Exotic Andreev bound states in topological superconductors

Yukio Tanaka (Nagoya University)

Yukawa Institute (2014)
Main collaborators

A. Yamakage (Nagoya)

K. Yada (Nagoya)

T. Hashimoto (Nagoya)

M. Sato (Nagoya)

T. Mizushima (Osaka)

S. Takami (Nagoya)
Andreev bound state
Classical example of Andreev bound state

ABS with nonzero energy

ABS has been known since 1963.

P.G. de Gennes and D. Saint-James


High transparent interface

Energy levels of Andreev bound state (nonzero energy)

\[ \varepsilon_n = \pm \frac{\pi v_F x}{2L} (n + 1/2), \quad n = 0, 1, 2, \ldots \]

\[ \Delta_0 \gg |\varepsilon_n| \]

\[ \Delta_0 \quad \text{magnitude of pair potential} \]

\[ v_F x \quad x \text{ component of Fermi velocity} \]
Andreev bound state
(non-topological and topological)

Andreev bound state with non zero energy (de Gennes, Saint James 1963)

Not edge state
Non topological

Mid gap (zero energy) Andreev bound state
Surface Andreev bound state
Edge state Topological

L. Buchholtz & G. Zwicknagl (81):, J. Hara & K. Nagai : Prog. Theor. Phys. 74 (86)
C.R. Hu : (94)
Well known example of Andreev bound states in $d$-wave superconductor

Phase change of pair potential is $\pi$

$$\Delta_+ \Delta_- < 0$$

ABS in $d$-wave
(110)direction

Zero energy

Flat dispersion!!

Surface

$E = 0$

$k_y$

Alff, Kashiwaya PRB (1998)

Tanaka Kashiwaya PRL 74 3451 (1995),
Advance in understanding of Andreev bound state

Solution of BdG equation (quasi classical approximation)

Topological aspects
Analogy to Quantum Hall, Quantunm spin Hall,
Topological insulators

X. L. Qi, S.C. Zhang, PRL 102, 187001 (2009), Schnyder et. al, PRB 78 195125 (2008)
Flat Andreev bound state and topology

Hamiltonian

\[ \mathcal{H} = \sum_k \left( c_{k \uparrow}^\dagger, c_{-k \downarrow} \right) \mathcal{H}(k) \begin{pmatrix} c_{k \uparrow} \\ c_{-k \downarrow}^\dagger \end{pmatrix} \]

\[ \mathcal{H}(k) = \begin{pmatrix} \varepsilon(k) & \Delta(k) \\ \Delta(k) & -\varepsilon(k) \end{pmatrix}, \]

\[ \Delta(k) = \begin{cases} \psi(k) = \psi(\bar{k}) & \text{for spin-singlet} \\ d_z(k) = -d_z(-k) & \text{for spin-triplet} \end{cases} \]

Winding number for fixed \( k_y \)

\[ w_1 d(k_y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \partial_{k_x} \theta(k). \]

\[ \cos \theta(k) = \frac{\varepsilon(k)}{\sqrt{\varepsilon(k)^2 + \Delta(k)^2}} \]

\[ \sin \theta(k) = \frac{\Delta(k)}{\sqrt{\varepsilon(k)^2 + \Delta(k)^2}}. \]

Sato, Tanaka, et al, PRB 83 224511 (2011)
Midgap Andreev bound state
(Winding number)

\[ w_{1d}(k_y) = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk_x \partial_{k_x} \theta(k) \]

\[ = -\frac{1}{2} \sum_{k_x; \varepsilon(k) = 0} \text{sgn}[\Delta(k)] \cdot \text{sgn}[\partial_{k_x} \varepsilon(k)] \]

Topological invariant defined in bulk

If we consider a simple Fermi surface

\[ w_{1d} = -\frac{1}{2} \text{sgn}[\partial_{k_x} \varepsilon(-k_x^0, y)] \left[ \text{sgn}[\Delta(-k_x^0, y)] - \text{sgn}[\Delta(k_x^0, y)] \right]. \]

\[ w_{1d} \not= 0 \quad \leftrightarrow \quad \Delta(-k_x^0, y) \Delta(k_x^0, y) < 0 \]

Conventional condition

Sato, Tanaka, et al, PRB 83 224511 (2011)
Winding number & Index theorem (1)

From the **bulk-edge correspondence**, there exists the gapless states on the edge only when integer $w_{1d}$ is nonzero.

**BdG Hamiltonian** has a symmetry (chiral symmetry)

$$\{ \mathcal{H}(k), \sigma_y \} = 0$$

Zero energy ABS is an eigenstate of $\sigma_y$.

Number of ZES where the eigenvalue of $\sigma_y$ is 1

$$n_0^{(+)}$$

Number of ZES where the eigenvalue of $\sigma_y$ is $-1$

$$n_0^{(-)}$$

**Index Theorem**

$$w_{1d} = (n_0^{(+)} - n_0^{(-)})$$

---

**Superconductor**

$x$  

$y$
(Topological) Andreev bound states

Non-centrosymmetric superconductor (NCS)

- $d_{xy}$-wave
  - Hu (94)
  - Tanaka Kashiwaya (95)

- Chiral $p$-wave $p_x + i p_y$-wave
  - Tanaka Kashiwaya (97)
  - Sigrist Honerkamp (98)

- NCS (Helical) $p^+ + s$-wave
  - Iniotakis (07)
  - Eschrig (08)
  - Tanaka (09)

Flat  Chiral  Helical
## Andreev bound state (topological edge state) and topological invariant

<table>
<thead>
<tr>
<th>Andreev bound state</th>
<th>Topological invariant</th>
<th>Time reversal symmetry</th>
<th>Materials</th>
<th>Theory of tunneling</th>
<th>Insulator (semi-metal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chiral</td>
<td>2d winding Number Z</td>
<td>×</td>
<td>Sr$_2$RuO$_4$ $^3$He A</td>
<td>PRB (1997)</td>
<td>QHS</td>
</tr>
<tr>
<td>Helical</td>
<td>$z_2$</td>
<td>∅</td>
<td>$s + p$-wave (NCS)</td>
<td>PRB (2007)</td>
<td>QSHS (2D Topological insulator)</td>
</tr>
<tr>
<td>Cone</td>
<td>3d winding Number Z</td>
<td>∅</td>
<td>$^3$He B</td>
<td>PRB (2003)</td>
<td>Topological insulator</td>
</tr>
</tbody>
</table>

$\text{Cu}_x\text{Bi}_2\text{Se}_3$
Topological insulator $\text{Bi}_2\text{Se}_3$

- Nonzero topological number $\mathbb{Z}_2$
- Helical Dirac Cone as a surface state
- Strong spin-orbit coupling

Crystal structure $\text{Bi}_2\text{Se}_3$

Electronic band structure of $\text{Bi}_2\text{Se}_3$ measured by ARPES
Electronic states of Bi$_2$Se$_3$

energy levels of the atomic orbitals in Bi$_2$Se$_3$

Zhang et al, Nature 09
Superconducting topological insulator

$Cu_xBi_2Se_3$

$Cu$ doped topological insulator

**Resistivity**

$\rho(\text{m}\Omega\text{cm})$

$T = 1.8\,\text{K}$

$H/H_{c1} = 1\,\text{T}$

$T_c = 3.8\,\text{K}$

Y.S.Hor et al., PRL 104, 057001 (2010)

**Specific heat**

$\gamma_s$

$\gamma_n$

$\Delta_0/T_c = 1.9$

$\Delta_0/T_c = 2.3$

M. Kriener et al., PRL 106, 127001 (2011)
Effective Hamiltonian of $\text{Cu}_x\text{Bi}_2\text{Se}_3$

Model Hamiltonian (Normal state) \[ H_0(k) = m \sigma_x + v(k_x \sigma_z s_y - k_y \sigma_z s_x) + v_z k_z \sigma_y \]

Model Hamiltonian (superconducting state) \[ H(k) = [H_0(k) - \mu] \tau_z + \hat{\Delta} \tau_x \]

Pauli matrix \[ \sigma : \text{orbital, } \quad s : \text{spin, } \quad \tau : \text{particle-hole} \]

$8 \times 8$ matrix

ARPES

Pauli matrix \[ \sigma : \text{orbital, } \quad s : \text{spin, } \quad \tau : \text{particle-hole} \]
Candidate of pair potentials

<table>
<thead>
<tr>
<th>Energy gap</th>
<th>irreducible representation</th>
<th>spin</th>
<th>Orbital parity</th>
<th>Matrix form</th>
</tr>
</thead>
<tbody>
<tr>
<td>Δ_{1a}</td>
<td>$A_{1g}$</td>
<td>singlet</td>
<td>even</td>
<td>$\Delta \sigma_x$</td>
</tr>
<tr>
<td>Δ_{1b}</td>
<td>$A_{1g}$</td>
<td>singlet</td>
<td>even</td>
<td>$\Delta \sigma_x$</td>
</tr>
<tr>
<td>Δ_{2}</td>
<td>$A_{1u}$</td>
<td>triplet</td>
<td>odd</td>
<td>$\Delta \sigma_y s_z$</td>
</tr>
<tr>
<td>Δ_{3}</td>
<td>$A_{2u}$</td>
<td>singlet</td>
<td>odd</td>
<td>$\Delta \sigma_z$</td>
</tr>
<tr>
<td>Δ_{4}</td>
<td>$E_u$</td>
<td>triplet</td>
<td>odd</td>
<td>$\Delta \sigma_y s_x$</td>
</tr>
</tbody>
</table>

Cu$_x$Bi$_2$Se$_3$ Effective orbital $p_z$ orbital (No momentum dependence)

Liang Fu, Erez Berg, PRL, 105, 097001 (2010)
## Topological natures of four pairings

<table>
<thead>
<tr>
<th>Pair potential</th>
<th>Irreducible representation</th>
<th>spin</th>
<th>orbital</th>
<th>Gap structure</th>
<th>Parity (orbital inversion)</th>
<th>Topological number</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_{1a}$</td>
<td>$\Delta$</td>
<td>$A_{1g}$</td>
<td>Singlet</td>
<td>Intra inter</td>
<td>full gap</td>
<td>even</td>
</tr>
<tr>
<td>$\Delta_{1b}$</td>
<td>$\Delta\sigma_x$</td>
<td>$A_{1u}$</td>
<td>triplet</td>
<td>inter</td>
<td>full gap</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_{2}$</td>
<td>$\Delta\sigma_y s_z$</td>
<td>$A_{1u}$</td>
<td>singlet</td>
<td>intra</td>
<td>Point node (z-direction)</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_{3}$</td>
<td>$\Delta\sigma_z$</td>
<td>$A_{2u}$</td>
<td>triplet</td>
<td>inter</td>
<td>Point node [x(y)-direction]</td>
<td>odd</td>
</tr>
</tbody>
</table>

Supplementary materials in
S. Sasaki et al PRL 107 217001 (2011)
Energy Gap function

Full Gap
spatial inversion odd

Point Node spatial inversion odd

spin-singlet orbital-even

spin-triplet inter-orbital

Yamakage et al., PRB Rapid (2012)
Bulk local density of state

\[\Delta_1: \text{singlet, full gap}\]

\[\Delta_2: \text{triplet, full gap}\]

\[\Delta_3: \text{singlet, point node}\]

\[\Delta_4: \text{triplet, point node}\]

Energy \( (E/\Delta) \)

LDOS

full gap

point node

\( E^2 \)
Surface state generated at $z=0$

STI (Superconducting topological insulator)
Obtained Dispersions of Andreev bound state

spin-triplet inter-orbital spatial inversion odd-parity

$\Delta_2$

(a) $E/\Delta$

Normal Cone

(Only positive spin helicity $k_x s_y - k_y s_x = +k$ states are shown.)

(b) $E/\Delta$

Caldera Cone

(solution of confinement condition $\psi(z=0)=0$)

(c) $E/\Delta$

Deformed Cone

(Only negative energy states are shown.)

Hsieh and Fu PRL 108 107005(2012); arXiv: 1109.3464

A. Yamakage, PRB, 85, 180509(R) (2012)
Structural transition of the dispersion of ABS

(b) caldera

(a) cone

transition point:

transition

$\Delta_2$

energy

$\mu = v^2_z/m_1$

L. Hao and T. K. Lee, PRB '11
T. H. Hsieh and L. Fu, PRL '12
Although original Hamiltonian is a $8 \times 8$ matrix, is it possible to make a compact analytical formula of Andreev bound state?

Yes. If we concentrate on the low energy excitation near the Fermi energy, it is possible.

Quasi-classical theory Yip (PRB 2013) Y. Nagai (2013)
<table>
<thead>
<tr>
<th>$\Delta_{1a}$</th>
<th>$E = \pm \sqrt{(c(k) + \eta(k))^2 + \Delta^2}$</th>
<th>No</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_{1b}$</td>
<td>$E = \pm \sqrt{(c(k) + \eta(k))^2 + \Delta^2 \frac{m(k)^2}{\eta(k)^2}}$</td>
<td>No</td>
</tr>
<tr>
<td>$\Delta_2$</td>
<td>$E = \pm \sqrt{(c(k) + \eta(k))^2 + \Delta^2 \frac{v_z^2k_z^2 + v_x^2k_x^2}{\eta(k)^2}}$</td>
<td>$E = \pm \Delta \frac{vk_\parallel}{\sqrt{m(k)^2 + v_z^2k_z^2 + v_x^2k_x^2}} \frac{m(k)}{\sqrt{m(k)^2 + v_z^2k_z^2}}$</td>
</tr>
<tr>
<td>$\Delta_3$</td>
<td>$E = \pm \sqrt{(c(k) + \eta(k))^2 + \Delta^2 \frac{v_\parallel^2}{\eta(k)^2}}$</td>
<td>No (along z-direction) \n(In other directions, yes)</td>
</tr>
<tr>
<td>$\Delta_4$</td>
<td>$E = \pm \sqrt{(c(k) + \eta(k))^2 + \Delta^2 \frac{v_z^2k_z^2 + v_x^2k_x^2}{\eta(k)^2}}$</td>
<td>$E = \pm \Delta \frac{vk_x}{\sqrt{m^2(k) + v_z^2k_z^2 + v_x^2k_x^2}} \frac{m(k)}{\sqrt{m^2(k) + v_z^2k_z^2}}$</td>
</tr>
</tbody>
</table>

$$H_0(k') = m \sigma_x + v (k_x \sigma_z s_y - k_y \sigma_z s_x) + v_z k_z \sigma_y + c(k)$$

$$m(k) = m_0 + m_1 k_z^2 + m_2 k_\parallel^2 \quad \eta(k) = \sqrt{m(k)^2 + v_z^2 k_z^2 + v_x^2 k_x^2}$$

$$c(k) = -\mu + c_1 k_z^2 + c_2 k_\parallel^2 \quad k_\parallel = \sqrt{k_x^2 + k_y^2}$$

Charge transport in normal metal / STI junctions

STI

$\Delta_1$, $\Delta_2$, $\Delta_3$, $\Delta_4$

z-axis

Normal metal

STI (Superconducting topological insulator)
Conductance between normal metal / superconducting topological insulator junction (numerical calculation)

$$\Delta_1$$

Similar to conventional spin-singlet s-wave superconductor

$$\Delta_2$$

Zero bias conductance peak is possible even for $$\Delta_2$$ case with full gap

Hsieh and Fu  PRL 108 107005(2012); arXiv: 1109.3464

A. Yamakage, PRB, 85, 180509(R) (2012)
Conductance between normal metal / STI junction

(numerical calculation)

(Spatial inversion odd-parity)

Point node case

Tunneling conductance strongly depends on the direction of nodes.

A. Yamakage, PRB, 85, 180509(R) (2012)

<table>
<thead>
<tr>
<th>Energy gap</th>
<th>irreducible representation</th>
<th>spin</th>
<th>Orbital parity</th>
<th>Matrix form</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_{1a}$ $\Delta_{1b}$</td>
<td>full gap</td>
<td>$A_{1g}$</td>
<td>singlet</td>
<td>even</td>
</tr>
<tr>
<td>$\Delta_2$</td>
<td>full gap</td>
<td>$A_{1u}$</td>
<td>triplet</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_3$</td>
<td>point node</td>
<td>$A_{2u}$</td>
<td>singlet</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_4$</td>
<td>point node</td>
<td>$E_u$</td>
<td>triplet</td>
<td>odd</td>
</tr>
</tbody>
</table>
## Conductance based on quasi-classical approximation

| \( \Delta_{1a} \) | \( T_S = T_N \frac{1 + T_N |\Gamma_{1a}|^2 + (1 - T_N)|\Gamma_{1a}|^4}{|1 - (1 - T_N)\Gamma_{1a}^2|^2} \) |
| \( \Delta_{1b} \) | \( T_S = T_N \frac{1 + T_N |\Gamma_{1b}|^2 - (1 - T_N)|\Gamma_{1b}|^4}{|1 - (1 - T_N)\Gamma_{1b}^2|^2} \) |
| \( \Delta_2 \) | \( T_S = \frac{T_N}{2} \left( \frac{1 + T_N |\Gamma_{2+}|^2 - (1 - T_N)|\Gamma_{2+}|^4}{|1 + (1 - T_N)\Gamma_{2+}^2|^2} + \frac{1 + T_N |\Gamma_{2-}|^2 - (1 - T_N)|\Gamma_{2-}|^4}{|1 + (1 - T_N)\Gamma_{2-}^2|^2} \right) \) |
| \( \Delta_3 \) | \( T_S = T_N \frac{1 + T_N |\Gamma_3|^2 - (1 - T_N)|\Gamma_3|^4}{|1 - (1 - T_N)\Gamma_3^2|^2} \) |

\[ \sigma_T(E) = \frac{\int_0^{\pi/2} d\theta \int_0^{2\pi} d\phi T_S \sin 2\theta}{\int_0^{\pi/2} d\theta \int_0^{2\pi} T_N \sin 2\theta} \]

\[ \gamma_{1a} = 1 \]

\[ \gamma_{1b} = \frac{m(k)}{\sqrt{m(k)^2 + v_z k_{\parallel}^2 + v^2 k_{\parallel}^2}} \]

\[ \gamma_{2\pm} = \frac{v_z k_{\parallel} \sqrt{m(k)^2 + v_z^2 k_{\parallel}^2 + v^2 k_{\parallel}^2} \pm im(k)vk_{\parallel}}{\sqrt{(m(k)^2 + v_z^2 k_{\parallel}^2 + v^2 k_{\parallel}^2)(m(k)^2 + v_z^2 k_{\parallel}^2)}} \]

\[ \gamma_3 = \frac{vk_{\parallel}}{\sqrt{m(k)^2 + v_z^2 k_{\parallel}^2 + v^2 k_{\parallel}^2}} \]
Conductance formula available in (single band) unconventional superconductors

(Tanaka and Kashiwaya PRL 74 3451 1995)

\[
\sigma_T(E) = \frac{\int_{-\pi/2}^{\pi/2} d\theta T_S(E, \theta) \cos \theta}{\int_{-\pi/2}^{\pi/2} d\theta T_N(\theta) \cos \theta}
\]

\[
T_S(E, \theta) = \frac{T_N(\theta)\{1 + T_N(\theta) |\Gamma_+|^2 + [T_N(\theta) - 1] |\Gamma_+\Gamma_-|^2\}}{1 + [T_N(\theta) - 1] |\Gamma_+\Gamma_-|^2 \exp[i(\phi_- - \phi_+)]^2},
\]

\[
\exp(i\phi_+) = \frac{\Delta(\theta_+)}{|\Delta(\theta_+)|} = \frac{\Delta_+}{|\Delta_+|} \quad \exp(i\phi_-) = \frac{\Delta(\theta_-)}{|\Delta(\theta_-)|} = \frac{\Delta_-}{|\Delta_-|}
\]

conventional s-wave \quad \exp[i(\phi_+ - \phi_-)] = 1

\[
\Gamma_{\pm} = \frac{E - \sqrt{E^2 - \Delta_{\pm}^2}}{|\Delta_{\pm}|}
\]

transparency \quad T_N(\theta) = \frac{\cos^2 \theta}{\cos^2 \theta + Z^2} \quad Z = \frac{mH}{(\hbar^2 k_F)}

\[
T_S(E, \theta) = 1 + |a(E, \theta)|^2 - |b(E, \theta)|^2,
\]
### Calculated tunneling spectroscopy of STI

<table>
<thead>
<tr>
<th>$\Delta_{1a(b)}$</th>
<th>U-shaped gap structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_2$</td>
<td>ZBCP or ZBCP splitting</td>
</tr>
<tr>
<td>$\Delta_3$</td>
<td>No ZBCP (ZBCP is possible from in-plane junction)</td>
</tr>
<tr>
<td>$\Delta_4$</td>
<td>ZBCP</td>
</tr>
</tbody>
</table>

Experiments by Sasaki can be explained by $\Delta_2$ or $\Delta_4$ pairing.

<table>
<thead>
<tr>
<th>Pair potential</th>
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<th>orbital</th>
<th>Gap structure</th>
<th>Parity (orbital inversion)</th>
<th>Topological number</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta_{1a}$</td>
<td>$\Delta_1$</td>
<td>$A_{1u}$</td>
<td>intra</td>
<td>full gap</td>
<td>even</td>
<td>No</td>
</tr>
<tr>
<td>$\Delta_{1b}$</td>
<td>$\Delta_{2u}$</td>
<td></td>
<td></td>
<td>full gap</td>
<td>odd</td>
<td>DIII $Z_2$</td>
</tr>
<tr>
<td>$\Delta_2$</td>
<td>$\Delta_{y s_x}$</td>
<td>$A_{1u}$</td>
<td>triplet</td>
<td>intra</td>
<td>Point node (z-direction)</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_3$</td>
<td>$\Delta_{y s_z}$</td>
<td>$A_{2u}$</td>
<td>singlet</td>
<td>intra</td>
<td>Point node (z-direction)</td>
<td>odd</td>
</tr>
<tr>
<td>$\Delta_4$</td>
<td>$\Delta_{y s_y}$ ($\Delta_{y s_y}$)</td>
<td>$E_u$</td>
<td>triplet</td>
<td>inter</td>
<td>Point node (z-direction)</td>
<td>odd</td>
</tr>
</tbody>
</table>

Yamakage, Yada, Sato, and Tanaka, Physical Review B 85 180509(R) 2012
Summary (1)
Theory of tunneling spectroscopy of STI

1. $\Delta_2$ and $\Delta_4$ are consistent with point-contact experiment by Ando’s group.

2. Zero-bias conductance peak is possible even in full-gap topological 3d superconductors, differently from the case of BW in $^3$He.

3. Structural transition of the energy dispersion of ABS.

4. Analytical formula of ABS and conductance for fitting experiment is available now.

Yamakage, Yada, Sato, and Tanaka, Physical Review B 85 180509(R) 2012
Tunneling spectroscopy

Conventional BCS

Sn

Cu\textsubscript{x}Bi\textsubscript{2}Se\textsubscript{3}

Ando’s group (Osaka)

S. Sasaki et al PRL 107 217001 (2011)
Status of tunneling experiments

Consistent with Ando’s group with ZBCP

Contradict with Ando’s group with full gap (STM)

Composition and crystal structures of the actual samples have not fully clarified yet.

We must need further experimental and theoretical research.
Conflicting report which does not support topological superconductivity

How to resolve this discrepancy?

- Self-consistent determination of pair potential
- Surface-Dirac cone stemming topological insulator
- Evolution of Fermi surface

Levy et al., PRL 110, 117001 (2013)

Mizushima, Yamakage, Sato, Tanaka, arXiv:1311.2768
Electron interaction and pair potentials in doped TI

Short-range electron density-density interaction
Fu and Berg, PRL 105, 097001 (2010)

\[
\mathcal{H}_{\text{int}} = U \left[ n_1^2(r) + n_2^2(r) \right] + 2V n_1(r)n_2(r)
\]

We have determined the spatial dependence of the pair potential.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Spatial dependence of pair potential and LDOS

**Bulk: non-topological s-wave pairing**

\[ \hat{\Delta}(z) = \Delta_{1a}(z) + \Delta_3(z)\sigma_z \quad V/U = 0.0 \quad k_F\xi = 12.5 \]

\[ \tilde{m}_2 = -0.066 \]

Inevitable mixture of additional component due to the orbital polarization.

The separation between the conduction band and Dirac Fermi momentum of the Dirac cone \(k_F^D\).

\[ \delta \equiv \left( k_F^D - k_F \right) / k_F \]

**The large magnitude of \(\delta\) induces the splitting of coherence peak of SDOS.**

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Orbital Polarization of surface Dirac cone (normal state)

Dispersion of surface Dirac cone

$$E(k_x, k_y) = \pm v \sqrt{k_x^2 + k_y^2}$$

Wave functions of surface Dirac cone

$$\varphi_D(z) = (e^{-\kappa_- z} - e^{-\kappa_+ z}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}_\sigma \otimes u_s(k_x, k_y)$$

$$\kappa_\pm = \frac{v_z}{2m_1} \pm \sqrt{\frac{m_0 + m_2k_x^2}{m_1} + \frac{v_z^2}{m_1}}$$

"Penetration depth" of the Dirac cone $\ell \equiv \kappa_-^{-1} \sim k_F^{-1}$

LDOS for orbital 1

LDOS for orbital 2

Orbital polarization within the penetration depth of the surface Dirac fermions
Orbital polarization at the surface (superconducting)

Wave functions of surface Dirac cone

$$\varphi_D(z) = (e^{-\kappa z} - e^{-\kappa + z}) \begin{pmatrix} 0 \\ 1 \end{pmatrix}_\sigma \otimes u_s(k_x, k_y)$$

orbital 1: bulk
orbital 2: bulk + surface Dirac cone

orbital polarization $\Rightarrow$ drives a surface parity mixing

$$\hat{\Delta}(z) = \Delta_{1a}(z) + \Delta_3(z)\sigma_z$$

orbital 1 $\Delta_{1a} - \Delta_3$
orbital 2 $\Delta_{1a} + \Delta_3 \approx \Delta_{\text{bulk}}$

$\Delta_3 < 0$ from SCF calculation

enhancement of $\Delta_{1a} \approx \Delta_{\text{bulk}} + |\Delta_3|$ at surface

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Surface superconducting gap (splitting of single coherent peak) results from the synergy effect between the orbital polarization of the surface Dirac cone and the parity mixing of the pair potential.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Simple U-shaped STM spectrum in Cu$_x$Bi$_2$Se$_3$ is not originated from bulk s-wave pairing in the presence of surface Dirac cone existing in normal state.

STS data does not exclude the possible topological superconductivity.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)

Levy et al., PRL 110, 117001 (2013)

Topological superconductors represent a newly predicted phase of matter that is topologically distinct from conventional superconducting condensates of Cooper pairs. As a manifestation of their topological character, topological superconductors support solid-state realizations of Majorana fermions at their boundaries. The recently discovered superconductor Cu$_x$Bi$_2$Se$_3$ has been theoretically proposed as an odd-parity superconductor in the time-reversal-invariant topological superconductor class, and point-contact spectroscopy measurements have reported the observation of zero-bias conductance peaks corresponding to Majorana states in this material. Here we report scanning tunneling microscopy measurements of the superconducting energy gap in Cu$_x$Bi$_2$Se$_3$ as a function of spatial position and applied magnetic field. The tunneling spectrum shows that the density of states at the Fermi level is fully gapped without any in-gap states. The spectrum is well described by the Bardeen-Cooper-Schrieffer theory with a momentum independent order parameter, which suggests that Cu$_{0.2}$Bi$_2$Se$_3$ is a classical s-wave superconductor contrary to previous expectations and measurements.
Bulk topological odd-parity pairing

$A_{1u}$ state

There is no mixing of additional components at the surface.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Evolution of the Fermi surface

Odd parity pairing $\Delta_2$

(a) $\mu = 0.40$  (b) $\mu = 0.45$  (c) $\mu = 0.50$  (d) $\mu = 0.65$  (e) $\mu = 0.80$

(f) $\mu = 0.40$  (g) $\mu = 0.45$  (h) $\mu = 0.50$  (i) $\mu = 0.65$  (j) $\mu = 0.80$

$N_s(E)/N_{n0}(0)$

$E/\Delta$

QCP

T. Hashimoto et al 2014
Surface DOS of $A_{1u}$ state
(Evolution of Fermi surface)

$\Delta_2$

U-shaped Fermi LDOS is possible by the evolution of the Fermi surface from spheroidal to cylinder

$n \simeq 10^{17}$ cm$^{-3}$

$n \simeq 10^{19}$ cm$^{-3}$

$n \simeq 10^{20}$ cm$^{-3}$

Lahoud, PRB2013
Calculation of conductance odd parity pairing by changing Fermi surface

\[ \Delta_2 \quad \mu_S = 0.6 \text{ eV} \]
\[ \Delta_2 \quad \mu_S = 3.0 \text{ eV} \]
\[ \Delta_2 \quad \mu_S = 6.0 \text{ eV} \]
Evolution of Fermi surface can produce U shaped gap like spectra in odd parity pairing. 

Cu$_x$Bi$_2$Se$_3$ is still a strong candidate of topological superconductor.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Summary of SCF calculation

(1) If a topologically trivial bulk s-wave pairing symmetry is realized, the resulting surface density of state hosts an extra coherent peak at the surface induced gap besides a conventional peak.

(2) No such surface parity for topological odd-parity superconductors

(3) The simple U-shaped scanning tunneling microscope spectrum in Cu$_x$Bi$_2$Se$_3$ does not originate from s-wave superconductivity.

(4) Bulk odd-parity pairing gives a consistent understanding on the ZBCP observed in the point-contact tunneling spectroscopy and the U-shaped form of STS in Cu$_x$Bi$_2$Se$_3$.

Mizushima, Yamakage, Sato, Tanaka, PRB 90 184516(2014)
Crossed surface flat bands of doped Weyl semimetal superconductors

Wyle semimetal

- Zero-gap semiconductor caused by band crossing
- Linear dispersion near the band crossing point
- Breaking the time reversal symmetry or the inversion symmetry is necessary

Nodal point is stable against the perturbation

- Topological insulator/normal insulator superlattice (Burkov and Balents, PRL(2011))
- Pyrochlore iridates (X. Wan, et al., PRB(2011))
- HgCr$_2$Se$_4$ (G. Xu, et al., PRL(2011))
Key feature of Weyl semimetal: Fermi arc

X. Wan, et al., PRB(2011)
Hamiltonian of Wyle superconductor

\[ \mathcal{H}_k = t \sin k_x \sigma_y \tau_z - t \sin k_y \sigma_x \tau_0 + (t_z \cos k_z - M) \sigma_z \tau_z + m(2 - \cos k_x - \cos k_y) \sigma_z \tau_z - \mu \sigma_0 \tau_z - \Delta \sigma_y \tau_y. \]

**M term:** Time reversal symmetry breaking

Weyl points at \((0, 0, \pm Q)\) where \(M = t_z \cos Q\)

On the north pole and south pole, the directions of spin are the same, and therefore, \(s\)-wave pair potential can not open a gap.

**Point nodes**

G. Y. Cho, J. H. Bardarson, Y.-M. Lu, and J. E. Moore

PRB(2012)
Surface states of superconducting Weyl semimetal

Dispersion of the surface state

Quasiparticle spectra at $E=0$

Bo Lu, K. Yada, M. Sato and Y. Tanaka  
FIG. 3. (color online) (a) Projection of Fermi surfaces (dark region) on $k_y - k_z$ surface BZ and Chern number at a given $k_z$ in the BZ. The Chern number $C_1(k_z)$ changes when $k_z$ crosses a plane including a point node (red cross). The amount of change is given by the monopole charge of the point node. (b) Flat bands of SABS and Fermi arcs (lines with arrows) in the surface BZ.

Surface Andreev bound states of superconducting Weyl semimetal

$^3$He A-phase (single fermi surface)

Doped Weyl semimetal $\neq$ $^3$He A-phase $\times$ 2

The existence of the nontrivial state
(Fermi arc from normal state Weyl semimetal)
Surface Andreev bound states of superconducting Weyl semimetal

Can not connect

magnetic mirror reflection symmetry

particle-hole symmetry

+ particle-hole symmetry

FIG. 4. (color online). Normalized tunneling conductance as a function of bias voltage ($eV/\Delta$) in $x$-axis. $m$ is set as (a): 0.8 and (b): 0.2. (c) shows the relation between the height of normalized ZBCP and $\chi$. Other parameters are as the same as in Fig.2.
Summary of topological superconductor in doped Weyl semimetal

(1) We have obtained anomalous dispersion of Andreev bound state in superconducting doped Weyl semimetal with Fermi arcs in normal state.

(2) The Fermi arcs enable to support crossed flat bands of Andreev bound state.

(3) This flat band produces large Zero bias conductance peak.

arXiv:1406.3804