Odd-Parity Superconductors
Nematic, Chiral and Topological

Liang Fu

Nordita, Stockholm
July 7, 2016

Collaboration

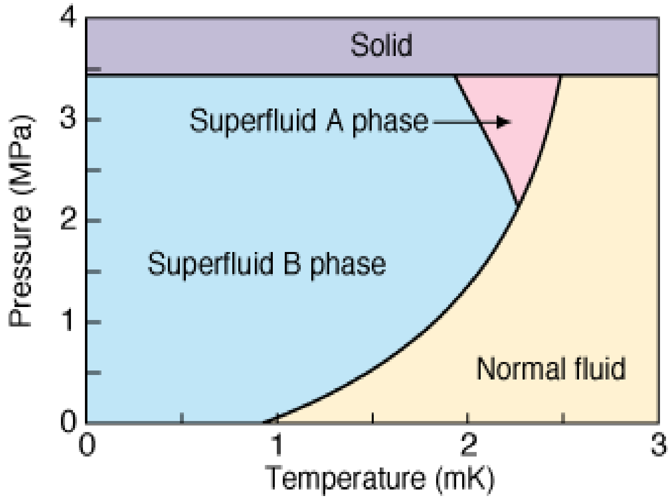
Vlad Kozii

Jorn Venderbos

Erez Berg

Odd-Parity Superconductors: $\Delta(k) = -\Delta(-k)$

p-wave superfluid He-3



- T-breaking A phase:
  point node in 3D; full gap in 2D
- T-invariant B phase: full gap
- Topological superfluid

(Candidate) Odd-Parity SCs: UPt_3 and Sr_2RuO_4

- Unconventional pairing symmetry
- Odd- vs even-parity debated

Odd-Parity Pairing and Spin-Orbit Coupling

Without SOC: odd-parity = spin triplet, meditated by spin fluctuations

SOC in inversion-symmetric materials:

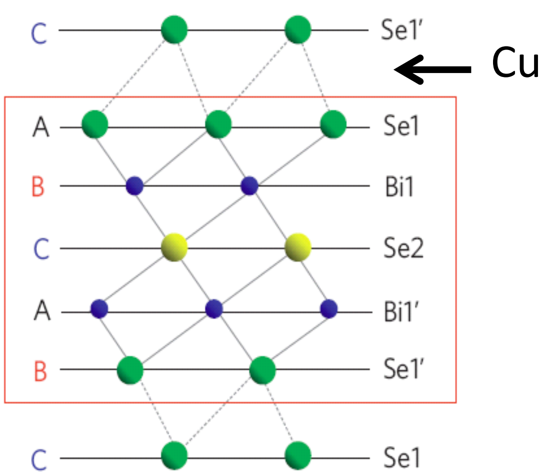
- bands are spin-orbit-entangled & doubly degenerate (pseudospin)
- odd-parity = pseudospin triplet

Odd-parity superconductivity with strong SOC ($\lambda_{SOC} \sim E_F$):

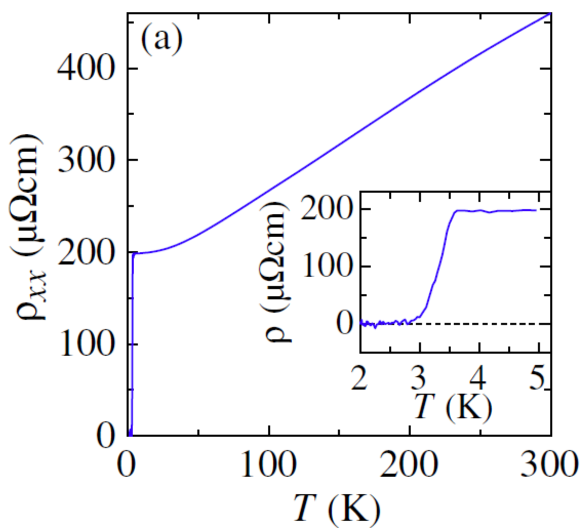
- does *not* require strong electron correlation
- can be meditated by electron-phonon interaction
- leads to new & topological phases absent in He-3

$Cu_xBi_2Se_3$

Bulk SC in a doped topological insulator: Cava et al., PRL (2010)

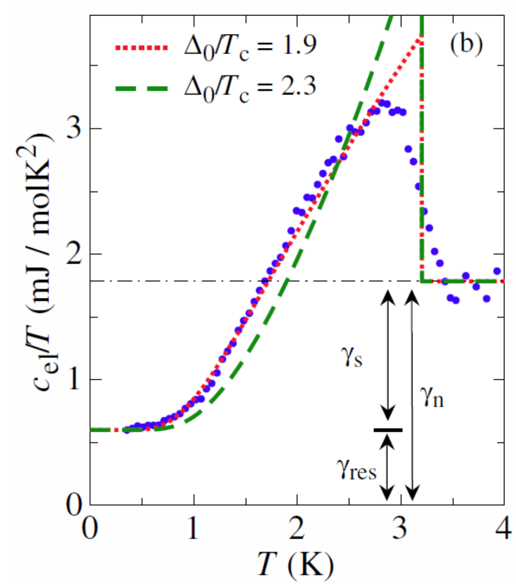


carrier density ~10^{20}



zero resistivity

Ando et al., PRL (2011)

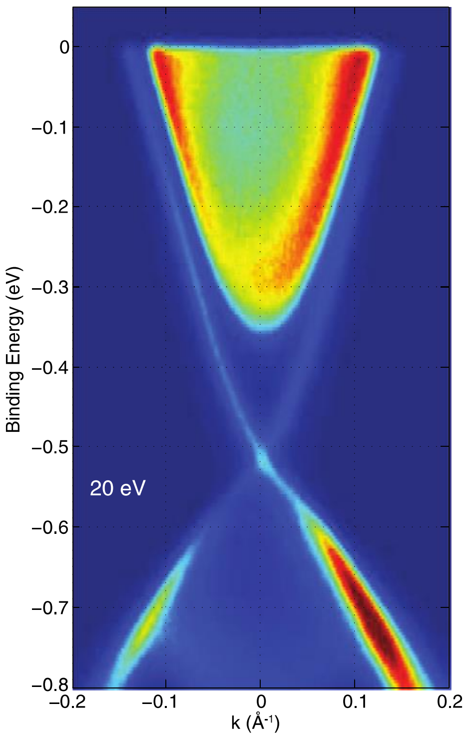


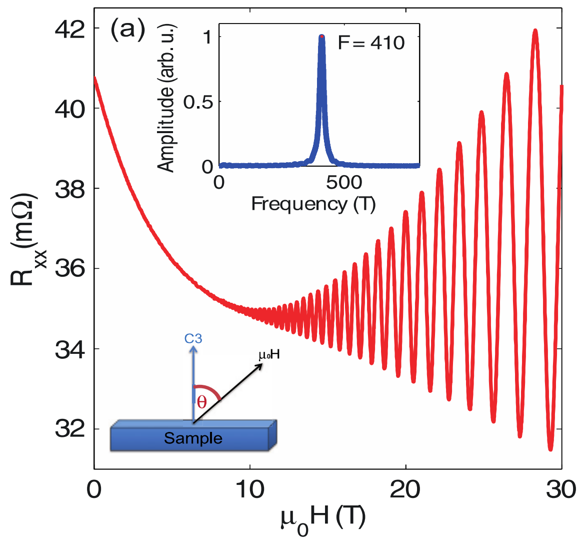
specific heat:

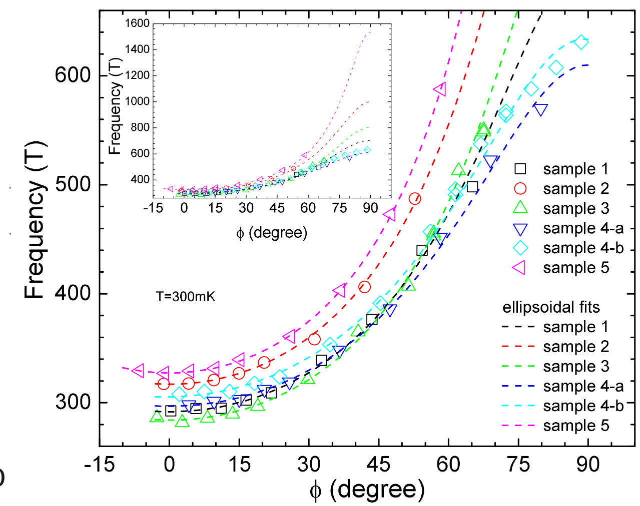
full gap or point node

Normal State Electronic Structure

ARPES and quantum oscillations: Dagan & Kanigel et al. PRB 13
Lu et al, PRB 14

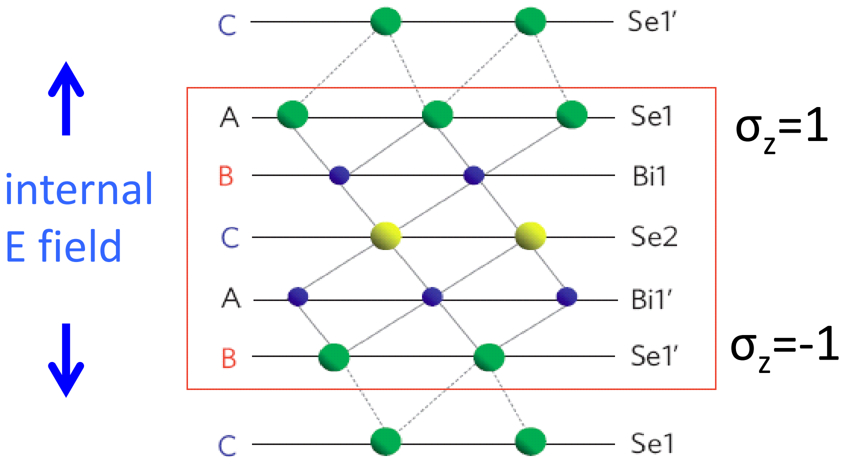


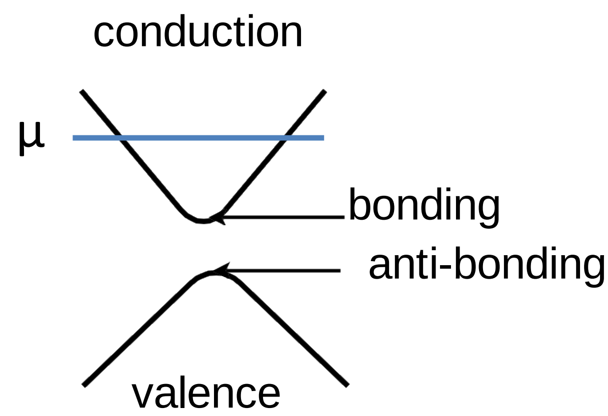




Single pocket: evolves from **closed** to **open** as electron density increases.

Spin-Orbit Coupling





Low-energy Hamiltonian: orbital (σ) and spin (s) LF & Berg, PRL 10

$$H_0 = \sum_k c_k^\dagger [m\sigma_x + v\underline{\sigma_z(k_x s_y - k_y s_x)} + v_z k_z \sigma_y - \mu] c_k$$

- staggered Rashba SOC from opposite E fields on top and bottom layers
- with inversion symmetry, SOC necessarily involves multiple orbitals

Pairing

Order parameters and pairing symmetries: LF & Berg, PRL 10

A_{1g} $\quad c^+_{1\uparrow} c^+_{1\downarrow} + c^+_{2\uparrow} c^+_{2\downarrow}$

A_{1u} $\quad c^+_{1\uparrow} c^+_{2\downarrow} + c^+_{1\downarrow} c^+_{2\uparrow}$

A_{2u} $\quad c^+_{1\uparrow} c^+_{1\downarrow} - c^+_{2\uparrow} c^+_{2\downarrow}$

E_u $\quad (c^+_{1\uparrow} c^+_{2\uparrow},\ c^+_{1\downarrow} c^+_{2\uparrow})$

odd-parity

- order parameters classified by representations of D_{3d} point group
- spin is locked to lattice by spin-orbit coupling

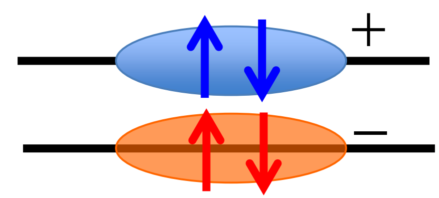
Pairing

Order parameters and pairing symmetries: LF & Berg, PRL 10

A_{1g} $\quad c^{+}_{1\uparrow} c^{+}_{1\downarrow} + c^{+}_{2\uparrow} c^{+}_{2\downarrow}$

$$\left.\begin{array}{ll} A_{1u} & c^{+}_{1\uparrow} c^{+}_{2\downarrow} + c^{+}_{1\downarrow} c^{+}_{2\uparrow} \\ A_{2u} & c^{+}_{1\uparrow} c^{+}_{1\downarrow} - c^{+}_{2\uparrow} c^{+}_{2\downarrow} \\ E_{u} & (c^{+}_{1\uparrow} c^{+}_{2\uparrow},\ c^{+}_{1\downarrow} c^{+}_{2\uparrow}) \end{array}\right] \text{odd-parity}$$

A_{2u} : sign-changing spin-singlet



odd-parity ≠ spin triplet

SOC is crucial for SC gap

- order parameters classified by representations of D_{3d} point group
- spin is locked to lattice by spin-orbit coupling

Pairing

Order parameters and pairing symmetries: LF & Berg, PRL 10

A_{1g} $\quad c^+_{1\uparrow} c^+_{1\downarrow} + c^+_{2\uparrow} c^+_{2\downarrow}$

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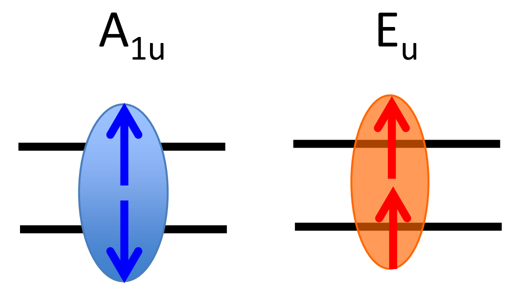
A_{2u} $\quad c^+_{1\uparrow} c^+_{1\downarrow} - c^+_{2\uparrow} c^+_{2\downarrow}$

E_u $\quad (c^+_{1\uparrow} c^+_{2\uparrow}, \; c^+_{1\downarrow} c^+_{2\uparrow})$

odd-parity



inter-orbital triplet
easy axis vs. plane

- order parameters classified by representations of D_{3d} point group
- spin is locked to lattice by spin-orbit coupling

Gap Functions in Band Basis

$\Delta_{\alpha\beta}(k)$

A_{1g}	$c^+_{1\uparrow} c^+_{1\downarrow} + c^+_{2\uparrow} c^+_{2\downarrow}$	Projection to band basis*	I
A_{1u}	$c^+_{1\uparrow} c^+_{2\downarrow} + c^+_{1\downarrow} c^+_{2\uparrow}$	$\Delta_{\alpha\beta}(k) c^+_{k,\alpha}\, \epsilon_{\beta\beta'} c^+_{-k,\beta'}$	$k \cdot \tau$
A_{2u}	$c^+_{1\uparrow} c^+_{1\downarrow} - c^+_{2\uparrow} c^+_{2\downarrow}$	$\longrightarrow$	$k_x \tau_y - k_y \tau_x$
E_u	$(c^+_{1\uparrow} c^+_{2\uparrow},\ c^+_{1\downarrow} c^+_{2\uparrow})$		$(k_x \tau_z - k_z \tau_x, k_y \tau_z - k_z \tau_y)$

Yip, PRB 13; Kozii & LF, PRL 15

Odd-parity pairing within SOC leads to p-wave gap functions distinct from He-3.

* d-vectors depend on band basis; use "manifestly covariant Bloch basis"

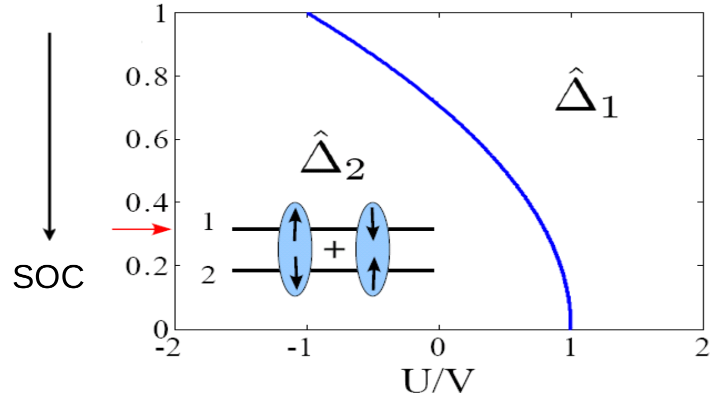
LF, PRL 15

Odd-Parity Pairing from Density Interaction

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

$$H_{int}(\mathrm{x}) = -U[n_1^2(\mathrm{x}) + n_2^2(\mathrm{x})] - 2Vn_1(\mathrm{x})n_2(\mathrm{x})$$

U: intra-orbital interaction V: inter-orbital interaction



Density interaction leads to pairing in even- and odd-parity channels, because strong SOC ($\lambda_{SOC} \sim E_F$) makes pairing interaction pseudospin-dependent.

Proof of principle: odd-parity pairing in electron-phonon superconductors

PRL **105,** 097001 (2010) PHYSICAL REVIEW LETTERS week ending 27 AUGUST 2010

Odd-Parity Topological Superconductors: Theory and Application to $Cu_xBi_2Se_3$

Liang Fu and Erez Berg

"We next study the pairing symmetry of the newly discovered superconductor $Cu_xBi_2Se_3$ within a two-orbital model, and find that a novel spin-triplet pairing with odd parity is favored by strong spin-orbit coupling. Based on our criterion, we propose that $Cu_xBi_2Se_3$ is a good candidate for a topological superconductor."

Support from electron-phonon calculations: Wan & Savrasov, Nat. Commun. 14

nature physics

ARTICLES

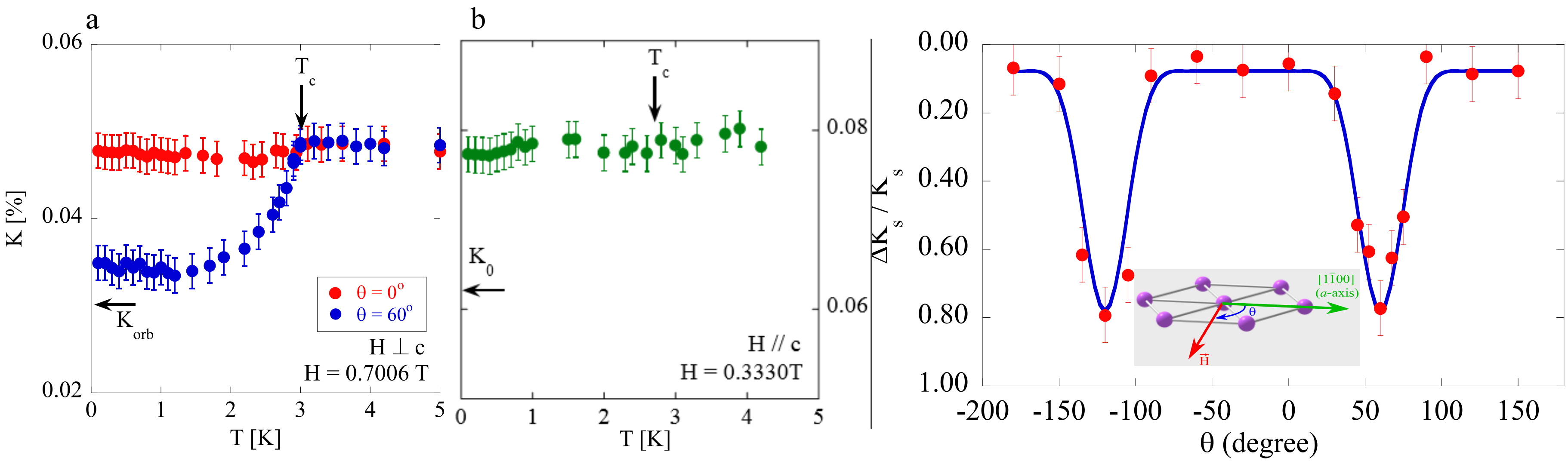
PUBLISHED ONLINE: 30 MAY 2016 | DOI: 10.1038/NPHYS3781

Spin-rotation symmetry breaking in the superconducting state of $Cu_xBi_2Se_3$

K. Matano[1], M. Kriener[2†], K. Segawa[2†], Y. Ando[2,3] and Guo-qing Zheng[1,4]*

NMR Knight Shift

Zheng et al, Nat. Phys. (2016)



Knight shift shows uniaxial anisotropy in SC state

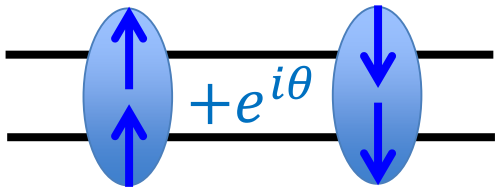
⇒ SC states spontaneously breaks three-fold rotational symmetry

first clear observation of rotational symmetry breaking in a SC

Rotation Symmetry Breaking from E_u Pairing

A_{1g}	$c^{+}_{1\uparrow} c^{+}_{1\downarrow} + c^{+}_{2\uparrow} c^{+}_{2\downarrow}$
A_{1u}	$c^{+}_{1\uparrow} c^{+}_{2\downarrow} + c^{+}_{1\downarrow} c^{+}_{2\uparrow}$
A_{2u}	$c^{+}_{1\uparrow} c^{+}_{1\downarrow} - c^{+}_{2\uparrow} c^{+}_{2\downarrow}$
E_u	$(c^{+}_{1\uparrow} c^{+}_{2\uparrow},\ c^{+}_{1\downarrow} c^{+}_{2\downarrow})$

"We find four different pairing symmetries in the $\boldsymbol{A_{1g}}$, $\boldsymbol{A_{1u}}$, $\boldsymbol{A_{2u}}$, and $\boldsymbol{E_u}$ representations of the $\boldsymbol{D_{3d}}$ group. The three ***A*** representations are one dimensional and the ***E*** representation is two dimensional. " LF & Berg, PRL 10



- Rotation symmetry breaking is only compatible with E_u pairing
- Anisotropic Knight shift requires locking of spin to the lattice by SOC.

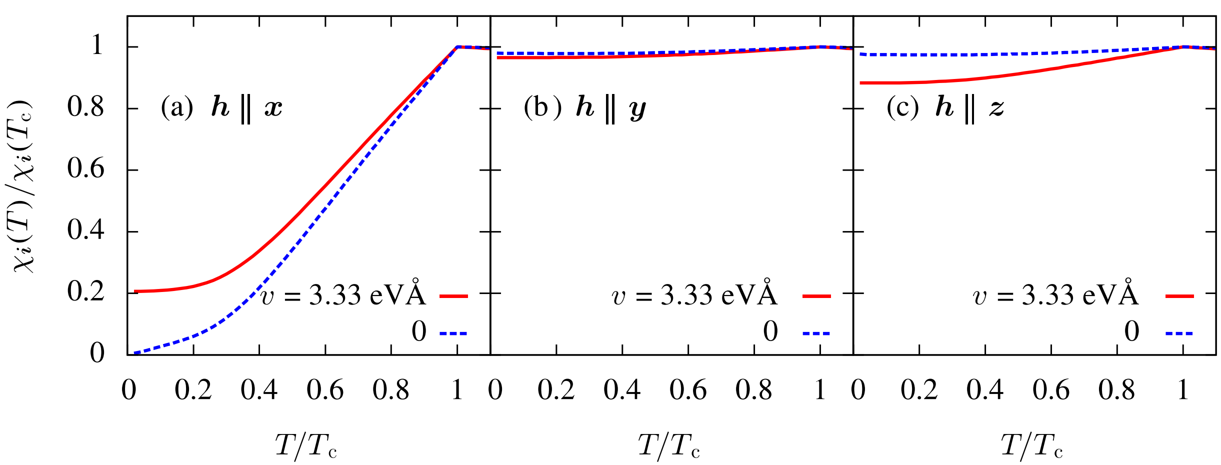
Bulk Electronic State of Superconducting Topological Insulator

Tatsuki HASHIMOTO, Keiji YADA, Ai YAMAKAGE, Masatoshi SATO, and Yukio TANAKA

Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

(Received November 27, 2012; accepted January 7, 2013; published online March 6, 2013)

"We calculate the temperature dependence of the specific heat and spin susceptibility for four promising superconducting pairings proposed by Fu and Berg … we obtain wide variations of the temperature dependence of spin susceptibility for each pairing, reflecting the spin structure of the Cooper pair."



- SOC in the two-orbital model is crucial for spin susceptibility

Odd-Parity Nematic Superconductor

Basis functions for Δ_4 pairing LF, PRB 14

$$\Psi_1 : i(c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} - c^\dagger_{1\downarrow} c^\dagger_{2\downarrow})$$
$$\Psi_2 : c^\dagger_{1\uparrow} c^\dagger_{2\uparrow} + c^\dagger_{1\downarrow} c^\dagger_{2\downarrow}$$

$(\Psi_1, \Psi_2) \sim (x,y)$

Real vs. complex order parameters:

- $\Psi = \cos\theta\, \Psi_1 + \sin\theta\, \Psi_2$ is T invariant and rotation breaking

  "nematic superconductor": new SC phase distinct from He3

  Ψ and $-\Psi$ correspond to the same superconducting state

  $|\Phi\rangle_{2N} = (\sum_k \Delta_k c^\dagger_k c^\dagger_{-k})^N |0\rangle$ => "odd-parity nematic SC"

- $\Psi_1 \pm i \Psi_2$ is rotation invariant and T breaking => chiral SC

Pinning the Two-Component Order Parameter

Ginzburg-Landau free energy $F = A(T - T_c)(|\eta_1|^2 + |\eta_2|^2) +$

quartic terms: $B_1(|\eta_1|^2 + |\eta_2|^2)^2 + B_2|\eta_1^* \eta_2 - \eta_1 \eta_2^*|^2$

Subsidiary nematic order: $(N_1, N_2) = (|\eta_1|^2 - |\eta_2|^2, \eta_1^* \eta_2 + \eta_2^* \eta_1)$

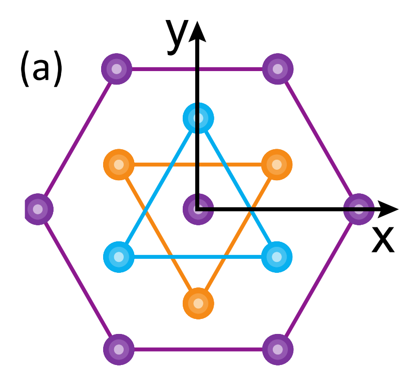
couples linearly to uniaxial strain $(\epsilon_{xx} - \epsilon_{yy}, 2\epsilon_{xy})$

- D_{3d} point group allows a sixth order term and selects easy axes in ab plane.

$$F^{(6)} = C_1(N_+^3 + N_-^3)$$

- pinning by symmetry-breaking field, e.g. uniaxial strain

$$F^{(2)} = h_1 N_1 + h_2 N_2$$

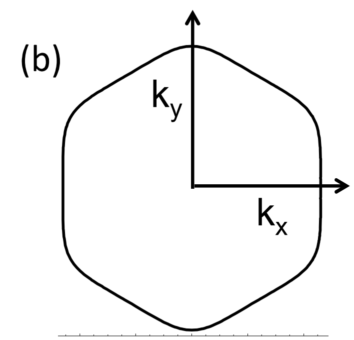


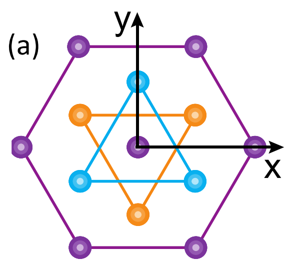
Anisotropic Gap Structures

Including crystal anisotropy: LF, PRB 14

$$H = H_0 + \lambda \sum_{\mathbf{k}} (k_+^3 + k_-^3) c_{\mathbf{k}}^\dagger \sigma_z s_z c_{\mathbf{k}},$$

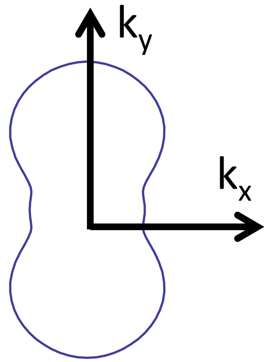
(hexagonal warping)





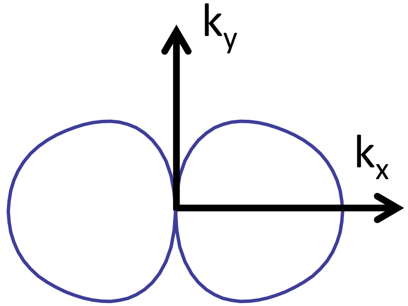
Quasi-particle gap

Ψ_2



T-invariant, full gap
=> topological SC

Ψ_1

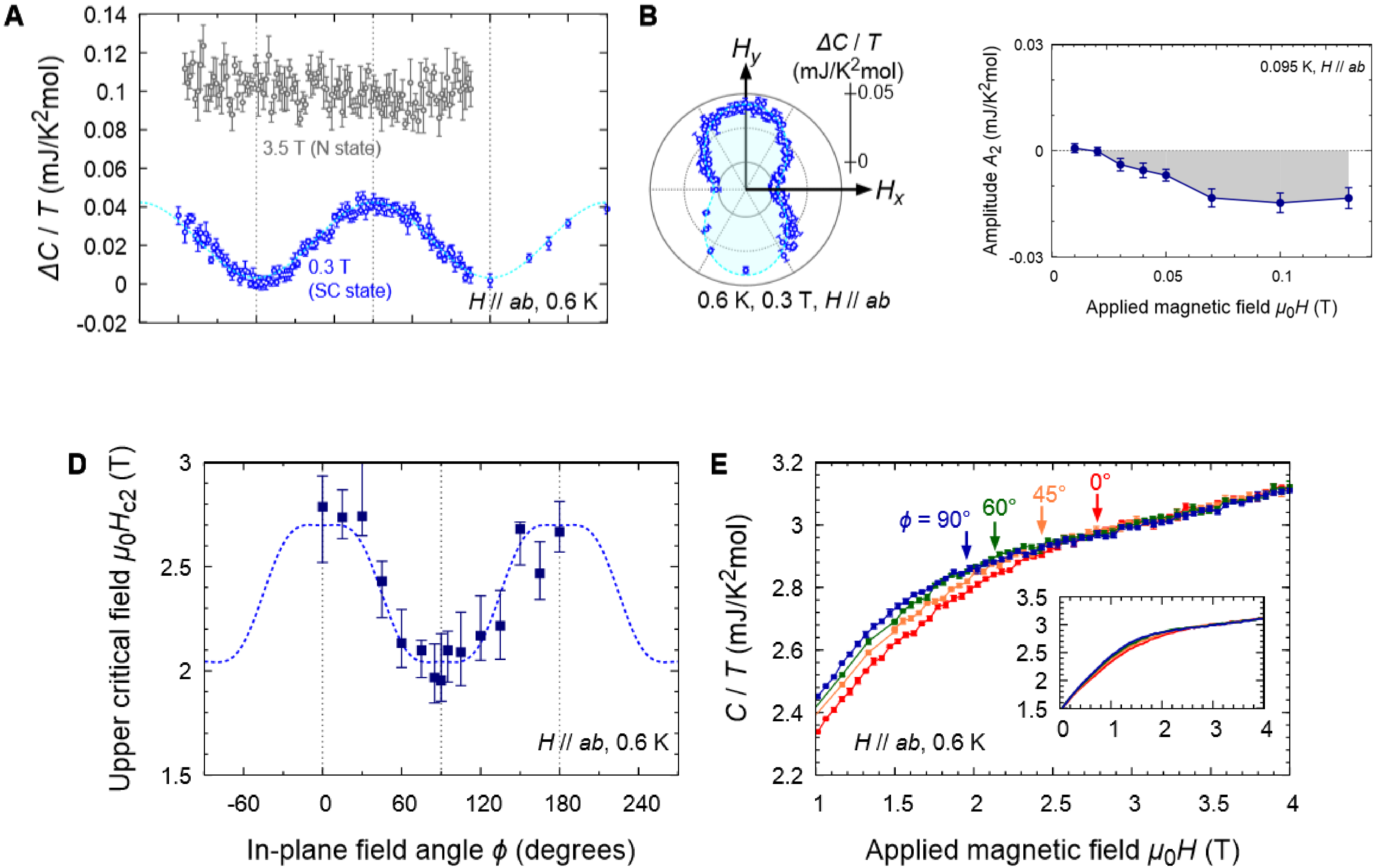


Point nodes protected by mirror
$\Rightarrow$ topological nodal SC

Thermodynamic evidence for nematic superconductivity in $Cu_xBi_2Se_3$

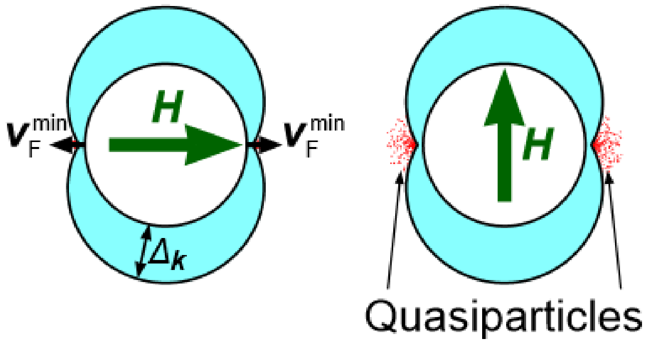
Shingo Yonezawa[1*], Kengo Tajiri[1], Suguru Nakata[1], Yuki Nagai[2], Zhiwei Wang[3,4], Koji Segawa[3,5], Yoichi Ando[3,4], Yoshiteru Maeno[1]

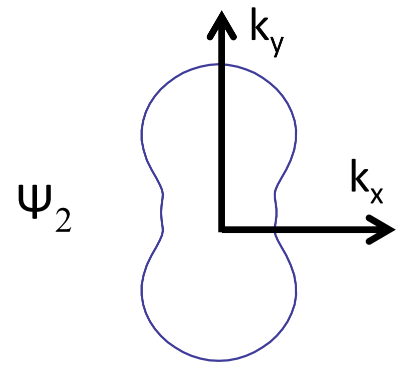
arXiv:1602.08941

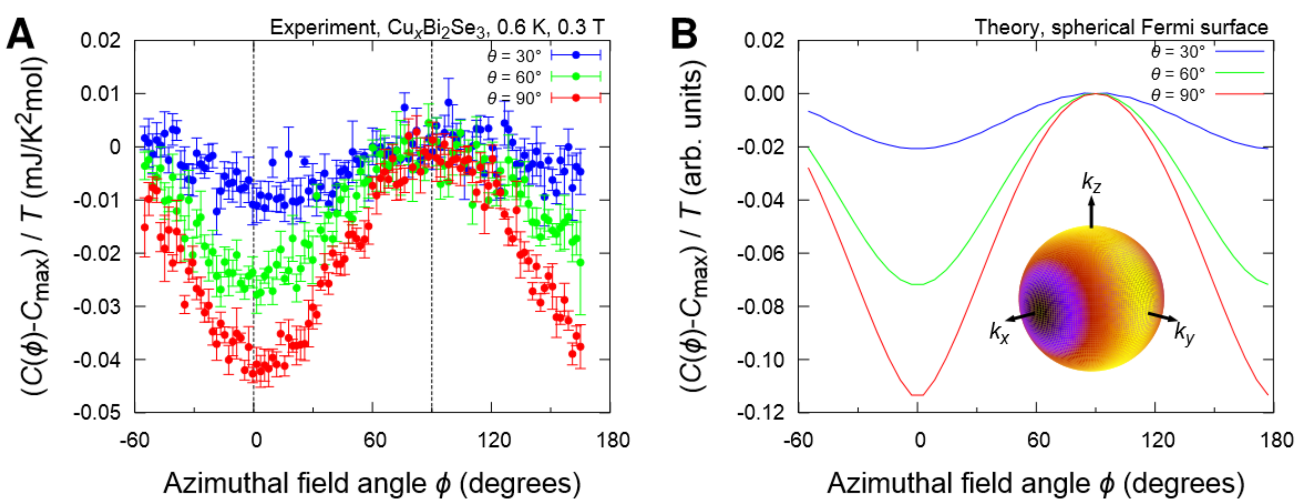


- Specific heat shows two-fold oscillation, down to H/Hc_2 = 1.5%

Field-Direction Dependent Specific Heat





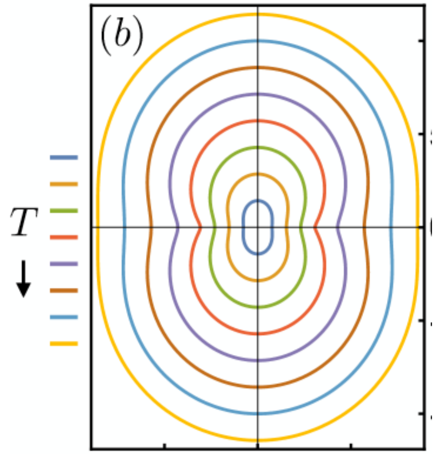


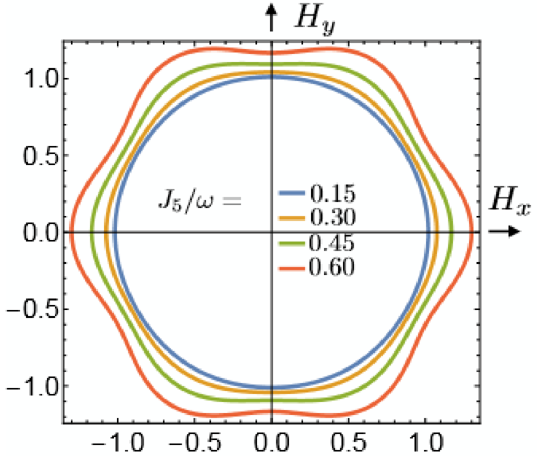
"From these agreements between experiment and theory, we conclude that the SC gap of $Cu_xBi_2Se_3$ is Δ_{4y}, possessing gap minima or nodes lying along the k_x direction"

Detecting Nematic Superconductivity

Basal plane anisotropy in thermodynamic, transport and spectroscopy

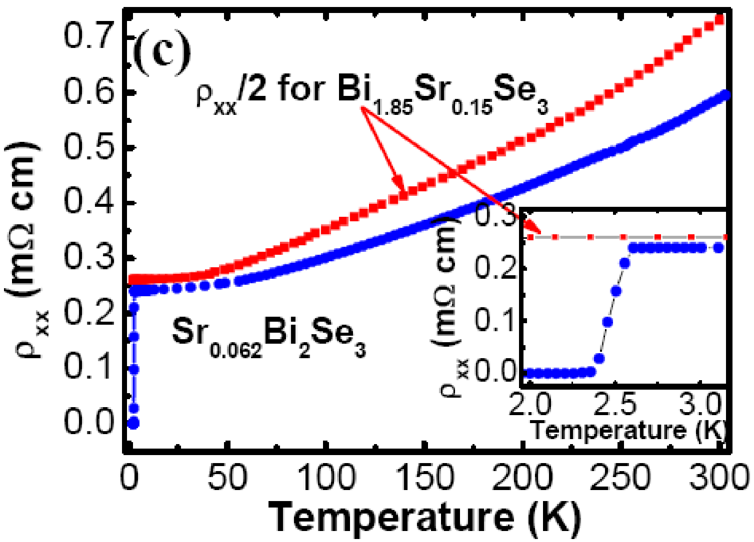
- gap anisotropy: directional tunneling, penetration depth,
  thermal conductivity in magnetic field (Nagai, PRB 12)
- vortex lattice anisotropy: neutron scattering, STM
- **upper critical field anisotropy** (Venderbos, Kozii, LF, arXiv:1603.03406)



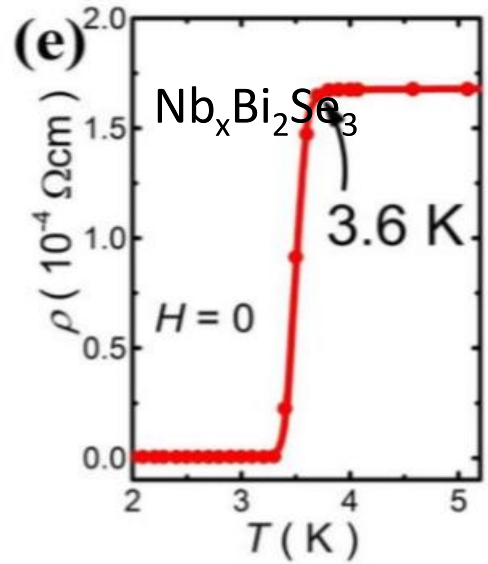


(b) $J_4/J_1 = 0.4$

$Sr_xBi_2Se_3$ & $Nb_xBi_2Se_3$



Zhang et al, J. Am. Chem. Soc. 15

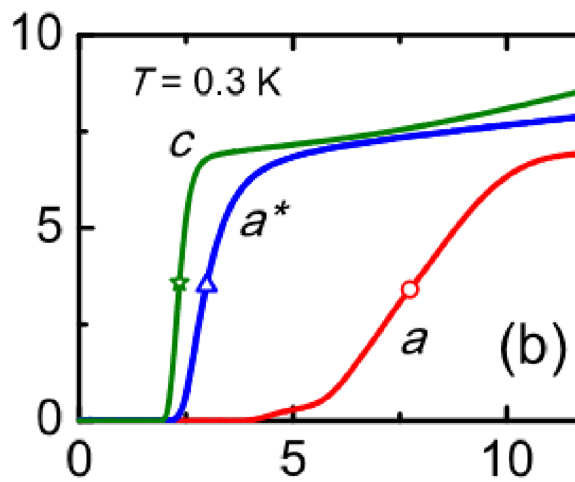


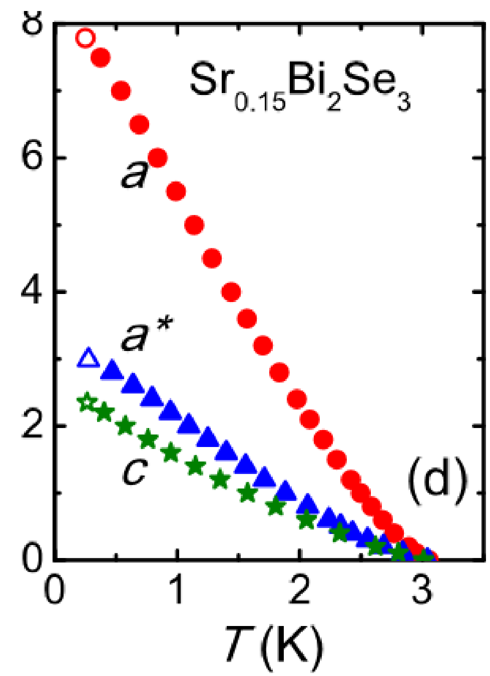
Hor et al, arXiv 15

Rotational symmetry breaking in the topological superconductor $Sr_xBi_2Se_3$ probed by upper critical field experiments

Y. Pan,[1,*] A. M. Nikitin,[1] G. K. Araizi,[1] Y. K. Huang,[1] and A. de Visser[1,†]

arXiv:1603.04197





- In-plane upper critical field shows twofold anisotropy

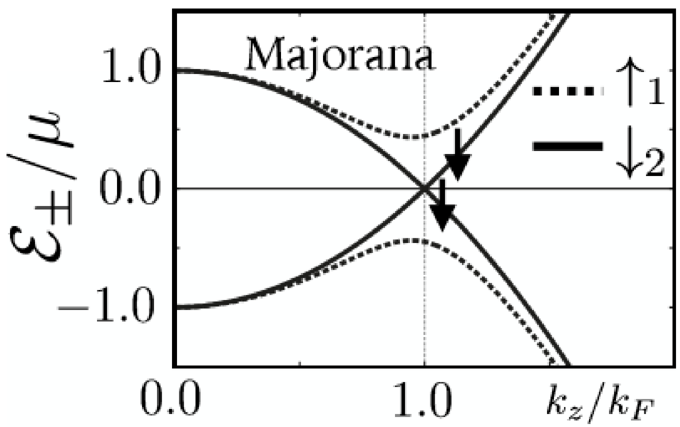
Doped topological insulators/semimetals with strong SOC ($\lambda_{SOC} \sim E_F$) may offer a new fertile ground for discovering odd-parity superconductivity.

Odd-Parity Chiral Superconductors

$\Psi_1 \pm i\,\Psi_2$ is a chiral state, with **non-unitary** gap function **due to SOC**

$$\Delta(k) = (k_x + i\,k_y)\,s_z - k_z\,s_+ \qquad \text{(distinct from He-3 A phase)}$$

- 3D closed Fermi surface: c-axis point nodes for spin ↓; full gap for spin ↑ nodal quasiparticles are **3D Majorana fermions**



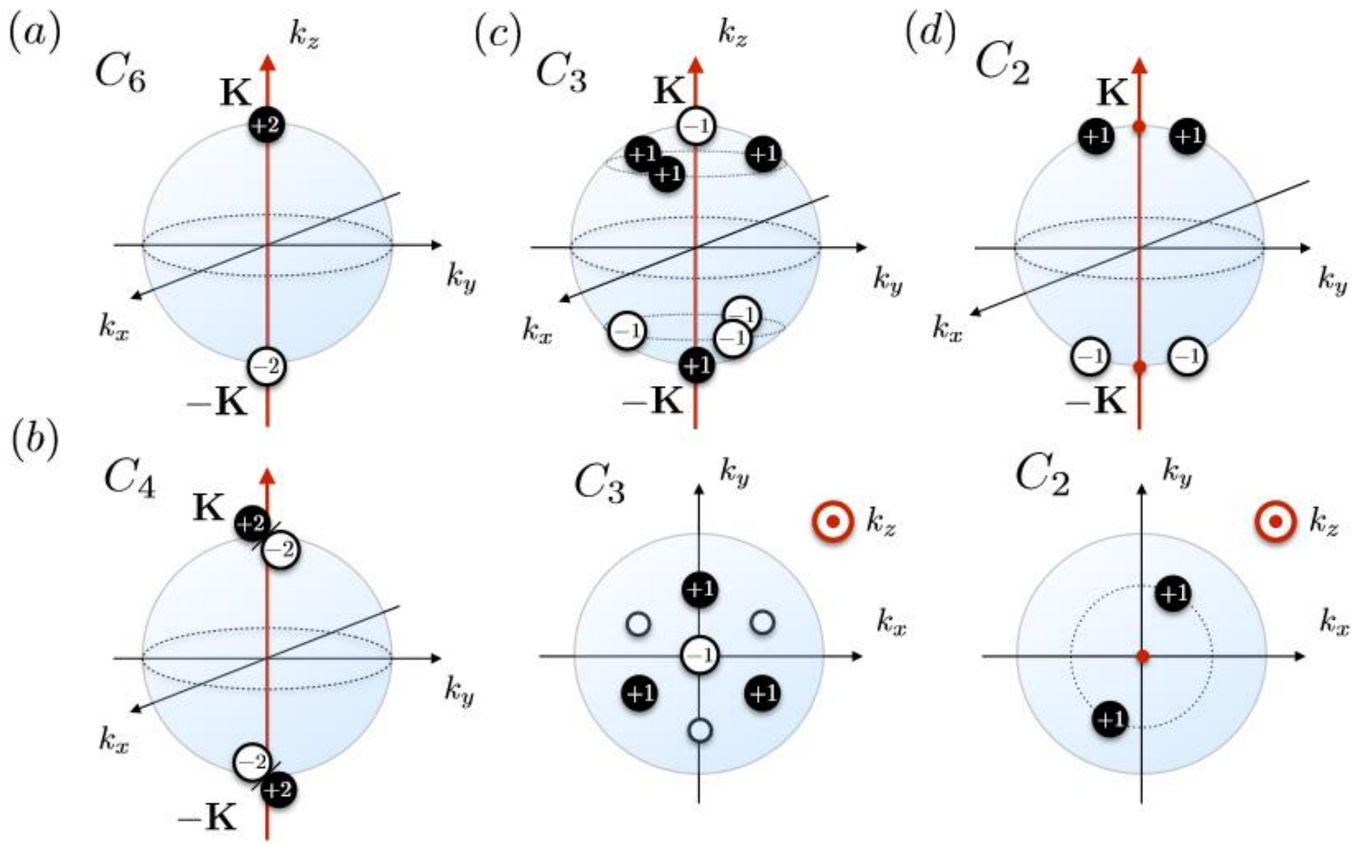
$$H_+ = \sum_{\vec q} \Psi^\dagger_{\vec q} \begin{pmatrix} v_F q_z & 0 & 0 & \lambda_c i q_- \\ 0 & -v_F q_z & \lambda_c i q_- & 0 \\ 0 & -\lambda_c i q_+ & v_F q_z & 0 \\ -\lambda_c i q_+ & 0 & 0 & -v_F q_z \end{pmatrix} \Psi_{\vec q},$$

$$\Psi_q^+ = \left(c^\dagger_{\vec K + \vec q}, c^\dagger_{-\vec K + \vec q}, c_{\vec K - \vec q}, c_{-\vec K - \vec q} \right)$$

- open Fermi surface: full gap, stack of 2D p + i p SC

Venderbos, Kozii, LF, arXiv:1512.04554

3D Majorana Fermions in Chiral Superconductors



Classification of MFs with different locations, dispersions & topological charges

Kozii, Venderbos, LF, to arXiv:1607…

Detecting Majorana Fermions by Anisotropic Spin Relaxation

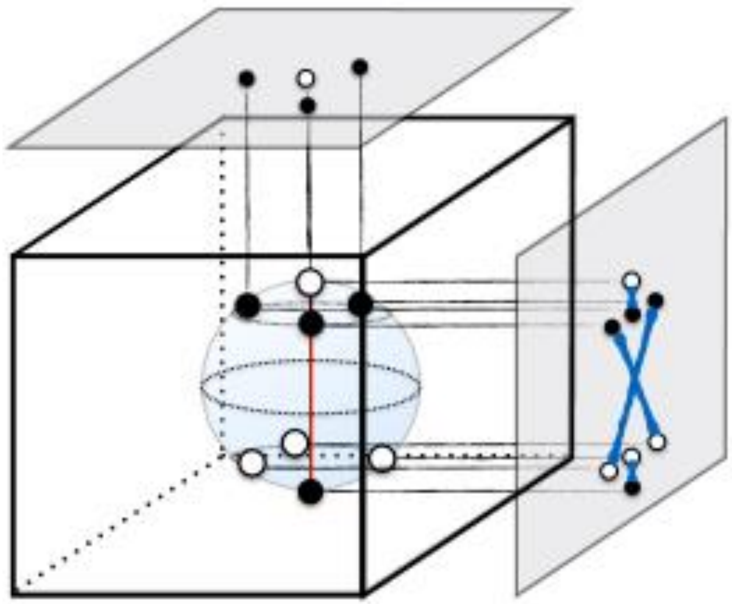
For quadratic Majorana nodes on rotation axis:

$$\frac{1}{T_1} = D_\perp T^3 S_\perp^2 + D_z T^3 \frac{T}{|\tilde{\Delta}_0|} S_z^2,$$

- Spin relaxation rate has different T-dependence for parallel and perpendicular nuclear spin components because gapless states near Majorana nodes are spin-polarized.

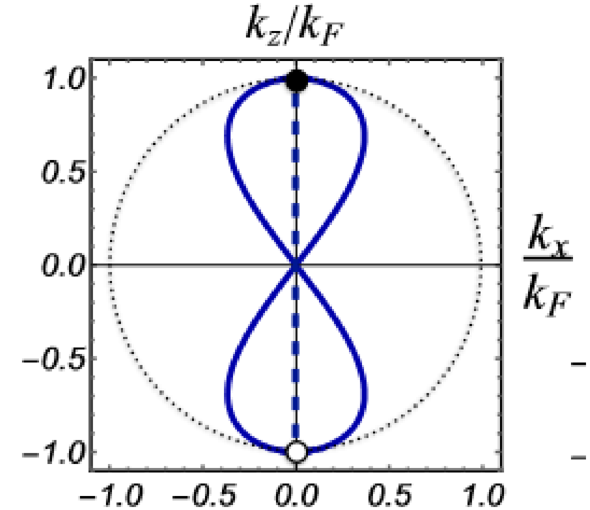
$$\mathcal{P} H_{\mathrm{hf}} \mathcal{P} = \gamma_N A_{\mathrm{hf}} \sum_{\mathbf{q}\mathbf{q}'} \hat{S}^z \left[g_{zz}^1 c_{\mathbf{q}1}^\dagger c_{\mathbf{q}'1} + g_{zz}^2 c_{\mathbf{q}2}^\dagger c_{\mathbf{q}'2} \right.$$
$$\left. + g_{zz}^3 c_{\mathbf{q}1}^\dagger c_{\mathbf{q}'2} + g_{zz}^{3*} c_{\mathbf{q}2}^\dagger c_{\mathbf{q}'1} \right],$$

Majorana Surface Arcs



3-fold symmetry

Linear Majorana nodes

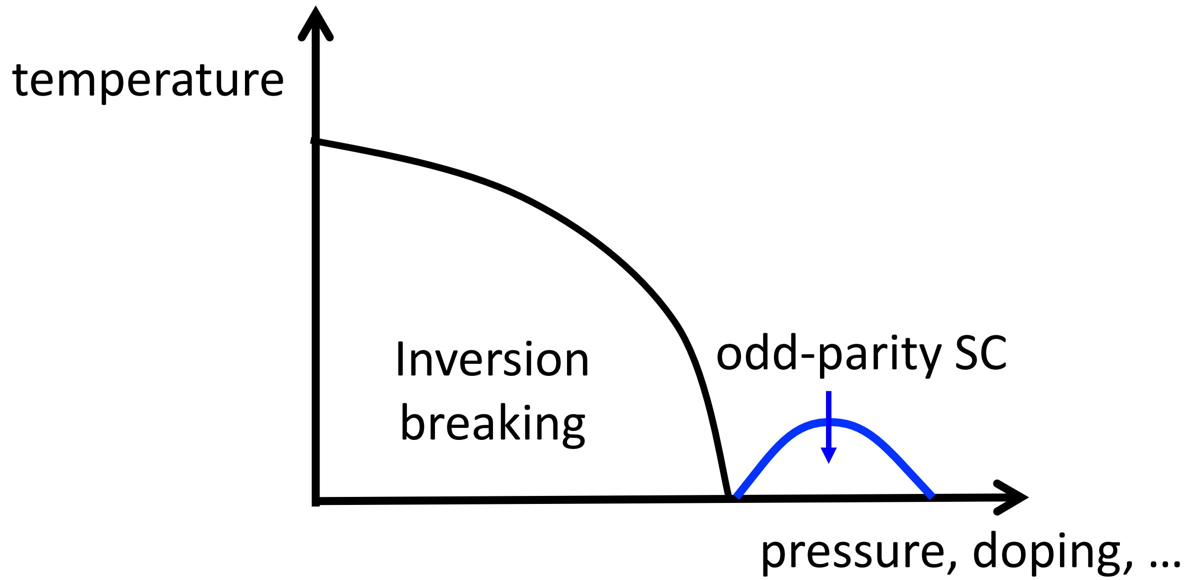


6-fold symmetry

Quadratic Majorana nodes

New Mechanism for Odd-Parity SC

Odd-parity pairing meditated by <u>parity</u> fluctuations in <u>spin-orbit-coupled</u> systems



superconductivity near inversion breaking structural distortion   Kozii & LF, PRL 15;

Inversion Breaking Coupled to Fermi Surface

Consider normal state with time-reversal (T) and inversion (P) symmetry

q=0 symmetry-breaking OPs: $\hat{Q} = \sum_k \Gamma_{\alpha\beta}(k) c^\dagger_{k\alpha} c_{k\beta}$

	T	P	$\Gamma(k)$	
nematic	$+$	$+$	$(k_x^2 - k_y^2) I$	
ferromagnet	$-$	$+$	$\vec{s}$	
current	$-$	$-$	$\vec{k} I$	
P-breaking orders	$+$	$-$	$\xi_{ij} k_i s_j$	*generalized spin current*

Spin-orbit interaction enables coupling between P-breaking orders and electrons on Fermi surface, with k- and (pseudospin)-dependent form factor.

LF, PRL 115, 026401 (2015)

Inversion-Breaking Particle-Hole Order Parameter

$$\hat{Q} = \sum_k \Gamma_{\alpha\beta}(k) c^\dagger_{k\alpha} c_{k\beta} \qquad \Gamma(k) = \xi_{ij} k_i s_j$$

- classified by representations of crystal point group
- symmetry operation acts jointly on momentum and spin

3D system with $O(3)$ symmetry	transformation property	
$\Gamma_1(\mathbf{k}) = (\hat{\mathbf{k}} \cdot \boldsymbol{\sigma})$	pseudoscalar	gyrotropic
$\Gamma_2^i(\mathbf{k}) = [\hat{\mathbf{k}} \times \boldsymbol{\sigma}]^i$	vector	ferroelectric
$\Gamma_3^{ij}(\mathbf{k}) = \hat{k}^i \sigma^j + \hat{k}^j \sigma^i - \frac{2}{3}(\hat{\mathbf{k}} \cdot \boldsymbol{\sigma})\delta^{ij}$	rank 2 tensor	multipolar

Consequences:

- P-breaking structural transition induces Fermi surface spin splitting

LF, PRL 115, 026401 (2015)

SC meditated by Parity Fluctuations

Parity fluctuations generate <u>k- and spin-dependent</u> effective interaction:

$$H_{\mathrm{eff}} = \sum_{\mathbf{q}} V_{\mathbf{q}} \hat{Q}(\mathbf{q}) \hat{Q}(-\mathbf{q}) \qquad V_{\mathbf{k}\pm\mathbf{k}'} = V_0 \mp V_1 \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}' + \ldots.$$

rewritten in pairing channel:

$$H_{\mathrm{p}} = V_0 (a_0 \hat{S}^\dagger \hat{S} + \sum_n a_n \sum_\mu \hat{F}_n^{\mu\dagger} \hat{F}_n^\mu)$$

- S denotes s-wave channel
- F's denote p-wave channels

$$\hat{F}^\dagger = \frac{1}{2} \sum_{\mathbf{k},\alpha\beta\gamma} \epsilon_{\beta\gamma} F_{\alpha\beta}(\mathbf{k}) c^\dagger_{\mathbf{k}\alpha} c^\dagger_{-\mathbf{k}\gamma}.$$ (form factor identical to particle-hole orders)

Vlad Kozii & LF, PRL 15

SC meditated by Parity Fluctuations

Attraction in both s-wave and the odd-parity pairing channel with the same symmetry as the fluctuating particle-hole order

$$H_{\mathrm{p}} = V_0 (a_0 \hat{S}^\dagger \hat{S} + \sum_n a_n \sum_\mu \hat{F}_n^{\mu\dagger} \hat{F}_n^\mu)$$ (a_n>0 is attractive)

Types of parity fluctuations

type of interaction	a_0	a_1	a_2	a_3	a_4
$\tilde{Q}_1(\mathbf{q})\tilde{Q}_1(\mathbf{q})$	1	1	-1	-1	0
$\tilde{Q}_2(\mathbf{q})\tilde{Q}_2(-\mathbf{q})$	1	-1	1	-1	0
$\tilde{Q}_3^i(\mathbf{q})\tilde{Q}_3^i(-\mathbf{q})$	1	$-1/2$	$-1/2$	1	$-1/4$

- Odd-parity pairing competes with s-wave; comparable pairing strengths.
- Coulomb interaction or Zeeman field suppresses s-wave, promotes odd-parity.

see also Wang, Cho, Hughes, Fradkin PRB 16

Summary and Outlook

Theoretical proposal: $Cu_xBi_2Se_3$ may be an odd-parity SC with strong SOC.

2016: NMR and field-dependent specific heat experiments discovered rotational symmetry breaking, providing strong evidence for odd-parity Δ_4 pairing with E_u symmetry.

Search for odd-parity chiral SCs with nonunitary gap & 3D Majorana fermions

Search for Majorana surface states---hallmark of topology

Microscopic pairing mechanisms