Topologically protected nodes: Application to Sr_2RuO_4 and UTe_2

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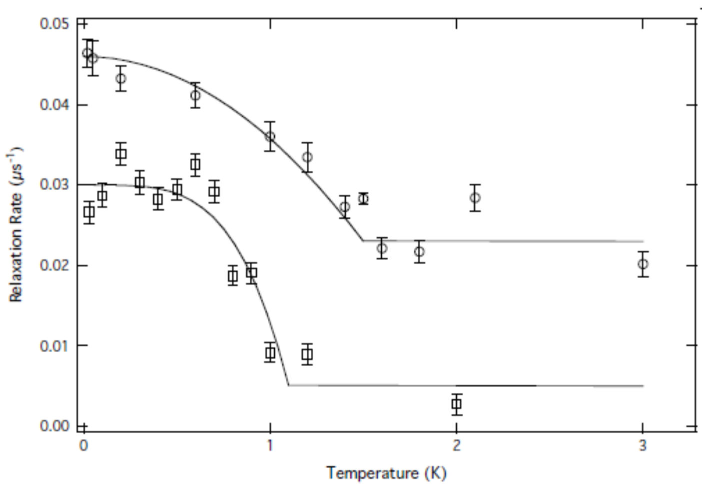
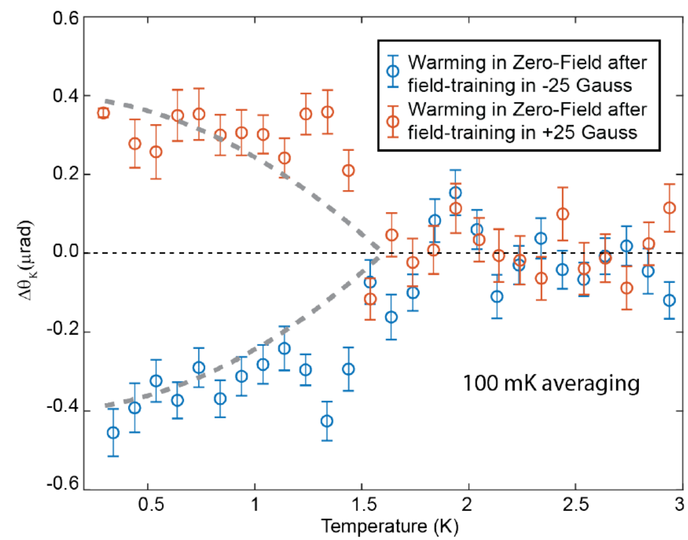
1- Key superconducting symmetries, pseudospin singlet and triplet pairing
2- Topological nodal classification
3- Bogoliubov Fermi surfaces in Sr_2RuO_4
4- Weyl superconductivity in UTe_2
5- New results from theory on UTe_2

NSF DMREF-1335215, PRL **118**, 127001 (2017), PRB **98**, 224509 (2018), PRL **121**, 157003 (2018), PRB **100**, 220504(R) (2019), PR Research **2**, 032023(R) (2020), arXiv:2002.02529

Why UTe_2 and Sr_2RuO_4?



Luke, Uemura Nature (1998)



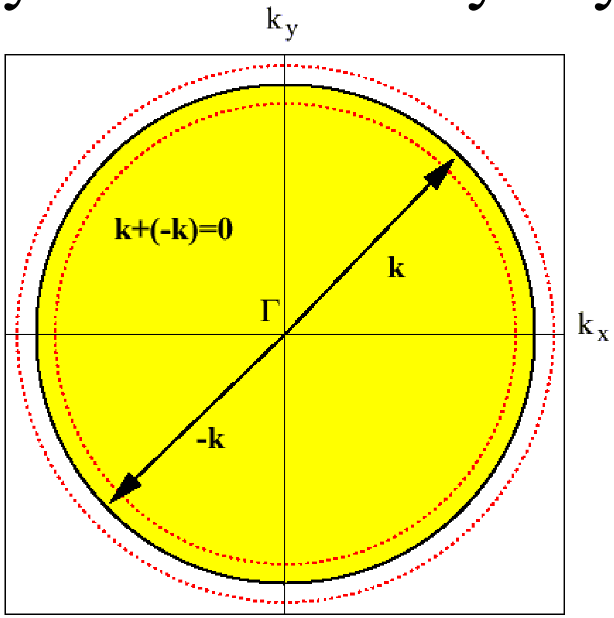
arXiv:2002.02529

Both are unconventional superconductors that spontaneously break time-reversal symmetry (“intertwined order”)

I will argue both have nodes that are not dictated by symmetry – but are topologically protected.

Superconductivity Symmetries

Superconductivity is stabilized by key symmetries:



- To ensure that states **k** and –**k** are on the Fermi surface requires symmetries (inversion, time-reversal): I or T
- Note that antiunitary $(IT)^2$=-1 and takes **k** to **k**, this ensures 2-fold degeneracy at each **k** (pseudospin).

Single Band Cooper Pairing

Pseudospin: Kramers degenerate fermions with same k: $|k,\uparrow\rangle, IT|k,\uparrow\rangle \equiv |k,\downarrow\rangle$

Pair these states at **k** and **–k**: Parametrization of the gap function $\Delta_{\mathbf{k},ss'}$

Even parity, pseudospin singlet:

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} 0 & \psi(\vec{k}) \\ -\psi(\vec{k}) & 0 \end{pmatrix} = i\sigma^y \psi(\vec{k})$$

Scalar wave function: $\psi(\vec{k})$ with $\psi(-\vec{k}) = \psi(\vec{k})$ even parity

Odd parity, pseudospin triplet:

$$\hat{\Delta}_{\vec{k}} = \begin{pmatrix} -d_x + id_y & d_z \\ d_z & d_x + id_y \end{pmatrix} = i\vec{d}(\vec{k}) \cdot \vec{\sigma}\sigma^y$$

Vector wave function: $\vec{d}(\vec{k})$ with $\vec{d}(-\vec{k}) = -\vec{d}(\vec{k})$ odd parity

Superconductivity, pairing states

Assume materials has time-reversal (T) and parity (I) symmetries

$$\Delta(\mathrm{k}) = [\psi(k) + \vec{d}(k) \bullet \vec{\sigma}](i\sigma_y) = \begin{pmatrix} -d_x + id_y & d_z + \psi \\ d_z - \psi & d_x + id_y \end{pmatrix}$$

Additional symmetry further dictates structure of Cooper pairs (and nodes):

D_{4h}

Γ	$\Delta(\mathrm{k})$
A_{1u}	$\vec{d}_{helical} = \hat{x}k_x + \hat{y}k_y$
B_{1g}	$\psi_{d-wave} = k_x^2 - k_y^2$
E_u	$\vec{d}_{chiral} = \hat{z}(k_x \pm ik_y)$
	$\vec{d}_{nematic} = \hat{z}k_x, \hat{z}k_y$
E_g	$\psi_{chiral} = k_z(k_x \pm ik_y)$
	$\psi_{nematic} = k_z k_x$

cuprates ← B_{1g}

$Cu_xBi_2Se_3$ ← $\vec{d}_{nematic}$

Sr_2RuO_4? ← E_g

E_u and E_g have two superconducting degrees of freedom – allows for multiple ground states

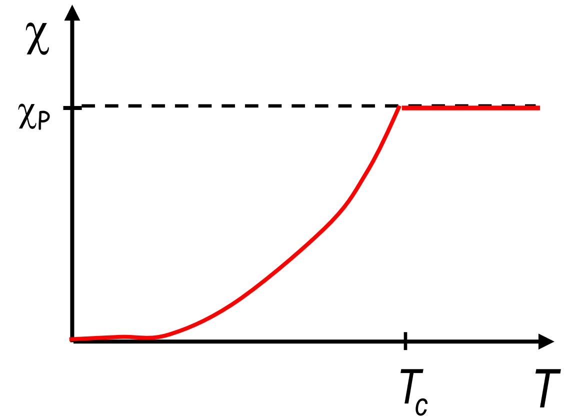
Spin susceptibility

For $\psi(\mathrm{k})$, $\chi=0$; for $\mathrm{d(k)}$, $\chi=\mathrm{cnst}$ if $\vec{d}\cdot\vec{H}=0$

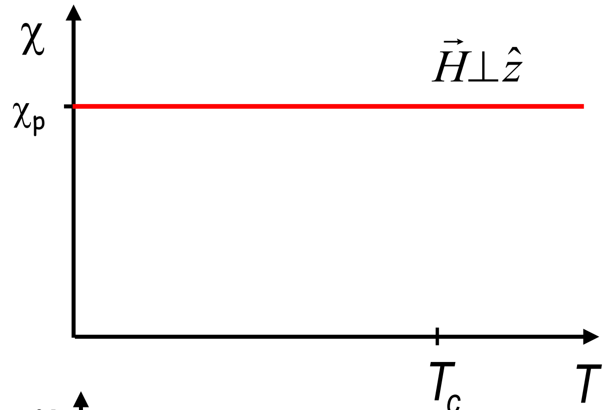
If $\vec{d}\cdot\vec{H}=0$, then no Pauli suppression of upper critical field.

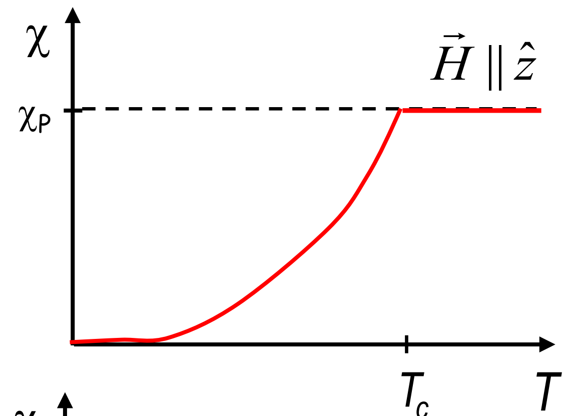
$$\psi_{d-wave}=k_x^2-k_y^2$$

$$\psi_{chiral}=k_z(k_x \pm ik_y)$$

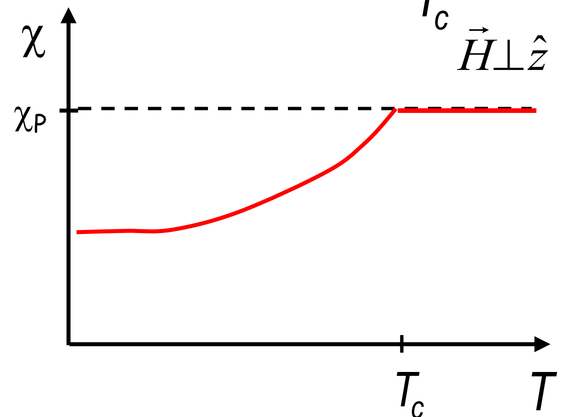


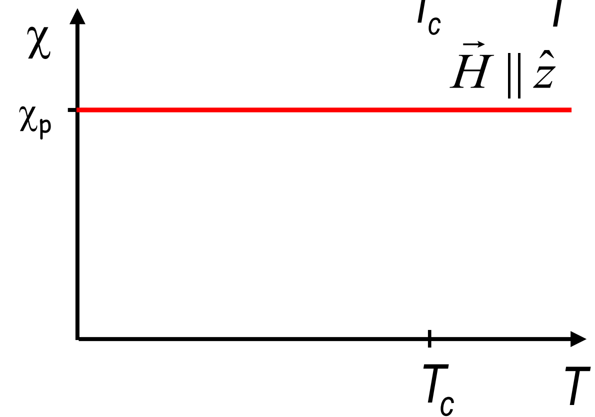
$$\vec{d}_{nematic}=\hat{z}k_x$$





$$\vec{d}_{helical}=\hat{x}k_x+\hat{y}k_y$$





Topological Nodal Classification

Many topological nodal classifications based on symmetries: Beri, Bzdusek, Fischer, Ryu, Sato, Yanase, Samokhin, Sato, Schynder, Shiozaki, Sigrist, Sumita, Ryu, Volovik, and Yanase

1- Includes key superconducting symmetries T and I and particle-hole symmetry C (all these take **k** to **–k**).

T. Bzdušek and M. Sigrist, PRB **96**, 155105 (2017)

2- Nodes classified by symmetries that take **k** to **k**

TI and CI and S= (CI)(TI)=CT (take k to k), 10-fold way (AZ classes)

label	Example	FS	line	point
DIII (even I, T yes)	$\psi_{d-wave} = k_x^2 - k_y^2$		2Z	
D (even I, T no)	$\psi_{chiral} = k_z(k_x \pm ik_y)$	Z_2		2Z
CII (odd I, T yes)	$\vec{d}_{helical} = \hat{x}k_x + \hat{y}k_y$			
C (odd I, T no)	$\vec{d}_{chiral} = \hat{z}(k_x \pm ik_y)$			Z

DFA, PMR Brydon, and C. Timm PRL **118**, 127001 (2017)

2D generalization: MH Fischer, M Sigrist, DFA, PRL **121**, 157003 (2018)

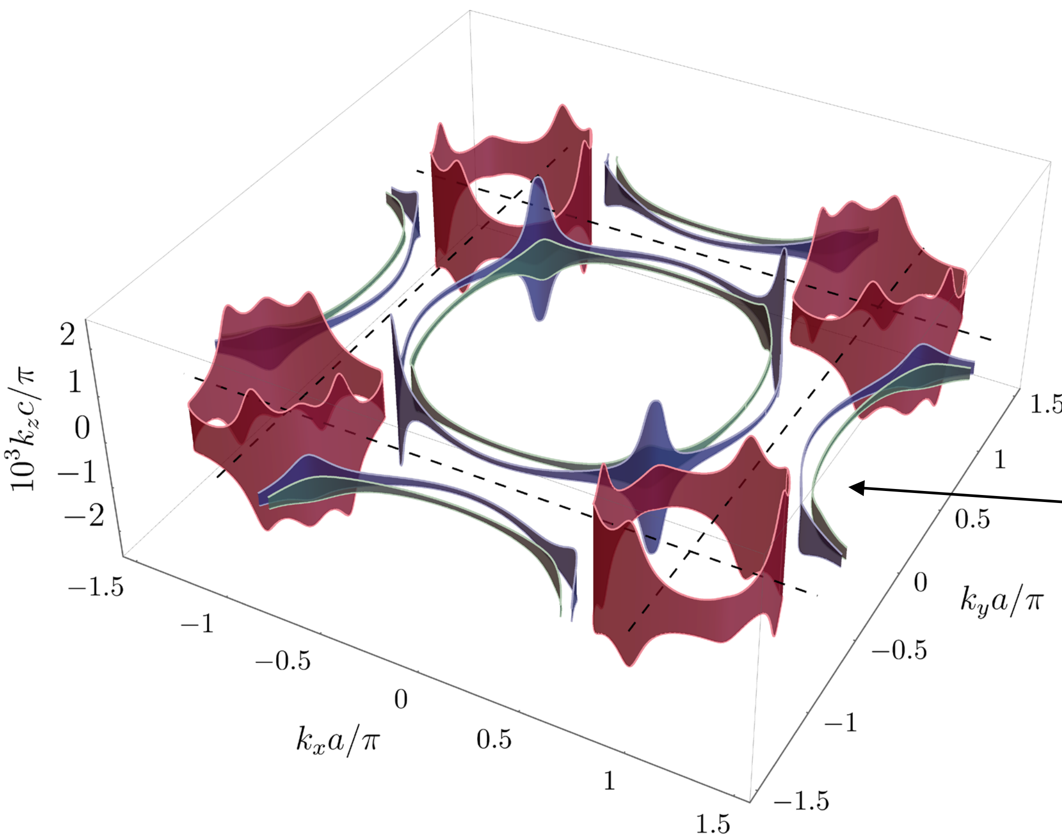
Bogoliubov Fermi Surfaces in Sr_2RuO_4

Joerg Schamlian and Andrew Mackenzie talks: singlet superconductor

Shear c_{66} modulus jump at Tc: Ghosh et al., arXiv:2002.06130and Benhabib et al., arXiv:2002.05916.

Chiral d-wave state: $\psi_{chiral} = k_z(k_x + ik_y)$

Based on a local Hund's rule pairing mechanism, find this state is stable



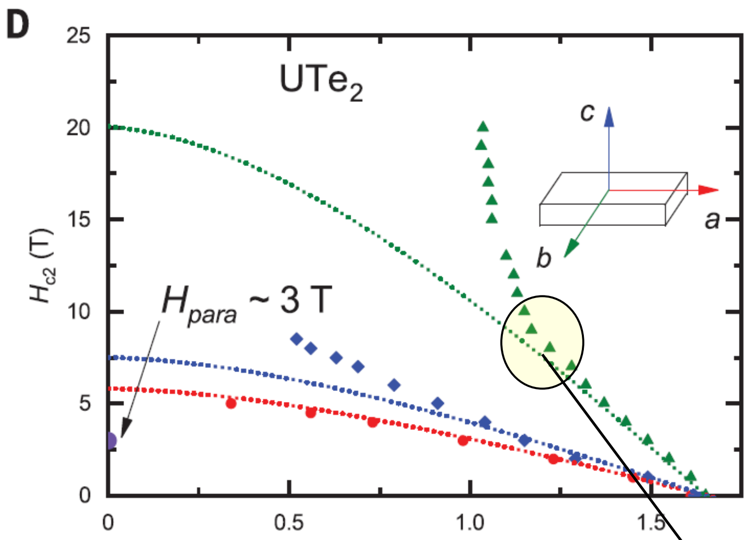
Even parity, broken time reversal: Z_2 protected Bogoliubov Fermi surfaces

H. Suh, H. Menke, PMR Brydon, A. Ramires, C. Timm, and DFA, PR Research **2**, 032023(R)

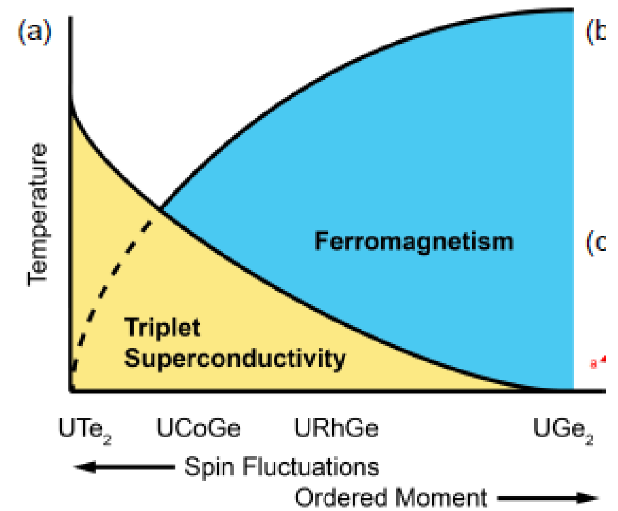
Weyl Superconductivity in UTe_2

arXiv:2002.02529

Superconducting UTe_2



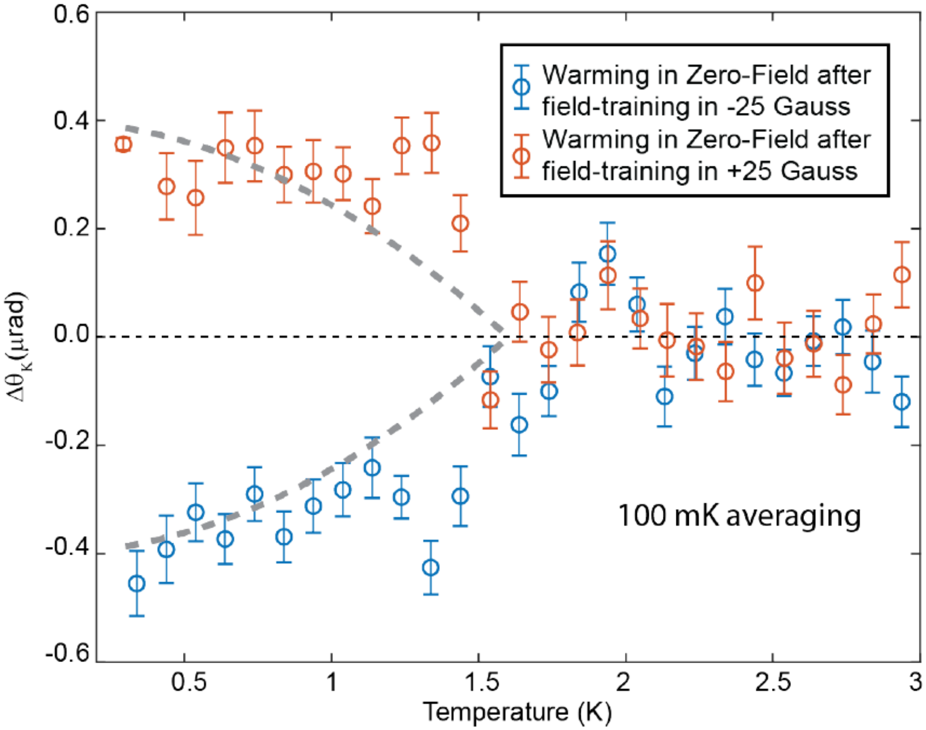
Ran et al, Science (2019)



Kink in Hc_2 – perhaps phase transition (Ishizuka et al., PRL (2019))

Spin-triplet likely, assumed here: what can we say about the order parameter? How about quasiparticle excitations?

Broken Time-reversal Symmetry



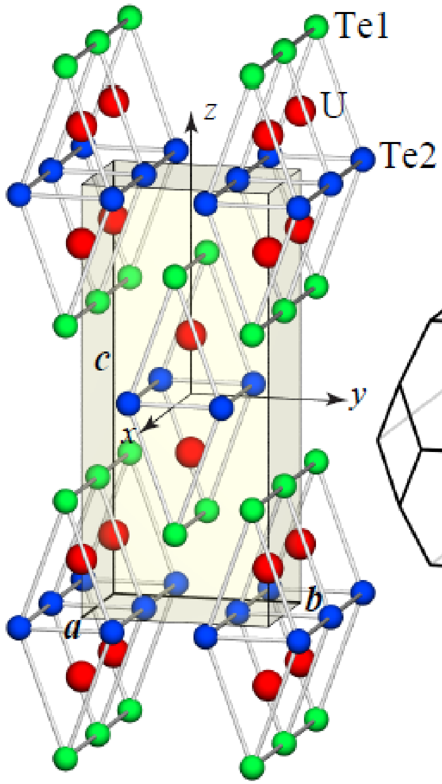
arXiv:2002.02529

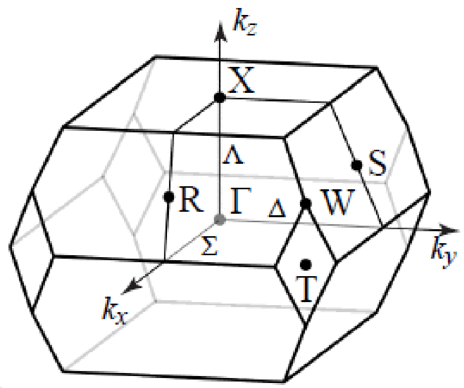
Polar Kerr is trained by field along c-axis

Also, next talk: chiral edge states (Vidya Madhavan)

To break time-reversal symmetry, need **two** components to the order parameter. Typically this requires symmetry.

Orthorhombic

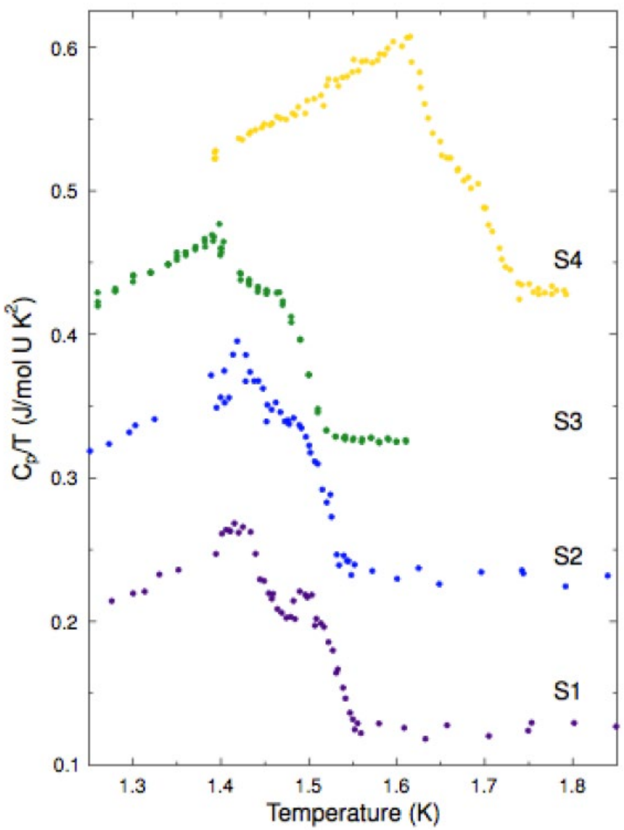




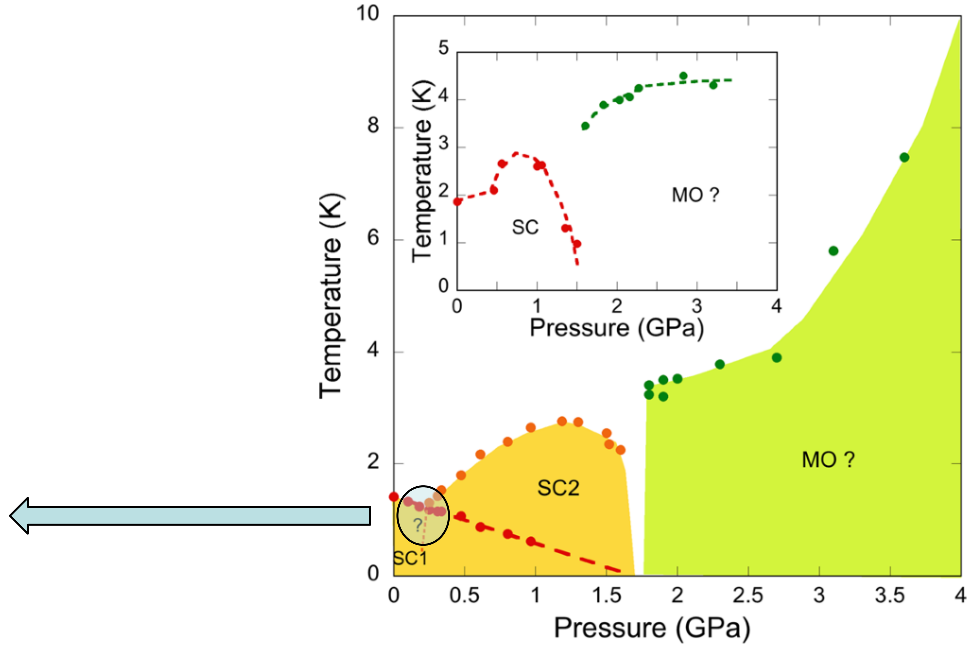
Γ	
A_u	$\vec{d}_A = a\hat{x}f_x + b\hat{y}f_y + c\hat{z}f_z$
B_{1u}	$\vec{d}_{B1} = a\hat{x}f_y + b\hat{y}f_x + c\hat{z}f_u$
B_{2u}	$\vec{d}_{B2} = a\hat{x}f_z + b\hat{y}f_u + c\hat{z}f_x$
B_{3u}	$\vec{d}_{B3} = a\hat{x}f_u + b\hat{y}f_z + c\hat{z}f_y$

Orthorhombic with point group D_{2h}. All **one** component order parameters. How can time-reversal symmetry be broken?

Multiple Superconducting Transitions



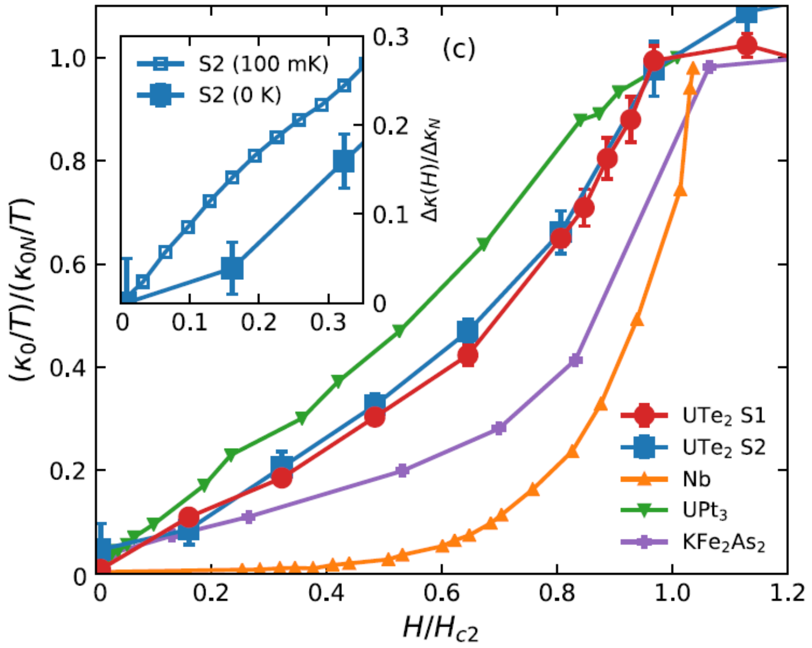
arXiv:2002.02529



Braithwaite et al.,Nat. Phys. Com. (2019).

Thomas et al. arXiv:2005.01659 the two Tc's cross at pressure Pc=0.2 GPa

Nodal excitations:



Suggests point nodes: B_{3u} or B_{2u} state based on assumed time-reversal invariance

Metz et al, PRB (2019)

Possible pairing states

We have time-reversal (T) and inversion (I) symmetries and D_{2h} point group

Little about details of Kondo Fermi liquid state (Z-point electron pocket, Miao et al., PRL 2020).

Γ	
A_u	$\vec{d}_A = \hat{x}f_x, \hat{y}f_y, \hat{z}f_z$
B_{1u}	$\vec{d}_{B1} = \hat{x}f_y, \hat{y}f_x, \hat{z}f_u$
B_{2u}	$\vec{d}_{B2} = \hat{x}f_z, \hat{y}f_u, \hat{z}f_x$
B_{3u}	$\vec{d}_{B3} = \hat{x}f_u, \hat{y}f_z, \hat{z}f_y$

$f_x \sim k_x (\sin k_x)$

$f_y \sim k_y (\sin k_y)$

$f_z \sim k_z (\sin k_z)$

$f_u \sim k_x k_y k_z$

Keep f - functions general but consistent with symmetry

Kerr training by c-axis field implies coupling: $iB_z(\psi_1\psi_2^* - \psi_2\psi_1^*)$

Two possibilities: i) $A_u + iB_{1u}$
ii) $B_{2u} + iB_{3u}$

Weyl Points?

- Under what conditions do Weyl points occur?
- Consider d_1+id_2:

$$E(k) = \pm\sqrt{(\varepsilon(k)-\mu)^2 + |d(k)|^2 \pm |q(k)|}$$

[where q=i(dxd*)]

$(\varepsilon(k)-\mu)^2$=0 $\quad |\Delta_\pm|^2 = |d|^2 \pm |q|$=0 or

$|\Delta_\pm| = |d_1|^2 + |d_2|^2 \pm 2|d_1 \times d_2|$ =0

$|d_1| = |d_2|$ and $d_1 \cdot d_2 = 0$

Together these define a line in momentum space. This line can intersect a Fermi surface at a point. *Weyl points can generically exist.*

$|d_1| = |d_2|$ and $d_1 \cdot d_2 = 0$

B_{2u}+iB_{3u} state

Weyl nodes can generically appear, need detailed a microscopic model

Insight from topological semimetals ($MoTe_2$): look in high-symmetry planes

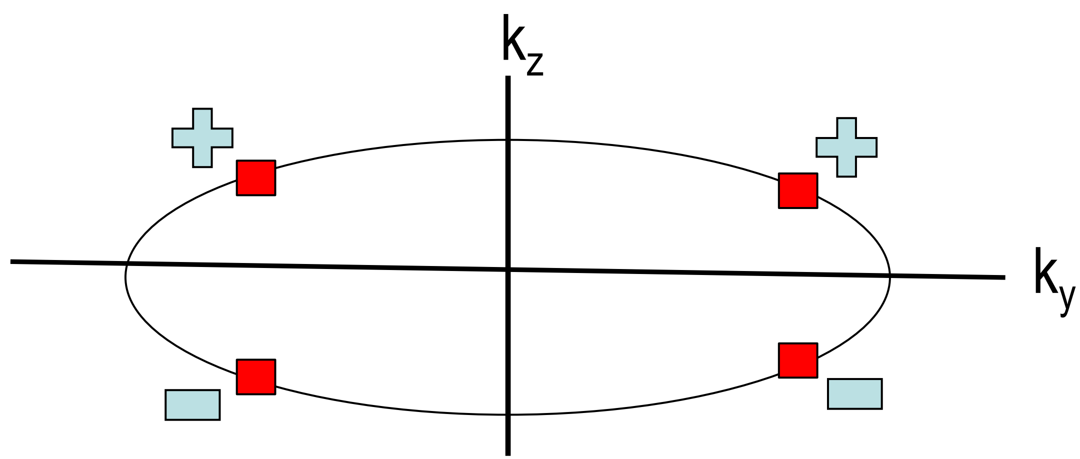
Γ	
A_{1u}	$\vec{d}_A = \hat{x}f_x, \hat{y}f_y, \hat{z}f_z$
B_{1u}	$\vec{d}_{B1} = \hat{x}f_y, \hat{y}f_x, \hat{z}f_u$
B_{2u}	$\vec{d}_{B2} = \hat{x}f_z, \hat{y}f_u, \hat{z}f_x$
B_{3u}	$\vec{d}_{B3} = \hat{x}f_u, \hat{y}f_z, \hat{z}f_y$

Consider k_x=0: f_x=f_u=0 $d_{B2} \cdot d_{B3} = 0$

$|d_1| = |d_2|$? Yes!

$$k_x = 0:\ |f_{z2}|^2 - |f_{z3}|^2 = |f_{y3}|^2$$

$$k_y = 0:\ |f_{z2}|^2 - |f_{z3}|^2 = -|f_{x2}|^2$$



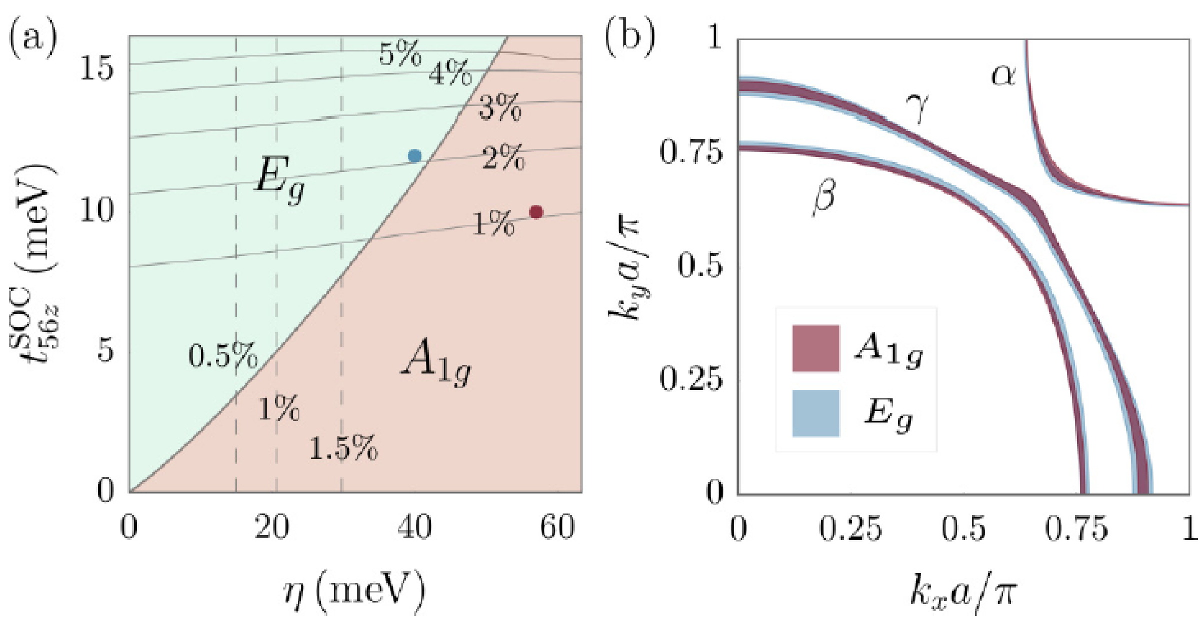
Weyl points occur:
Surface Fermi arcs
See Madhavan talk

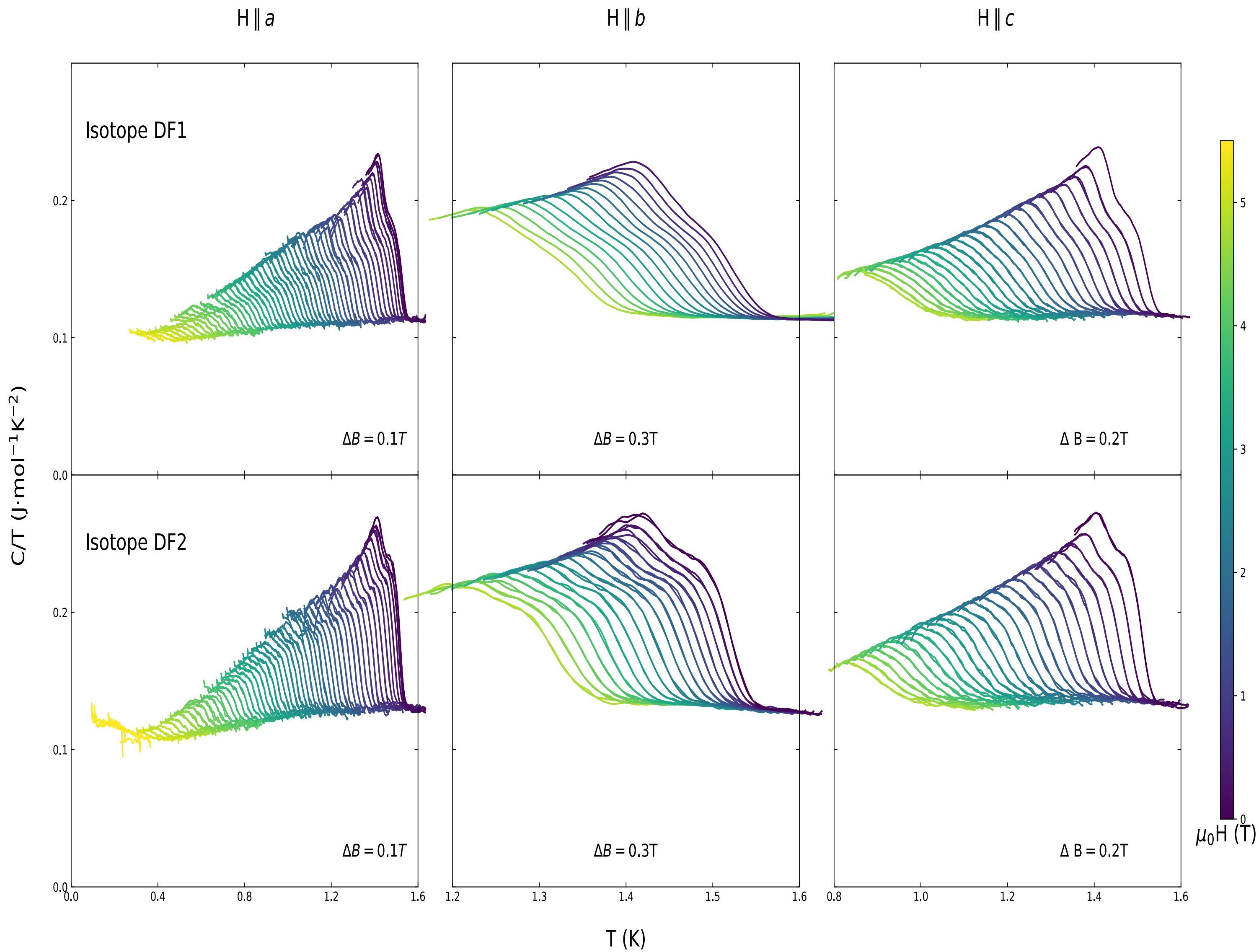
Conclusions:

- Topologically protected nodes can appear in even and odd-parity broken time-reversal
- Z_2 protected Bogoliubov Fermi surfaces possible in Sr_2RuO_4.
- Two transitions and broken time-reversal symmetry in UTe_2 suggests $B_{2u}+iB_{3u}$ or A_u+iB_{1u} order parameters.
- Likely has at least four singly-charged Weyl nodes with associated surface Fermi arcs.

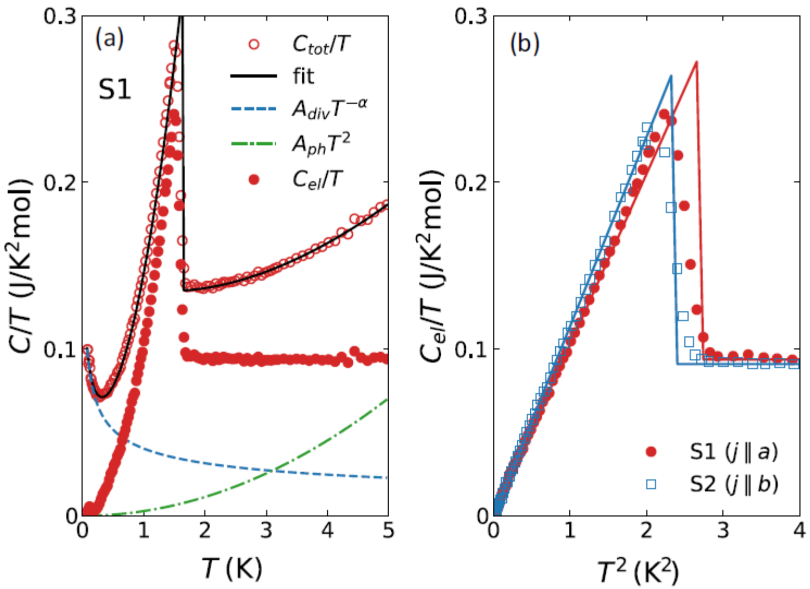
E_g state in Sr_2RuO_4

U'-J on-site attractive interaction (see also Puetter and Kee, Euro. Phys. Lett 2012)
Spin-orbit and c-axis dispersion




H ∥ a
H ∥ b
H ∥ c
Isotope DF1
Isotope DF2
ΔB = 0.1T
ΔB = 0.3T
Δ B = 0.2T
ΔB = 0.1T
ΔB = 0.3T
Δ B = 0.2T
C/T (J·mol⁻¹K⁻²)
T (K)
μ0H (T)

UTe_2 Specific Heat

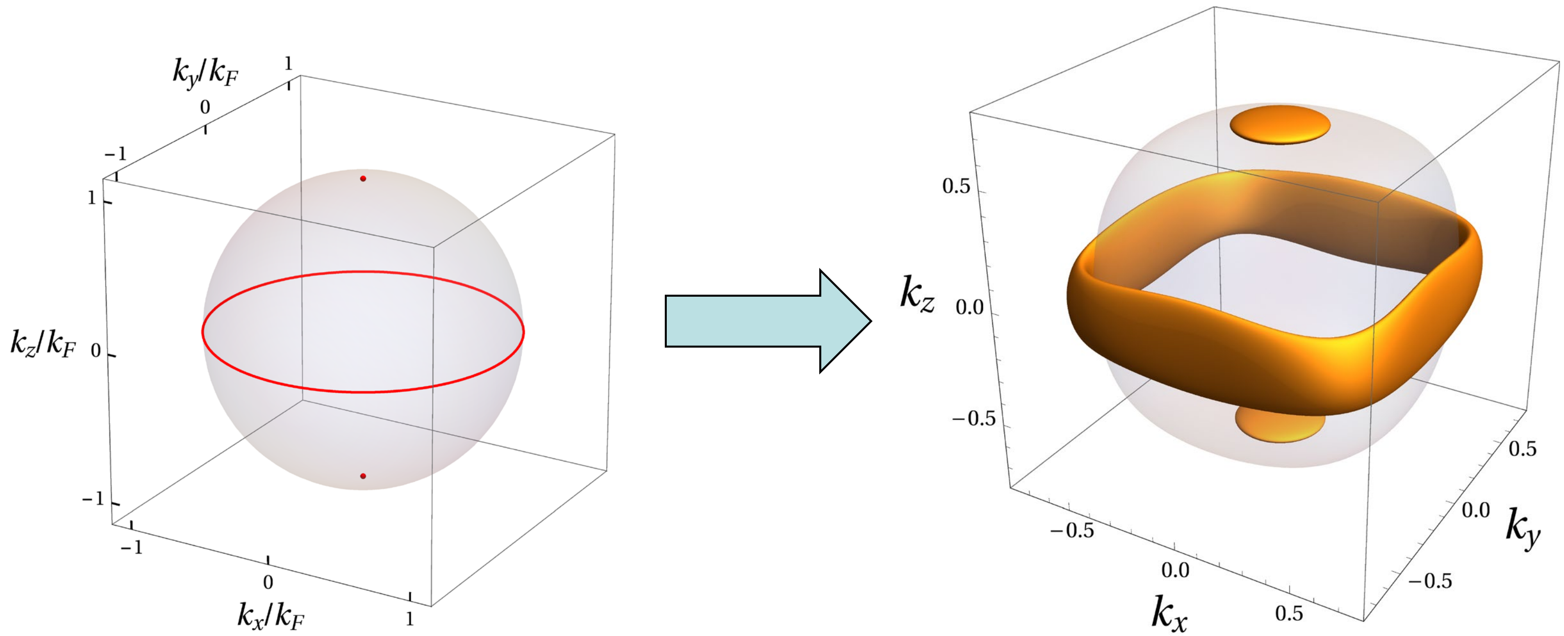


Metz et al, PRB (2019)

Key Surprise:

In clean *even parity* superconductors with spontaneous *time-reversal symmetry breaking*, the excitation spectrum is either

i) Fully gapped
ii) Has topologically protected Bogoliubov Fermi surfaces



Usual Single band theory does not have Bogoliubov Fermi surfaces, they appear once multiple bands are included. PRL 118, 127001 (2017), PRB (2018).

Topological Protection

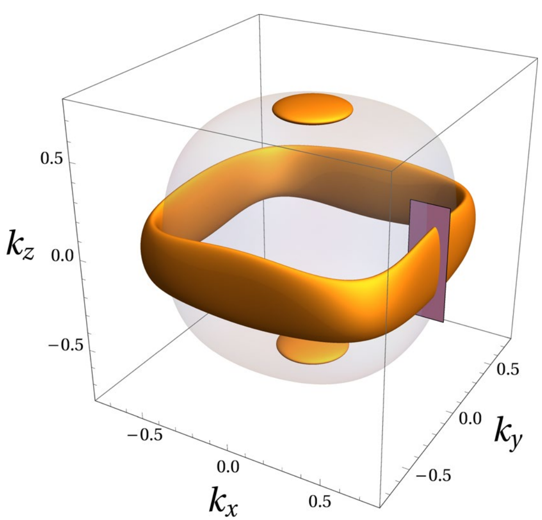
Kobayshi et al PRB (2014), Zhao et al PRL (2016),
Bzdusek and Sigrist PRB (2017).

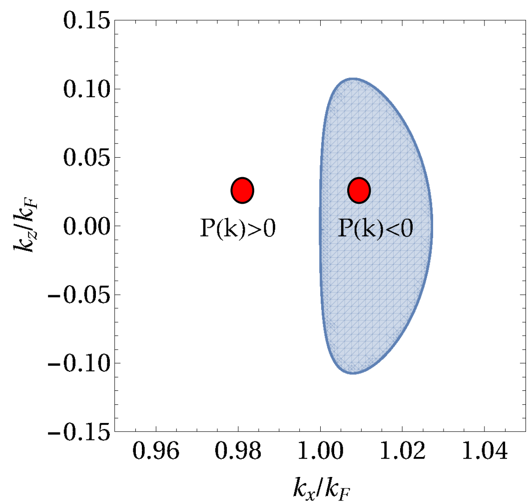
If (**CI**)^2=1,then: Fermi surfaces can be topologically protected with a Z_2 invariant.

We find Z_2 invariant is defined through the Pfaffian.

$$Pf(H_{BdG}) = \sqrt{Det(H_{BdG})} = \varepsilon_+^2\varepsilon_-^2 + \Delta_0^2(\varepsilon_+\varepsilon_- + \beta^2 k_z^2 k_x^2 + \beta^2 k_z^2 k_y^2)$$

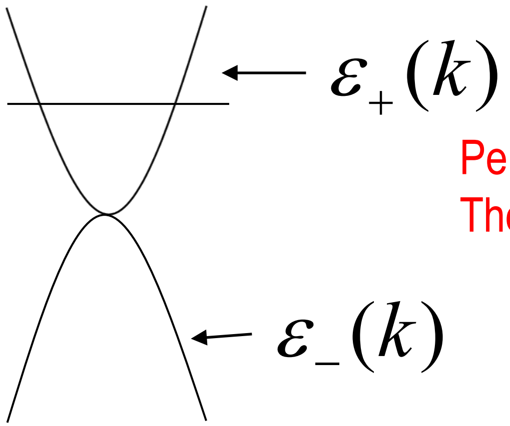
$$(-1)^\delta = Pf[H_{BdG}(k_{in})]Pf[H_{BdG}(k_{out})]$$ If δ=1, then topologically non-trivial





Fermi surface is stable to any perturbation that preserves CI symmetry.

Physical Origin of Bogoliubov Fermi surfaces



Perturbation Theory

$$H_{BdG,+} = \begin{pmatrix} \widetilde{H}_{N,+}(k) & \Delta_+(k) \\ \Delta_+^t(k) & -\widetilde{H}_{N,+}^T(-k) \end{pmatrix}$$

$$\Delta_+(k) = \psi(k) i\sigma_y \propto k_z(k_x + ik_y)$$

$$\widetilde{H}_{N,+} = \varepsilon_+(k) + \gamma(k) + \vec{h}(k)\cdot\vec{\sigma}$$

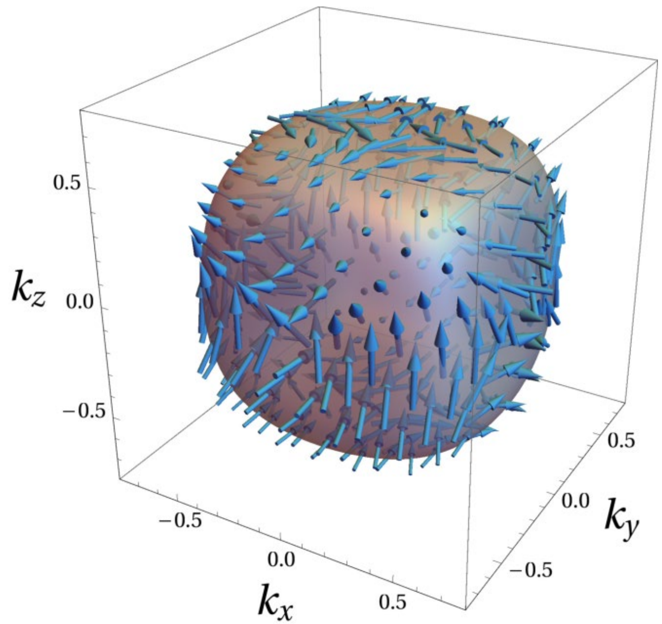
$$E_k = \pm|\vec{h}| \pm \sqrt{(\varepsilon_+ + \gamma - \mu)^2 + |\psi(k)|^2}$$

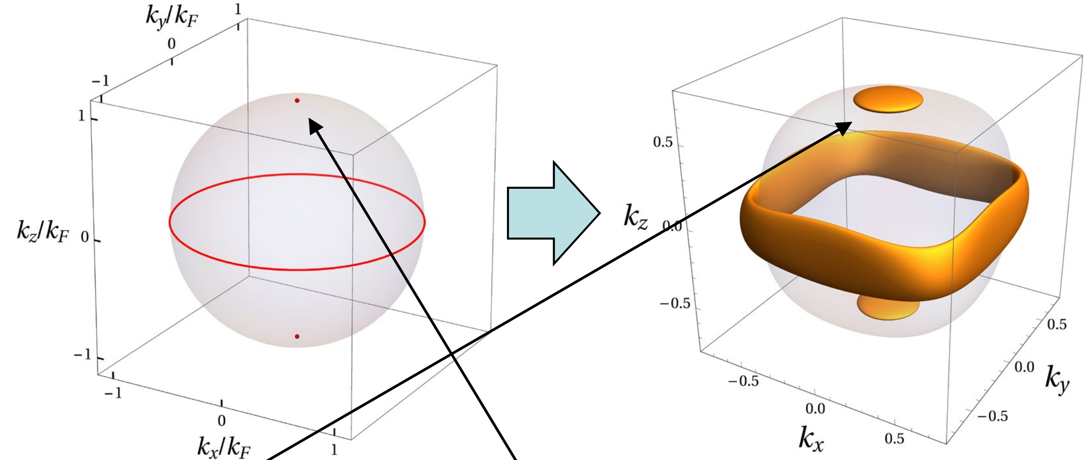
The superconductor has created an internal pseudospin magnetic field

$$|\vec{h}| \cong \frac{\Delta_0^2}{\varepsilon_+ - \varepsilon_-}$$

This field gives the Bogoliubov Fermi surfaces

Pseudospin magnetic field





$$E_k = \pm|\vec{h}| \pm \sqrt{(\varepsilon_+ + \gamma - \mu)^2 + |\psi(k)|^2}$$

h(k) will exist whenever the superconductor breaks time-reversal – the spectrum does not need to be nodal.