From Odd-Parity Pairing to Topological Superconductivity

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Outline

1. superconductivity in $Cu_xBi_2Se_3$
   - spin-orbit coupling drives odd-parity pairing

2. topological superconductors
   - criterion and experimental signature

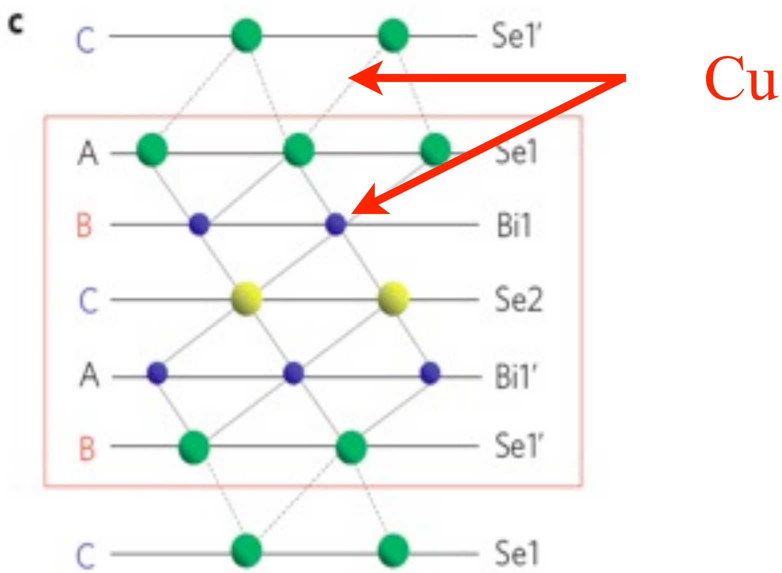
3. recent developments
   - unusual surface Andreev bound states
   - recent experiments on $Cu_xBi_2Se_3$

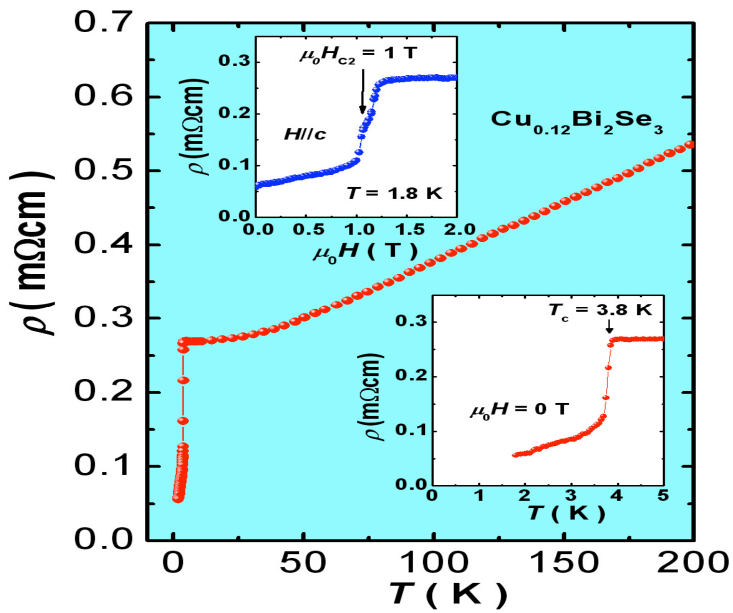
References:

1. LF & Berg, PRL 105, 097001(2010)
2. Hsieh & LF, arXiv 1109.3464
3. Qi & LF, 2011

Superconductivity in $Cu_xBi_2Se_3$

Hor et al, PRL 104, 057001 (2010)



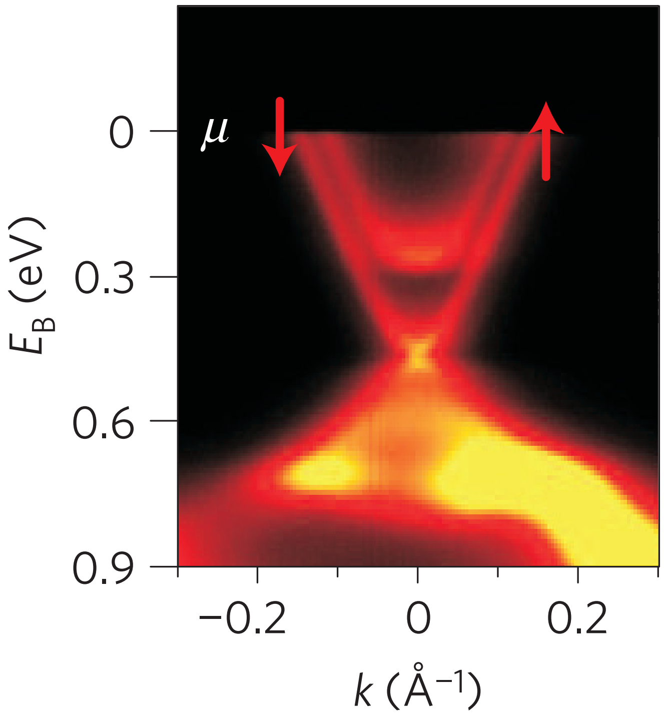


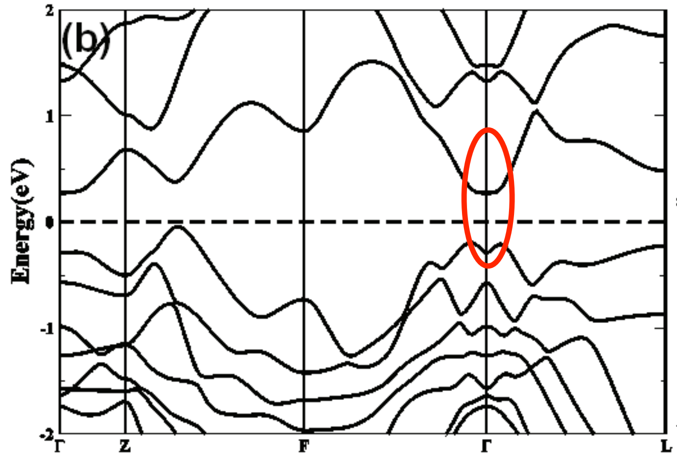
- doped semiconductor
- interstitial Cu: donor
- substitutional Cu on Bi: acceptor
- carrier density ~10^{20} cm^{-3}

- Tc up to 3.8K
- type-II: Hc2 ~ 1.7T(c-axis), 3.6T(ab)

Band Structure

ARPES on $Cu_xBi_2Se_3$: (Wray et al, Nature Physics 2010)





(Zhang et al, 2009)

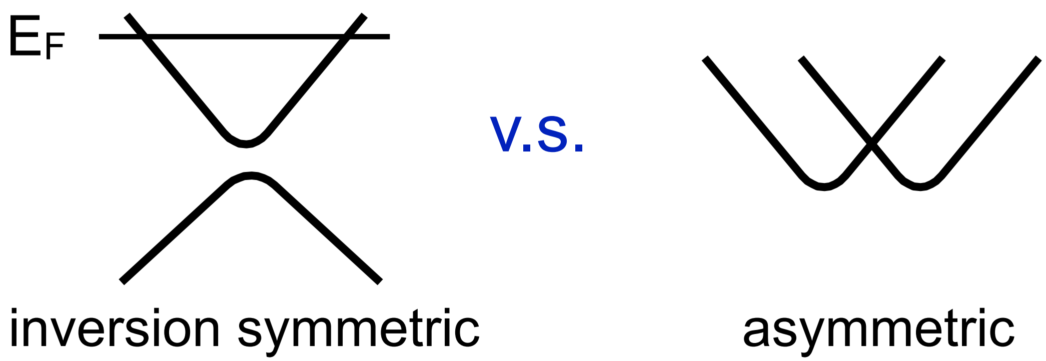
- rigid band shift due to electron doping by Cu
- Fermi energy E_F ~ 0.25eV from band bottom
- 3D Fermi surface centered at Γ: $k_F \sim 0.1A^{-1}$

Key Features

inversion symmetry + strong spin-orbit coupling

Consequences:

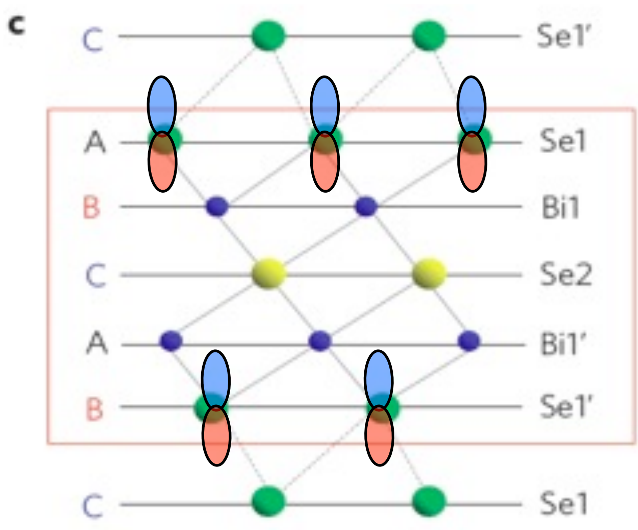
- energy bands are doubly degenerate & spin-orbital mixed
- spin-orbit coupling is hidden in wavefunction: dispersion not enough

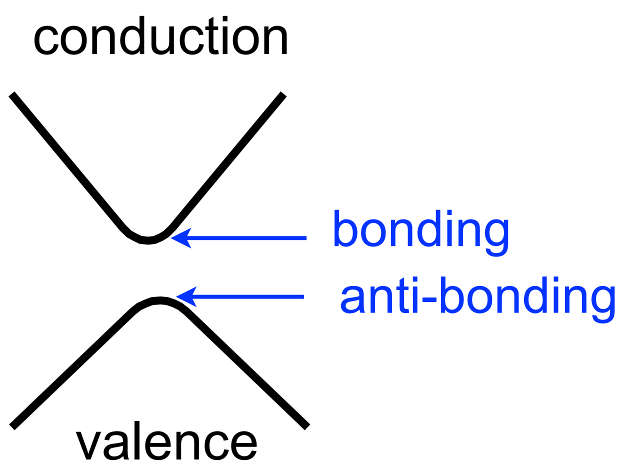


- at least two-orbitals to describe wavefunctions on Fermi surface

Previously overlooked material class for unconventional superconductors

k.p Hamiltonian





- Wannier functions: two Se-Bi p_z orbitals (σ_z) & electron spin (s_z)
- 4×4 k.p Hamiltonian dictated by symmetries:

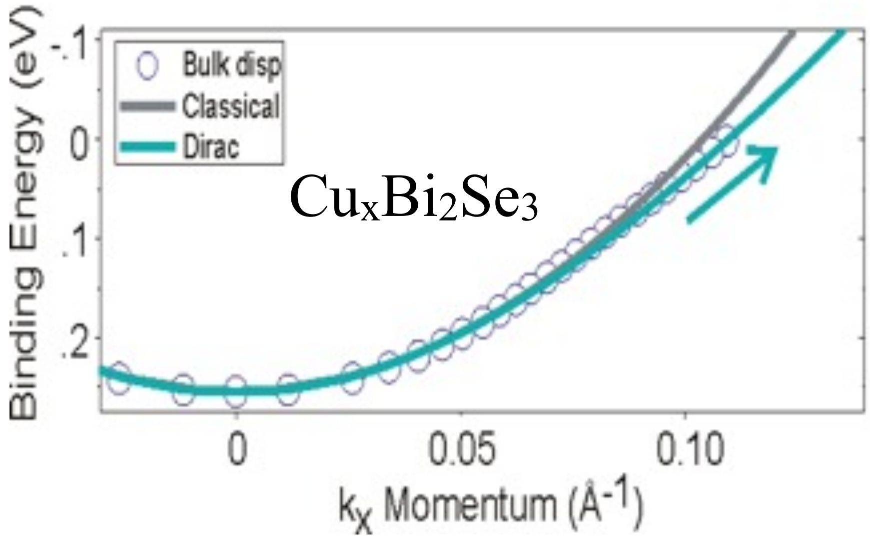
$$H_0(\mathbf{k}) = \underline{m\sigma_x + v_z k_z \sigma_y} + \underline{v(k_x\sigma_z s_y - k_y \sigma_z s_x)}$$

inter-layer hopping
Su-Heeger-Schrieffer model

intra-layer Rashba spin-orbit
with opposite electric fields

LF & Berg, PRL 10; Liu et al, PRB 10; tight-binding: Hsieh & LF, arXiv 11

k.p Hamiltonian



Relativistic dispersion:

$$E(\mathbf{k}) = \sqrt{m^2 + v^2 k^2}$$

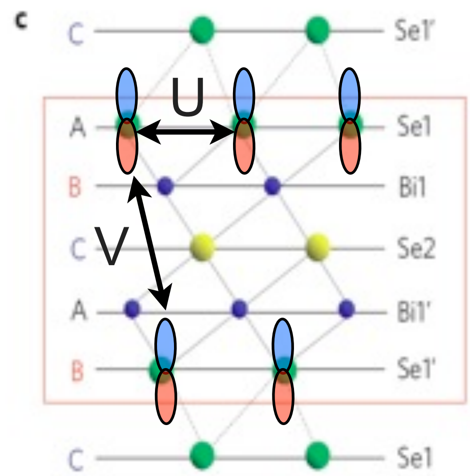
Parameters: (Hasan et al, PRB 11)

m=0.15eV, v=6eVA

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

- spin-orbit mixing is momentum dependent
- spin-orbit strength depends on doping: comparable to Fermi energy in superconducting doping. strongest!

Model Study of Paring Symmetry



Superconductivity is likely phonon-meditated.

Effective Hamiltonian:

$$H = \int d\mathbf{k} c^\dagger_{\mathbf{k}} (H_0(\mathbf{k}) - \mu) c_{\mathbf{k}} + \int d\mathbf{x} H_{int}(\mathbf{x}).$$

$$H_{int}(\mathbf{x}) = -U[n_1^2(\mathbf{x}) + n_2^2(\mathbf{x})] - 2V n_1(\mathbf{x}) n_2(\mathbf{x}).$$

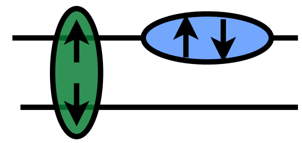
U: intra-orbital interaction V: inter-orbital interaction

- short range density-density interaction
- minimal modification of BCS theory of single band SC
- U and V are treated as phenomenological parameters

Classification of Paring Symmetry

Pairing order parameter: $\langle c^\dagger_{m\alpha}(\mathbf{x}) c^\dagger_{n\beta}(\mathbf{x}) \rangle$ (m,n: orbital & α,β: spin)

- classified by representation of crystal point group D_{3d}
- even- and odd-parity pairing under inversion (1↔2)



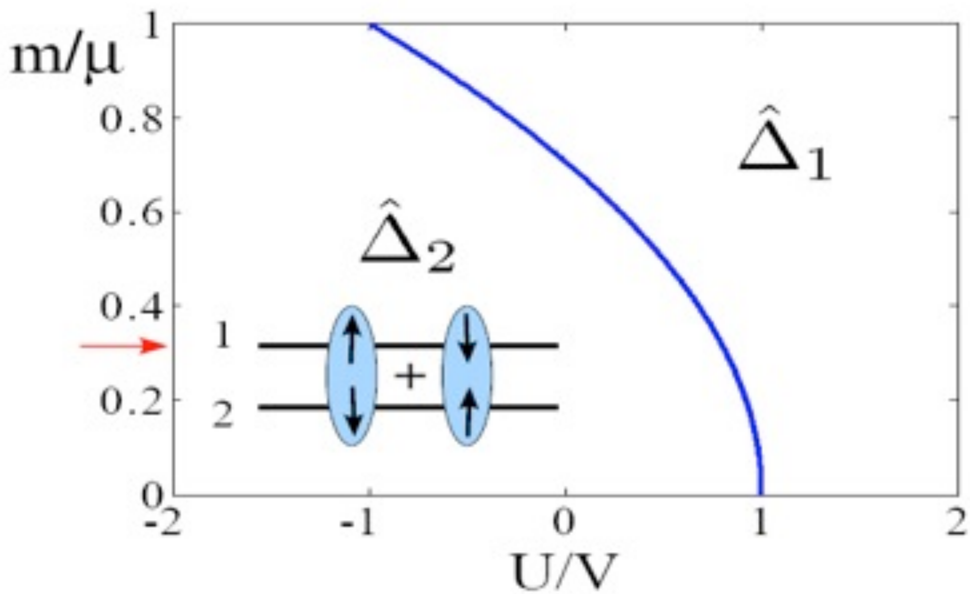
intra-orbital

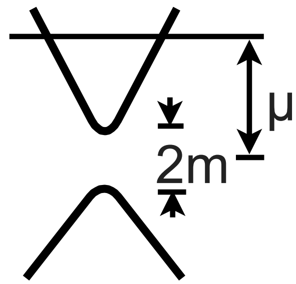
	• pairing	• C_3 rotation	• inversion	• mirror	
$c_{1\uparrow}c_{1\downarrow} + c_{2\uparrow}c_{2\downarrow}$	singlet	$+$	$+$	$+$	A_{1g}
$c_{1\uparrow}c_{1\downarrow} - c_{2\uparrow}c_{2\downarrow}$	singlet	$+$	$-$	$+$	A_{2u}

inter-orbital

	pairing	C_3 rotation	inversion	mirror	
$c_{1\uparrow}c_{2\downarrow} - c_{1\downarrow}c_{2\uparrow}$	singlet	$+$	$+$	$+$	A_{1g}
$c_{1\uparrow}c_{2\downarrow} + c_{1\downarrow}c_{2\uparrow}$	triplet	$+$	$-$	$-$	A_{1u}
$(c_{1\uparrow}c_{2\uparrow}, c_{1\downarrow}c_{2\downarrow})$	triplet	(x, y)	$(-, -)$	$(+, -)$	E_u

Odd-Parity Pairing





U: intra-orbital
V: inter-orbital (attractive)

Δ_1 : spin singlet, even-parity

Δ_2 : inter-orbital spin triplet, odd-parity

- m/μ: doping-dependent spin-orbit; U/V: interaction
- two phases are fully gapped & TR-invariant.
- Δ_2 pairing wins for attractive U and V:
  electron-phonon + spin-orbit realizes unconventional pairing symmetry.
- Δ_2 realizes a topological superconducting phase

Topological Superconductor

- definition: a fully gapped superconductor which cannot be smoothly (w/o gap closing) connected to the strong coupling BEC regime.

(see Read & Green 00)

- mean-field definition and classification

(Schynder, Ryu, Furusaki & Ludwig 08; Kitaev; 08; Qi et a, 09; Volovik et al)

symmetry class	d=2	d=3	superconducting analog of
D (T-breaking)	Z	0	quantum Hall state
→ DIII (T-invariant)	Z_2	Z	topological insulator

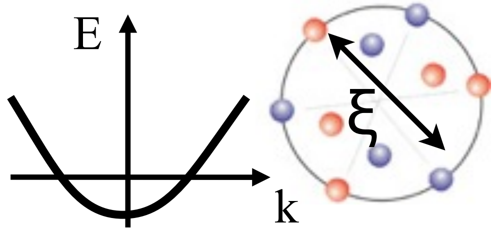
- bulk-boundary correspondence: gapless surface excitations

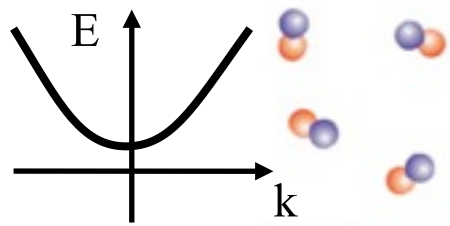
where to find a topological superconductor?

Pairing Symmetry

Even-parity $\Delta(c^\dagger_{k\uparrow}c_{-k\downarrow} - c^\dagger_{k\downarrow}c_{-k\uparrow})$ gap = $\sqrt{(E_k-\mu)^2+\Delta_k^2}$

BCS: $\mu>0$ —— **crossover** ——→ BEC: $\mu<0$

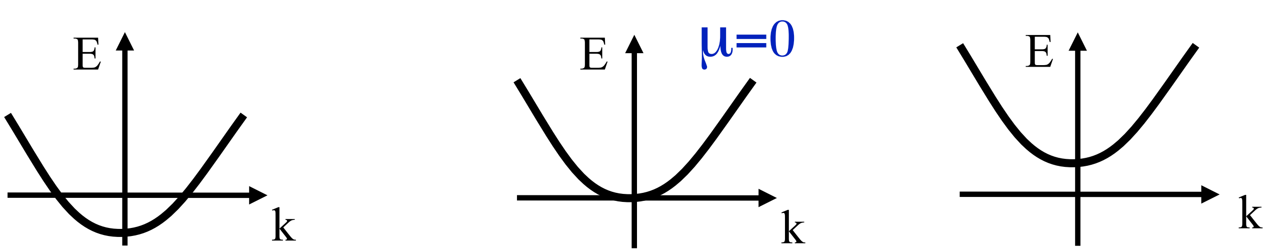




- gap is finite across BCS-BEC: topologically trivial.

Odd-parity $\Delta_k(c^\dagger_{k\uparrow}c_{-k\downarrow} + c^\dagger_{k\downarrow}c_{-k\uparrow}),\ \Delta_k \propto k$

BCS —— **transition** ——→ BEC



- gap closing at $\mu=0$; phase transition from BCS to BEC; BCS is topological.

topological superconductivity ≈ odd-parity pairing

Pairing Symmetry

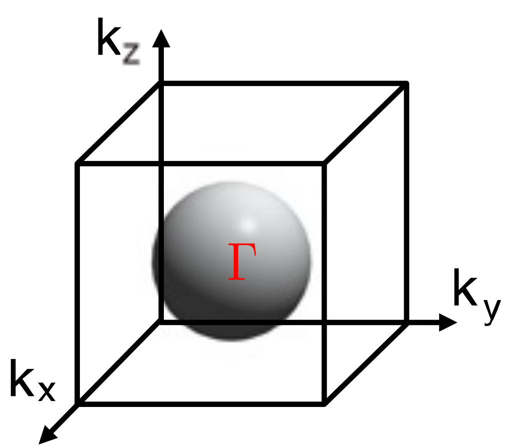
the key to topological superconductors

Criterion for fully-gapped TR-invariant topological superconductor (class DIII) with inversion symmetry:

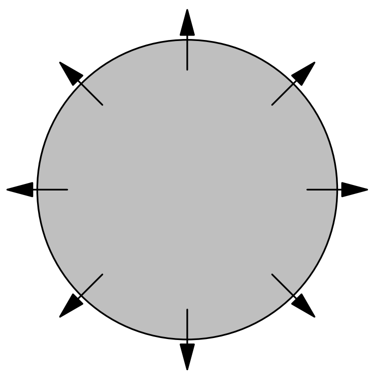
0. Odd-Parity Pairing ***and***
1. Fermi surface encloses an odd # of TR-invariant momenta ***or***
2. d-vector has a nonzero winding number over Fermi surfaces

(LF & Berg, PRL 10; LF & Kane, PRB 07)
(Yang Qi & LF, 11)

1.



2.

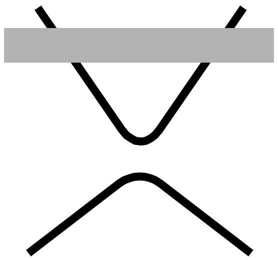


d-vector defined by pairing

$$\psi^{\dagger}_{k\alpha}[\vec{d}(k)\cdot\vec{s}(is_y)]_{\alpha\beta}\psi^{\dagger}_{-k\beta}$$

α, β: pseudo-spin

Δ_2 phase: electronic analog of superfluid He-3



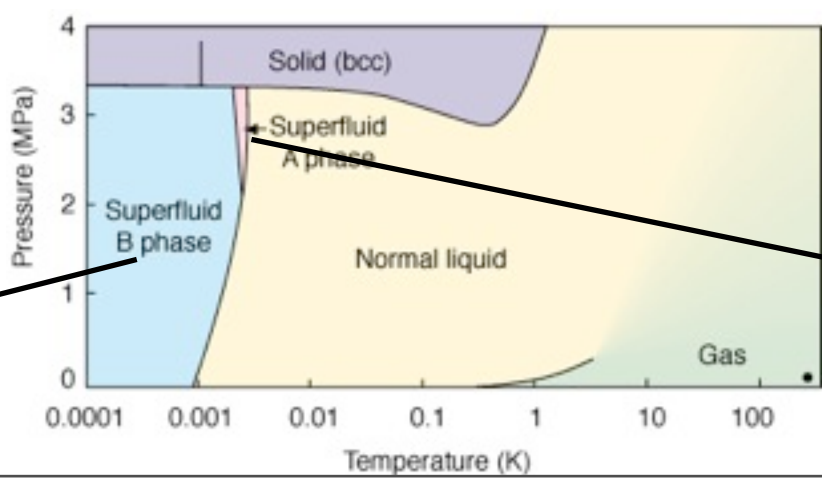
pairing gap << Fermi energy =>

pairing order parameter can be expressed in terms of states at Fermi surface ψ_{k1} and ψ_{k2} (pseudospin).

$$c_{1\uparrow}c_{2\downarrow} + c_{1\downarrow}c_{2\uparrow} \quad \Longrightarrow \quad \psi_k \begin{pmatrix} k_z & k_y + ik_x \\ k_y - ik_x & -k_z \end{pmatrix} (is_y \psi_{-k})$$

- k-dependence comes from electron wavefunction.
- pseudospin triplet pairing, analogous to He-3 BW phase
- Δ_2 pairing realizes a topological superconductor phase in class DIII.

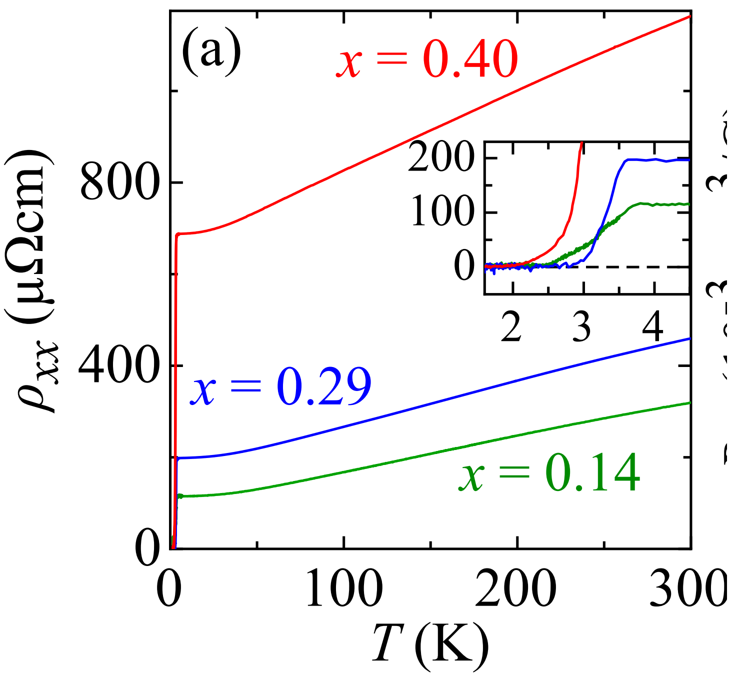
T-invariant:
3D $Cu_xBi_2Se_3$ (?)

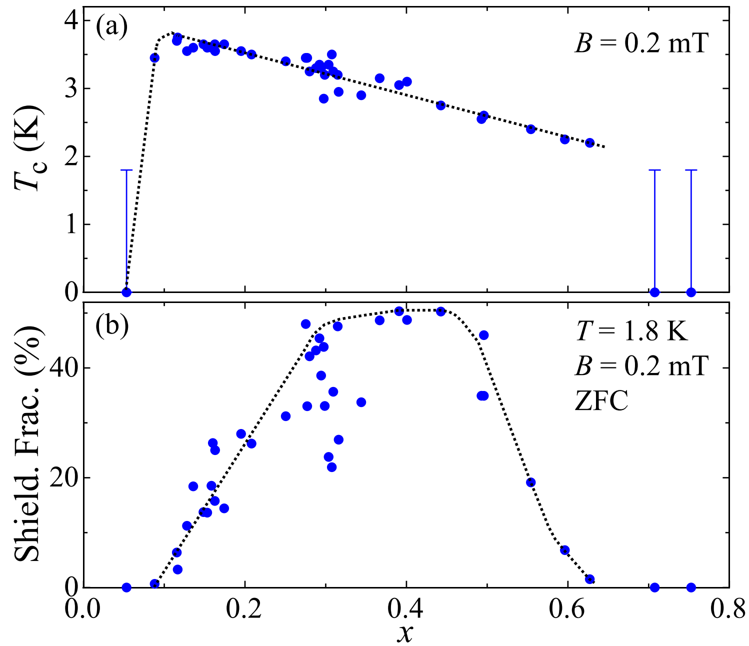


T-breaking chiral superfluid:
quasi-2D Sr_2RuO_4 (?)

Recent Developments: improved samples

Ando et al, PRB 84, 54513 (2011)



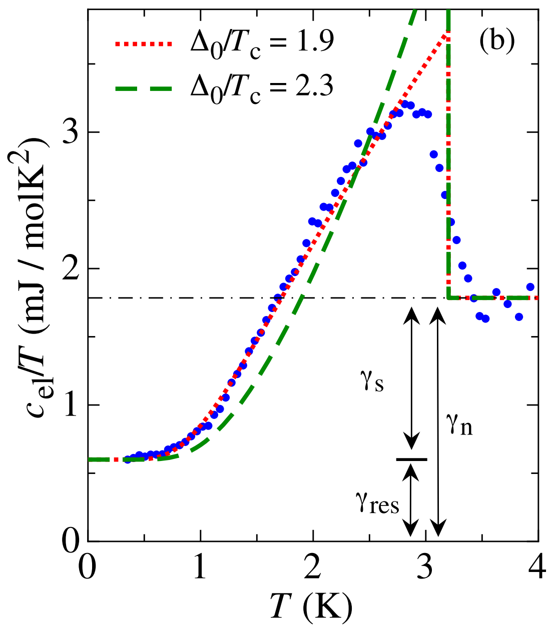


- Electrochemical synthesis
- Zero resistivity observed at 2.8 K
- Shielding fraction > 50%

- Tc versus doping
- carrier density from R_H = 2% electron doping
- inhomogeneous SC

Experimental Test of Pairing Symmetry

Ando et al, PRL 106, 127004 (2011)



- exponential T-dependence at low T (residual C/T due to normal region)
- consistent with full pairing gap
- rule out other pairing with nodes

Δ = 7.3K, Δ/T_c = 2.3

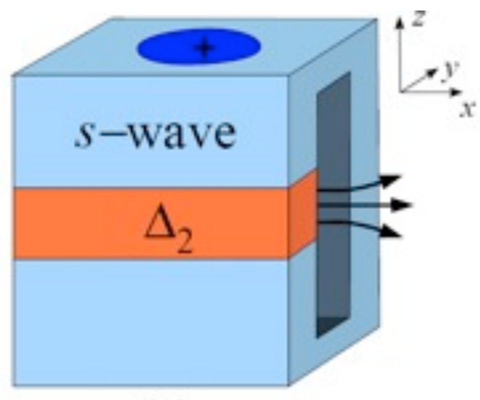
$$\xi_0 = \hbar v_F/\pi\Delta_0 = 24 \text{ nm}$$

$$\ell = \hbar k_F/(\rho_0 n e^2) = 25 \text{ nm}.$$

Phase sensitive test of pairing symmetry is needed.

- superconducting loop is a π junction
- trap flux: Φ= h/4e

c.f. Liu et al 2004, expt on Sr_2RuO_4



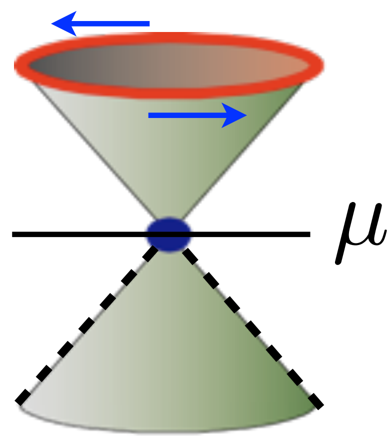
Surface Andreev Bound States

hallmark of topological superconductor

Bulk-boundary correspondence:

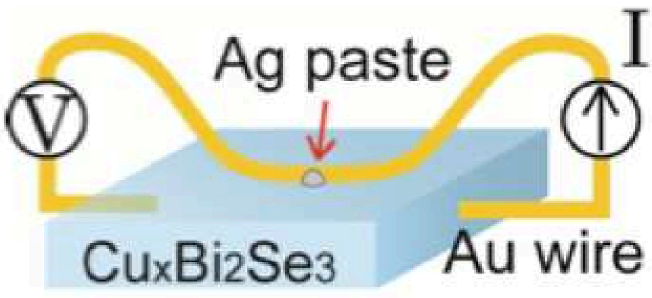
- gapless surface Andreev bound state with linear dispersion at k=0
- Bogoliubov quasiparticles are 2+1D itinerant Majorana fermions
  half of Dirac fermion in topological insulator
- low-energy Hamiltonian near k=0

$$H_{surf} = -iv\gamma^T(\partial_x\sigma_x + \partial_y\sigma_z)\gamma$$

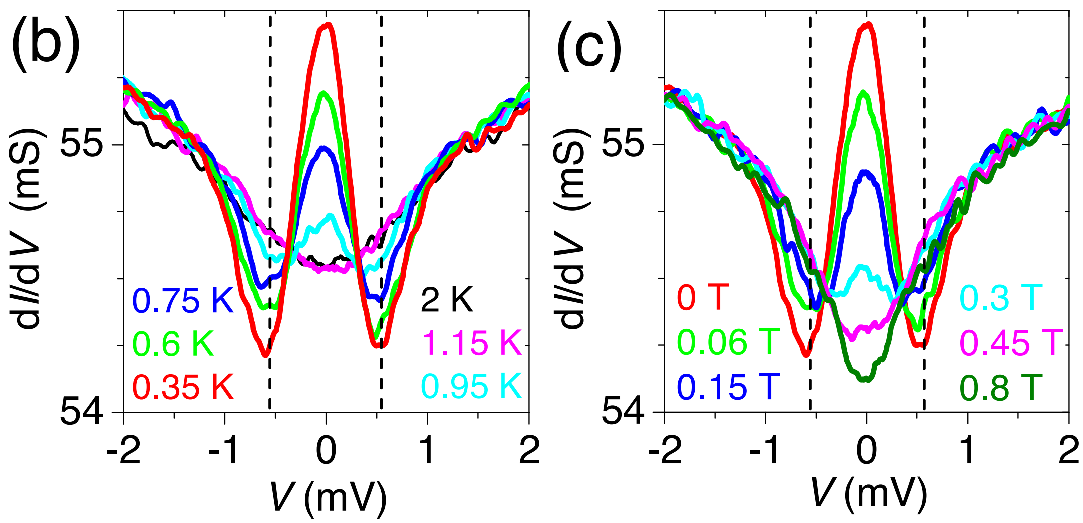


- detection by tunneling or ARPES

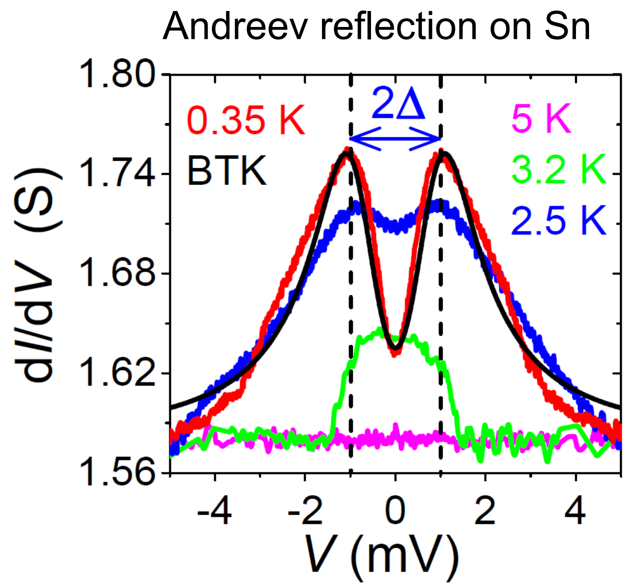
Point-Contact Spectroscopy on $Cu_xBi_2Se_3$



Ando et al, arXiv 1108.1101;
PRL in the press



V.S.



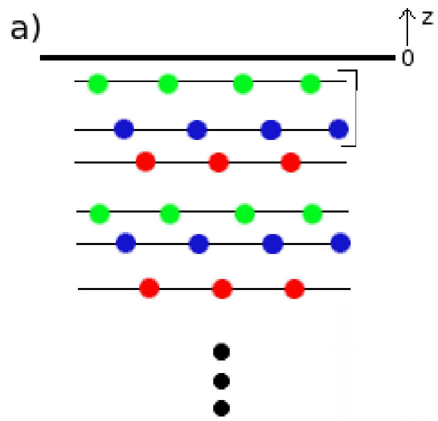
- zero-bias conductance peak within superconducting gap
- suppressed by magnetic field along z-direction
- strong indication of unconventional pairing

Surface Andreev Bound States

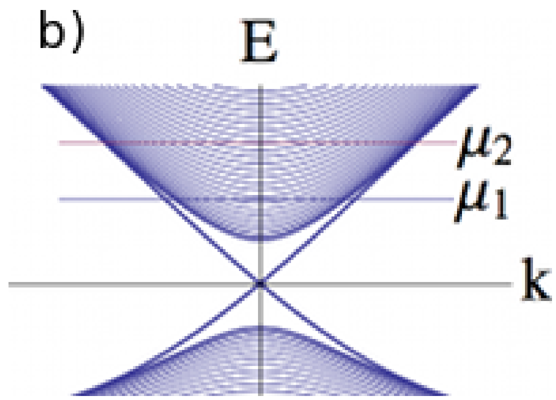
$$H_{\rm BdG} = [m\sigma_x + v_z(-i\partial_z)\sigma_y + v(k_x\sigma_z s_y - k_y\sigma_z s_x) - \mu]\tau_z + \Delta_2\sigma_y s_z\tau_x$$

boundary condition:

$$\sigma_z\psi(z=0) = \psi(z=0)$$



surface states (Δ_2 =0):



normal state:

Topological insulator surface states at k=0 exist if v_z m <0

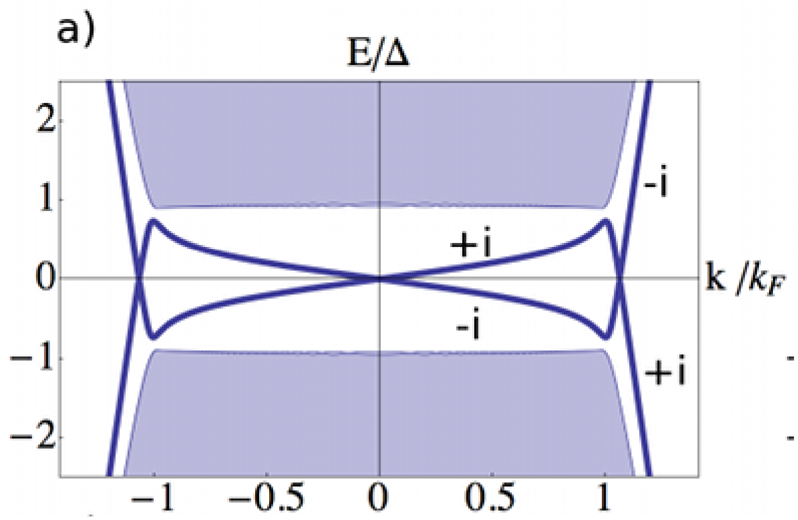
$$\psi_\pm(\mathbf{k}_{||}, z) \;=\; e^{z/l}(1,0)_\sigma \otimes (1, \pm i e^{i\phi})_s,$$

Hsieh & LF, arXiv 1109.3464

Surface Andreev Bound States

$$H_{\mathrm{BdG}} = [m\sigma_x + v_z(-i\partial_z)\sigma_y + v(k_x\sigma_z s_y - k_y\sigma_z s_x) - \mu]\tau_z + \Delta_2\sigma_y s_z\tau_x$$

superconducting state: ($\Delta_2 \neq 0$):



- linearly dispersing Majorana surface Andreev bound states near k=0:

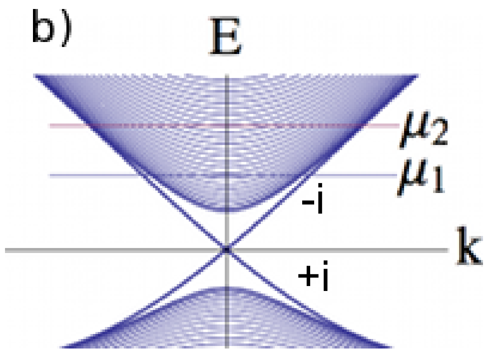
$$\psi^{\alpha}_{k=0} = e^{z\cdot\Delta/|v_z|}(\sin(k_F z - \theta), \sin(k_F z))_{\sigma}\,[(1,-\alpha)_s, i\mathrm{sgn}(v_z)(1,\alpha)_s]_{\tau}\,,$$

$$\tilde{v} = v\cdot(\Delta/\mu)\cdot\mathrm{sgn}(v_z)m/\mu \propto -v \qquad\qquad \alpha = \pm 1$$

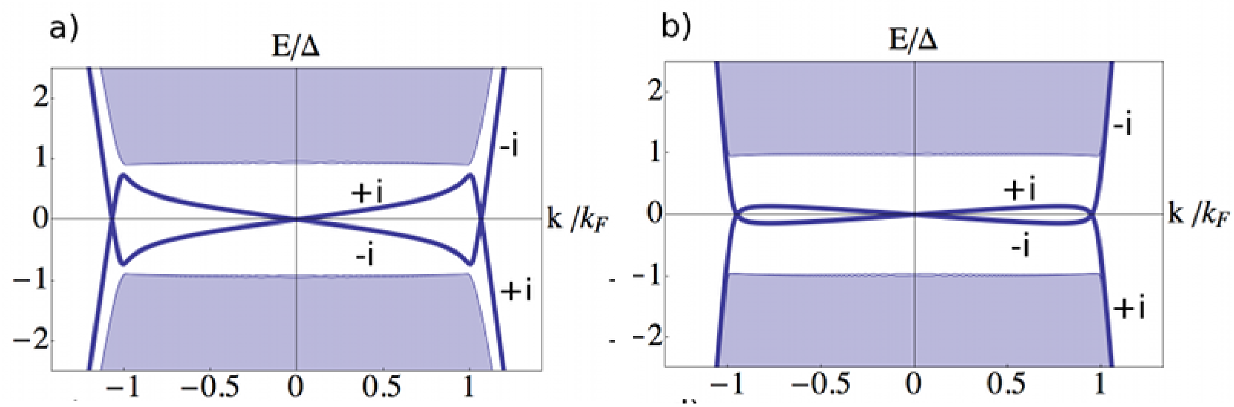
- second surface Andreev band crossing near k_F !

Surface Andreev Bound States

surface states ($\Delta_2 = 0$):



surface Andreev bound states ($\Delta_2 \neq 0$):

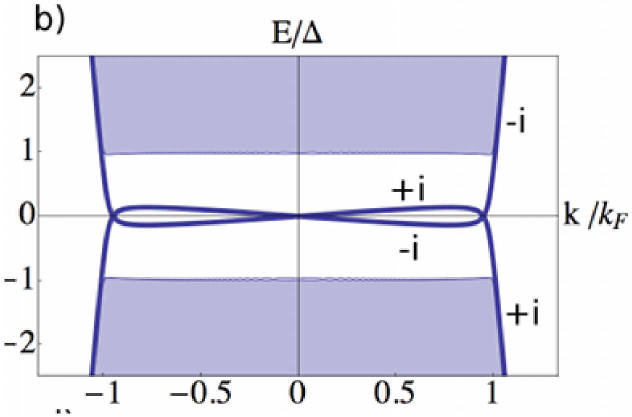


- odd-parity pairing does not gap surface states of doped topological insulator
=> gapless surface Andreev bound states near k_F

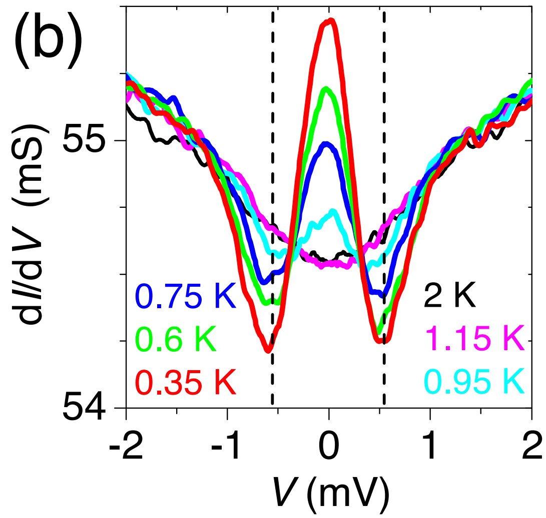
- second crossing remains even if surface states do not exist at Fermi energy
=> a new type of Andreev states: defy quasi-classical description

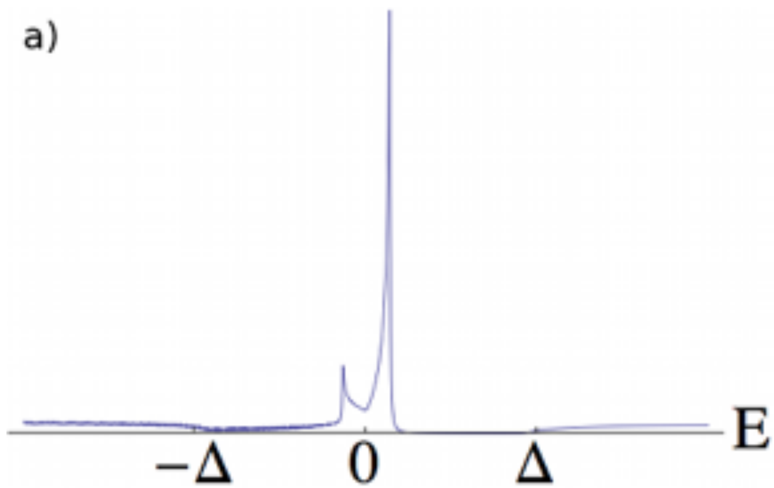
- protected by mirror helicity: a bulk topological invariant

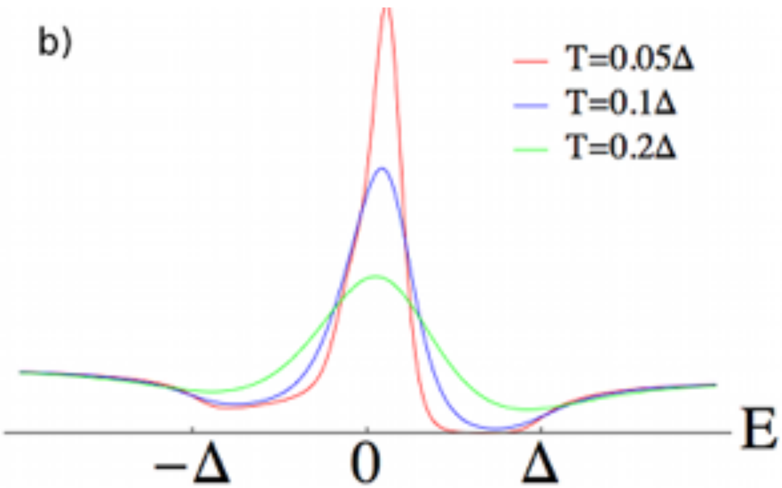
Local Tunneling Density of State



$m/\mu = 0.3$







- double peaks due to Van-Hove singularity at turning points
- thermal broadening results in one zero-bias peak and dip at gap edge
- Prediction: peak splits into two at lower temperature for clean surface

Conclusion Outlook

Conclusion:

1. unconventional pairing & topological superconductivity can be driven by strong spin-orbit coupling.

2. a promising candidate: Cu-doped Bi_2Se_3
   - more to be done: STM, NMR, phase-sensitive test ...

More candidates?

- doped topological insulator: Bi_2Te_3 under pressure, $TlBiTe_2$ ...
- doped normal semiconductor: PbTe, SnTe ...