Novel Quantum States in Condensed Matter 2017 Nov. 17, 2017

Multipole Superconductivity and Unusual Gap Closing
— Application to Sr_2IrO_4 and UPt_3 —

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SS, T. Nomoto, & Y. Yanase, Phys. Rev. Lett. **119**, 027001 (2017).
S. Kobayashi, SS, Y. Yanase, & M. Sato, in preparation.
SS & Y. Yanase, in preparation.

Outline

1. Introduction
2. Method: Superconducting gap classification
   based on space group symmetry
3. Result 1: Condition for nonsymmorphic line nodes
   (a) Complete classification
   (b) Application: Sr_2IrO_4
4. Result 2: j_z-dependent point nodes in UPt_3
5. Conclusion

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Superconducting gap classification (point group)

- Most studies: gap classification based on **crystal point group** symmetry
- Classification theory by Sigrist & Ueda (1991)
  - (1) **Most simple basis** of OP for each point group
  - (2) Gap or node @ specific ***k***
- Ex.) Point group D_{6h}

  Γ_1^- (A_{1u}): $k_x\hat{x} + k_y\hat{y}, k_z\hat{z}$

  Line node @ $k_z = 0$

  → No line node with SOC

  Blount's theorem (1985): "No line node for odd-parity SC w/ SOC"

Classification for D_{6h}

Irreducible representation Γ	Basis functions
	(a)
Γ_1^+	$\psi(\Gamma_1^+;\mathbf{k})=1,\ k_x^2+k_y^2,\ k_z^2$
Γ_2^+	$\psi(\Gamma_2^+;\mathbf{k})=k_xk_y(k_x^2-3k_y^2)(k_y^2-3k_x^2)$
Γ_3^+	$\psi(\Gamma_3^+;\mathbf{k})=k_zk_x(k_x^2-3k_y^2)$
Γ_4^+	$\psi(\Gamma_4^+;\mathbf{k})=k_zk_y(k_y^2-3k_x^2)$
Γ_5^+	$\psi(\Gamma_5^+,1;\mathbf{k})=k_xk_z$ $\psi(\Gamma_5^+,2;\mathbf{k})=k_yk_z$
Γ_6^+	$\psi(\Gamma_6^+,1;\mathbf{k})=k_x^2-k_y^2$ $\psi(\Gamma_6^+,2;\mathbf{k})=2k_xk_y$
	(b)
Γ_1^-	$\mathbf{d}(\Gamma_1^-;\mathbf{k})=\hat{\mathbf{x}}k_x+\hat{\mathbf{y}}k_y,\hat{\mathbf{z}}k_z$
Γ_3^-	$\mathbf{d}(\Gamma_3^-;\mathbf{k})=\hat{\mathbf{z}}k_x(k_x^2-3k_y^2)$, $k_z[(k_x^2-k_y^2)\hat{\mathbf{x}}-2k_xk_y\hat{\mathbf{y}}]$
Γ_4^-	$\mathbf{d}(\Gamma_4^-;\mathbf{k})=\hat{\mathbf{z}}k_y(k_y^2-3k_x^2)$, $k_z[(k_y^2-k_x^2)\hat{\mathbf{y}}-2k_xk_y\hat{\mathbf{x}}]$
Γ_5^-	$\mathbf{d}(\Gamma_5^-,1;\mathbf{k})=\hat{\mathbf{x}}k_z,\hat{\mathbf{z}}k_x$ $\mathbf{d}(\Gamma_5^-,2;\mathbf{k})=\hat{\mathbf{y}}k_z,\hat{\mathbf{z}}k_y$
Γ_6^-	$\mathbf{d}(\Gamma_6^-,1;\mathbf{k})=\hat{\mathbf{x}}k_x-\hat{\mathbf{y}}k_y$ $\mathbf{d}(\Gamma_6^-,2;\mathbf{k})=\hat{\mathbf{x}}k_y-\hat{\mathbf{y}}k_x$

M. Sigrist & K. Ueda, RMP (1991)

Superconducting gap classification (space group)

- Recent study: importance of **space group** symmetry
  (Point group) + (Translation)

- Classification theory based on (magnetic) space group
  (1) Choosing specific ***k*** at first
  (2) The presence or absence of Cooper pair w.f.

- Ex.) Space group $P6_3/mmc$ (D_{6h}^4) + TRS
  M. R. Norman (1995)
  T. Micklitz & M. R. Norman (2009)

  A_{1u}: $k_z = 0 \rightarrow$ Gap, $k_z = \pi \rightarrow$ **Line node**
  Incompatible w/ Blount's theorem due to nonsymmorphic symmetry

- **Unusual gap structures beyond Sigrist-Ueda method !**

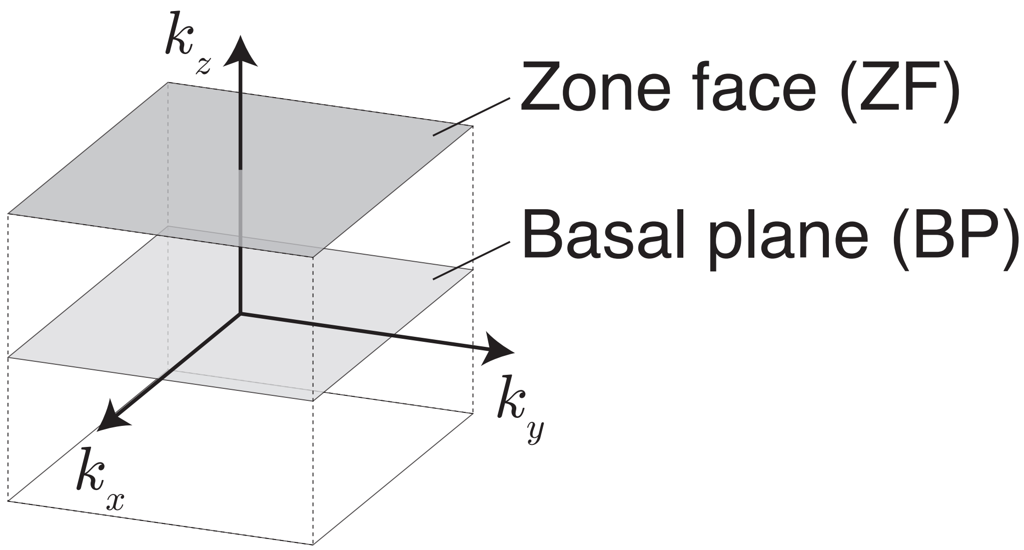
Results by space group & Unsolved questions

- Nontrivial line nodes by nonsymmorphic symmetry
  - UPt_3, $UCoGe$, UPd_2Al_3 T. Micklitz & M. R. Norman (2009, 2017) T. Nomoto & H. Ikeda (2017)

Nonsymmorphic symmetry

↓

Difference in reps. of gap between BP and ZF



→ **What is the condition for nontrivial line nodes ?**

- Only a few & less-known studies of point nodes

→ **Do point nodes peculiar to crystal group exist ?**

Abstract of this study

Aim 1

Investigate **the condition for nonsymmorphic line nodes**

Aim 2

Consider **crystal symmetry-protected point nodes**

Method

Gap classification based on **space group** symmetry

Result 1

Complete classification

- Application: Sr_2IrO_4

Result 2

j_z-dependent point nodes

- Application: UPt_3

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Gap classification (Flow)

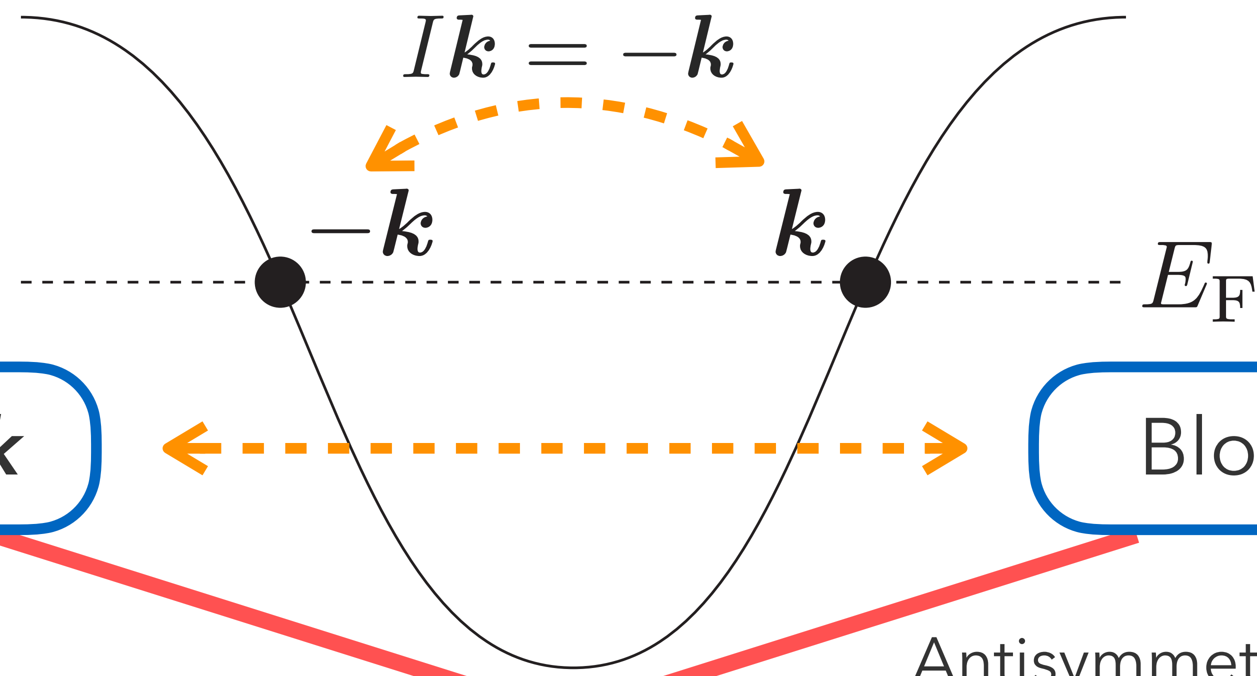
Magnetic space group

- **Centrosymmetric**

High-symmetry ***k***-point →

Little group

- Small representation
  = Bloch state at ***k***



Bloch state at **−*k*** ↔ Bloch state at ***k***

Antisymmetric direct product (**Mackey-Bradley theorem**)

↓

Representation of Cooper pair wave function

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System for classification of line nodes

- Gap classification: **inversion**
- On high-sym. ***k***-plane: **mirror (glide)** & primitive lattice

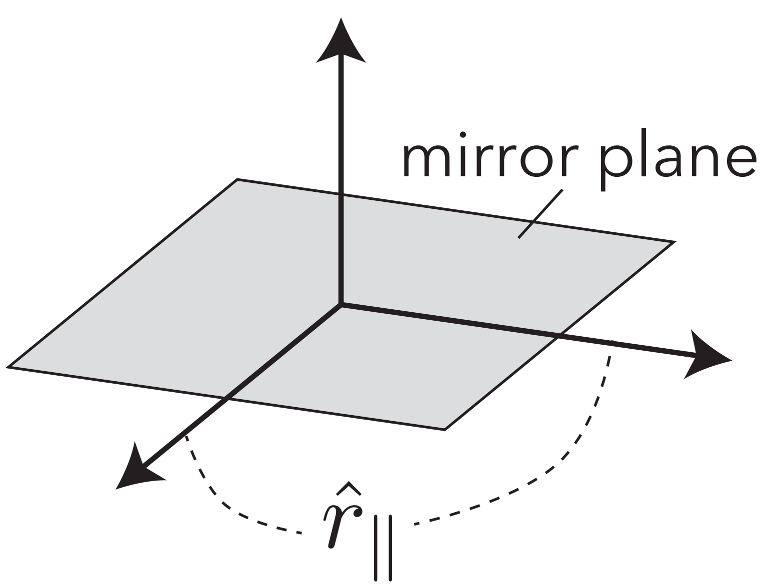
→ Space group contains C_{2h}:

$$G = \begin{cases} \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\mathbf{0}\}T + \{\sigma_\perp|\mathbf{0}\}T & \text{(i) Rotation + Mirror} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel\}T & \text{(ii) Rotation + Glide} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\perp\}T & \text{(iii) Screw + Mirror} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T & \text{(iv) Screw + Glide} \end{cases}$$

Note)

- $\{p|\boldsymbol{a}\}\boldsymbol{r} = p\boldsymbol{r} + \boldsymbol{a}$: space group operator
- T : translation group
- $\boldsymbol{\tau}_\perp, \boldsymbol{\tau}_\parallel$: non-primitive translation

→ **Nonsymmorphic**



Magnetic space group *M*

- Ferromagnetic (FM)

  $M = G$ (Unitary space group)

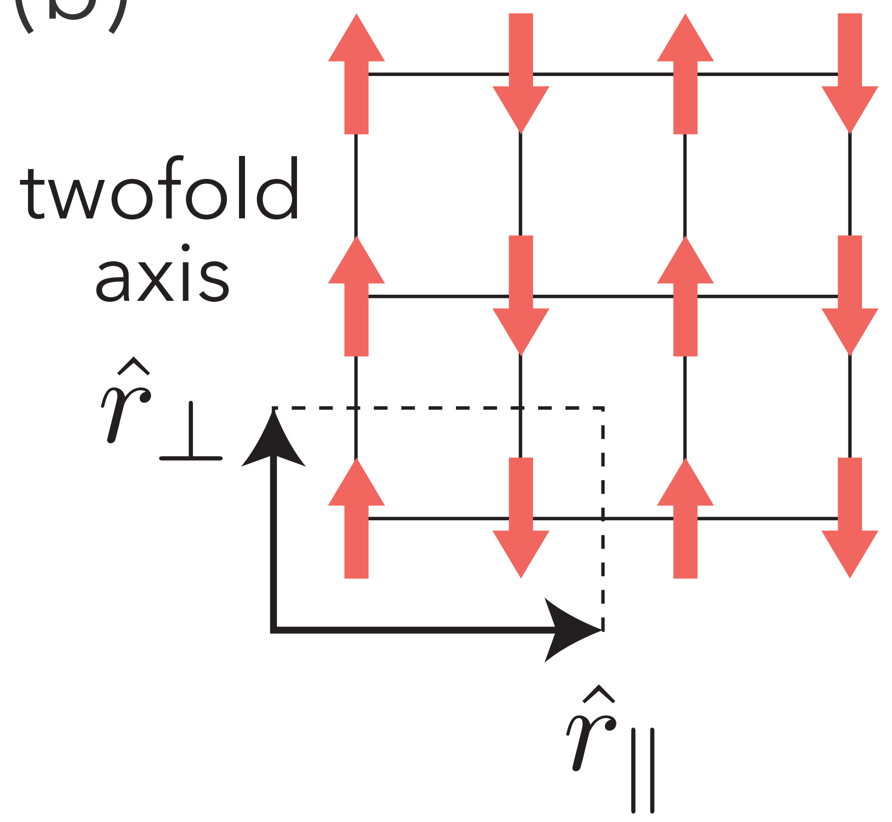
- Paramagnetic (PM) or Antiferromagnetic (AFM)

  $M = G + \tilde{\theta} G$

- Anti-unitary operator:

$$\tilde{\theta} = \begin{cases} \{\theta|\mathbf{0}\} & \text{(a) PM} \\ \{\theta|\boldsymbol{\tau}_{\parallel}\} & \text{(b) AFM 1} \\ \{\theta|\boldsymbol{\tau}_{\perp}\} & \text{(c) AFM 2} \\ \{\theta|\boldsymbol{\tau}_{\parallel} + \boldsymbol{\tau}_{\perp}\} & \text{(d) AFM 3} \end{cases}$$

(b)



Classification results by IRs of C_{2h}

$$G = \begin{cases} \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\mathbf{0}\}T + \{\sigma_\perp|\mathbf{0}\}T & \text{(i)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel\}T & \text{(ii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\perp\}T & \text{(iii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T & \text{(iv)} \end{cases}$$

$$\tilde{\theta} = \begin{cases} \{\theta|\mathbf{0}\} & \text{(a)} \\ \{\theta|\boldsymbol{\tau}_\parallel\} & \text{(b)} \\ \{\theta|\boldsymbol{\tau}_\perp\} & \text{(c)} \\ \{\theta|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\} & \text{(d)} \end{cases}$$

	G	$\tilde{\theta}$	BP $(k_\perp = 0)$	ZF $(k_\perp = \pi)$	
FM	(i), (ii)	-	A_u	A_u	
	(iii), (iv)	-		B_u	← UCoGe [1]
PM AFM	(i), (ii)	(a), (b)	$A_g + 2A_u + B_u$	$A_g + 2A_u + B_u$	
	(i), (ii)	(c), (d)		$B_g + 3A_u$	← Sr_2IrO_4
	(iii), (iv)	(a), (b)		$A_g + 3B_u$	← UPt_3 [2]
	(iii), (iv)	(c), (d)		$B_g + A_u + 2B_u$	← UPd_2Al_3 [1], Sr_2IrO_4

[1] T. Nomoto & H. Ikeda (2017) / [2] T. Micklitz & M. R. Norman (2009)

Non-primitive translation ⊥ mirror (glide) plane
→ **Nonsymmorphic line node (gap opening) !**

T. Micklitz & M. R. Norman (2017)

Application to centrosymmetric space groups

$$G = \begin{cases} \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\mathbf{0}\}T + \{\sigma_\perp|\mathbf{0}\}T & \text{(i)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel\}T & \text{(ii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\perp\}T & \text{(iii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T & \text{(iv)} \end{cases}$$

Monoclinic

No.	SG	$\perp = y$
10	$P2/m$	(i)
11	$P2_1/m$	(iii)
13	$P2/c$	(ii)
14	$P2_1/c$	(iv)

UPd_2Al_3 (No. 11)

UCoGe (No. 14)

Orthorhombic

No.	SG	$\perp = x$	$\perp = y$	$\perp = z$
47	$Pmmm$	(i)	(i)	(i)
48	$Pnnn$	(ii)	(ii)	(ii)
49	$Pccm$	(ii)	(ii)	(i)
50	$Pban$	(ii)	(ii)	(ii)
51	$Pmma$	(iii)	(i)	(ii)
52	$Pnna$	(ii)	(iv)	(ii)
53	$Pmna$	(i)	(ii)	(iv)
54	$Pcca$	(iv)	(ii)	(ii)
55	$Pbam$	(iv)	(iv)	(i)
56	$Pccn$	(iv)	(iv)	(ii)
57	$Pbcm$	(ii)	(iv)	(iii)
58	$Pnnm$	(iv)	(iv)	(i)
59	$Pmmn$	(iii)	(iii)	(ii)
60	$Pbcn$	(iv)	(ii)	(iv)
61	$Pbca$	(iv)	(iv)	(iv)
62	$Pnma$	(iv)	(iii)	(iv)
63	$Cmcm$	-	-	(iii)
64	$Cmca$	-	-	(iv)
65	$Cmmm$	-	-	(i)
66	$Cccm$	-	-	(i)
67	$Cmma$	-	-	(ii)
68	$Ccca$	-	-	(ii)

Sr_2IrO_4 (This talk) (No. 54)

Tetragonal

No.	SG	$\perp = z$	$\perp = x, y$
83	$P4/m$	(i)	-
84	$P4_2/m$	(i)	-
85	$P4/n$	(ii)	-
86	$P4_2/n$	(ii)	-
123	$P4/mmm$	(i)	(i)
124	$P4/mcc$	(i)	(ii)
125	$P4/nbm$	(ii)	(ii)
126	$P4/nnc$	(ii)	(ii)
127	$P4/mbm$	(i)	(iv)
128	$P4/mnc$	(i)	(iv)
129	$P4/nmm$	(ii)	(iii)
130	$P4/ncc$	(ii)	(iv)
131	$P4_2/mmc$	(i)	(i)
132	$P4_2/mcm$	(i)	(ii)
133	$P4_2/nbc$	(ii)	(ii)
134	$P4_2/nnm$	(ii)	(ii)
135	$P4_2/mbc$	(i)	(iv)
136	$P4_2/mnm$	(i)	(iv)
137	$P4_2/nmc$	(ii)	(iii)
138	$P4_2/ncm$	(ii)	(iv)

Cubic

No.	SG	$\perp = x, y, z$
200	$Pm\bar{3}$	(i)
201	$Pn\bar{3}$	(ii)
205	$Pa\bar{3}$	(iv)
221	$Pm\bar{3}m$	(i)
222	$Pn\bar{3}n$	(ii)
223	$Pm\bar{3}n$	(i)
224	$Pn\bar{3}m$	(ii)

Hexagonal

No.	SG	$\perp = z$	$\perp = [1\!-\!10], [120], [210]$
175	$P6/m$	(i)	-
176	$P6_3/m$	(iii)	-
191	$P6/mmm$	(i)	(i)
192	$P6/mcc$	(i)	(ii)
193	$P6_3/mcm$	(iii)	(i)
194	$P6_3/mmc$	(iii)	(ii)

UPt_3 (No. 194)

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What is Sr_2IrO_4 ?

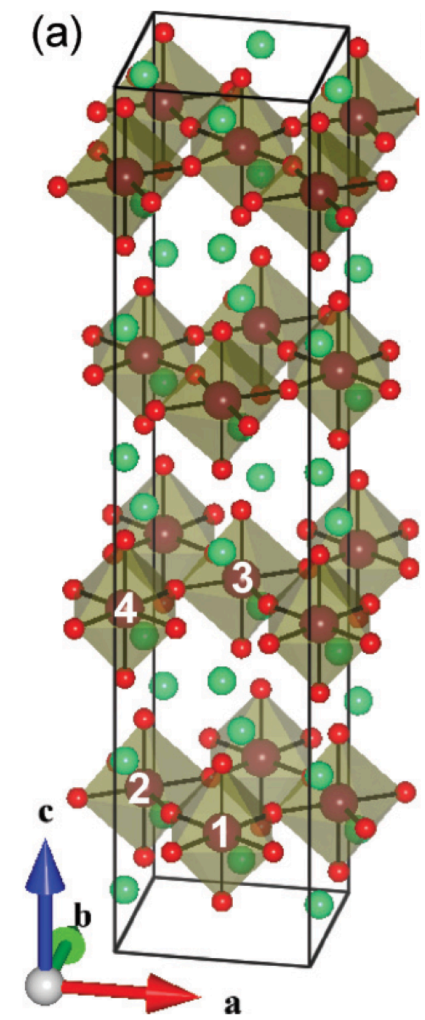
- A layered perovskite insulator
- **Nonsymmorphic** lattice: $I4_1/acd$ or $I4_1/a$
- Locally parity violation on Ir sites

  → **Sublattice-dependent ASOC**
- Many similarities to high-T_c cuprate
  - Pseudogap & *d*-wave gap under doping

    Y. K. Kim *et al.* (2014, 2016) / Y. J. Yan *et al.* (2015)
  - Theory of *d*-wave superconductivity

    H. Watanabe *et al.* (2013)

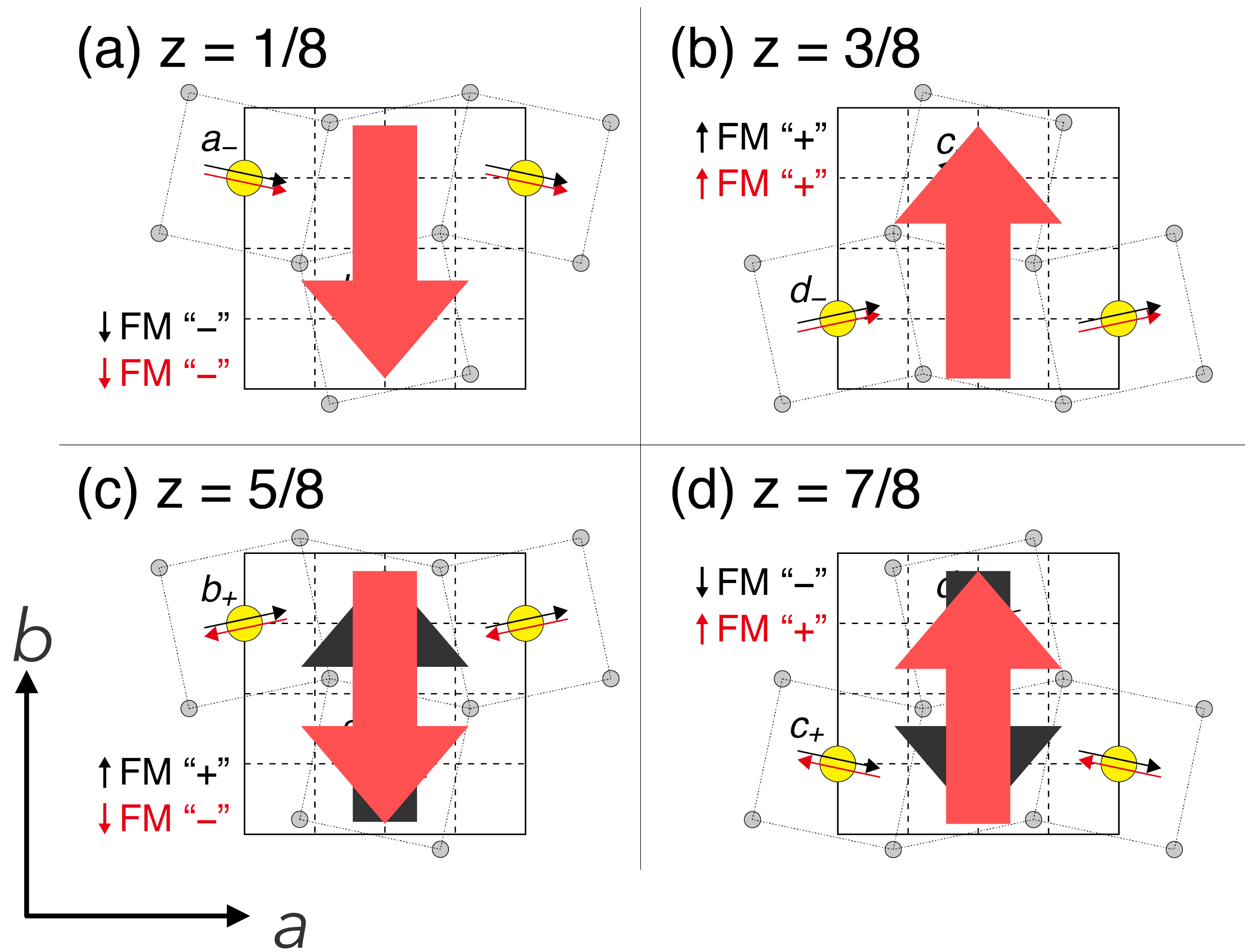
    → Expectation for (high-T_c) **superconductivity** !
  - J_{eff} = 1/2 antiferromagnet



F. Ye *et al.* (2013)

Magnetic structures on Ir site

- Canted moments: AFM along *a* axis & FM along *b* axis



SS, T. Nomoto, & Y. Yanase
PRL **119**, 027001 (2017)

−++− pattern
B. J. Kim *et al.* (2009)

Symmetry analysis
- B_{1g} representation of D_{4h}
- Even-parity **magnetic octupole**

Unusual gap structures

−+−+ pattern
L. Zhao *et al.* (2016)

Symmetry analysis
- E_u representation of D_{4h}
- Odd-parity **magnetic quadrupole**

FFLO superconductivity

Gap classification (1)

- Magnetic space group in −++− state ($P_I cca$)

$$M_{-++-} = G_{-++-} + \{\theta|\boldsymbol{\tau}_x + \boldsymbol{\tau}_y + \boldsymbol{\tau}_z\}G_{-++-},$$

$$G_{-++-} = \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2z}|\boldsymbol{\tau}_x + \boldsymbol{\tau}_z\}T + \{\sigma_z|\boldsymbol{\tau}_x + \boldsymbol{\tau}_z\}T$$
$$+ \{C_{2x}|\boldsymbol{\tau}_z\}T + \{\sigma_x|\boldsymbol{\tau}_z\}T + \{C_{2y}|\boldsymbol{\tau}_x\}T + \{\sigma_y|\boldsymbol{\tau}_x\}T$$

- Comparison with general classification
  - $k_z = 0,\ \pi/c$: (iv) Screw + Glide, (d) AFM 3
  - $k_{x,y} = 0,\ \pi/a$: (ii) Rotation + Glide, (d) AFM 3

$$G = \begin{cases} \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\mathbf{0}\}T + \{\sigma_\perp|\mathbf{0}\}T & \text{(i)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel\}T & \text{(ii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\perp\}T & \text{(iii)} \\ \{E|\mathbf{0}\}T + \{I|\mathbf{0}\}T + \{C_{2\perp}|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T + \{\sigma_\perp|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\}T & \text{(iv)} \end{cases}$$

$$\tilde{\theta} = \begin{cases} \{\theta|\mathbf{0}\} & \text{(a)} \\ \{\theta|\boldsymbol{\tau}_\parallel\} & \text{(b)} \\ \{\theta|\boldsymbol{\tau}_\perp\} & \text{(c)} \\ \{\theta|\boldsymbol{\tau}_\parallel + \boldsymbol{\tau}_\perp\} & \text{(d)} \end{cases}$$

Gap classification (2)

- Representations decomposed by IRs of C_{2h}

G	$\tilde{\theta}$	BP $(k_\perp = 0)$	ZF $(k_\perp = \pi)$	
(i), (ii)	-	A_u	A_u	
(iii), (iv)	-		B_u	
(i), (ii)	(a), (b)	$A_g + 2A_u + B_u$	$A_g + 2A_u + B_u$	
(i), (ii)	(c), (d)		$B_g + 3A_u$	$\leftarrow k_{x,y} = 0,\ \pi/a$
(iii), (iv)	(a), (b)		$A_g + 3B_u$	
(iii), (iv)	(c), (d)		$B_g + A_u + 2B_u$	$\leftarrow k_z = 0,\ \pi/c$

- Induction to D_{4h} space

$k_z = 0,\ \pi/c$

$$\begin{cases} A_{1g} + A_{2g} + B_{1g} + B_{2g} + 2A_{1u} \\ \quad + 2A_{2u} + 2B_{1u} + 2B_{2u} + 2E_u & \text{BP} \\ 2E_g + A_{1u} + A_{2u} + B_{1u} + B_{2u} + 4E_u & \text{ZF} \end{cases}$$

$k_{x,y} = 0,\ \pi/a$

$$\begin{cases} A_{1g} + B_{1g} + E_g + 2A_{1u} \\ \quad + A_{2u} + 2B_{1u} + B_{2u} + 3E_u & \text{BP} \\ A_{2g} + B_{2g} + E_g + 3A_{1u} + 3B_{1u} + 3E_u & \text{ZF} \end{cases}$$

Gap classification (3)

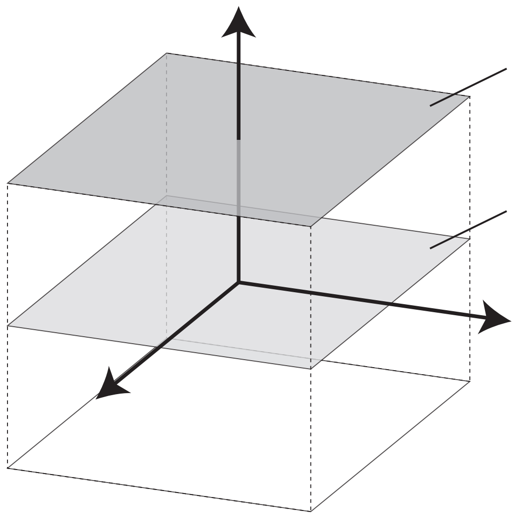
- $k_z = 0,\ \pi/c$: horizontal

s-wave, d-wave

$$\begin{cases} A_{1g} + A_{2g} + B_{1g} + B_{2g} + 2A_{1u} \\ \quad + 2A_{2u} + 2B_{1u} + 2B_{2u} + 2E_u & \text{BP} \\ 2E_g + A_{1u} + A_{2u} + B_{1u} + B_{2u} + 4E_u & \text{ZF} \end{cases}$$

- $k_{x,y} = 0,\ \pi/a$: vertical

$$\begin{cases} A_{1g} + B_{1g} + E_g + 2A_{1u} \\ \quad + A_{2u} + 2B_{1u} + B_{2u} + 3E_u & \text{BP} \\ A_{2g} + B_{2g} + E_g + 3A_{1u} + 3B_{1u} + 3E_u & \text{ZF} \end{cases}$$



Nontrivial gap structures !

	$k_z = 0$	$k_z = \pi/c$	$k_{x,y} = 0$	$k_{x,y} = \pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap

Numerical calculation

- Gap structure obtained by group theory

	$k_z=0$	$k_z=\pi/c$	$k_{x,y}=0$	$k_{x,y}=\pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap

Demonstration
by numerical calculation

Effective J_{eff} = 1/2 model

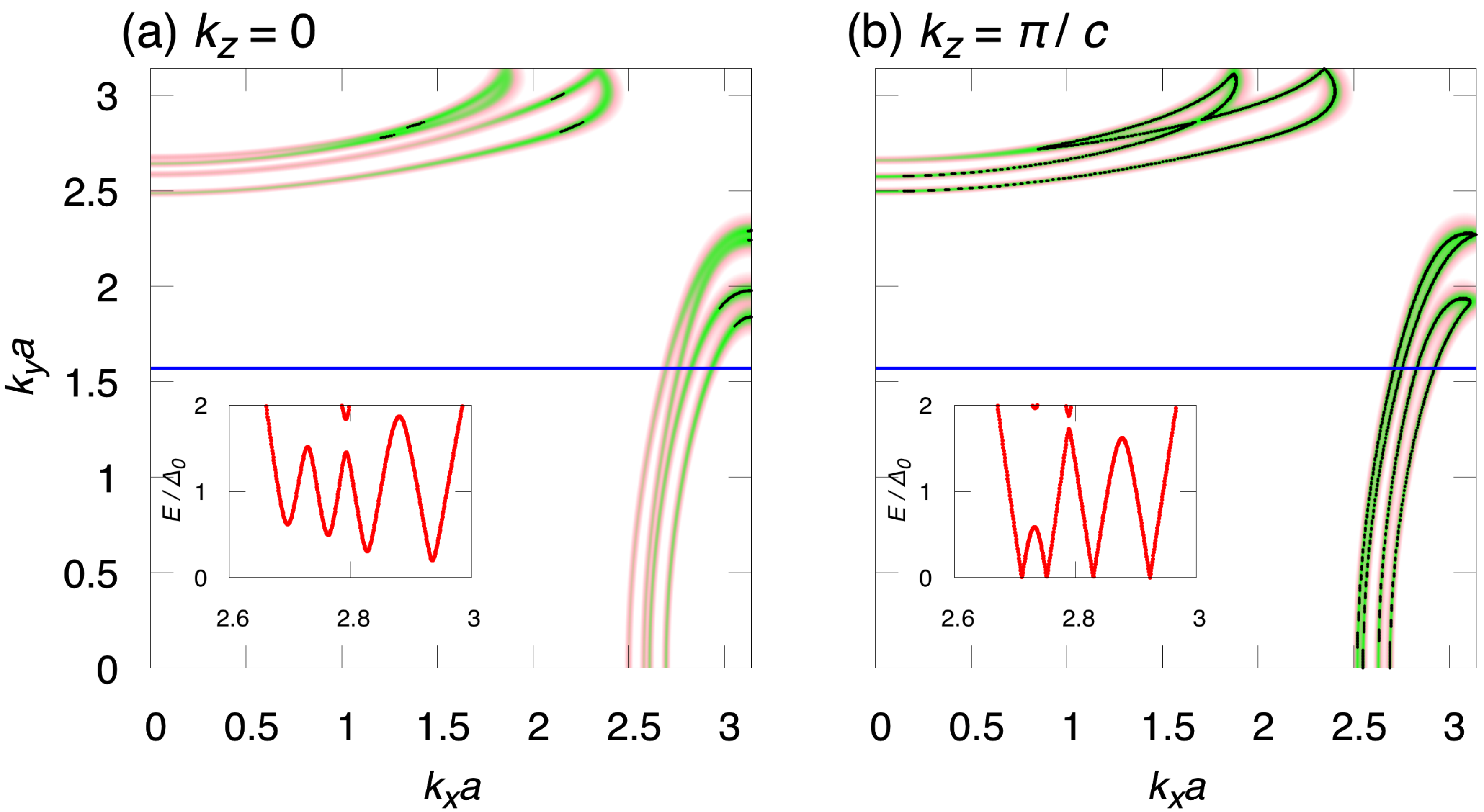
- 3D single-orbital tight-binding model
- 8 Ir atoms / unit cell & 3 types of ASOC
- Mean-field theory: $\hat{\Delta}^{(s)}(\boldsymbol{k})=\Delta_0 i\hat{\sigma}_y^{(\mathrm{spin})}\otimes\hat{1}_2$

$$\hat{\Delta}^{(d)}(\boldsymbol{k})=\Delta_0\sin\frac{k_x a}{2}\sin\frac{k_y a}{2}i\hat{\sigma}_y^{(\mathrm{spin})}\hat{\sigma}_x^{(\mathrm{sl})}\otimes\hat{1}_2$$

Numerical results (*s*-wave & horizontal plane)

- Calculation using effective J_{eff} = 1/2 model

	$k_z = 0$	$k_z = \pi/c$	$k_{x,y} = 0$	$k_{x,y} = \pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap

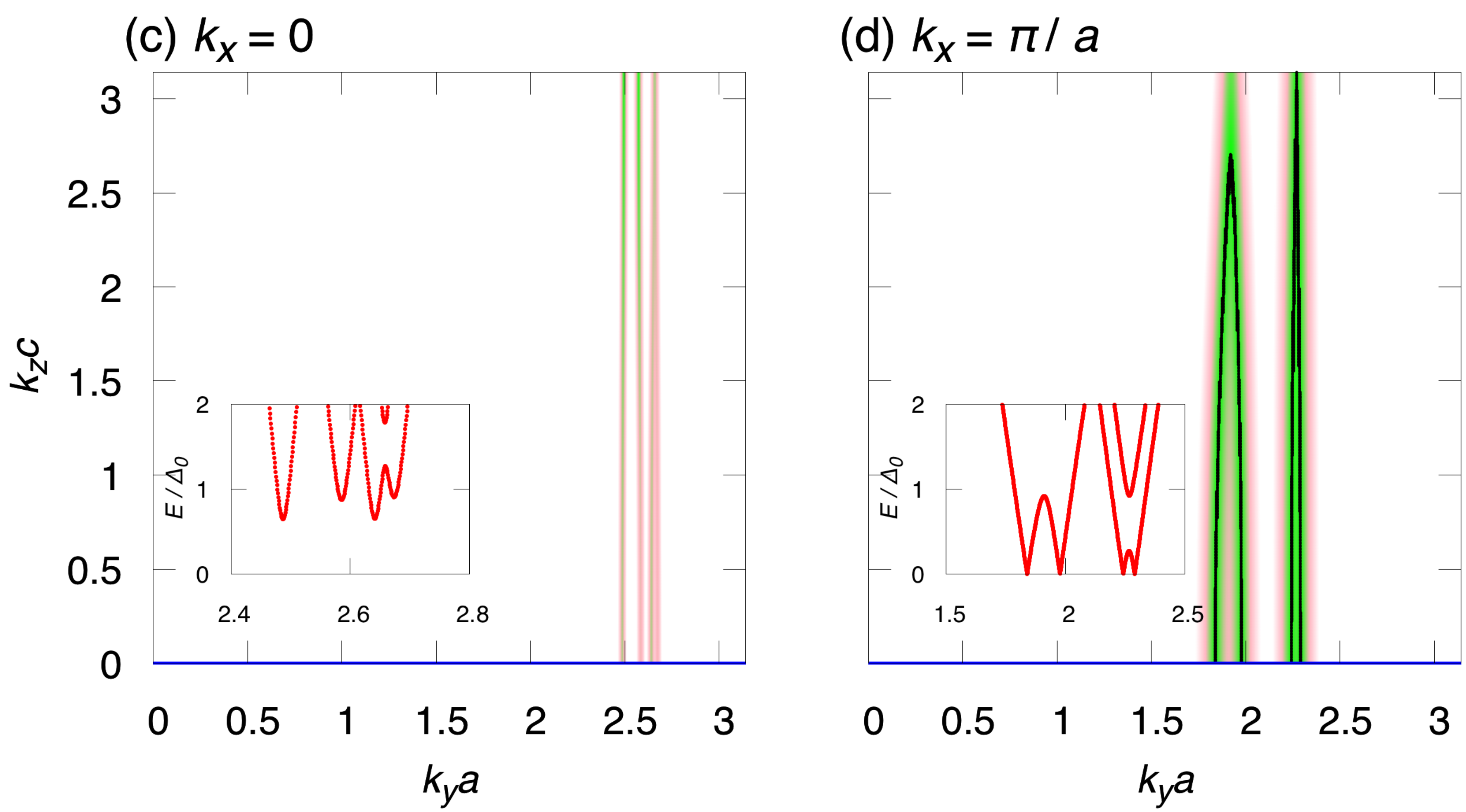


Nontrivial **line nodes** protected by **nonsymmophic symmetry !**

Numerical results (*s*-wave & vertical plane)

- Calculation using effective J_{eff} = 1/2 model

	$k_z = 0$	$k_z = \pi/c$	$k_{x,y} = 0$	$k_{x,y} = \pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap

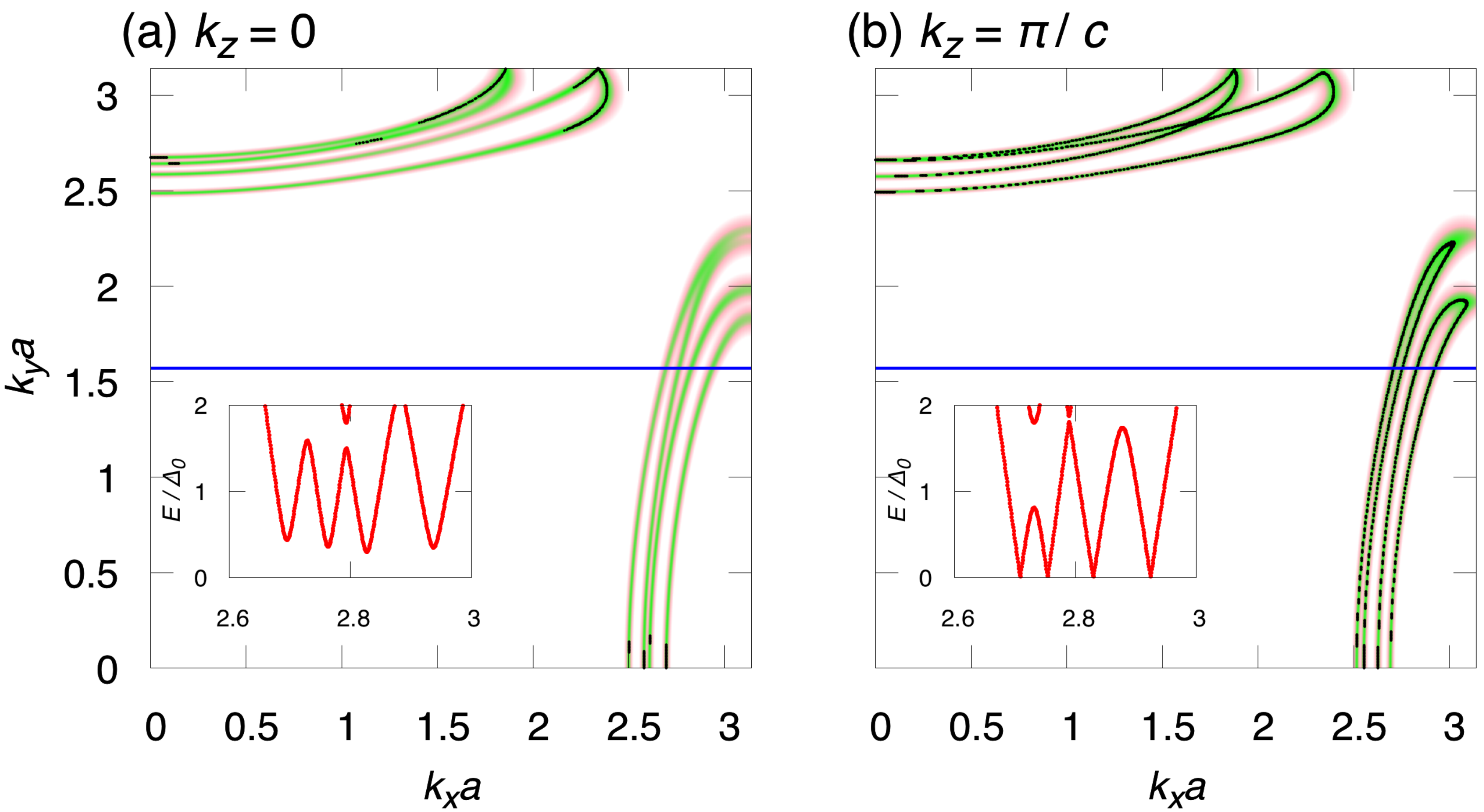


Nontrivial **line nodes** protected by **nonsymmophic symmetry !**

Numerical results (*d*-wave & horizontal plane)

- Calculation using effective J_{eff} = 1/2 model

	$k_z = 0$	$k_z = \pi/c$	$k_{x,y} = 0$	$k_{x,y} = \pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap

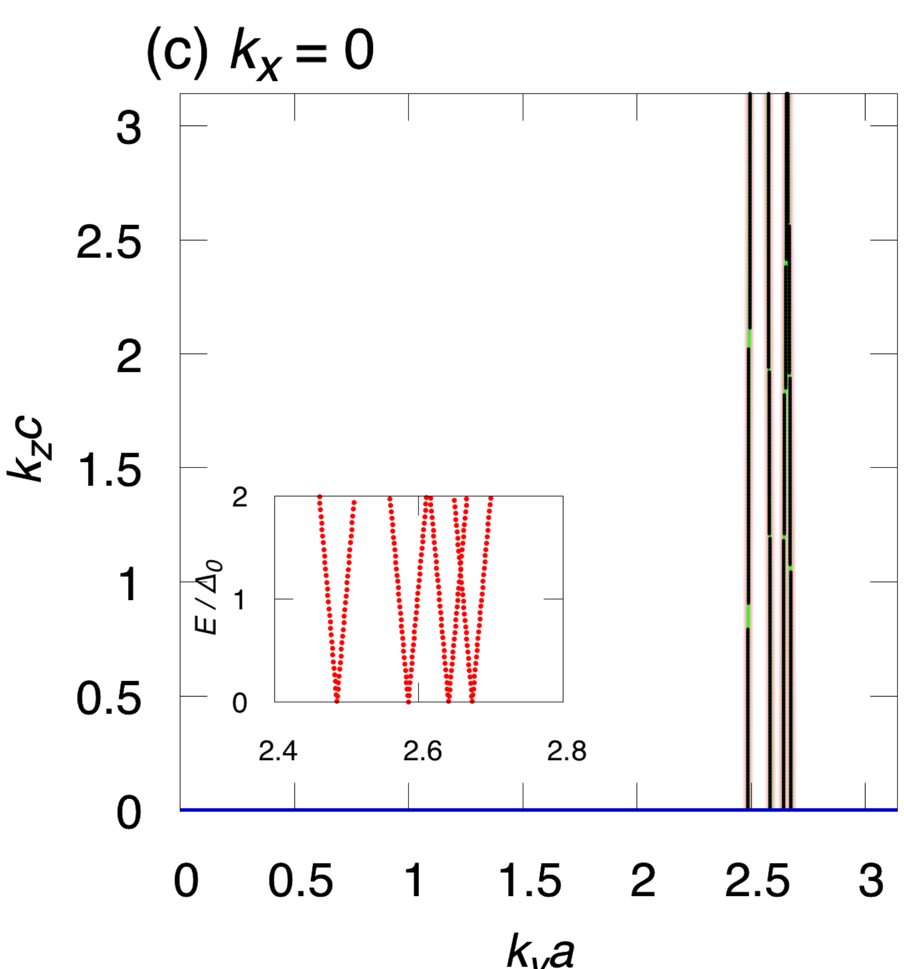


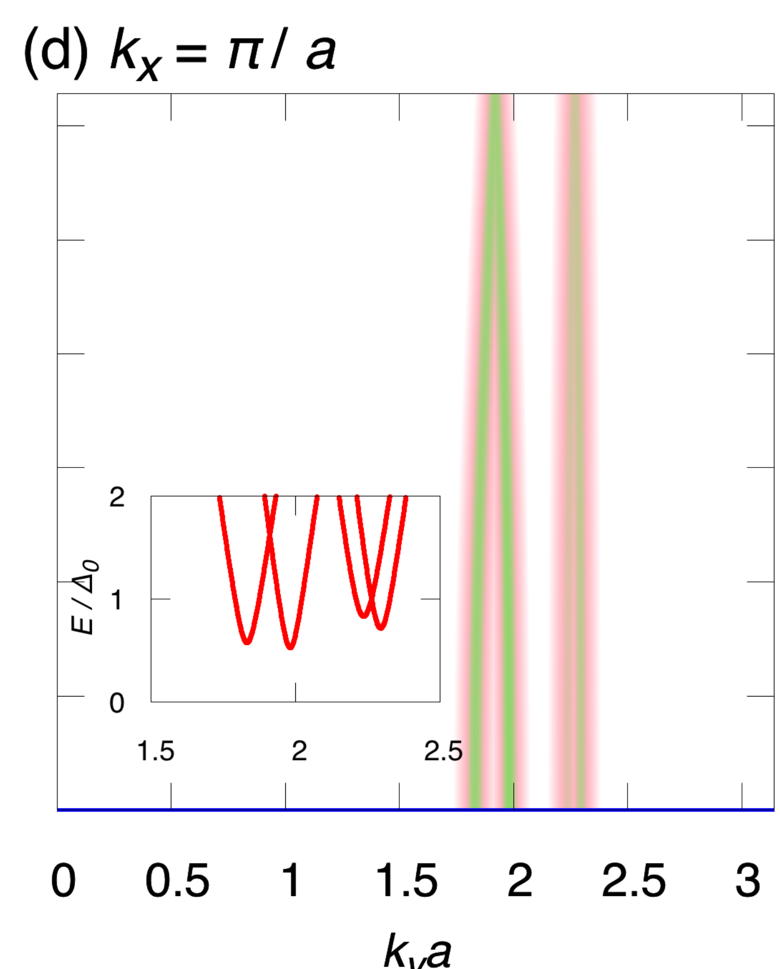
Nontrivial **line nodes** protected by **nonsymmophic symmetry !**

Numerical results (*d*-wave & vertical plane)

- Calculation using effective $J_{\text{eff}} = 1/2$ model

	$k_z = 0$	$k_z = \pi/c$	$k_{x,y} = 0$	$k_{x,y} = \pi/a$
A_{1g} (s-wave)	gap	node	gap	node
B_{2g} (d-wave)	gap	node	node	gap





Nontrivial **gap opening** protected by **nonsymmophic symmetry !**

Usual *d*-wave OP: vanishes on **ZF** and BP

Outline

1. Introduction
2. Method: Superconducting gap classification based on space group symmetry
3. Result 1: Condition for nonsymmorphic line nodes
   (a) Complete classification
   (b) Application: Sr_2IrO_4
4. **Result 2: j_z-dependent point nodes in UPt_3**
5. Conclusion

Symmetry-protected point nodes

- Previous subject: Complete classification of line nodes

  Gap classification on high-symmetry **plane**

- This subject: unusual "j_z-dependent" point nodes

  Gap classification on high-symmetry **line**

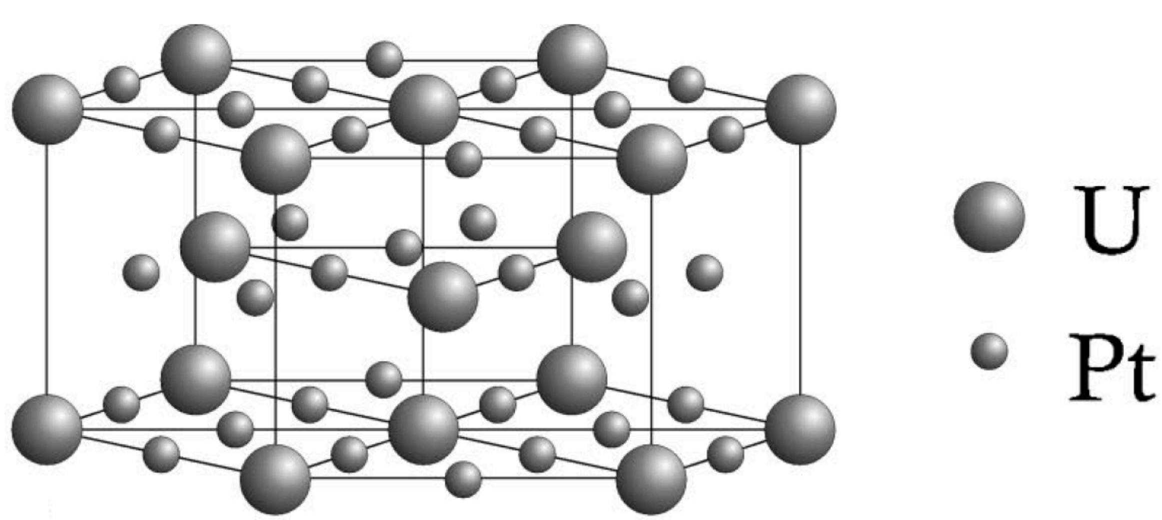
Consider ***n*-fold axis** in BZ (n = 2, 3, 4, 6)

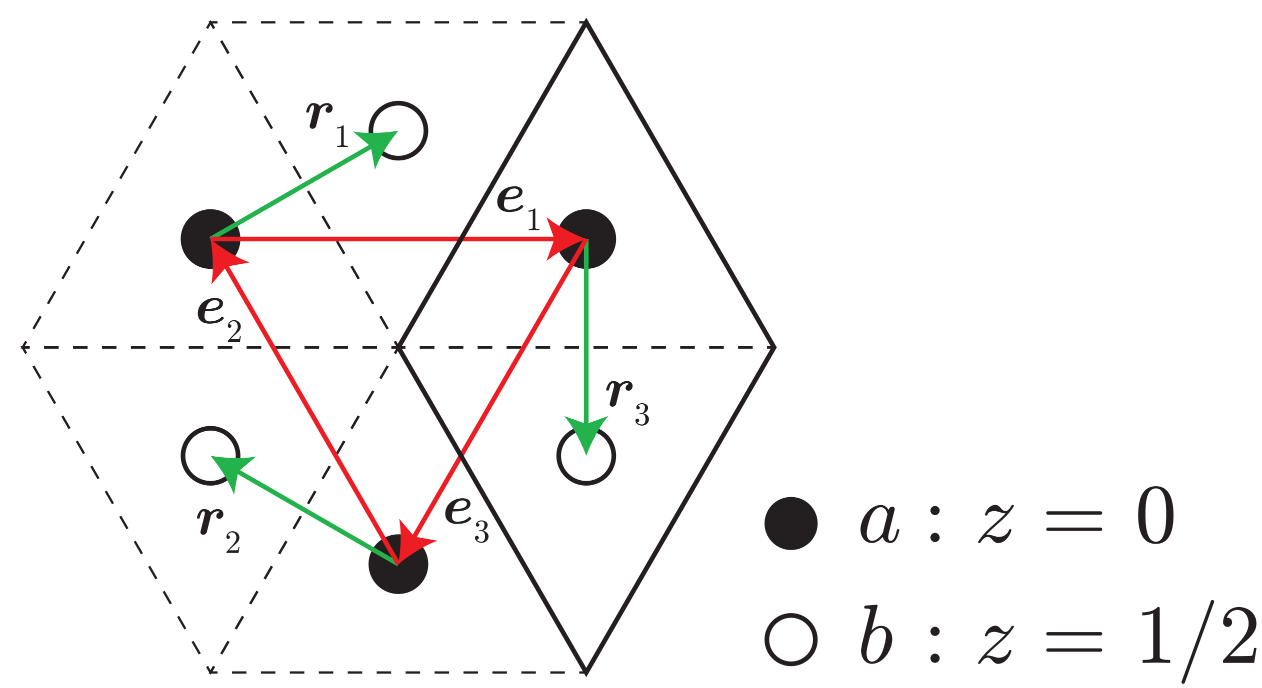
A example of unconventional result: 3-fold line of UPt_3

Crystal symmetry of UPt_3

- Point group: D_{6h} → Globally centrosymmetric
- Site symmetry: D_{3h} → Local parity violation

  → **Sublattice-dependent ASOC** (Zeeman-type)





Two uranium sublattices (*a* & *b*)

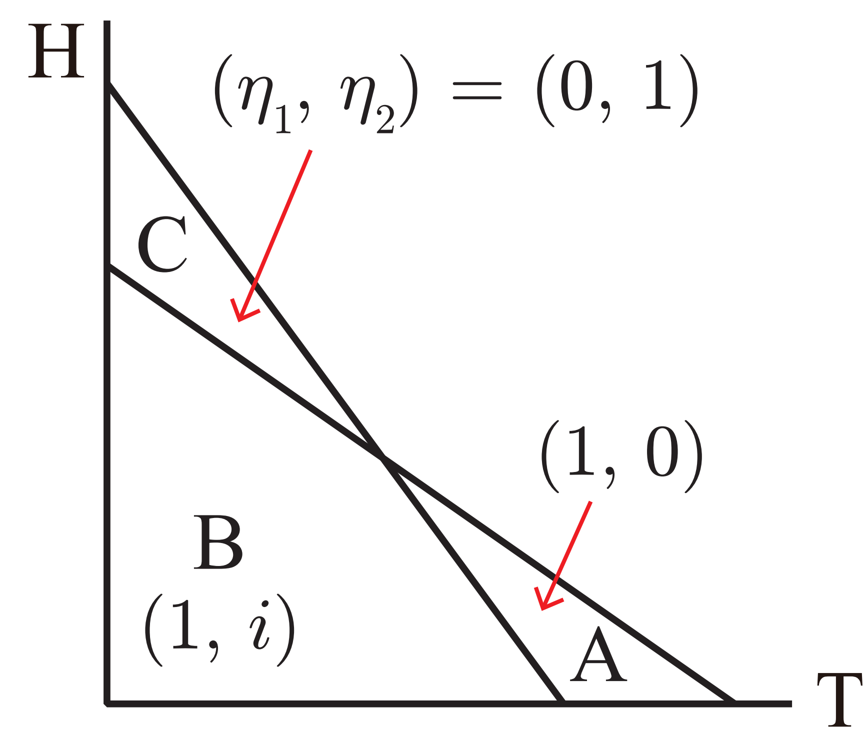
Symmetry of superconductivity in UPt_3

- Multiple SC phases — R. A. Fisher *et al.* (1989), S. Adenwalla *et al.* (1990)

  → Multi-component E_{2u} **order parameter**:

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

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



- Consistency with experiments:
  - Phase diagram
  - Broken TRS in B phase
  - Hybrid gap structure
  - Weak in-plane anisotropy in $H_{c2}(\theta)$
  - Suppression in $H_{c2} \parallel c$

Fermi surfaces of UPt_3

- First-principle study
  → *Γ*-FSs, *A*-FSs, & *K*-FSs
- *K*-FSs: NOT sufficiently studied
  (cf. Weyl nodes on *Γ*- & *A*-FSs based on E_{2u})

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Nonsymmorphic Weyl superconductivity in UPt_3 based on E_{2u} representation

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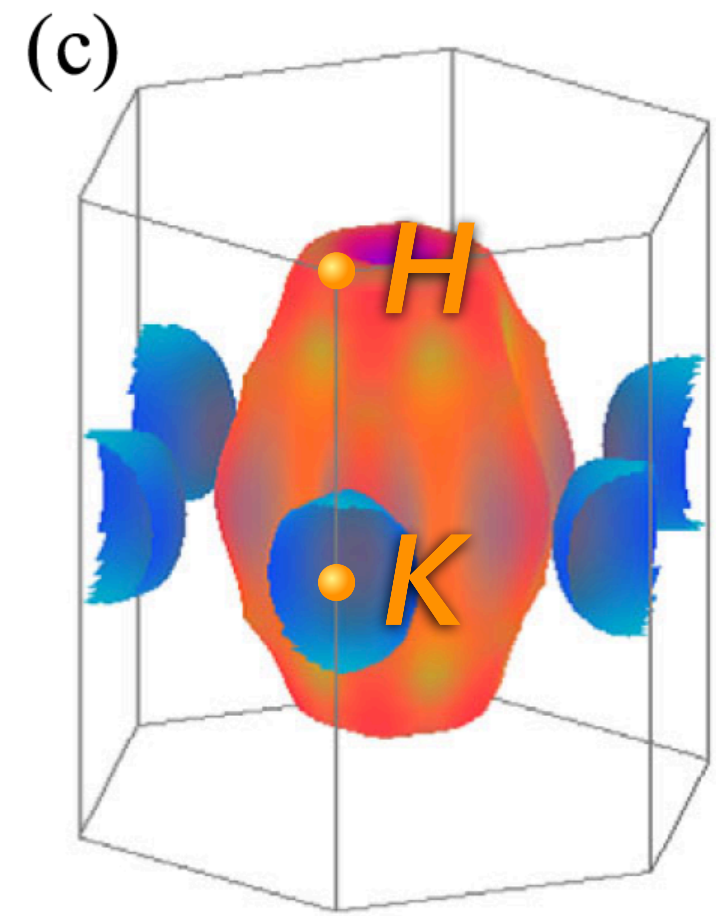


T. Nomoto & H. Ikeda (2016)

- *K*-*H* line: **3-fold rotation** symmetry

Investigate **superconducting gap structure** on the ***K*-*H*** line of UPt_3 !

Gap classification on *K-H* line

- Little group on *K-H* line: $\mathcal{M}^{\boldsymbol{k}}/T \simeq C_{3v} + \{\theta I|\mathbf{0}\}C_{3v}$
- Gap classification

Bloch state

$$\chi[\gamma^{\boldsymbol{k}}(m)]$$

C_{3v}	E	C_3	C_3^2	$3\sigma_v$
$E_{1/2}$	2	1	-1	0
$E_{3/2}$	2	-2	2	0

***j*$_z$ = ±1/2, ±3/2**

Cooper pair

$$\chi[P^{\boldsymbol{k}}(m)]$$

D_{3d}	E	C_3, C_3^2	$3C_2'$	I	IC_3, IC_3^2	$3\sigma_v$
$P_1^{\boldsymbol{k}}$	4	1	2	-2	1	0
$P_2^{\boldsymbol{k}}$	4	4	2	-2	-2	0

$$P_1^{\boldsymbol{k}} = A_{1g} + A_{1u} + E_u$$

$$P_2^{\boldsymbol{k}} = A_{1g} + 2A_{1u} + A_{2u}$$

Two nonequivalent representations of Cooper pair depending on Bloch-state **angular momentum *j*$_z$** !

Gap structure

- Order parameter: **E_{2u}** representation of D_{6h}

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

- Compatibility relations between D_{6h} and D_{3d}

(IR of D_{6h})	A_{1u}	A_{2u}	B_{1u}	B_{2u}	E_{1u}	E_{2u}
(IR of D_{6h})$\downarrow D_{3d}$	A_{1u}	A_{2u}	A_{2u}	A_{1u}	E_u	E_u

- Irreducible decomposition

$$P_1^{\boldsymbol{k}} = A_{1g} + A_{1u} + E_u$$ → Gap (normal: $E_{1/2}$)

$$P_2^{\boldsymbol{k}} = A_{1g} + 2A_{1u} + A_{2u}$$ → Point node (normal: $E_{3/2}$)

Next problem:

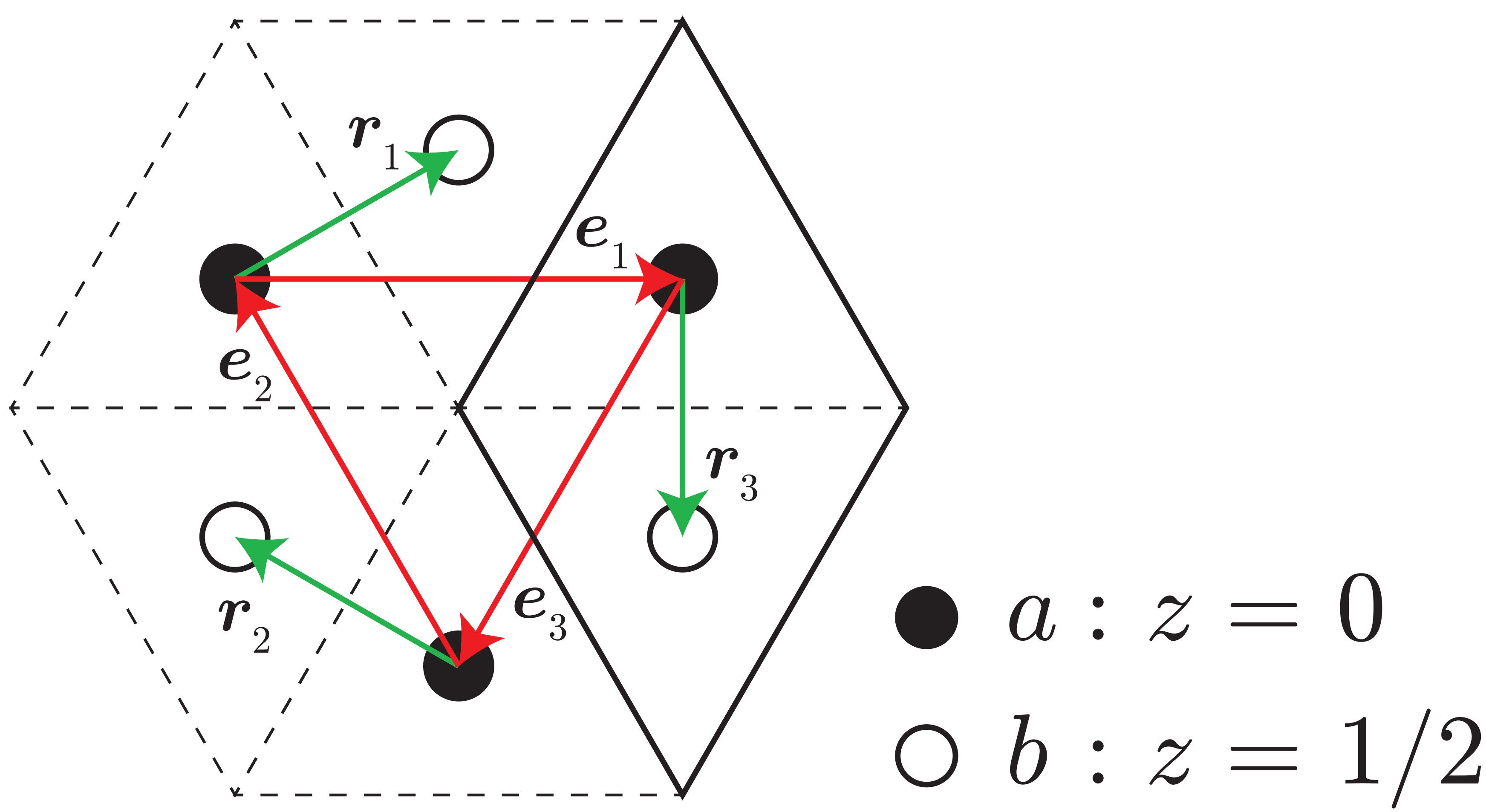
Which normal state is realized on *K-H* line ?

Effective model of UPt_3

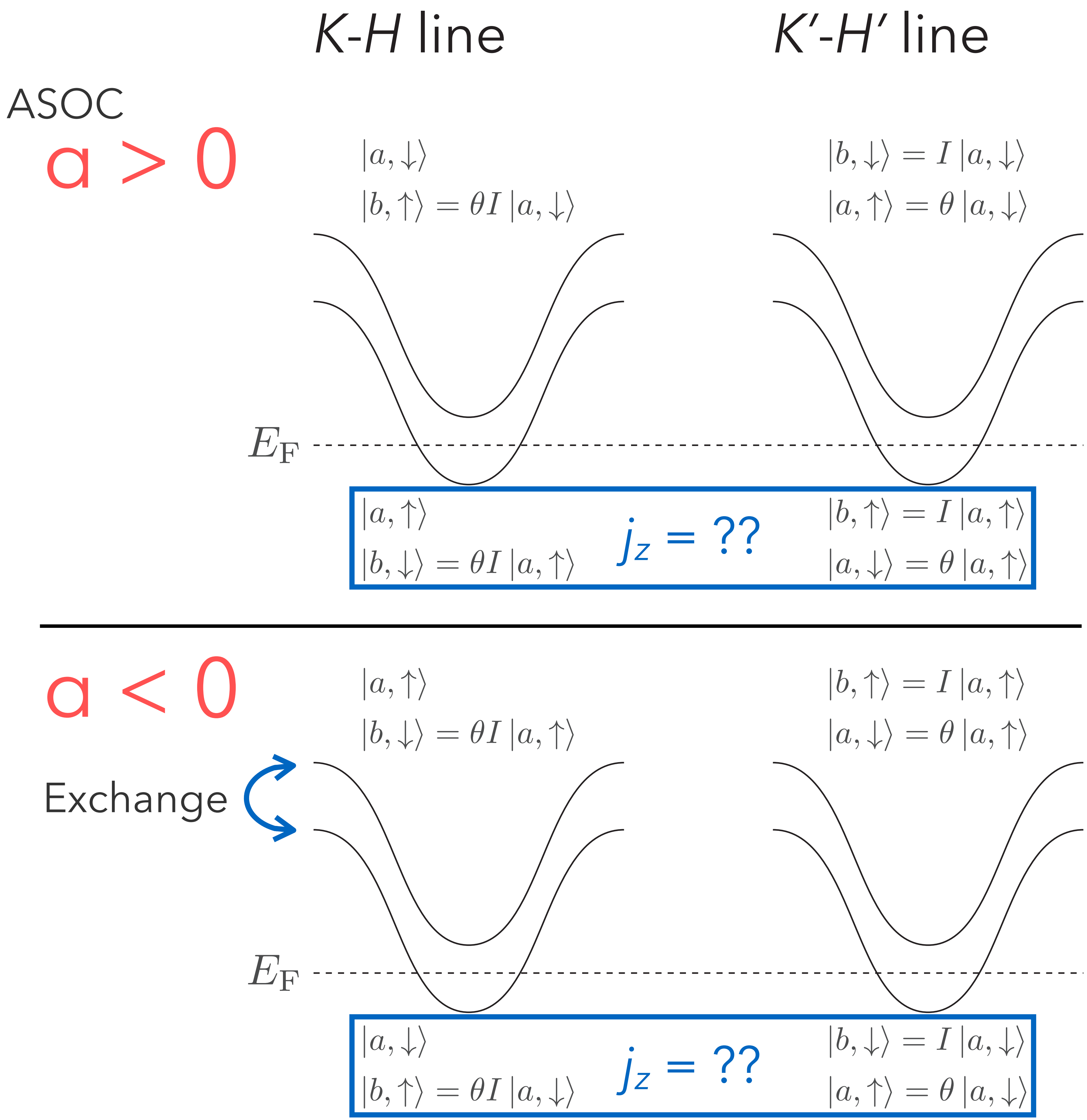
- 3D single-orbital tight-binding model by Yanase

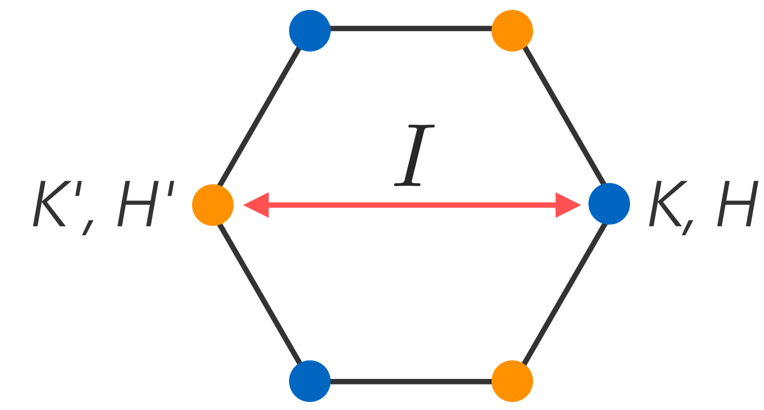
  Y. Yanase, PRB (2016, 2017)

  - Two uranium sublattices (*a* & *b*)
  - Zeeman-type ASOC



j_z-dependent gap structure





orbital spin **perm.**

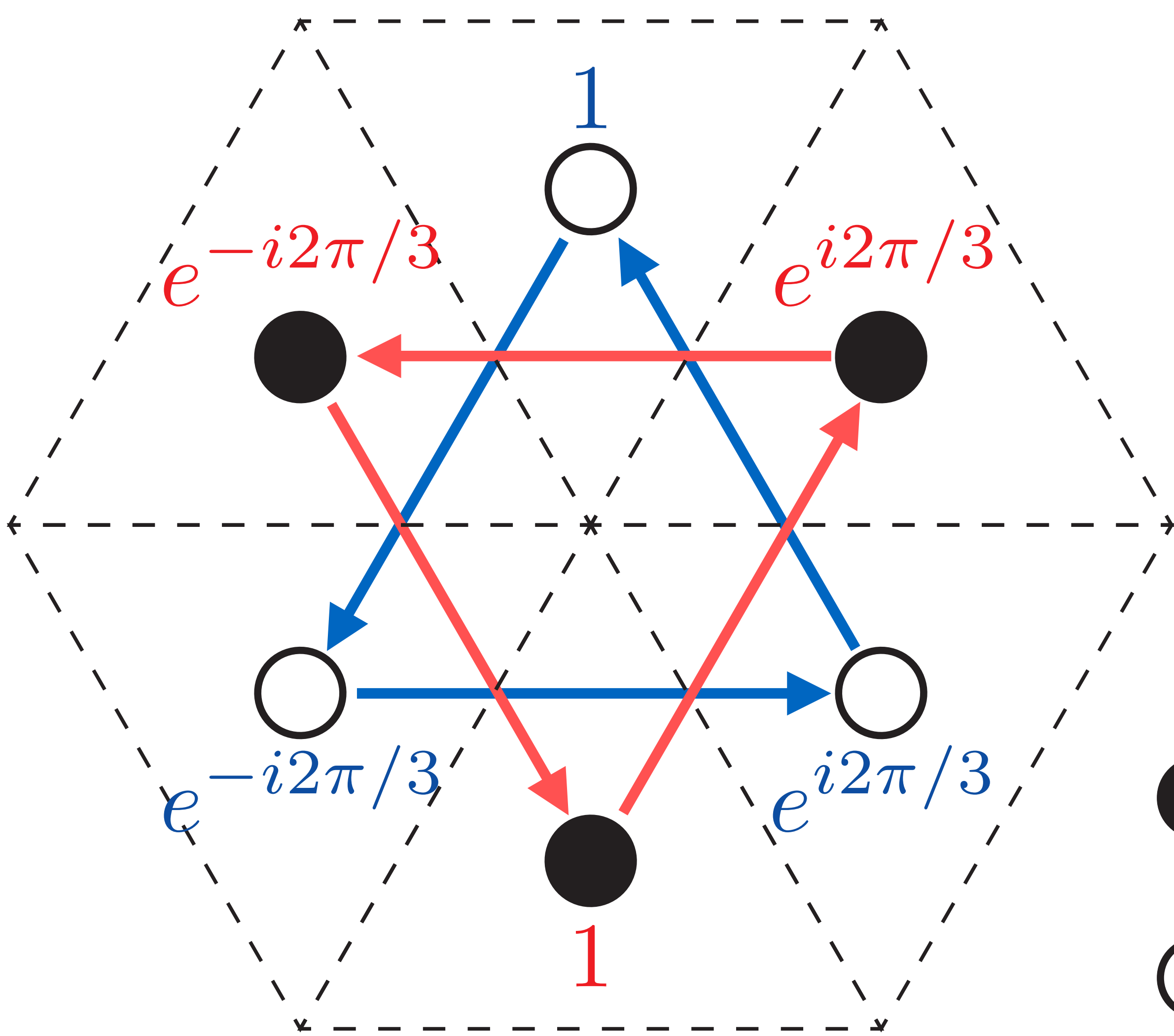
$$j_z = l_z + s_z + \lambda_z$$

$$= 0 \pm 1/2 + ??$$

Effective orbital angular momentum

- Bloch function on each site has a phase factor $e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
- Phase factor by 3-fold rotation at K point ...

Note) Opposite phase factor at $\underline{K'}$ point



Effective angular momentum by site permutation !

● a : $e^{+i2\pi/3} \rightarrow \lambda_z = +1$

○ b : $e^{-i2\pi/3} \rightarrow \lambda_z = -1$

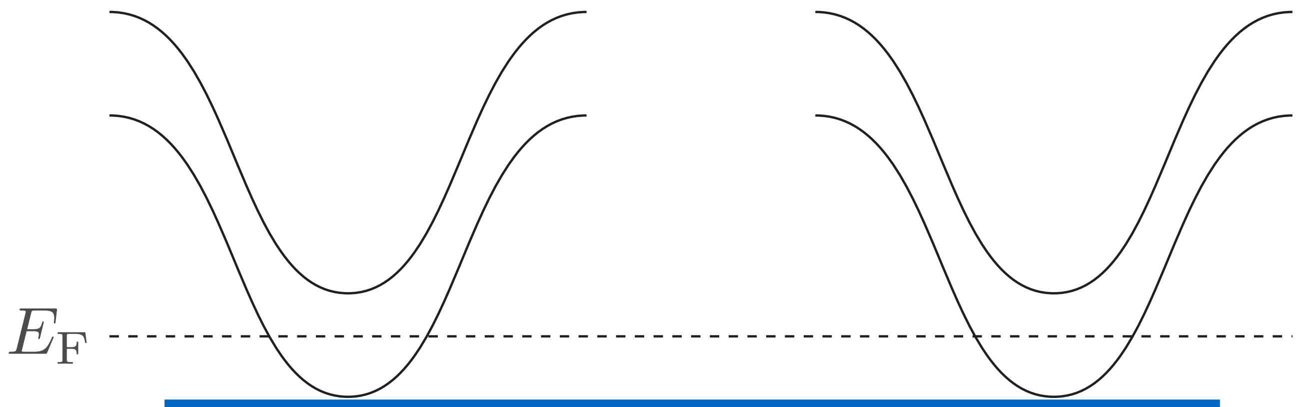
j_z-dependent gap structure

K-H line	K'-H' line
$(a:\lambda_z=+1,\ b:\lambda_z=-1)$	$(a:\lambda_z=-1,\ b:\lambda_z=+1)$

ASOC

$\alpha > 0$

K-H line	K'-H' line
$\lvert a,\downarrow\rangle$	$\lvert b,\downarrow\rangle = I\lvert a,\downarrow\rangle$
$\lvert b,\uparrow\rangle = \theta I\lvert a,\downarrow\rangle$	$\lvert a,\uparrow\rangle = \theta\lvert a,\downarrow\rangle$



K-H line		K'-H' line
$\lvert a,\uparrow\rangle$	$E_{3/2}$	$\lvert b,\uparrow\rangle = I\lvert a,\uparrow\rangle$
$\lvert b,\downarrow\rangle = \theta I\lvert a,\uparrow\rangle$		$\lvert a,\downarrow\rangle = \theta\lvert a,\uparrow\rangle$

orbital spin **perm.**

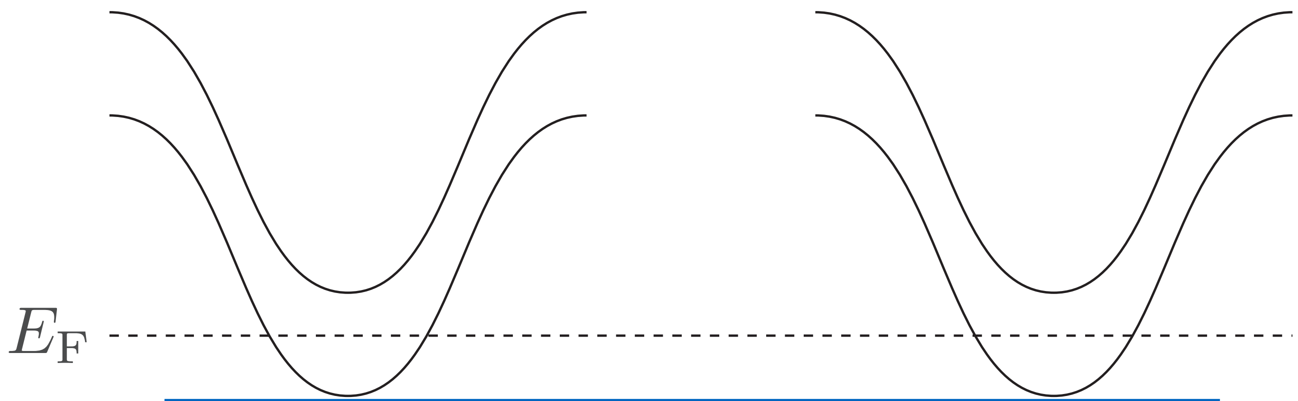
$$j_z = l_z + s_z + \lambda_z$$

$$= 0 \pm 1/2 \pm 1$$

→ **Point node**

$\alpha < 0$

K-H line	K'-H' line
$\lvert a,\uparrow\rangle$	$\lvert b,\uparrow\rangle = I\lvert a,\uparrow\rangle$
$\lvert b,\downarrow\rangle = \theta I\lvert a,\uparrow\rangle$	$\lvert a,\downarrow\rangle = \theta\lvert a,\uparrow\rangle$



K-H line		K'-H' line
$\lvert a,\downarrow\rangle$	$E_{1/2}$	$\lvert b,\downarrow\rangle = I\lvert a,\downarrow\rangle$
$\lvert b,\uparrow\rangle = \theta I\lvert a,\downarrow\rangle$		$\lvert a,\uparrow\rangle = \theta\lvert a,\downarrow\rangle$

$$j_z = 0 \pm 1/2 \mp 1$$

→ **Gap**

Numerical results

- E_{2u} order parameter by Yanase Y. Yanase, PRB (2016, 2017)

Intra-sublattice *p*-wave

Inter-sublattice *d*+*f*-wave

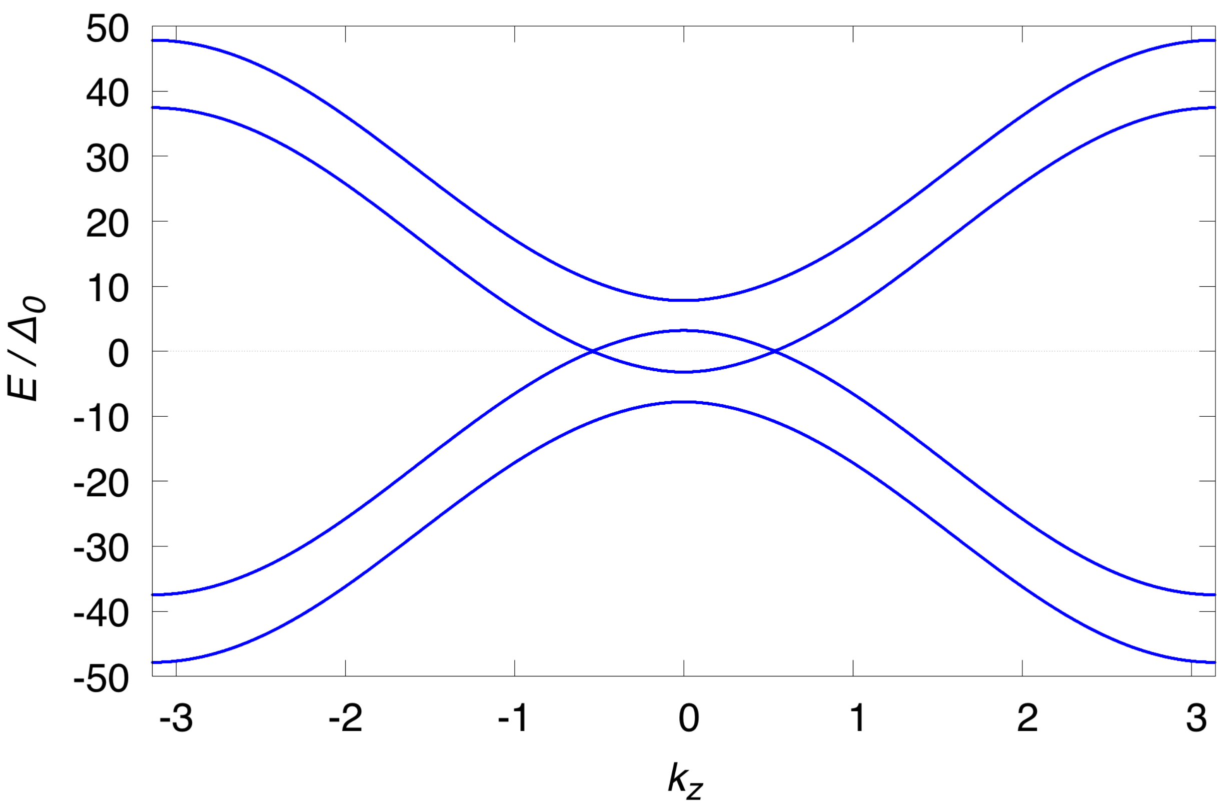
\+ **Inter-sublattice *p*-wave**

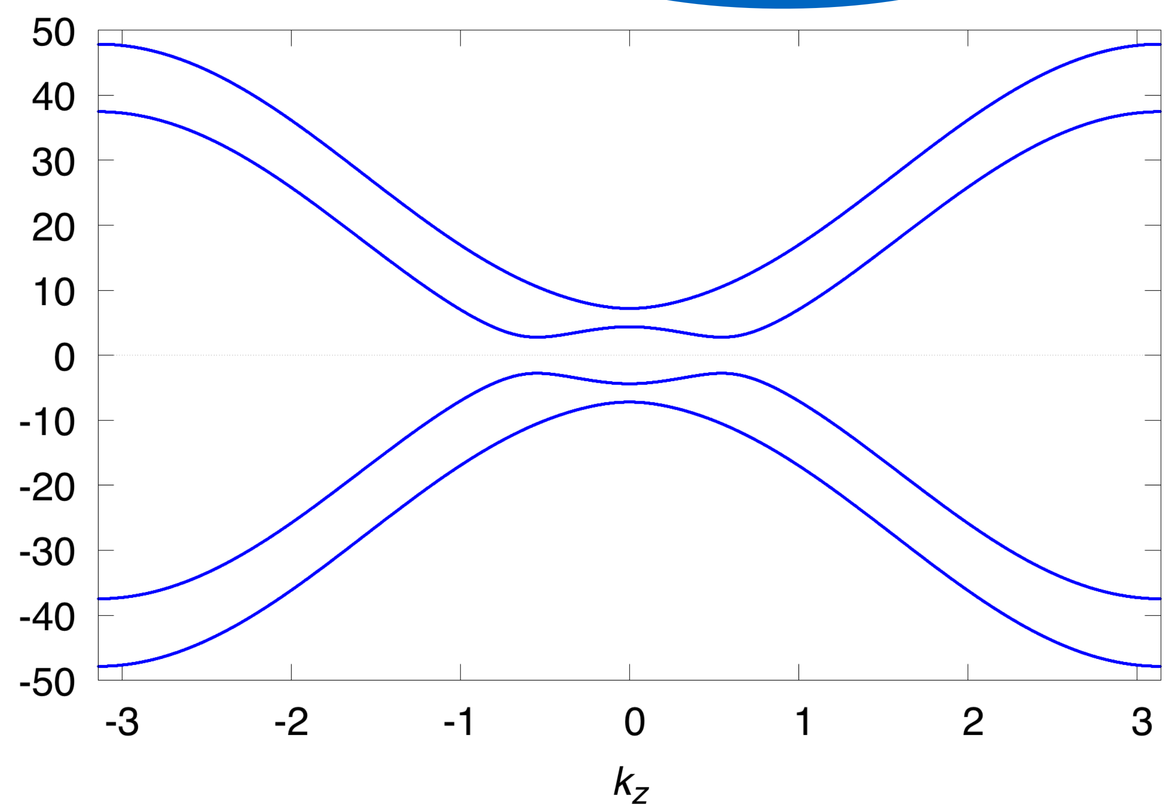
Disappear on *K*-*H* line...

***ab initio* study by J. Ishizuka**

$\alpha > 0$: $E_{3/2}$ → Point node

$\alpha < 0$: $E_{1/2}$ → Gap





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Conclusions

- Gap structures beyond the Sigrist-Ueda method
- Classification on high-symmetry plane in BZ:
  - **Line nodes protected by nonsymmorphic symmetry** due to non-primitive translation ⊥ mirror plane
  - Application to **magnetic octupole** state in Sr_2IrO_4
- Classification on high-symmetry line in BZ:
  - ***j_z*-dependent point nodes (gap opening)** on *K*-*H* line of UPt_3
  - This result is general on **3- or 6-fold axis**