \( H_{\text{imp}} = V \delta(r) = (U \tau^z \sigma^0 - J \tau^0 S \cdot \sigma) \delta(r) \)

Assume only the spin-up level is on resonance: \( U = JS(= g) \).

- **Zero energy states** exist in the strong coupling limit.

\[ \mu = 0 \]

\[ E_{\pm} = \pm \frac{\pi v^2}{g \ln \left( \frac{v \Lambda}{\Delta_0} \right)} \]

- Momentum cutoff \( \Lambda (\gg \Delta_0/v) \)
- Valid for large \( g \)

(There also exist pair states with negative energy.)
Magnetic + scalar impurity

Impurity potential \[ H_{\text{imp}} = V \delta(r) = (U \tau^z \sigma^0 - J \tau^0 \mathbf{S} \cdot \mathbf{\sigma}) \delta(r) \]

Assume only the spin-up level is on resonance: \( U = JS(= g) \).

• **Zero energy states** exist in the strong coupling limit.

Intermediate \( \mu \)
\[
\lim_{g \to \infty} E_{\pm} = \pm \Delta_0 \left( \frac{\Delta_0}{2\mu} - \frac{3\Delta_0^3}{8\mu^3} + O \left( \frac{\Delta_0^5}{\mu^5} \right) \right) \quad |\mu| \gg \Delta_0
\]

(There also exist pair states with negative energy.)
Difference from Majorana zero modes

<table>
<thead>
<tr>
<th></th>
<th>Impurity bound states</th>
<th>Majorana zero modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Localized at ...</td>
<td>Impurity</td>
<td>Vortex (magnetic flux)</td>
</tr>
<tr>
<td>Locked at zero energy?</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Appear in pairs?</td>
<td>Yes</td>
<td>No</td>
</tr>
</tbody>
</table>

Further differences will be found if we look at wave functions.
Wave function

Solve the Bogoliubov-de Gennes equation:  

\[ (H_0 + H_{\text{imp}})\chi(\mathbf{r}) = E\chi(\mathbf{r}) \]

\[ H_{\text{imp}} = V\delta(\mathbf{r}) = (U\tau^z\sigma^0 - J\tau^0 \mathbf{S} \cdot \mathbf{\sigma})\delta(\mathbf{r}) \]

\[ \frac{\mu}{\Delta_0} = 0, \quad U = JS_z = 100 \]

\[ \frac{\mu}{\Delta_0} = 50, \quad U = JS_z = 100 \]
Wave function

\[ \mu / \Delta_0 = 0, \ U = J S_z = 100 \]

\[ |\Psi|^2 \]

\[ r / \xi \]

\[ \chi^+_{z}(r) \simeq (K_0(r/\xi), 0; 0, -ie^{-i\phi} e^{i\theta} K_1(r/\xi))^T \]

\[ \chi^-_{z}(r) \simeq (ie^{i\phi} e^{-i\theta} K_1(r/\xi), 0; 0, K_0(r/\xi))^T \]

\[ K_n(r/\xi) \approx e^{-r/\xi} \sqrt{\pi \xi / (2r)} : \text{modified Bessel function} \quad r \geq \xi \]
Wave function

\[ \mu / \Delta_0 = 0, \quad U = J S_z = 100 \]

\[ |\Psi|^2 \]

\[ r / \xi \]

Only electron components

\[ \chi_\uparrow (r) \simeq (F_0(r), i\text{sgn}(\mu)e^{i\theta}F_1(r); 0, 0)^T \]

\[ \chi_\downarrow (r) \simeq (0, 0; i\text{sgn}(\mu)e^{-i\theta}F_1(r), F_0(r))^T \]

\[
\begin{align*}
F_0(r) &= \xi \sqrt{2\pi k_F / r} e^{-r/\xi} \cos(k_F r - \pi/4) \\
F_1(r) &= -\xi \sqrt{2\pi k_F / r} e^{-r/\xi} \cos(k_F r + \pi/4)
\end{align*}
\]
Wave function

Two length scales:

- Coherence length $\xi = \nu / \Delta_0$ (decay)
- Fermi wavelength $\lambda_F = 2\pi / k_F$ (oscillations)
Local density of states (LDOS)

STM measurement

\[ N(E, \mathbf{r}) = N_{\uparrow}(E, \mathbf{r}) + N_{\downarrow}(E, \mathbf{r}) \]

\[ N_\sigma(E, \mathbf{r}) = \sum_n \left[ |u_{n,\sigma}|^2 \delta(E - E_n) + |v_{n,\sigma}|^2 \delta(E + E_n) \right] \]

Spin-averaged LDOS

- Oscillation for large doping

\[ \mu/\Delta_0 = 0, \quad U = J S_z = 100 \]

\[ \mu/\Delta_0 = 50, \quad U = J S_z = 100 \]
Local density of states (LDOS)

STM measurement

\[ N(E, \mathbf{r}) = N_{\uparrow}(E, \mathbf{r}) + N_{\downarrow}(E, \mathbf{r}) \]

\[ N_{\sigma}(E, \mathbf{r}) = \sum_{n} \left[ |u_{n,\sigma}|^2 \delta(E - E_n) + |v_{n,\sigma}|^2 \delta(E + E_n) \right] \]

Spin-resolved LDOS

- At large doping:

\[ \chi = (u_{\uparrow}, u_{\downarrow}; v_{\downarrow}, -v_{\uparrow})^T \]

\[ S_z \neq 0 \quad \text{and} \quad S_x \neq 0 \]
Spin accumulation

Response to external magnetic field \( S = \frac{1}{2} \sigma \tau_0 \)

\( S_z \neq 0 \) \hspace{1cm} \( S_x \neq 0 \)

\( <S_z> \)

\( <S_x> \)

Insensitive to external magnetic field

\( U = J S = 100 \)
## Difference from Majorana zero modes

<table>
<thead>
<tr>
<th></th>
<th>Impurity bound states</th>
<th>Majorana zero modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Localized at ...</td>
<td>Impurity</td>
<td>Vortex (magnetic flux)</td>
</tr>
<tr>
<td>Locked at zero energy?</td>
<td>No</td>
<td>Yes</td>
</tr>
<tr>
<td>Appear in pairs?</td>
<td>Yes, but may be degenerate.</td>
<td>No</td>
</tr>
<tr>
<td>Oscillation of LDOS?</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(spin-averaged)</td>
<td>Yes/No (depending on $\mu$)</td>
<td>No</td>
</tr>
<tr>
<td>(spin-resolved)</td>
<td>Yes</td>
<td>Yes</td>
</tr>
<tr>
<td>Energy shift under $B$ field?</td>
<td>Yes/No ($B$ field direction)</td>
<td>No</td>
</tr>
</tbody>
</table>
Summary

<table>
<thead>
<tr>
<th>Impurity bound states</th>
<th>Majorana zero modes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Localized at ...</td>
<td>Impurity</td>
</tr>
<tr>
<td>Locked at zero energy?</td>
<td>No</td>
</tr>
<tr>
<td>Appear in pairs?</td>
<td>Yes, but may be degenerate.</td>
</tr>
<tr>
<td>Oscillation of LDOS?</td>
<td>(spin-averaged) Yes/No (depending on $\mu$)</td>
</tr>
<tr>
<td></td>
<td>(spin-resolved) Yes</td>
</tr>
<tr>
<td>Energy shift under $B$ field?</td>
<td>Yes/No ($B$ field direction)</td>
</tr>
</tbody>
</table>

- Differences in measureable quantities.
- Clues for experimental detection of Majorana zero modes.