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Classification theory of topological crystalline gapless superconductivity

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SS & Y. Yanase, Phys. Rev. B **97**, 134512 (2018).
S. Kobayashi, SS, Y. Yanase, & M. Sato, Phys. Rev. B **97**, 180504(R) (2018).
SS, T. Nomoto, K. Shiozaki, & Y. Yanase, Phys. Rev. B **99**, 134513 (2019).

Topology in gapped systems

- Topological invariant: defined for **gapped** Hamiltonian
  - *e.g.*) insulators, fully gapped SCs
- Classification by **symmetry** and **dimensionality**
  - Onsite symmetry: 10 **Altland-Zirnbauer (AZ) classes**

    A. Altland & M. R. Zirnbauer, PRB (1997)
    - TRS, PHS, & CS
    - *"Topological periodic table"*

      A. P. Schnyder *et al.* (2008)
      A. Kitaev (2009) / S. Ryu *et al.* (2010)

TRS	PHS	CS	AZ class
0	0	0	A
0	0	1	AIII
+1	0	0	AI
+1	+1	1	BDI
0	+1	0	D
−1	+1	1	DIII
−1	0	0	AII
−1	−1	1	CII
0	−1	0	C
+1	−1	1	CI

	d												
Cartan	0	1	2	3	4	5	6	7	8	9	10	11	…
Complex case:													
A	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	…
AIII	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	0	$\mathbb{Z}$	…
Real case:													
AI	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	…
BDI	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	…
D	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	…
DIII	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	…
AII	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	…
CII	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	…
C	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	0	…
CI	0	0	0	$2\mathbb{Z}$	0	$\mathbb{Z}_2$	$\mathbb{Z}_2$	$\mathbb{Z}$	0	0	0	$2\mathbb{Z}$	…

Topology in gapped systems

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  - Onsite symmetry: 10 **Altland-Zirnbauer (AZ) classes**
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    - TRS, PHS, & CS
    - *"Topological periodic table"* A. P. Schnyder *et al.* (2008) A. Kitaev (2009) / S. Ryu *et al.* (2010)
  - Crystal symmetry: **point groups**, **space groups**
    - *"Topological crystalline insulators"* L. Fu (2011)
    - Various methods

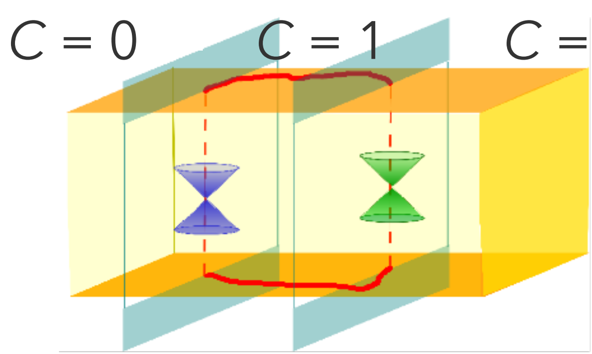
      Symmetry-based indicator: H. C. Po *et al.* (2017), H. Watanabe *et al.* (2018)
      Topological quantum chemistry: B. Bradlyn *et al.* (2017)
      Atiyah-Hirzebruch spectral sequence: K. Shiozaki *et al.* (2018)

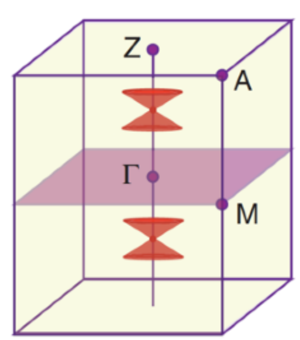
Topology in gapless systems

- Topology is useful even for **gapless** Hamiltonian

Semimetals

- Jumps of topological # in BZ = **Topological gapless points**
  - Weyl points (Chern #)
  - Dirac points on a C_n-axis

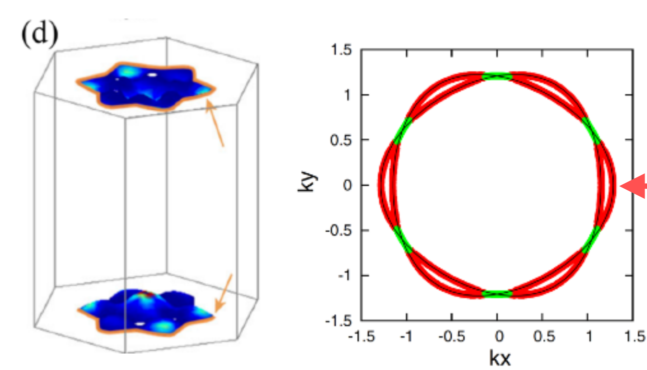




Yang-Nagaosa (2014)

Nodal superconductors

- Gapless points = **SC nodes**
  - **Unusual nodes** due to crystal symmetry Norman (1995) Nomoto-Ikeda (2017)
  - Topological protection ?



Nomoto-Ikeda(2016) / Yanase (2016)

Bulk property	Normal	Superconducting
Gapped	Topological insulators	(Fullgap) topological SCs
Gapless	Topological semimetals	????

Motivation

(a) SS-Yanase, PRB (2018). / Kobayashi-SS-Yanase-Sato, PRB (2018).
(b) SS-Nomoto-Shiozaki-Yanase, PRB (2019).

Background: gapless physics

- Semimetal case:
  - **Gapless points** characterized by a **topological invariant**
  - **Crystal sym.** → an **additional invariant** of gapless points
- Nodal SC case: examples of **symmetry-protected nodes**

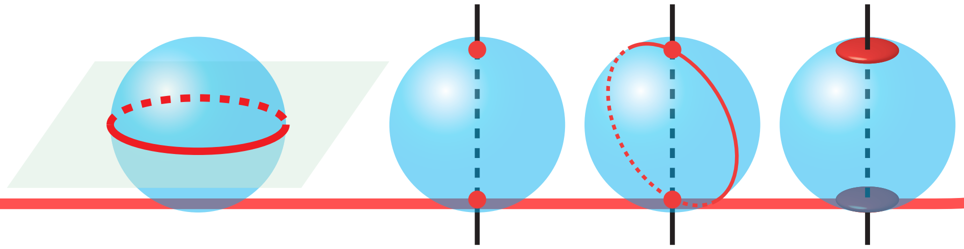
- *Do SC nodes meet topology ?*
- *Do crystal symmetries give an invariant of nodes ?*

Aim

Topologically classify symmetry-protected SC nodes for centrosymmetric superconductors

(a) (Line) nodes on high-symmetry plane

(b) Nodes on high-symmetry line



Collaborators

(a) SS-Yanase, PRB (2018). / Kobayashi-SS-Yanase-Sato, PRB (2018).
(b) SS-Nomoto-Shiozaki-Yanase, PRB (2019).

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Youichi Yanase

Supervisor
- Superconductivity
- SCES
- Multipole physics

(a)

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Shingo Kobayashi

Clifford algebra

Quantum field theory

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Masatoshi Sato

(b)

Dept. of Appl. Phys., The Univ. of Tokyo
Takuya Nomoto

Group theory

K-theory, cohomology

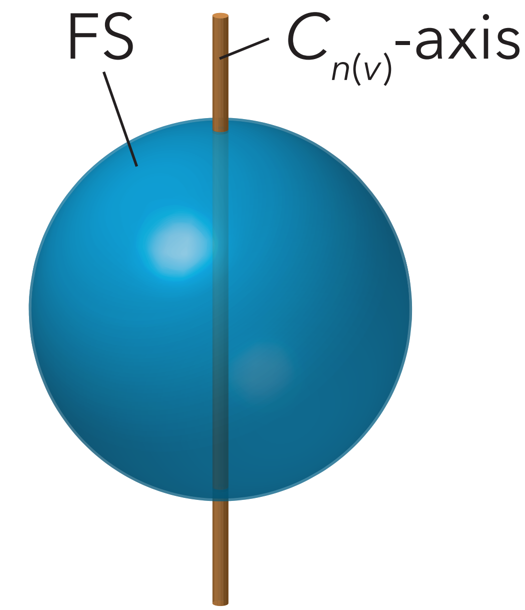
YITP, Kyoto Univ.
Ken Shiozaki

Methods

- High-sym. $\boldsymbol{k}$ → normal Bloch state α_1, α_2, ...

ex.) C_2-axis

IRs	E	C_2	
α_1	1	$+i$	~ spin up
α_2	1	$-i$	~ spin down

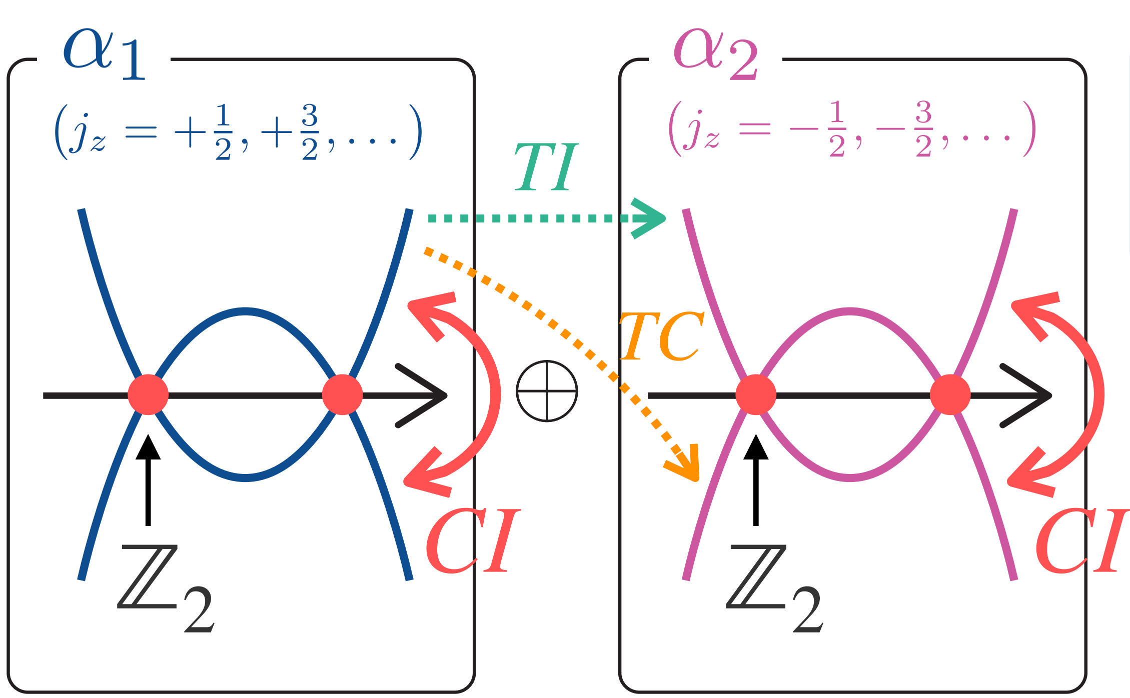


- Symmetry of SC order parameter

→ maps of (pseudo-) TRS, PHS, & CS among α_1, α_2, ...

ex.) B_g sym.
I: inversion,
T: TRS, C: PHS

$H_{\mathrm{BdG}}(\boldsymbol{k}) \sim$



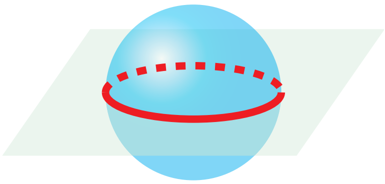
PHS w/ $(CI)^2 = +E$: **class D → Classification = $\mathbb{Z}_2$**

"Emergent" AZ class
→ Topological invariant !

Main results

(a) SS-Yanase, PRB (2018). / Kobayashi-SS-Yanase-Sato, PRB (2018).
(b) SS-Nomoto-Shiozaki-Yanase, PRB (2019).

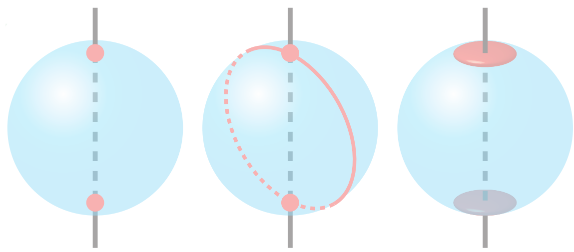
(a) For mirror- or glide-invariant SCs:



- Complete classification on **high-symmetry planes** for all symmorphic & nonsymmorphic symmetries
- No unusual node beyond previous examples

UPt_3: Norman (1995), Micklitz-Norman (2009), Kobayashi-Yanase-Sato (2016), Nomoto-Ikeda (2016)
CrAs: Micklitz-Norman (2017) / UCoGe, UPd_2Al_3: Nomoto-Ikeda (2017) / Sr_2IrO_4: SS-Nomoto-Yanase (2017)

(b) For rotation-invariant SCs:

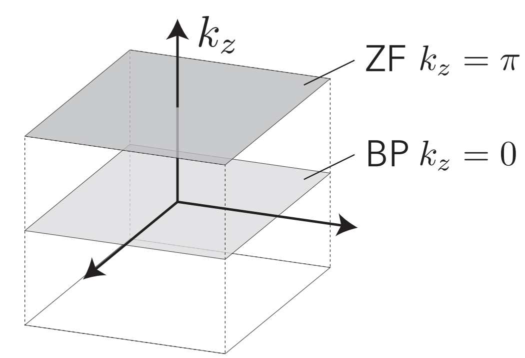


- Classification on **high-symmetry axes** *only* for symmorphic symmetries
- **Novel type of gap structure** on C_3- and C_6-axes

Complete classification on mirror- or glide-planes

S. Kobayashi, SS, Y. Yanase, & M. Sato, Phys. Rev. B **97**, 180504(R) (2018).

- Nontrivial results: differences between BP & ZF
  - **Nonsymmorphic (screw and/or AFM) sym.**
    → unusual node structures on ZF

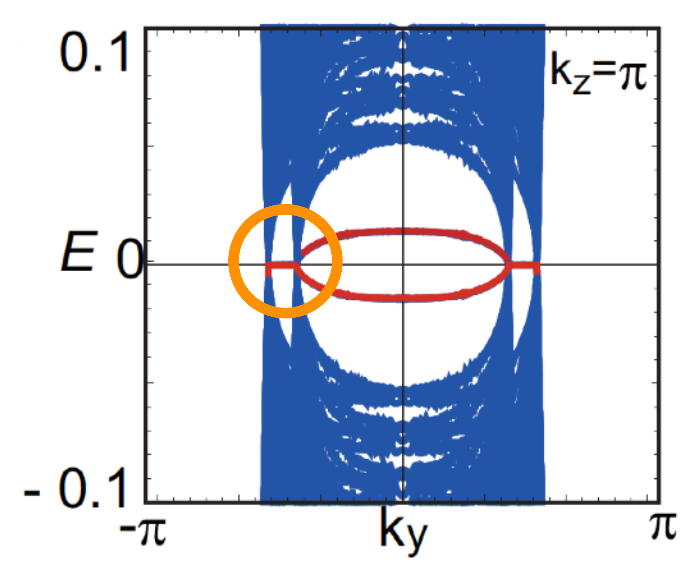


Symmetry of SC order parameter

	Cases	A_g BP	A_g ZF	B_g BP	B_g ZF	A_u BP	A_u ZF	B_u BP	B_u ZF
Rotation / PM	(a)	$0 \rightarrow$	0	(ii) $\mathbb{Z}_2 \rightarrow$	$\mathbb{Z}_2$	$0 \rightarrow$	0		
Screw / PM	(b)	$0 \rightarrow$	0	(ii) $\mathbb{Z}_2 \rightarrow$	$2\mathbb{Z}$	(i) $0 \rightarrow$	$2\mathbb{Z}$	$0 \rightarrow$	0
Rotation / AFM	(c)	(iii) $0 \rightarrow$	$2\mathbb{Z}$	(iii) $\mathbb{Z}_2 \rightarrow$	0	$0 \rightarrow$	0	(i) $0 \rightarrow$	$2\mathbb{Z}$
Screw / AFM	(d)	(iii) $0 \rightarrow$	$\mathbb{Z}_2$	(iii) $\mathbb{Z}_2 \rightarrow$	0	$0 \rightarrow$	0	$0 \rightarrow$	0

UPt_3 (Norman's zero)
UCoGe, CrAs?
Sr_2IrO_4
UPd_2Al_3

- Edge mode: **Majorana flat band**



Classification of 59 space groups

SS & Y. Yanase, Phys. Rev. B **97**, 134512 (2018).

(a)

	No.	Short	⊥= y
	10	$P2/m$	(RM)
UPd_2Al_3	11	$P2_1/m$	(SM)
	13	$P2/c$	(RG)
UCoGe	14	$P2_1/c$	(SG)

(b)

	No.	Short	⊥= x	⊥= y	⊥= z
	47	$Pmmm$	(RM)	(RM)	(RM)
	48	$Pnnn$	(RG)	(RG)	(RG)
	49	$Pccm$	(RG)	(RG)	(RM)
	50	$Pban$	(RG)	(RG)	(RG)
	51	$Pmma$	(SM)	(RM)	(RG)
	52	$Pnna$	(RG)	(SG)	(RG)
	53	$Pmna$	(RM)	(RG)	(SG)
Sr_2IrO_4	54	$Pcca$	(SG)	(RG)	(RG)
	55	$Pbam$	(SG)	(SG)	(RM)
	56	$Pccn$	(SG)	(SG)	(RG)
	57	$Pbcm$	(RG)	(SG)	(SM)
	58	$Pnnm$	(SG)	(SG)	(RM)
	59	$Pmmn$	(SM)	(SM)	(RG)
	60	$Pbcn$	(SG)	(RG)	(SG)
	61	$Pbca$	(SG)	(SG)	(SG)
UCoGe, CrAs	62	$Pnma$	(SG)	(SM)	(SG)
	63	$Cmcm$	N/A	N/A	(SM)
	64	$Cmca$	N/A	N/A	(SG)
	65	$Cmmm$	N/A	N/A	(RM)
	66	$Cccm$	N/A	N/A	(RM)
	67	$Cmma$	N/A	N/A	(RG)
	68	$Ccca$	N/A	N/A	(RG)

(c)

No.	Short	⊥= z	⊥= x,y
83	$P4/m$	(RM)	N/A
84	$P4_2/m$	(RM)	N/A
85	$P4/n$	(RG)	N/A
86	$P4_2/n$	(RG)	N/A
123	$P4/mmm$	(RM)	(RM)
124	$P4/mcc$	(RM)	(RG)
125	$P4/nbm$	(RG)	(RG)
126	$P4/nnc$	(RG)	(RG)
127	$P4/mbm$	(RM)	(SG)
128	$P4/mnc$	(RM)	(SG)
129	$P4/nmm$	(RG)	(SM)
130	$P4/ncc$	(RG)	(SG)
131	$P4_2/mmc$	(RM)	(RM)
132	$P4_2/mcm$	(RM)	(RG)
133	$P4_2/nbc$	(RG)	(RG)
134	$P4_2/nnm$	(RG)	(RG)
135	$P4_2/mbc$	(RM)	(SG)
136	$P4_2/mnm$	(RM)	(SG)
137	$P4_2/nmc$	(RG)	(SM)
138	$P4_2/ncm$	(RG)	(SG)

(d)

	No.	Short	⊥= z	⊥= [1−10],[120],[210]
	175	$P6/m$	(RM)	N/A
	176	$P6_3/m$	(SM)	N/A
	191	$P6/mmm$	(RM)	(RM)
	192	$P6/mcc$	(RM)	(RG)
	193	$P6_3/mcm$	(SM)	(RM)
UPt_3	194	$P6_3/mmc$	(SM)	(RG)

(e)

No.	Short	⊥= x,y,z
200	$Pm\bar{3}$	(RM)
201	$Pn\bar{3}$	(RG)
205	$Pa\bar{3}$	(SG)
221	$Pm\bar{3}m$	(RM)
222	$Pn\bar{3}n$	(RG)
223	$Pm\bar{3}n$	(RM)
224	$Pn\bar{3}m$	(RG)

Main results

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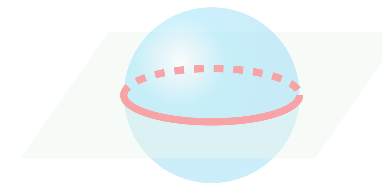
(b) SS-Nomoto-Shiozaki-Yanase, PRB (2019).



(a) For mirror- or glide-invariant SCs:

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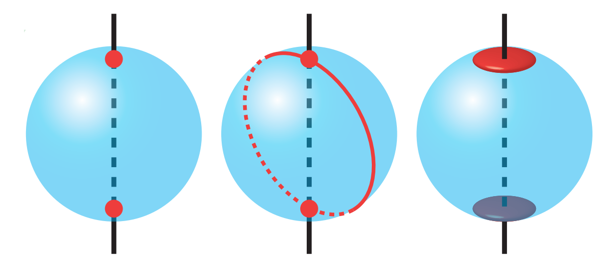
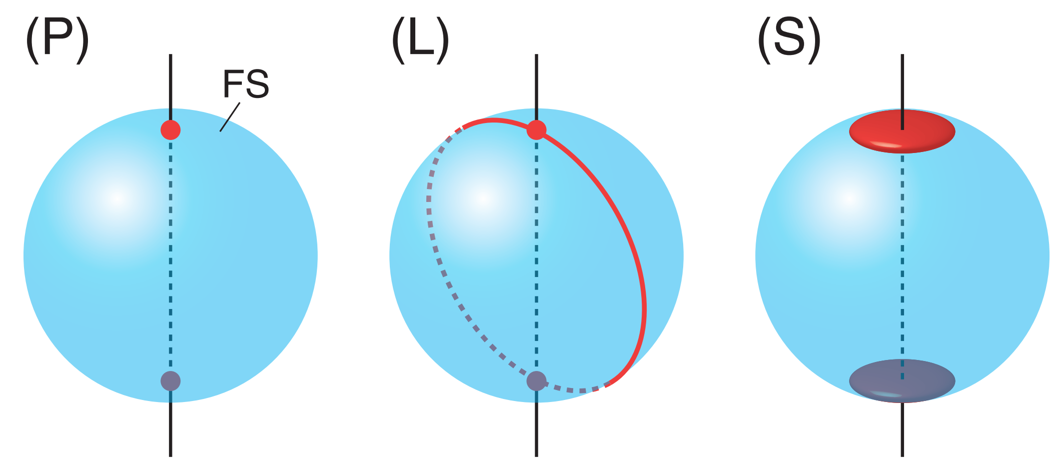


- Classification on **high-symmetry axes** *only* for symmorphic symmetries
- **Novel type of gap structure** on C_3- and C_6-axes

Classification on symmorphic $C_{n(v)}$-axes

SS, T. Nomoto, K. Shiozaki, & Y. Yanase, PRB **99**, 134513 (2019).

- **Four types** of gap structure
  - (G) Fullgap
  - (P) Point nodes
  - (L) Line nodes
  - (S) Bogoliubov FSs



Novel j_z-dependent feature for C_3 & C_6

→ Examples: SrPtAs (even) & UPt_3 (odd)

(a) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_2$, $\alpha = \pm 1/2$

IR of C_{2h}	EAZ	Classification
A_g	AIII	0 (G)
A_u	AIII	0 (G)
B_g	D	$\mathbb{Z}_2$ (L)
B_u	C	0 (G)

(b1) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_3$, $\alpha = +(-)1/2$

IR of S_6	EAZ	Classification
A_g	AIII	0 (G)
A_u	AIII	0 (G)
${}^2E_g({}^1E_g)$	D	$\mathbb{Z}_2$ (S)
${}^1E_g({}^2E_g)$	A	$\mathbb{Z}$ (S)
${}^2E_u({}^1E_u)$	C	0 (G)
${}^1E_u({}^2E_u)$	A	$\mathbb{Z}$ (P)

(b2) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_3$, $\alpha = \pm 3/2$

IR of S_6	EAZ	Classification
A_g	DIII	0 (G)
A_u	CII	0 (G)
${}^{1,2}E_g$	A	$\mathbb{Z}$ (S)
${}^{1,2}E_u$	A	$\mathbb{Z}$ (P)

(c) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_4$, $\alpha = +(-)1/2, +(-)3/2$

IR of C_{4h}	EAZ	Classification
A_g	AIII	0 (G)
A_u	AIII	0 (G)
B_g	A	$\mathbb{Z}$ (L)
B_u	A	$\mathbb{Z}$ (P)
${}^2E_g({}^1E_g)$	D	$\mathbb{Z}_2$ (S)
${}^1E_g({}^2E_g)$	A	$\mathbb{Z}$ (S)
${}^2E_u({}^1E_u)$	C	0 (G)
${}^1E_u({}^2E_u)$	A	$\mathbb{Z}$ (P)

(d1) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_6$, $\alpha = +(-)1/2, +(-)5/2$

IR of C_{6h}	EAZ	Classification
A_g	AIII	0 (G)
A_u	AIII	0 (G)
B_g	A	$\mathbb{Z}$ (L)
B_u	A	$\mathbb{Z}$ (P)
${}^1E_{1g}({}^2E_{1g})$	D	$\mathbb{Z}_2$ (S)
${}^2E_{1g}({}^1E_{1g})$	A	$\mathbb{Z}$ (S)
${}^1E_{1u}({}^2E_{1u})$	C	0 (G)
${}^2E_{1u}({}^1E_{1u})$	A	$\mathbb{Z}$ (P)
${}^{1,2}E_{2g}$	A	$\mathbb{Z}$ (S)
${}^{1,2}E_{2u}$	A	$\mathbb{Z}$ (P)

(d2) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_6$, $\alpha = \pm 3/2$

IR of C_{6h}	EAZ	Classification
A_g	AIII	0 (G)
A_u	AIII	0 (G)
B_g	D	$\mathbb{Z}_2$ (L)
B_u	C	0 (G)
${}^{1,2}E_{1g}$	A	$\mathbb{Z}$ (S)
${}^{1,2}E_{1u}$	A	$\mathbb{Z}$ (P)
${}^{1,2}E_{2g}$	A	$\mathbb{Z}$ (S)
${}^{1,2}E_{2u}$	A	$\mathbb{Z}$ (P)

(e) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{2v}$, $\alpha = 1/2$

IR of D_{2h}	EAZ	Classification
A_g	CI	0 (G)
A_u	CI	0 (G)
B_{1g}	BDI	$\mathbb{Z}_2$ (L)
B_{1u}	BDI	$\mathbb{Z}_2$ (P)
B_{2g}	BDI	$\mathbb{Z}_2$ (L)
B_{2u}	CI	0 (G)
B_{3g}	BDI	$\mathbb{Z}_2$ (L)
B_{3u}	CI	0 (G)

(f1) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{3v}$, $\alpha = 1/2$

IR of D_{3d}	EAZ	Classification
A_{1g}	CI	0 (G)
A_{1u}	CI	0 (G)
A_{2g}	BDI	$\mathbb{Z}_2$ (L)
A_{2u}	BDI	$\mathbb{Z}_2$ (P)
2D IRs	see (b1)	

(f2) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{3v}$, $\alpha = 3/2$

IR of D_{3d}	EAZ	Classification
A_{1g}	AIII	0 (G)
A_{1u}	C	0 (G)
A_{2g}	D	$\mathbb{Z}_2$ (L)
A_{2u}	AIII	0 (G)
2D IRs	see (b2)	

(g) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{4v}$, $\alpha = 1/2, 3/2$

IR of D_{4h}	EAZ	Classification
A_{1g}	CI	0 (G)
A_{1u}	CI	0 (G)
A_{2g}	BDI	$\mathbb{Z}_2$ (L)
A_{2u}	BDI	$\mathbb{Z}_2$ (P)
B_{1g}	AI	$\mathbb{Z}$ (L)
B_{1u}	AI	$\mathbb{Z}$ (P)
B_{2g}	AI	$\mathbb{Z}$ (L)
B_{2u}	AI	$\mathbb{Z}$ (P)
2D IRs	see (c)	

(h1) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{6v}$, $\alpha = 1/2, 5/2$

IR of D_{6h}	EAZ	Classification
A_{1g}	CI	0 (G)
A_{1u}	CI	0 (G)
A_{2g}	BDI	$\mathbb{Z}_2$ (L)
A_{2u}	BDI	$\mathbb{Z}_2$ (P)
B_{1g}	AI	$\mathbb{Z}$ (L)
B_{1u}	AI	$\mathbb{Z}$ (P)
B_{2g}	AI	$\mathbb{Z}$ (L)
B_{2u}	AI	$\mathbb{Z}$ (P)
2D IRs	see (d1)	

(h2) $\bar{\mathcal{G}}^{\boldsymbol{k}} = C_{6v}$, $\alpha = 3/2$

IR of D_{6h}	EAZ	Classification
A_{1g}	CI	0 (G)
A_{1u}	CI	0 (G)
A_{2g}	BDI	$\mathbb{Z}_2$ (L)
A_{2u}	BDI	$\mathbb{Z}_2$ (P)
B_{1g}	BDI	$\mathbb{Z}_2$ (L)
B_{1u}	CI	0 (G)
B_{2g}	BDI	$\mathbb{Z}_2$ (L)
B_{2u}	CI	0 (G)
2D IRs	see (d2)	

Background of SrPtAs

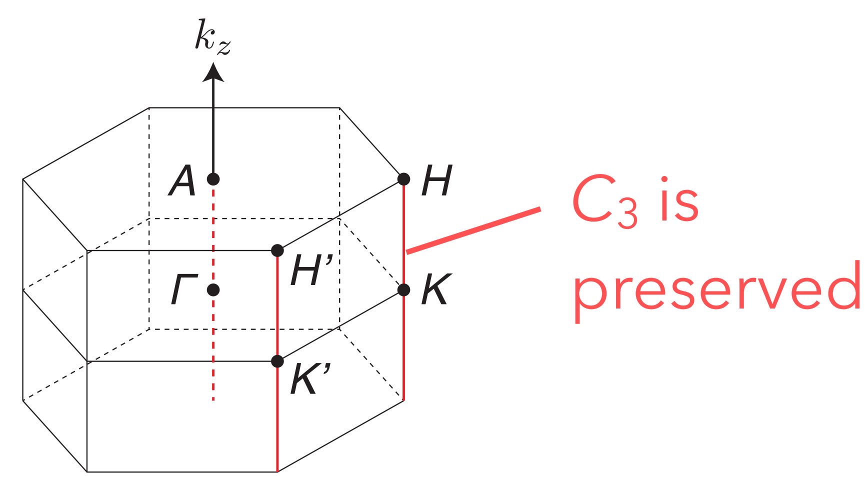
- SrPtAs: a pnictide SC w/ a hexagonal lattice (D_{6h})
- Pairing symmetry is still under debate
- **Even-parity chiral *d*-wave (E_{2g})** order parameter

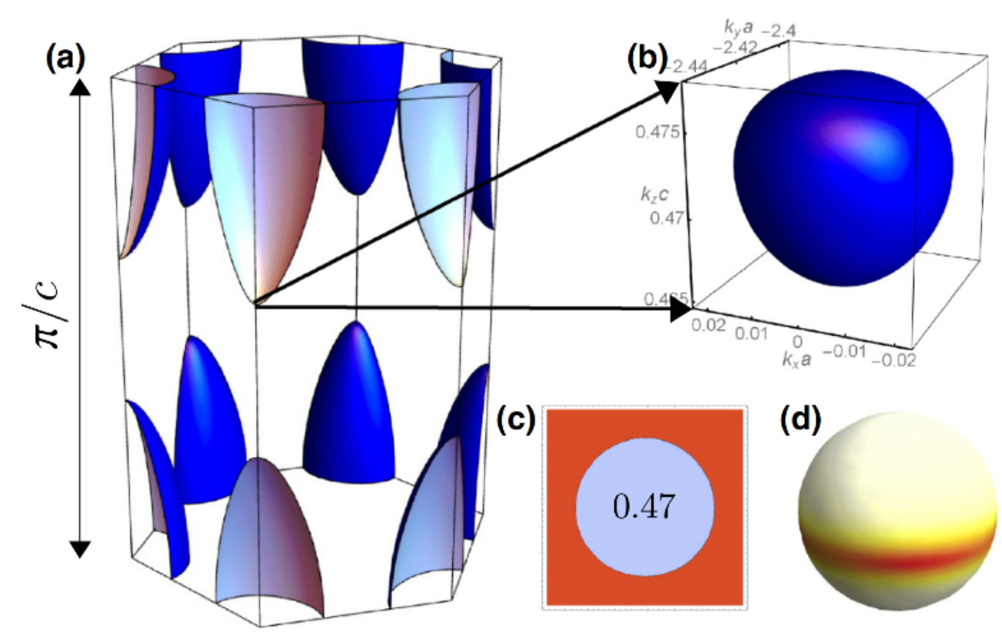
M. H. Fischer *et al.* (2014, 2015)

$$C_3 \hat{\Delta}_\pm(\boldsymbol{k}) C_3^T = e^{\pm i 2\pi/3} \hat{\Delta}_\pm(\boldsymbol{k})$$

  - **TRS broken & C_3 preserved** by choosing one of "±"
  - **Surface nodes** on *K*-*H* line

D. F. Agterberg *et al.*, PRL (2017)
T. Bzdušek & M. Sigrist, PRB (2017)

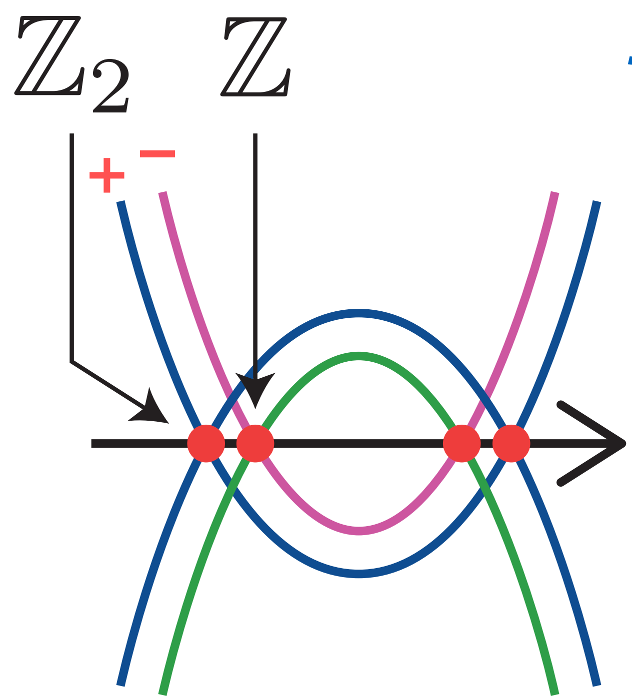




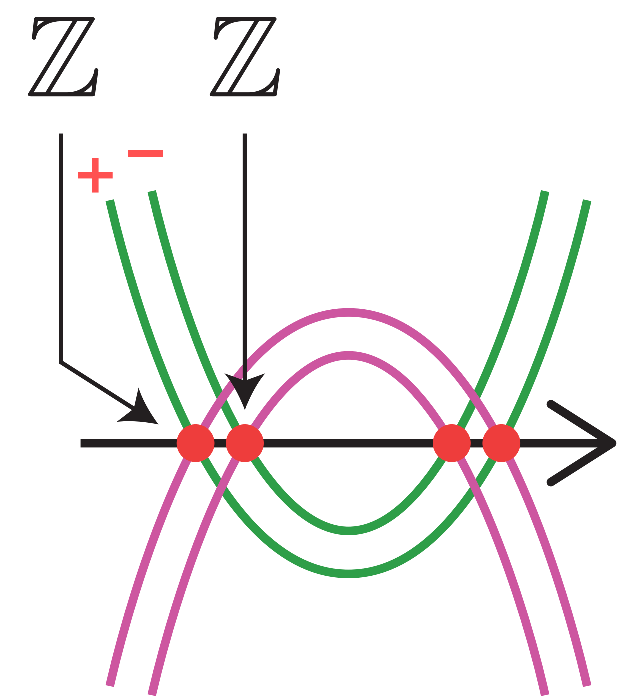
Results for even-parity SrPtAs

- **j_z-dependent topological protection** on *K*-*H* line

$j_z = \pm 1/2$



$j_z = \pm 3/2$

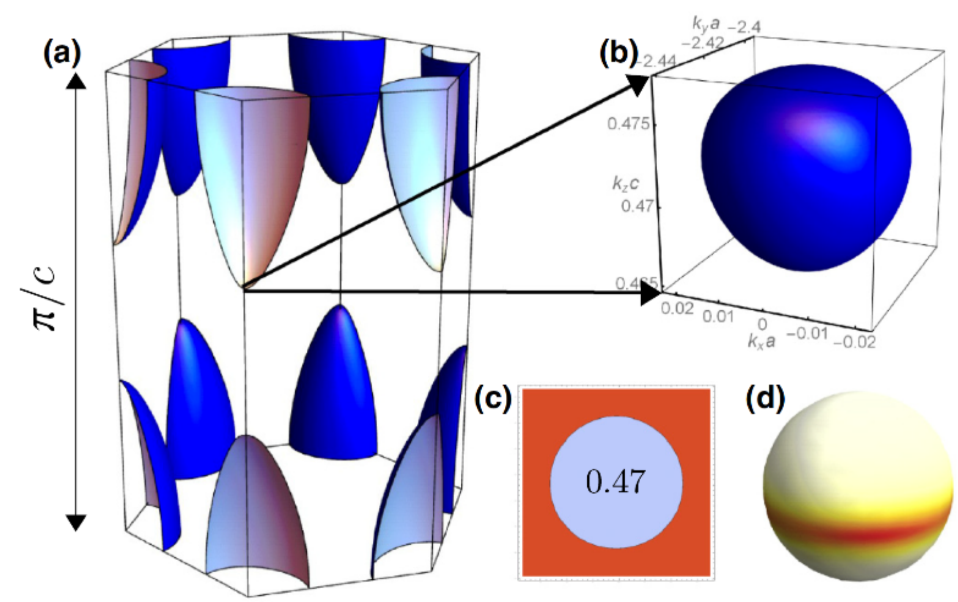


- Nodes on *K*-*H* line

  = Parts of **Bogoliubov FSs**

  irrespective of j_z

  D. F. Agterberg *et al.*, PRL (2017)
  T. Bzdušek & M. Sigrist, PRB (2017)



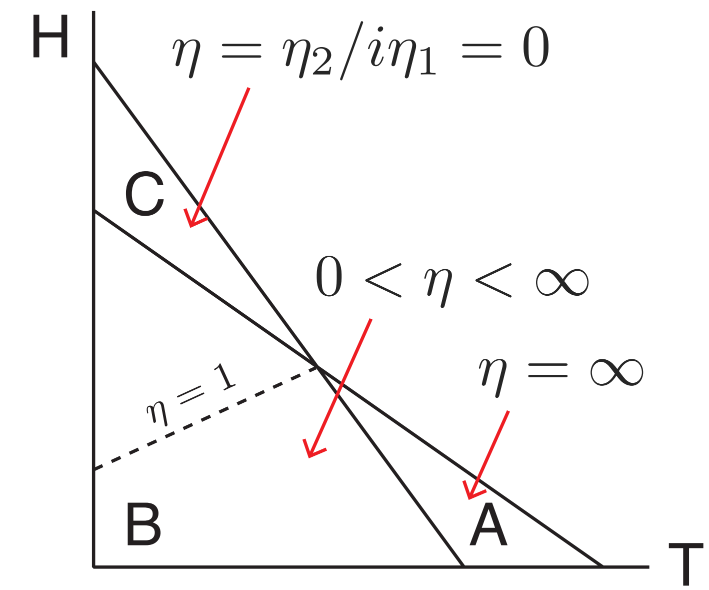
Background of UPt_3

- UPt_3: a heavy-fermion SC w/ a hexagonal lattice (D_{6h})
- Multiple SC phases: **odd-parity E_{2u} order parameter**

R. A. Fisher *et al.* (1989) / S. Adenwalla *et al.* (1990)

R. Joynt & L. Taillefer, RMP (2002)

$$\hat{\Delta}(\boldsymbol{k}) = \eta_1 \hat{\Gamma}_1^{E_{2u}} + \eta_2 \hat{\Gamma}_2^{E_{2u}}$$



  - **TRS broken** in B phase
  - **C_3 preserved** on η = 1

- First-principles study of UPt_3

T. Nomoto & H. Ikeda, PRL (2016)

→ *Γ*-FSs, *A*-FSs, & *K*-FSs

  - *K*-FSs: NOT sufficiently studied

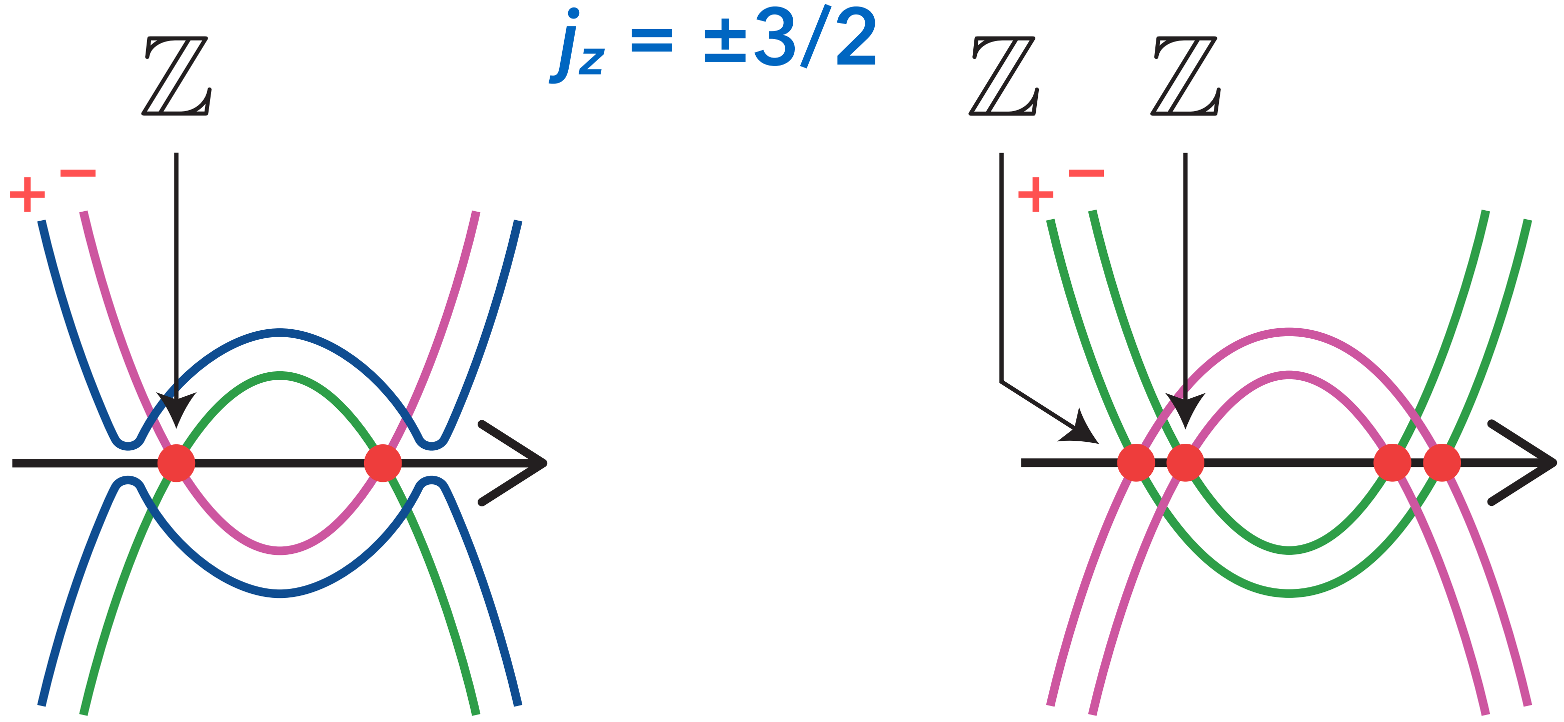
(c)

Results for odd-parity UPt_3

- j_z-dependent node structures on *K-H* line

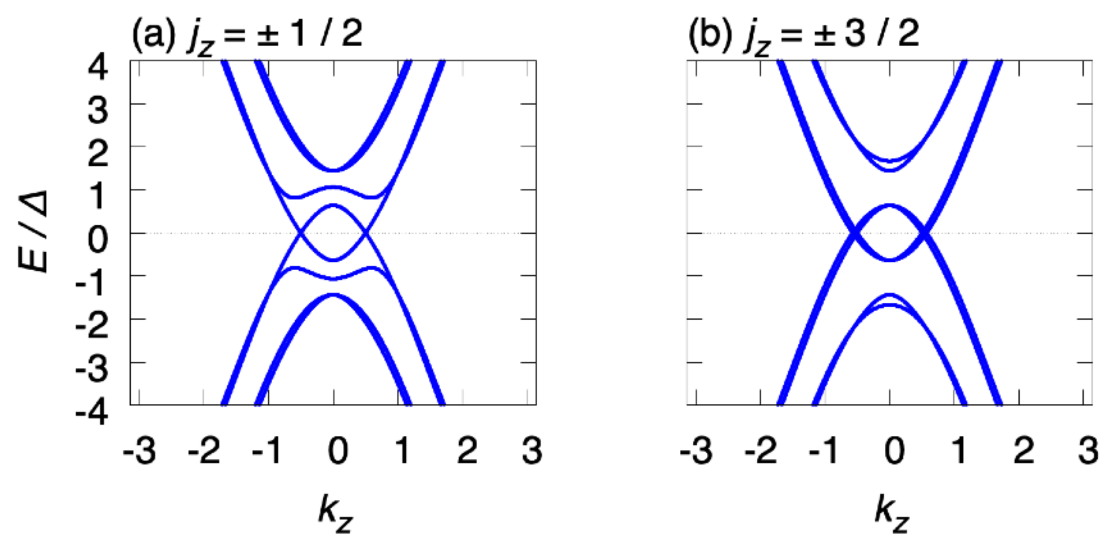
$j_z = \pm 1/2$ $j_z = \pm 3/2$

Perfectly non-unitary pairing



- Nodes on *K-H* line = **Point nodes depending on j_z**
- **Novel type of nodes !**
- Numerical calc.

Model: Y. Yanase (2016)



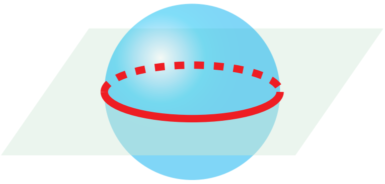
Conclusion

SS & Y. Yanase, Phys. Rev. B **97**, 134512 (2018).
S. Kobayashi, SS, Y. Yanase, & M. Sato, Phys. Rev. B **97**, 180504(R) (2018).
SS, T. Nomoto, K. Shiozaki, & Y. Yanase, Phys. Rev. B **99**, 134513 (2019).

- *Do SC nodes meet topology ?* → Yes !
- *Do crystal symmetries give an invariant of nodes ?* → Yes !
- Classification of **topological crystalline SC nodes**

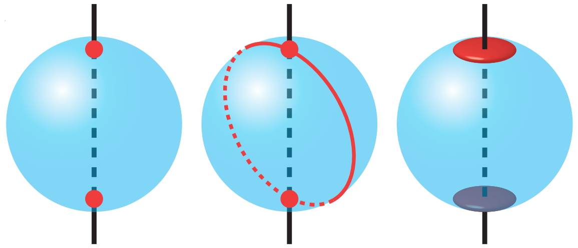
(a) For mirror or glide symmetry

- **Complete classification**
- Condition for **Majorana flat band**



(b) For rotation symmetry

- **Novel j_z-dep. node protections or structures on C_3 & C_6**
- Applications: SrPtAs & UPt_3



- **All nodes are topological ?**