Designing 2D topological SC's

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ICTP 08.11.2015
Q. Topological Superconductor material?

Bulk

1D proximity

2D proximity?
Designing 2D topological SC's

• 2D topological SC
  – odd-parity SC of spinless fermions
  – Majorana bound state
  – Strategies: 1) interaction, 2) spinlessness

• T-inv topo-SC at a Metal/Quantum Spin Ice interface

• Modulated topo-SC in group VI TMD (e.g., MoS2)
Strategy I

- Manipulate the pairing interaction: target (ferromagnetic) spin fluctuation
Topological Superconductivity in Metal/Quantum-Spin-Ice Heterostructures

Jian-Huang She, Choonghyun Kim, Craig Fennie, Michael Lawler, E-AK (in preparation, 2015)
Q. Proof of principle for non-phonon mechanism?
Literature on spin-fluctuation mediated superconductivity

260,000 results on google scholar......

Spin-fluctuation-mediated even-parity pairing in heavy-fermion superconductors
Abstract It is shown that the anisotropic even-parity pairings are assisted and the odd-parity as well as the isotropic even-parity pairings are impeded by antiferromagnetic spin fluctuations which are observed in heavy-fermion solids.
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Anisotropic Superfluidity in He 3: A Possible Interpretation of Its Stability as a Spin-Fluctuation Effect
Abstract It is proposed that the paramagnon effects which enhance Tc for triplet pairing in He 3 are also important in selecting the particular component of the triplet p-wave state observed. It is found that the component favored is the original Anderson-Morel state.
Cited by 459 Related articles All 5 versions Web of Science: 360 Cite Save More
Proof of Principle Example for spin-fluctuation mediated SC?
Fundamental Challenge of non-Phonon mechanism

Phonon driven

Lattice of superconducting material

Spin-fluctuation driven

Lattice of superconducting material

Absence of separation of scales!
Challenges

Experimental

• The electrons and the glue cannot be separately controlled.

• Other ordering phenomena.

Theoretical

• Strongly correlated fermions, i.e. the sign problem.
Strategy?

The germ theory of disease. II.

Koch develops through sterility techniques and semisolid media to facilitate **bacterial isolation**. He also introduces theoretical criteria to define the role of bacteria in disease.
Strategy?
Separate the "glue" from "charge:
Heterostructure!

\[ \langle S_i(t) S_j(0) \rangle \neq 0 \]

spin-fluctuating insulator
Criteria for the substrate

1. No long range order $<S>=0$
2. Strong dynamic spin fluctuation $<S_iS_j>$
Quantum fluctuations in spin-ice-like Pr$_2$Zr$_2$O$_7$

K. Kimura$^1$, S. Nakatsuji$^{1,2}$, J.-J. Wen$^3$, C. Broholm$^{3,4,5}$, M.B. Stone$^5$, E. Nishibori$^6$ & H. Sawa$^6$

- Elastic neutron: pinch points (spin-ice like)
- Inelastic neutron: over 90% weight
• No order down to 20mK
• Dynamic fluct. upto ~3K
Structural Criteria for the Metal

1. Chemical stability
2. Lattice matching: $A_2B_2O_7$
3. No orphan bonds: (111) direction
Electronic Criteria for the Metal

1. Simple metal without ordering possibilities.
2. Wave function penetration for coupling.
3. Odd # of Fermi surface around high symmetry points for Topo SC.
Effective Continuum Theory

\[ H_c = \sum_{k\alpha} \left( \frac{\hbar^2 k^2}{2m} - E_F \right) \psi^\dagger_{\alpha}(k) \psi_{\alpha}(k) \]

\[ H_K(t) = J_K v_{\text{cell}} \sum_{a\alpha\beta} \int d^2r \psi^\dagger_{\alpha}(r) \sigma^a_{\alpha\beta} \psi_{\beta}(r) S_a(r_\perp = r, z = 0, t) \]

- Integrate out spins >> Effective e-e interaction

\[ H_{\text{int}}(t) = \left( \frac{J_K^2 v_{\text{cell}}^2}{\hbar} \right) \sum_{ab} \int dt' \int d^2r d^2r' s_a(r, t) \langle S_a(r, 0, t) S_b(r', 0, t') \rangle s_b(r', t') \]

\[ s_a(r, t) = \sum_{\alpha\beta} \psi^\dagger_{\alpha}(r, t) \sigma^a_{\alpha\beta} \psi_{\beta}(r, t) \]
Dominant Pairing Channel

- Key properties of the static spin structure factor

\[ S_{ab}(q) = \delta_{ab} - \left(1 - \frac{1}{1 + q^2 \xi^2}\right) \frac{q_a q_b}{q^2} \]

1. "spin-orbit" coupling
2. \( J_z = L_z + S_z \) conserved.
3. spin "mirror" symm: \( S_{ab}(q) = S_{ba}(q) \)
   -> singlet - triplet decoupled.

- Purely repulsive interaction in the singlet channel
Transition Temperature

• Spin dynamics

\[ T_c \sim \tau^{-1} e^{-1/\lambda} \]
\[ \lambda \sim \frac{J_K^2}{(E_F J_{ex})} \]
\[ \tau^{-1} \sim 2J_{ex} \sim 0.17 \text{meV} \]

• Parameters for our proposal

\[ E_F \sim 300 \text{meV}, \quad J_K \sim 10 \text{meV}, \quad \lambda \sim O(1) \]

• \( T_c \sim 1.5 \text{K} \)
1. $^3\text{He-B}$ type but 2D.
2. Overwhelmingly dominant.
Microscopic Proposal

\[ \text{Pr}_2\text{Zr}_2\text{O}_7/\text{Y}_2\text{Sn}_{2-x}\text{Sb}_x\text{O}_7 \ (111) \]

Non-magnetic

s-electrons:
large overlap,
isotropic FS.
Band structure for the Proposal

$Pr_2Zr_2O_7/Y_2Sn_{2-x}Sb_xO_7 \ (111)$

$x=0.2$

- Isotropic single pocket centered at $\Gamma$-point
Wave function penetration
Full Lattice Model for the proposal

- Effective Continuum theory is valid.
- Ferromagnetic fluctuation is dominant.
- Overwhelmingly dominant p-wave instability.
Earlier Proposal: Excitonic mechanism

- Little (64), Ginzburg (70), Bardeen (73)

Metal

- Unstable against exchange.
- Intrinsically s-wave.

Semi-conductor
Topological Superconductivity in Metal/Quantum-Spin-Ice Heterostructures

- Proof of principle for the spin-fluctuation SC.
- First T-inv Topo SC.
- Huge phase space.
Acknowledgements

Jian-huang She  Choonghyun Kim  Criag Fennie  Michael Lawler
Strategy II

• Manipulate the band structure
Modulated topological superconductivity in group-VI TMDs

Yi-Ting Hsu, Abolhassan Vaezi, E-AK (in preparation, 2015)
Q. What if the band structure is spin-split?
Spinless fermion via **real space** splitting

- TI surface states
- Proximity induce topo SC

Fu & Kane, PRL (2008)
Xu et al, Nat.Phys 10, 943 (2014)
Spinless fermion via $k$-space splitting?
Monolayer group VI TMD's

MoS$_2$, WS$_2$, MoSe$_2$, WSe$_2$

No inversion center! => Gap $\sim$2eV, spin-orbit coupling
Band-selective spin-splitting

- Partially filled crystal-field-split d-bands
  - Conduction band $|d_{z^2}\rangle : l_z=0$
  - Valence band $\frac{1}{\sqrt{2}}(|d_{x^2-y^2}\rangle \mp i|d_{xy}\rangle) : l_z=\pm 1$

- Spin-orbit coupling

$\vec{L} \cdot \vec{S}$

150~460meV
Confirmation of the band structure

Iwasa group N. Nano (2014)
k-space spin-split FS?

p-doped group VI- TMD!
Juice for superconductivity?

- d electrons => expect correlation effects
- n-doped TMD's

J.T. Ye et al. (Science 2012)
p-doped TMD

Moderate correlation (d-electron) +

k-space spin-split Fermi surfaces

Topological SC?

Yi-Ting Hsu

Abolhassan Vaezi
Triplet
\[ L = \pm 1 \]
\[ \vec{q} = -\vec{K} \]

Intra-pocket pairing

Inter-pocket pairing

Singlet + Triplet

\[ \vec{q} = \vec{K} \]
\[ L = 1 \]
Possible ground states

A. intra-pocket pairing

All electrons spin down

\[ L = \pm 1 \]

Triplet
Spatially modulated
Topo p+ip

Top view

All electrons spin up

\[ \vec{q} = -\vec{K} \quad \vec{q} = \vec{K} \]

B. inter-pocket pairing

All electrons spin down

Singlet+Triplet

\[ q = 0 \]

Top view

All electrons spin up

\[ \vec{q} = 0 \]
Perturbative Renormalization Group

- Microscopic interaction
  @ the UV limit:

- On-site repulsion $U$ (e-e)
  + Electron-phonon (e-phonon)
Effective interactions @

\[ E = \Lambda_0 < W \]

Pairing interaction for intra-pocket pair: \( g_1(E) \)

Pairing interaction for inter-pocket pair: \( g_2(E) \pm g_3(E) \)
$U > e$-ph case RG flow

Intra-pocket pairing: $g_1(E)$
Inter-pocket pairing: $g_2(E) \pm g_3(E)$

$g_1$ diverges negatively

$E = W$: Microscopic interactions
$E = \Lambda_0$: Effective interactions
$E \rightarrow 0$: Dominant instability
$U > e$-ph case RG flow

Effective interactions $E = \Lambda_0$

$E \rightarrow 0$ - Dominant instability

$g_1(E)$ diverges negatively

Intra-pocket pairing is dominant
Intra- v.s. Inter- pocket pairing

\[ \Leftrightarrow \text{e-e repulsion v.s. e-\text{ph} interaction} \]

- U only harms
- e-ph usually gives \( q=0 \) pairing

\[ U > \text{e-ph} \implies \text{intra-pocket pairing wins!} \]
Signature of

1. Spatially modulated phase (FF): phase sensitive measurement

2. Triplet spin response: Knight shift

3. Majorana bound state and edge states
Possible Materials

Transition metal dichalcogenides

\[
\begin{array}{cccc}
\alpha & \Delta & t & 2\lambda \\
\hline
\text{MoS}_2 & 3.193 & 1.66 & 1.10 & 0.15 \\
\text{WS}_2 & 3.197 & 1.79 & 1.37 & 0.43 \\
\text{MoSe}_2 & 3.313 & 1.47 & 0.94 & 0.18 \\
\text{WSe}_2 & 3.310 & 1.60 & 1.19 & 0.46 \\
\end{array}
\]

SOC-induced spin split
Topological properties for intra-pocket pairing

A. Chiral $p + ip$, breaks TRS

\[ p_x + ip_y \]

\[ K' \]

\[ K \]

\[ p_x + ip_y \]

Z-type topo sc:
integer spin degenerate edge modes

B. Non-chiral $p + ip$, preserves TRS

\[ p_x - ip_y \]

\[ K' \]

\[ K \]

\[ p_x + ip_y \]

$\Rightarrow Z_2$-type topo sc protected by TRS:
counter-propagating edge modes with spin up and down
Acknowledgements

Yi-Ting Hsu

Abolhassan Vaezi
Designing 2D topological SC's

- Control interaction
- Spinless fermion through k-space splitting
Funding