Nodal excitations in superconductors: insight from symmetry and topology

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1- Motivation

2- Review of “classical” single-band case: nodes from group theory

3- Topological nodal classification based on *superconducting symmetries*

4- Surprise from classification: Bogoliubov Fermi surfaces

5- Bogoliubov Fermi surfaces: materials, microscropic description, and topological protection.

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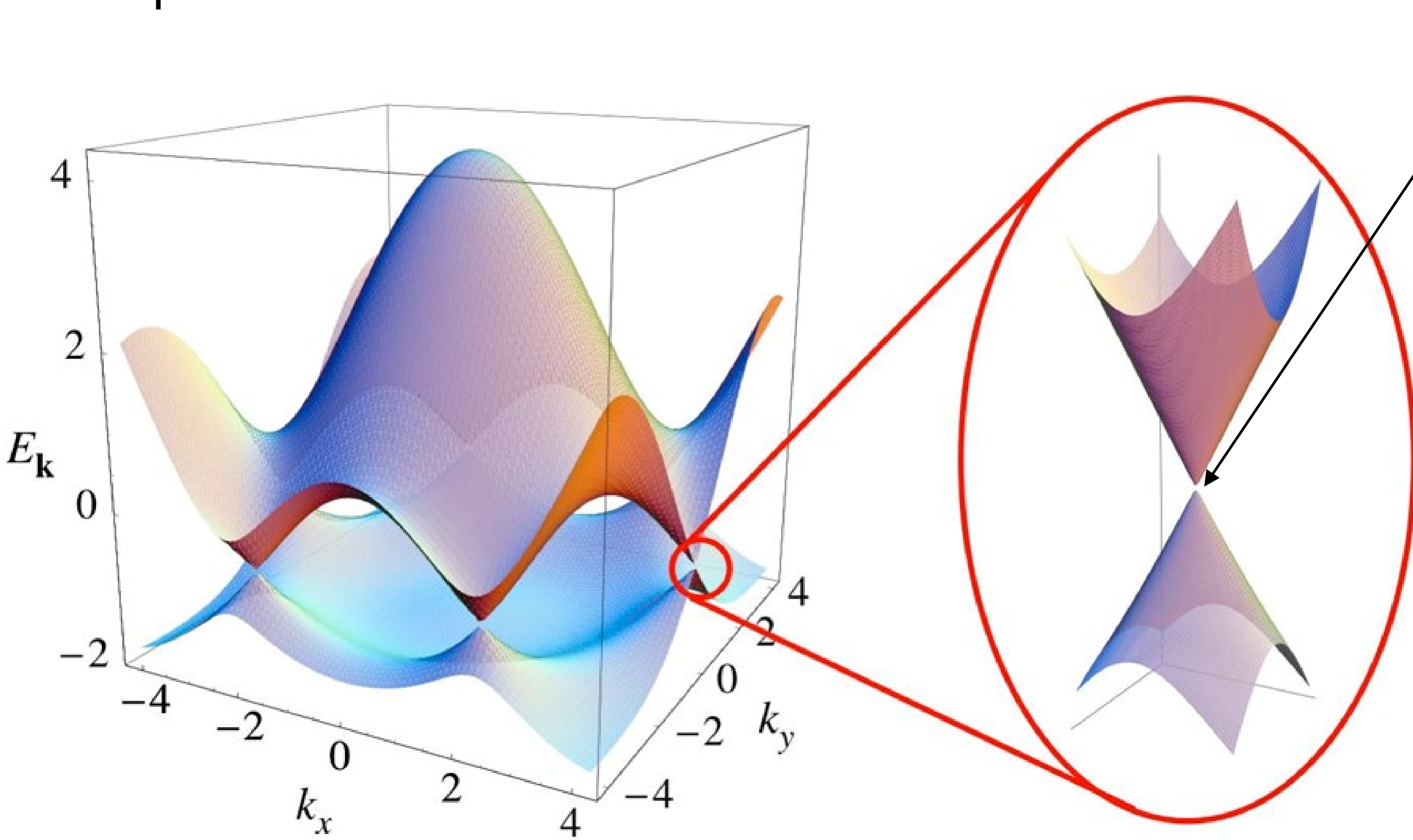
Nodal superconductors: similarities to nodal-metals

Protected by "sub-lattice" aka chiral symmetry
(Ryu and Hatsugai PRL 89, 077002, 2002)

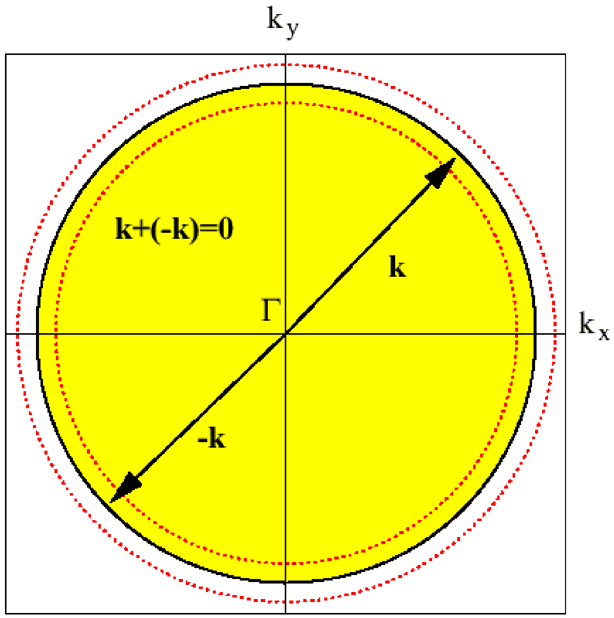
Graphene:

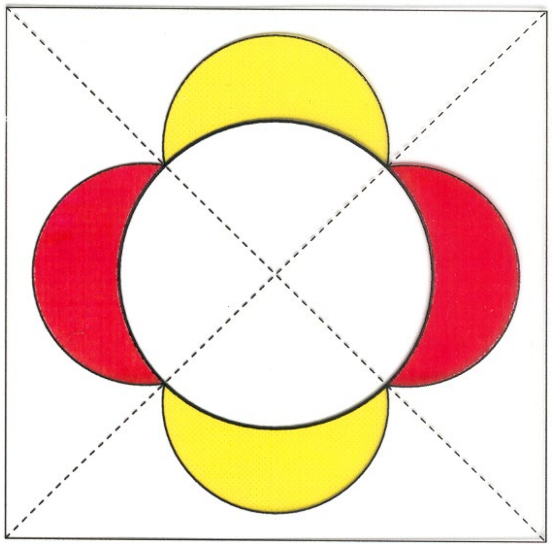


Chiral symmetry gives "flat-band" edge states (true in d-wave SC as well)

Basic Superconductivity

- Fermi sea unstable to formation of Cooper Pairs

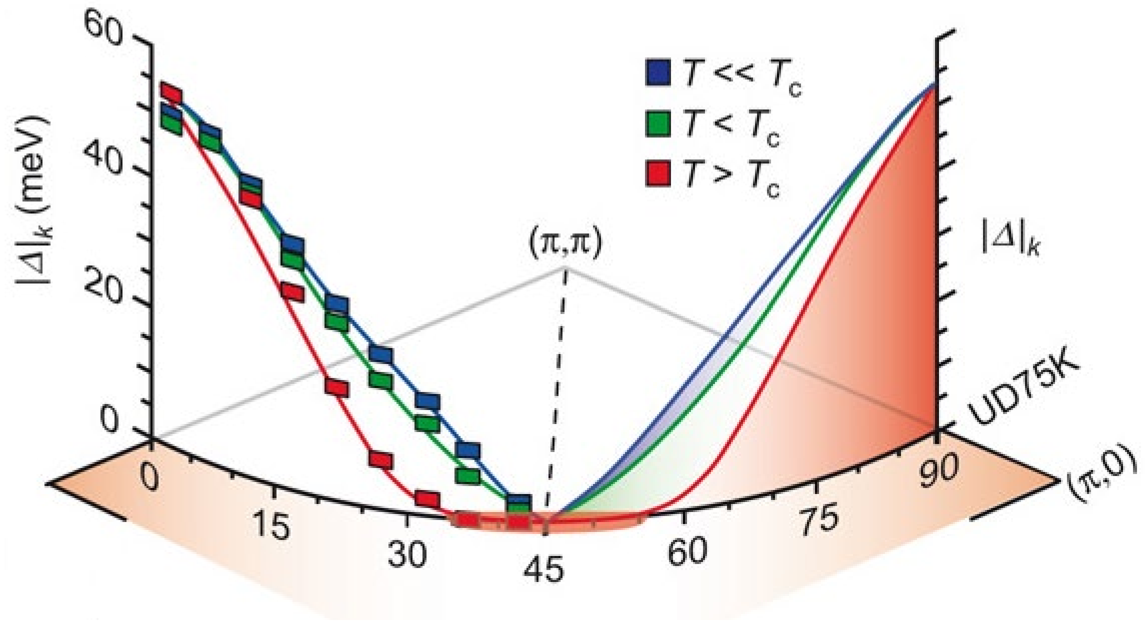




d-wave

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

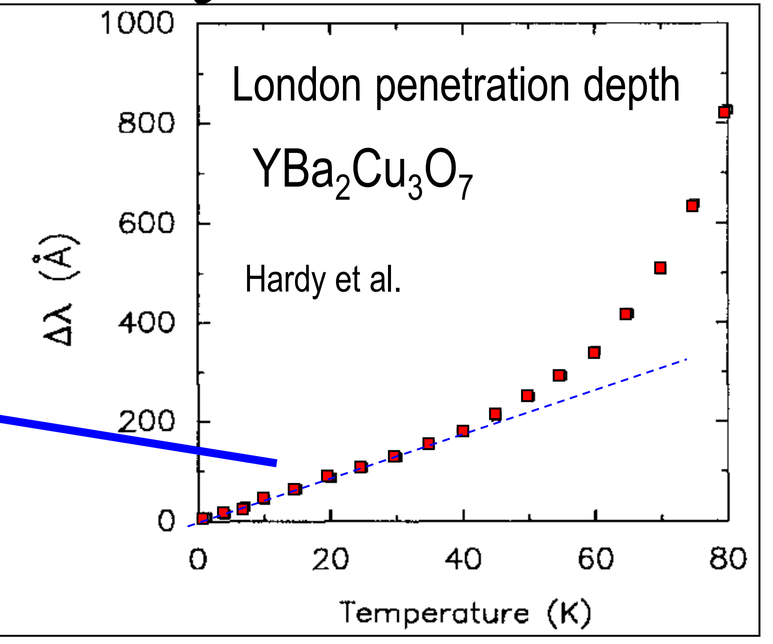
ARPES: cuprates



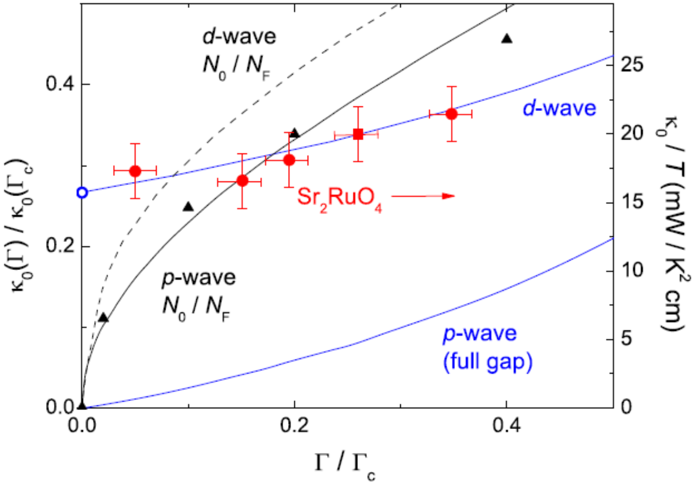
Z.X. Shen

Cuprates-Thermodynamics

Low temperature behavior reveals low energy excitations



In many lower Tc superconductors, nodes are identified this way.



Thermal conductivity: Sr_2RuO_4

$$\frac{\kappa}{T} \propto cnst + T$$

d-wave like

Tanatar, PRL (2001), Hassinger, PRX (2017)

Single Band Cooper Pairing

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

Parametrization of the gap function $\Delta_{\boldsymbol{k},ss'}$

Even parity, spin 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

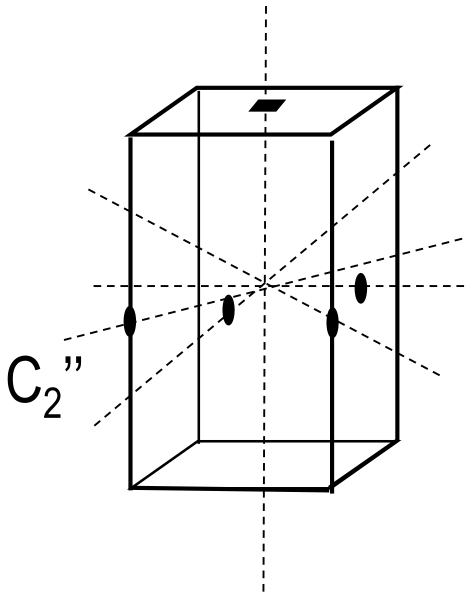
Odd parity, spin triplet:

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

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

Origin of Gap Structures: Group Theory

Point group: D_{4h}



D_{4h} contains inversion

→ even and odd representations

Character table for D_4

Γ	E	C_2	$2C_4$	$2C_2'$	$2C_2''$
A_1	1	1	1	1	1
A_2	1	1	1	-1	-1
B_1	1	1	-1	1	-1
B_2	1	1	-1	-1	1
E	2	-2	0	0	0

d-wave (B_1)

Even parity labelled with g (pseudo-spin singlet)
Odd parity labelled with u (pseudo-spin triplet)

Example of a tetragonal crystal with spin orbit coupling

Point group: D_{4h}

4 one-dim., 1 two-dim. representation
even (g) / odd (u) parity

Γ	$\psi(\vec{k})$	Γ	$\vec{d}(\vec{k})$
A_{1g}	1	A_{1u}	$\hat{x}k_x + \hat{y}k_y$
A_{2g}	$k_x k_y (k_x^2 - k_y^2)$	A_{2u}	$\hat{y}k_x - \hat{x}k_y$
B_{1g}	$k_x^2 - k_y^2$	B_{1u}	$\hat{x}k_x - \hat{y}k_y$
B_{2g}	$k_x k_y$	B_{2u}	$\hat{y}k_x + \hat{x}k_y$
E_g	$\{k_x k_z, k_y k_z\}$	E_u	$\{\hat{z}k_x, \hat{z}k_y\}$ $\{\hat{x}k_z, \hat{y}k_z\}$

Conventional: A_{1g}

Unconventional: everything else

only one representation is relevant for the superconducting phase transition

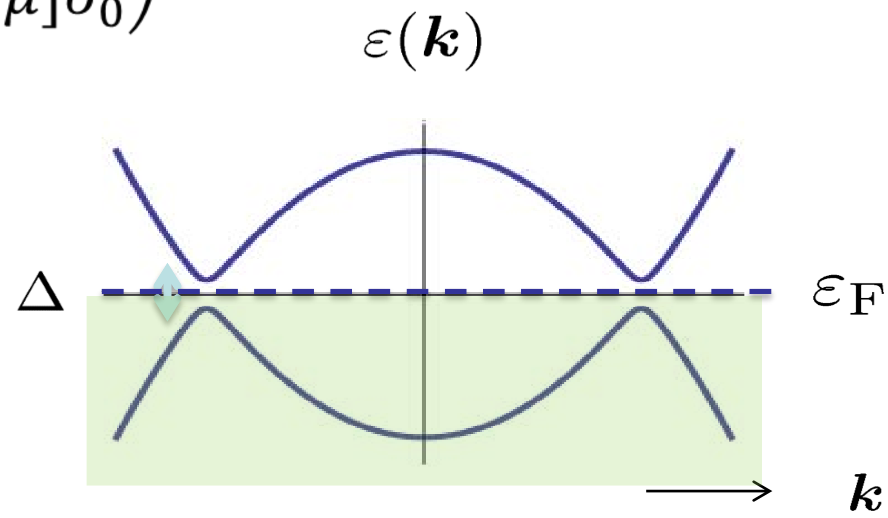
Excitation Spectrum: Single Band

Gor'kov and Volovik (1986), Rice, Sigrist and Ueda (1991).

$$\Delta(k) = \psi(k)U_T = \psi(k)i\sigma_y$$ Even parity $$T = i\sigma_y K = U_T K$$

$$\Delta(k) = \vec{d}(k)\cdot\vec{\sigma}U_T$$ Odd parity

$$H_{BdG} = \begin{pmatrix} [\varepsilon(k)-\mu]\sigma_0 & \Delta(k) \\ \Delta^t(k) & -[\varepsilon(k)-\mu]\sigma_0 \end{pmatrix}$$



built in charge conjugation **C** symmetry (always present even with more bands)

$$CH(k)C^{-1} = -H(-k)$$

C$= K\tau_x$ Anti-unitary

Excitation spectrum

$$H_{BdG} = \begin{pmatrix} [\varepsilon(k) - \mu]\sigma_0 & \Delta(k) \\ \Delta^t(k) & -[\varepsilon(k) - \mu]\sigma_0 \end{pmatrix}$$

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

$$E(k) = \pm\sqrt{(\varepsilon(k) - \mu)^2 + |\vec{d}(k)|^2} \qquad (\vec{d} \times \vec{d}^* = 0)$$

For nodes $E(k) = 0$

$(\varepsilon(k) - \mu)^2 = 0$ Means **k** is on Fermi surface

If ψ(k) vanishes on a line in **k**-space, get point nodes.
If ψ(k) vanishes on a plane in **k**-space, get line nodes.

This offers no way to generate Fermi surfaces in a single band SC system

URu_2Si_2 Example

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

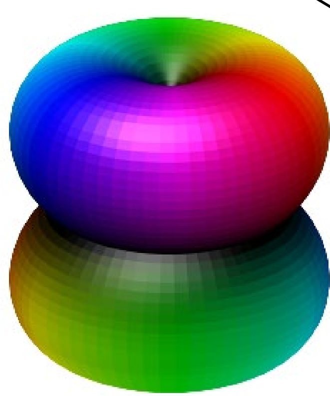
$(\varepsilon(k)-\mu)^2=0$ Here consider a spherical Fermi surface

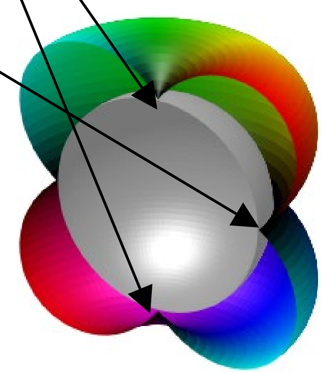
Consider: $\psi(k)=k_z(k_x+ik_y)$ (breaks time reversal symmetry)

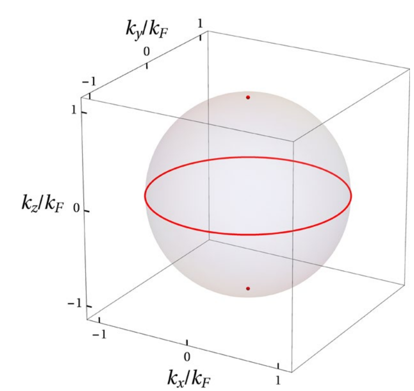
$$|\psi(k)|^2 = k_z^2(k_x^2+k_y^2)$$

$\psi(k)=0$ along line kx=ky=0, <u>Weyl point nodes</u> (+-2) (boundary arc states)

$\psi(k)=0$ on plane kz=0, <u>line nodes</u>

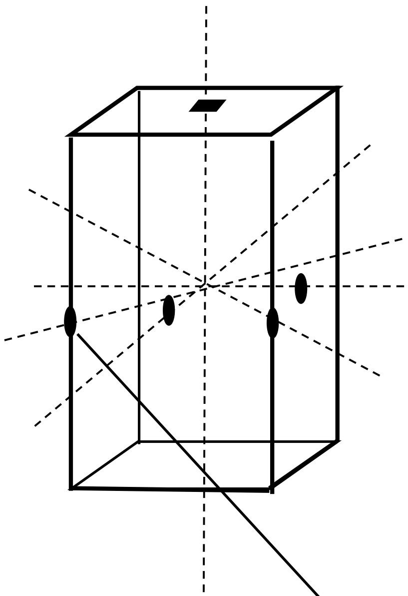






Traditional Origin of Nodes: Group Theory

Point group: D_{4h}



D_{4h} contains inversion

⇨ even and odd representations

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B_2	1	1	-1	-1	1
E	2	-2	0	0	0

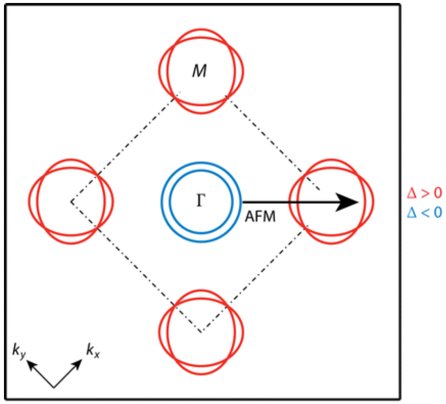
$$\psi(k) = \psi_0(k_x^2 - k_y^2)$$

Gor'kov Volovik (1987)

$$\psi(kx, ky) \overset{C_2''}{\longmapsto} \psi(ky, kx) = -\psi(kx, ky) \Longrightarrow \psi(k,k) = 0$$

Spin-singlet wavefunction, so only k rotates under C_2''

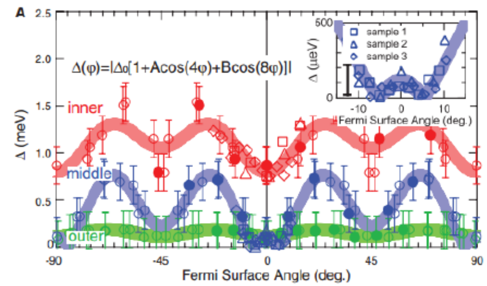
ARPES: Fe-based superconductors



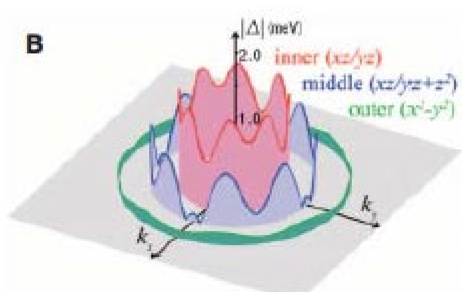
Huang D, Hoffman JE. 2017.
Annu. Rev. Condens. Matter Phys. 8:311–36

KFe_2As_2

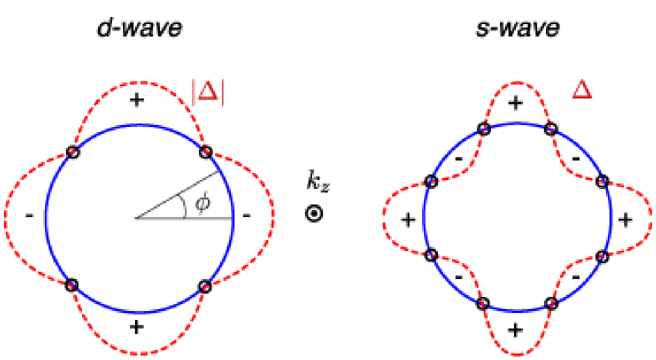
Around Γ point



Common mechanism: repulsive inter-pocket scattering (Mazin, Kuroki, Hirschfeld, Chubukov).

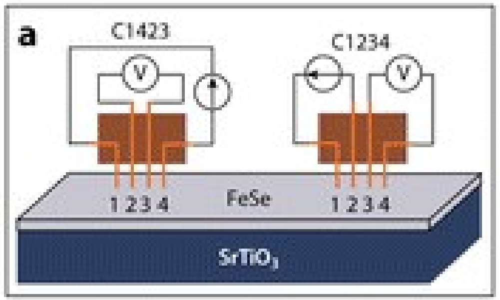


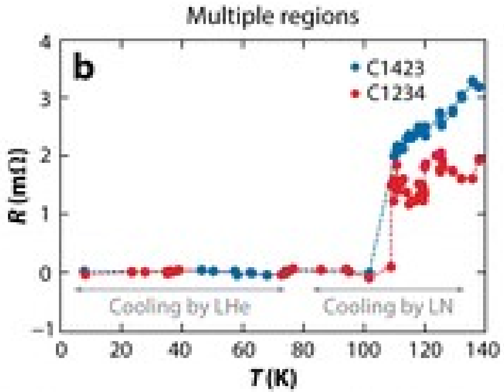
Okazaki *et al*, Science **337** p1314 (2012)



Accidental nodes: not dictated by symmetry

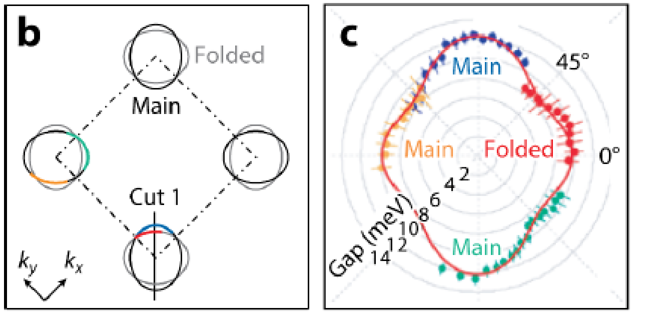
Superconductivity in monolayer FeSe





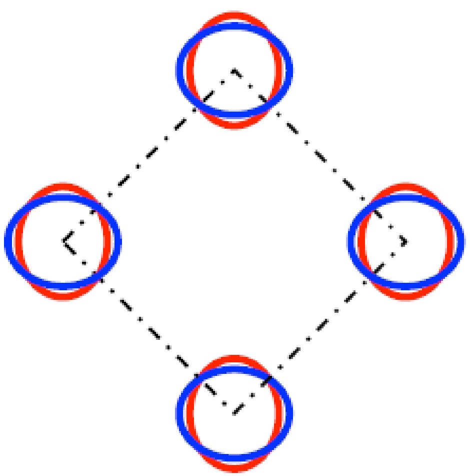
Ge et al Nature Materials14, 285 (2015).

Highest Tc in Fe superconductor family



Zhang et al, Phys. Rev. Lett. 117, 117001

FeSe seems "s-wave" – where have e-e interactions gone?



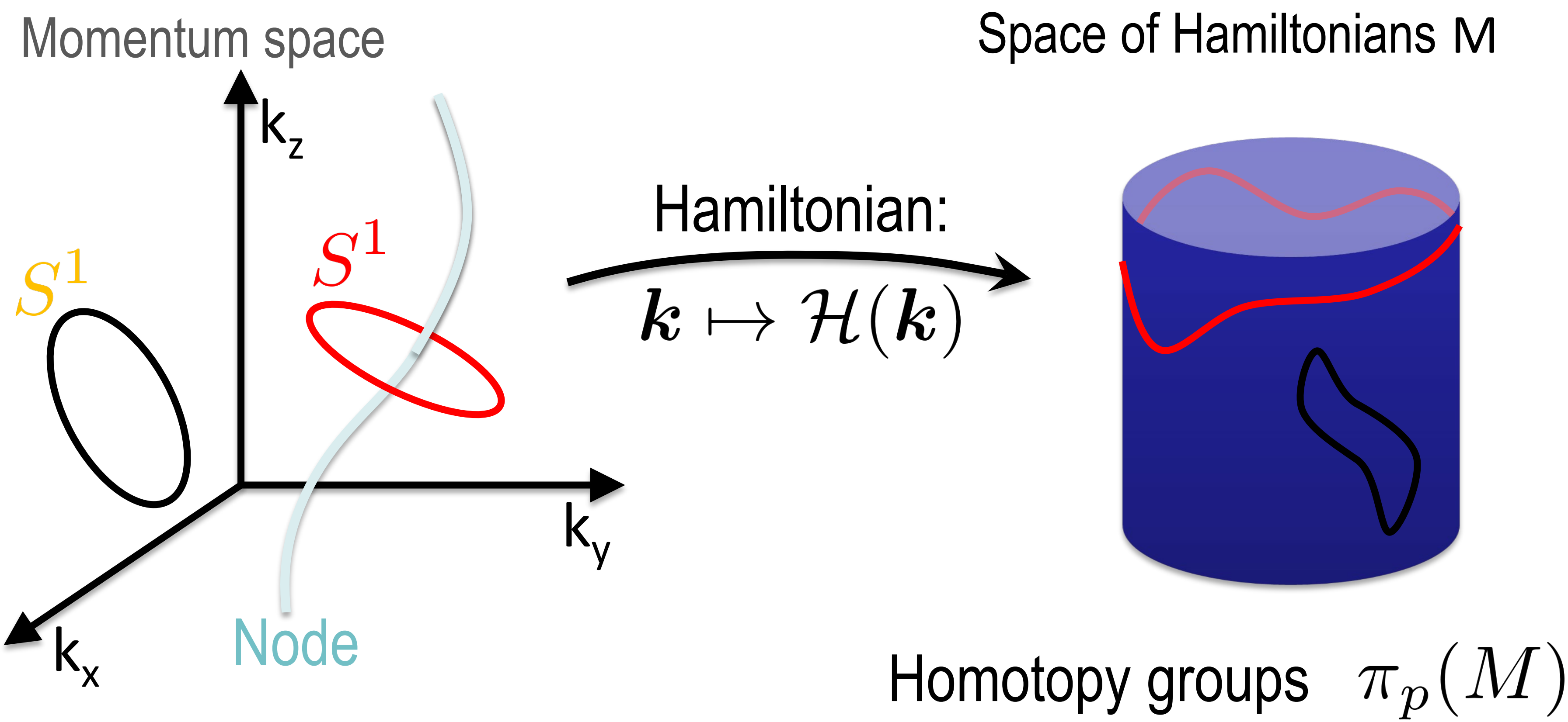
Gap changes signs on the two ellipses: *this is a d-wave state.*

Where have the nodes gone?

Homotopic Classification of Nodes In 3D

Homotopic Classification of Nodes

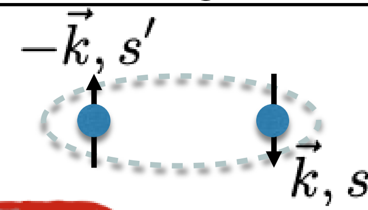
1- Identify relevant symmetries and symmetry classes
2- In each class find the dimensionality of nodes (co-dimension arguments)
3- Identify topological invariants associated with nodes:



Symmetry choice from T. Bzdušek and M. Sigrist, Phys. Rev. B **96**, 155105 (2017)

Superconducting Nodal Symmetries

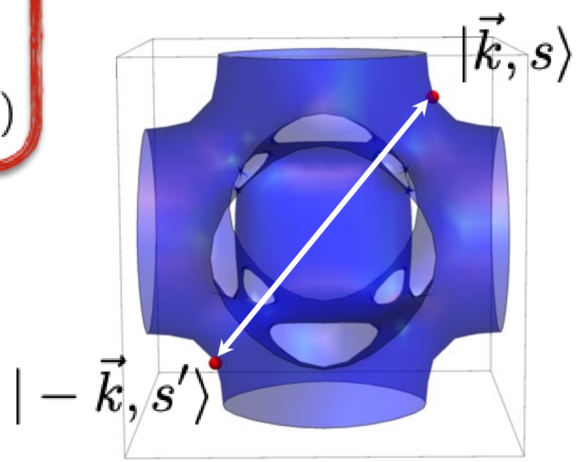
- Superconducting pairs:



weak coupling instability

$\longleftrightarrow$ equal energy of $|\vec{k}, s\rangle$ & $|-\vec{k}, s'\rangle$

- Key symmetries: T and I   Anderson, PRB (1984)



For nodal classification, want symmetries that take k to k.
Should also include C (particle-hole).
Key symmetries: TI and CI and S= (CI)(TI)=CT.

$$TI\ H(k)\ (TI)^{-1} = H(k) \qquad (TI)^2 = \pm 1 \qquad \text{AU}$$

$$CI\ H(k)\ (CI)^{-1} = -H(k) \qquad (CI)^2 = \pm 1 \qquad \text{AU}$$

$$S\ H(k)\ (S)^{-1} = -H(k) \qquad S^2 = 1 \qquad \text{U}$$

Same symmetry conditions as Altland-Zirnbauer classes: ten-fold way

“Bulk classes” vs. “nodal classes”

(invariants of gapped systems)

Symmetries local in **r-space**:

- Time reversal T
- Particle-hole C (charge conjugation)
- Chiral S (sublattice)

Altland-Zirnbauer classes

(charges of nodes in gapless systems)

Symmetries local in **k-space**:

- Composition TI
- Composition CI
- Chiral S

(where I is spatial inversion)

ten “AZ+I” classes

T. Bzdušek and M. Sigrist, Phys. Rev. B **96**, 155105 (2017)

Nodal "AZ+I" Classes

Node Dimension: Consider class DIII

Minimal model has pseudospin (σ) and particle-hole (τ) symmetry:

$$H = \sum c_{ij}(k)\sigma_i\tau_j$$

$S = \tau_z$ CI= $\tau_x K$ TI= $i\tau_y K$

$$S\,H(k)\,(S)^{-1} = -H(k)$$
$$CI\,H(k)\,(CI)^{-1} = -H(k)$$
$$TI\,H(k)\,(TI)^{-1} = H(k)$$

label	TI	CI	S
A	$\times$	$\times$	$\times$
AIII	$\times$	$\times$	1
AI	+1	$\times$	$\times$
BDI	+1	+1	1
D	$\times$	+1	$\times$
DIII	−1	+1	1
AII	−1	$\times$	$\times$
CII	−1	−1	1
C	$\times$	−1	$\times$
CI	+1	−1	1

Imply: only $c_{xy}(k)$ and $c_{yy}(k)$ are non-zero

$$E = \pm\sqrt{c_{xy}^2 + c_{yy}^2} = 0$$

This has codimension δ=2, allowing line nodes in 3D

Nodal "AZ+I" SC Classes

Not all "AZ+I"classes can be reached in superconductors since:

1- All superconductors have C symmetry

2- All superconductors also have I symmetry (not obvious)

3- Superconductor can break T (though not normal state), when present T^2=-1

$I\,H(k)\,(I)^{-1} = H(-k)$ For even parity: I=τ_0, for odd parity I=τ_z

Charge on S^0 S^1 S^2 in **k**-space.

label	TI	CI	S	π_0	π_1	π_2
DIII (even I)	-1	+1	1		2Z	
D (even I)	X	+1	X	Z_2		2Z
CII (odd I)	-1	-1	1			
C (odd I)	X	-1	X			Z

Line Nodes

Point Nodes

Surprise is Bogoliubov Fermi surfaces: not found in single-band superconductors

Point nodes are classified by Chern number (surface arcs), point nodes by winding number (flat band Majorana surface states).