NHSCP2014, Jun. 27, 2014, ISSP, Tokyo

Chiral superconducting state of Sr_2RuO_4 and URu_2Si_2 in the magnetic field

Niigata University
Youichi Yanase

Group members

D3

Tomohiro Yoshida
"Locally non-centrosymmetric SC"

Daisuke Maruyama
"Electron correlation in non-centrosymmetric metal"

D2

Shuhei Takamastu
"Spin-triplet SC in Sr_2RuO_4"
"Chiral SC in URu_2Si_2"

D1

Yasuharu Nakamura
"Multi-orbital SC in $SrTiO_3/LaAlO_3$ interface"

M2

Tatsuya Watanabe
Takanori Hitomi

Contents

(1) Spin-active chiral superconductivity in Sr_2RuO_4

(a) Spin-orbit coupling in spin-triplet Cooper pairs

(b) Phase diagram for H//[001]

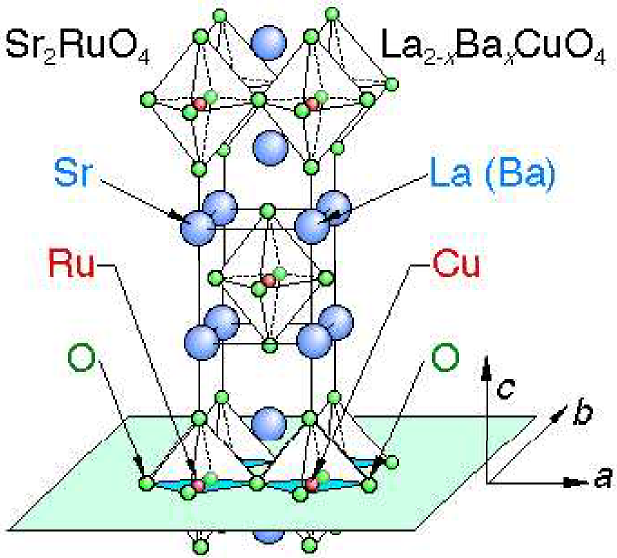
(2) “Hidden order” and chiral superconductivity in URu_2Si_2

Signature of broken rotation symmetry in the SC state

Spin-active chiral SC in Sr_2RuO_4

Spin-triplet superconductor: Sr_2RuO_4

Discovery of SC: Maeno *et. al*. (1994)



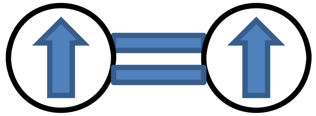
Evidences for the spin-triplet p-wave SC

Mackenzie and Maeno: RMP (2003)

Maeno *et. al*.: JPSJ (2012)

Internal degree of freedom

Spin: S=1



Vector order parameter "d-vector"

$$\vec{d}(k) = (d_{\mathrm{x}}(k), d_{\mathrm{y}}(k), d_{\mathrm{z}}(k))$$

Orbital: D_{4h} symmetry

(k_x, k_y) or $k_x \pm ik_y$

→ 3 X 2 = 6 component SC

→ Chiral p-wave SC at H=0: $\vec{d}(k) = (k_x \pm ik_y)\hat{z}$

Question: Does the SC state change in the magnetic field ?

Yes! for a small spin-orbit coupling. No, for a large spin-orbit coupling.

Microscopic theory of spin-orbit coupling in Sr_2RuO_4

Y. Y.-Ogata (2003)

Band structure of Sr_2RuO_4

Band calculation：Singh, Oguchi

dHvA measurement：Mackenzie et al.

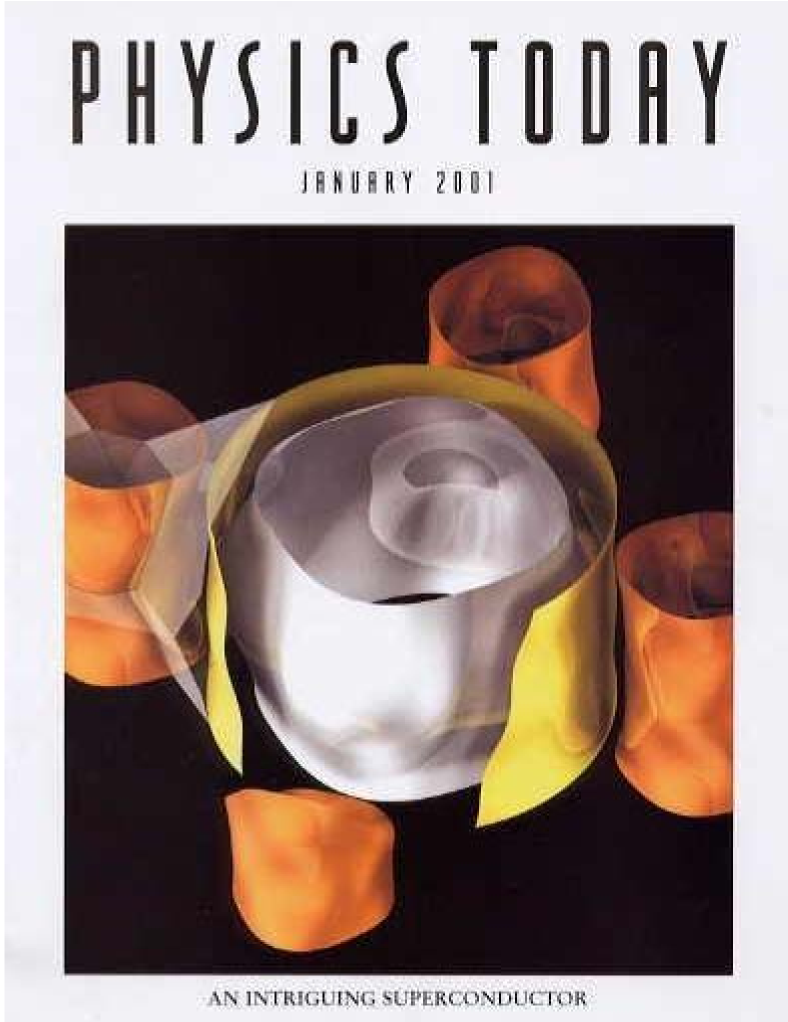
↓ Tight-binding approximation

Three-orbital Hubbard model

$$H = H_0 + H_{\rm LS} + H_{\rm I}$$

H_0: Kinetic energy
$H_{\rm LS}$: LS coupling
$H_{\rm I}$: Coulomb interaction

Semi -microscopic theory:
Ng-Sigrist (2000)



Maeno-Rice-Sigrist (2001)

General properties of spin-orbit coupling

Hierarchy of energy scales in (3d,4d) transition metal oxides

Transition temperature (T_c: ～1K) << LS coupling (λ: ～100K) << Fermi energy (E_F: ～10000K)

Perturbation expansion with respect to λ

Centrosymmetric system (Sr_2RuO_4)

$$F = F_0 \cancel{+ O(\lambda/T_c) + O(\lambda^2/T_c^2) + \ldots} + O(\lambda/E_F) + O(\lambda^2/E_F^2) + \ldots$$

Non-Centrosymmetric system (Li_2Pt_3B, $CePt_3Si$ *etc.*)

$$F = F_0 + O(\lambda/T_c) + O(\lambda^2/T_c^2) + \ldots + O(\lambda/E_F) + O(\lambda^2/E_F^2) + \ldots$$

Spin-orbit coupling of Cooper pairs is small in Sr_2RuO_4.
Most of other theories are not satisfactory.

Selection rules

Y.Y. - Takamatsu - Udagawa (2014)

(I) Selection rules coming from the symmetry of local orbital.

(II) Exact for electron correlation.

(III) Independent of the mechanism of Cooper pairing.

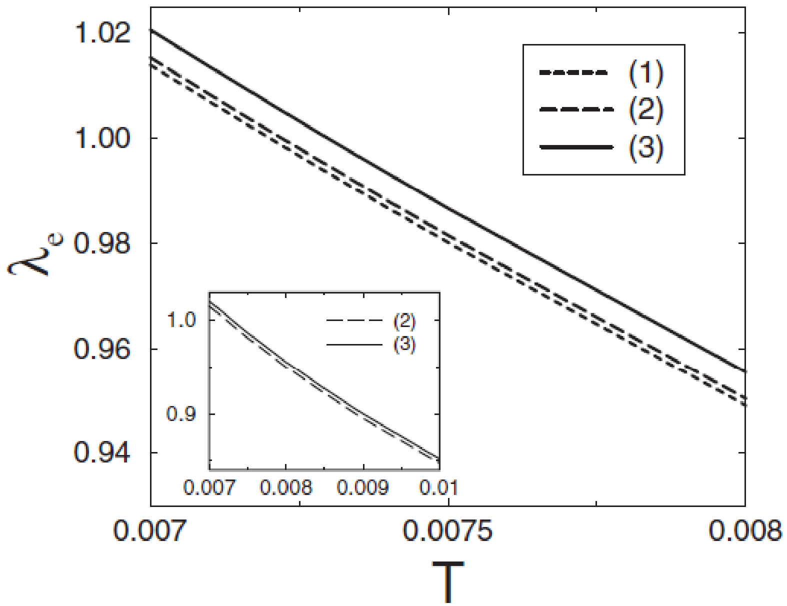
These results are valid for other models too.

Crystal structure	Tetragonal (ex. Sr_2RuO_4)		Hexagonal (ex. Na_xCoO_2)		
Local orbital	d_{xy}	d_{yz} d_{zx}	E_g		A_{1g}
Symmetry of SC	P-wave		P-wave	F-wave	P, F
d-vector	d//c	d//ab	d//ab	both	both
S.-O. coupling in Cooper pairs	$O(\lambda^2/F_F^2)$	$O(\lambda/E_F)$	$O(\lambda/E_F)$	$O(\lambda^2/F_F^2)$	$O(\lambda^2/F_F^2)$

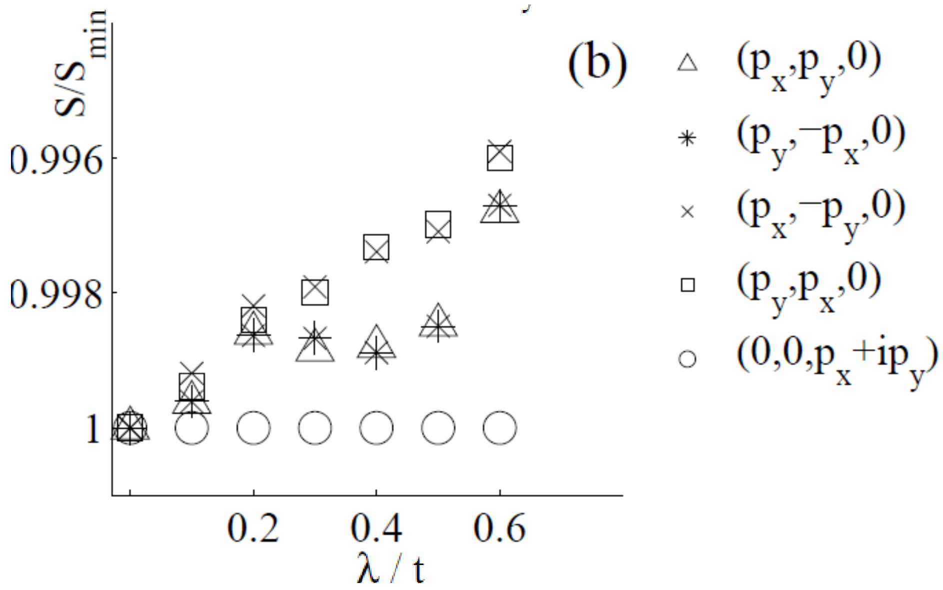
S.-O coupling of Cooper pairs = $\eta = (T_{c1} - T_{c2})/T_{c1}$

Numerical calculations

Perturbation theory
Y. Y. and Ogata (2003)



Functional renormalization group
Wang et. al. (2013)

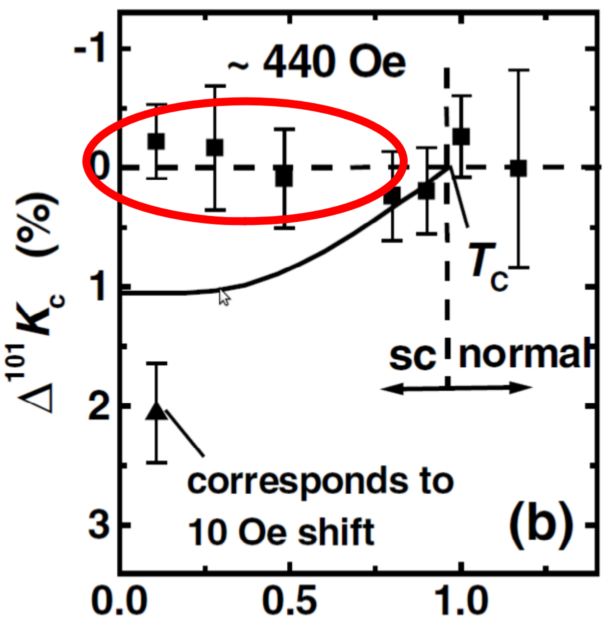


- ✓ Chiral p-wave SC driven by quasi-2D γ-Fermi surface
- ✓ Small spin-orbit coupling ($\eta < 0.01$)

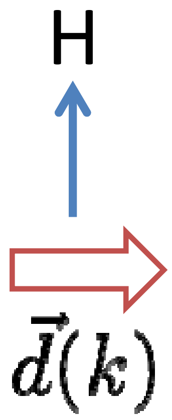
➡ Muitiple SC phases in magnetic fields

Experimental evidences for small spin-orbit coupling

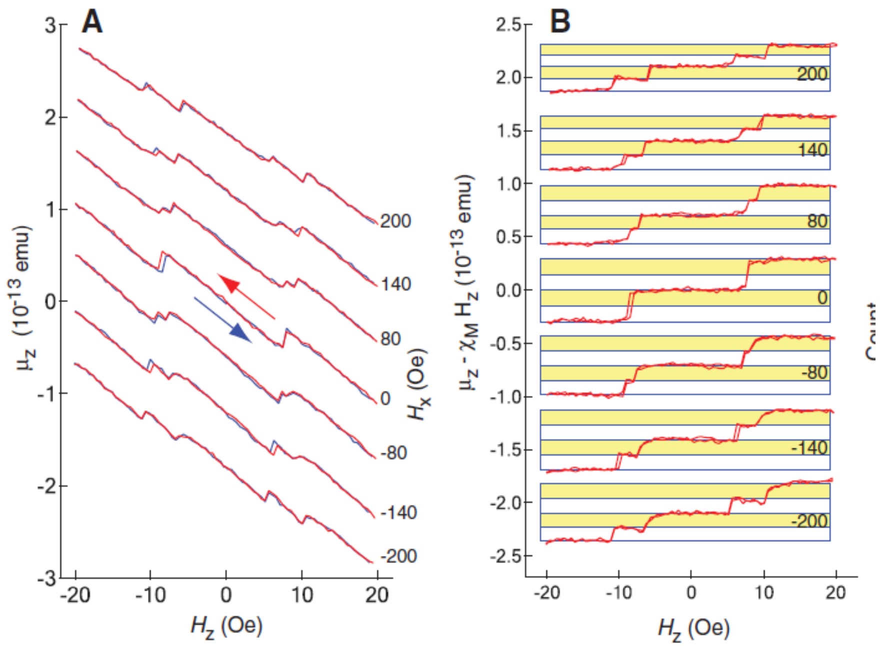
NMR Knight shift



H. Murakawa, *et al.*, PRL (2004)



Half-quantized flux



Jang et al. (2011)

Rotation of d-vector in magnetic fields

Small spin-orbit coupling of Cooper pairs

Raghu-Kapitulnik-Kivelson (2010): SC in (d_{yz},d_{zx})-orbitals → Moderate spin-orbit coupling

What occurs in the magnetic field ?

H // [001] Spin: $\vec{d}(k) = (d_{\rm x}(k), d_{\rm y}(k), \cancel{d_{\rm z}(k)})$

Chirality: $k_{\rm x} \pm i k_{\rm y}$

→ 2 × 2 = 4 component order parameters

4-component GL model

$$f = \sum_{s=\uparrow\uparrow,\downarrow\downarrow} (f_{s,{\rm xy}} + f_s^{(1)}) + f^{(2)}$$

$$\begin{aligned} f_{s,{\rm xy}} = {} & \alpha\left(|\Delta_{s,{\rm x}}|^2 + |\Delta_{s,{\rm y}}|^2\right) + \beta_1\left(|\Delta_{s,{\rm x}}|^2 + |\Delta_{s,{\rm y}}|^2\right)^2/2 \\ & + \beta_2(\Delta_{s,{\rm x}}\Delta^*_{s,{\rm y}} - {\rm c.c.})^2/2 + \beta_3|\Delta_{s,{\rm x}}|^2|\Delta_{s,{\rm y}}|^2 \\ & + \xi_1^2\left[|D_{\rm x}\Delta_{s,{\rm x}}|^2 + |D_{\rm y}\Delta_{s,{\rm y}}|^2\right] + \xi_2^2\left[|D_{\rm x}\Delta_{s,{\rm y}}|^2 + |D_{\rm y}\Delta_{s,{\rm x}}|^2\right] \\ & + \xi_3^2\left\{\left[(D_{\rm x}\Delta_{s,{\rm x}})(D_{\rm y}\Delta_{s,{\rm y}})^* + (D_{\rm x}\Delta_{s,{\rm y}})(D_{\rm y}\Delta_{s,{\rm x}})^*\right] + {\rm c.c.}\right\} \end{aligned}$$

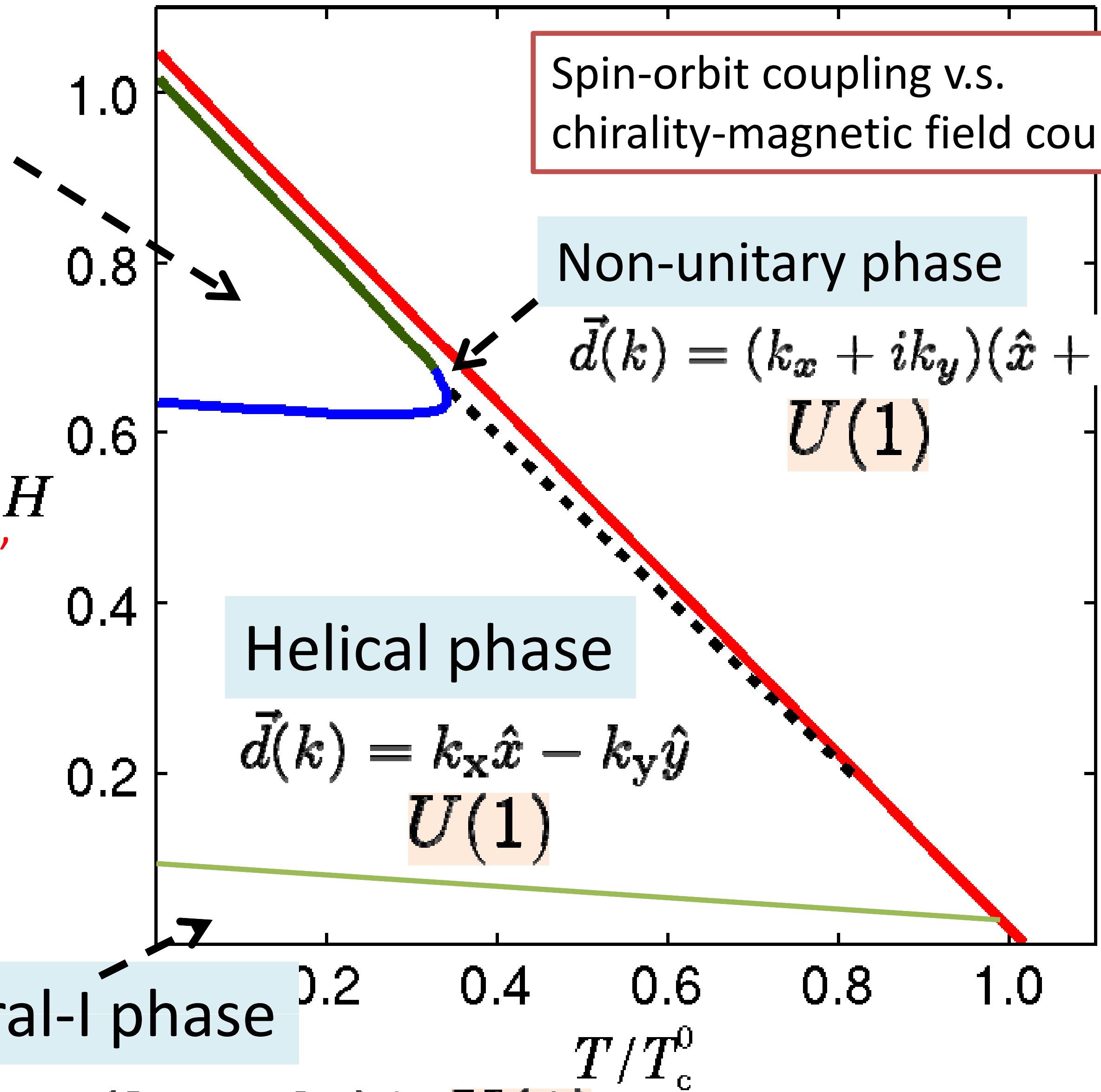
$$f_{\rm s}^{(1)} = \epsilon s(i\Delta_{s,{\rm x}}\Delta^*_{s,{\rm y}} + {\rm c.c.})$$

S.-O. coupling coming from (d_{yz},d_{zx})-orbitals

$$f^{(2)} = \delta\left[(\Delta_{\uparrow\uparrow,{\rm x}}\Delta^*_{\downarrow\downarrow,{\rm x}} - \Delta_{\uparrow\uparrow,{\rm y}}\Delta^*_{\downarrow\downarrow,{\rm y}}) + {\rm c.c.}\right]$$

S.-O. coupling coming from d_{xy}- and (d_{yz},d_{zx})-orbitals

SC phases in H//[001] (ε=-0.015, δ=-ε/4)



Spin-orbit coupling v.s. chirality-magnetic field coupling

(Spin-active) Chiral-II phase

$\vec{d}(k) = (k_x + ik_y)\hat{x}$

$U(1) \times U(1)$

"Fractional vortex lattice"

Non-unitary phase

$\vec{d}(k) = (k_x + ik_y)(\hat{x} + i\hat{y})$

$U(1)$

Helical phase

$\vec{d}(k) = k_x\hat{x} - k_y\hat{y}$

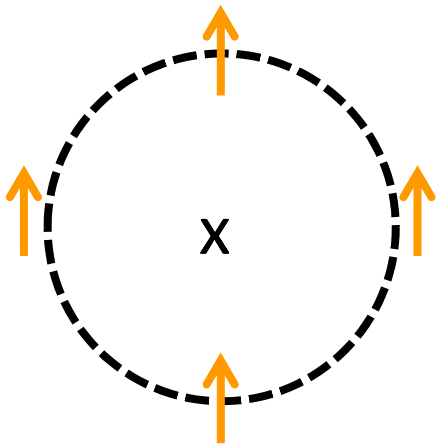
$U(1)$

Chiral-I phase

$\vec{d}(k) = (k_x + ik_y)\hat{z}$ $U(1)$

Vortex in spin-active SC

Integer vortex



$\Phi_0 = hc/2|e|$

Order parameter manifold

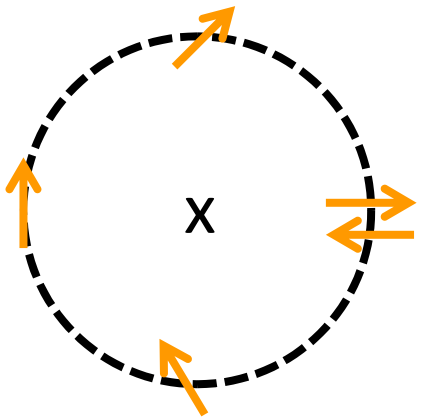
$U(1)$ -symmetry

Topological index (Vortex)

$\pi_1(S^1) = Z$

Quantized vortex

Fractional vortex



$\Phi_0/2 = hc/4|e|$

$$\boldsymbol{d} = \Delta e^{i\varphi}(\cos\alpha\hat{x} + \sin\alpha\hat{y})$$

Ivanov (2001)

A novel topological defect with Majorana Fermion and non-Abelian statistics

Order parameter manifold

$U(1) \times U(1)$ -symmetry

Topological index (Skyrmion)

$\pi_2(S^2) = Z$

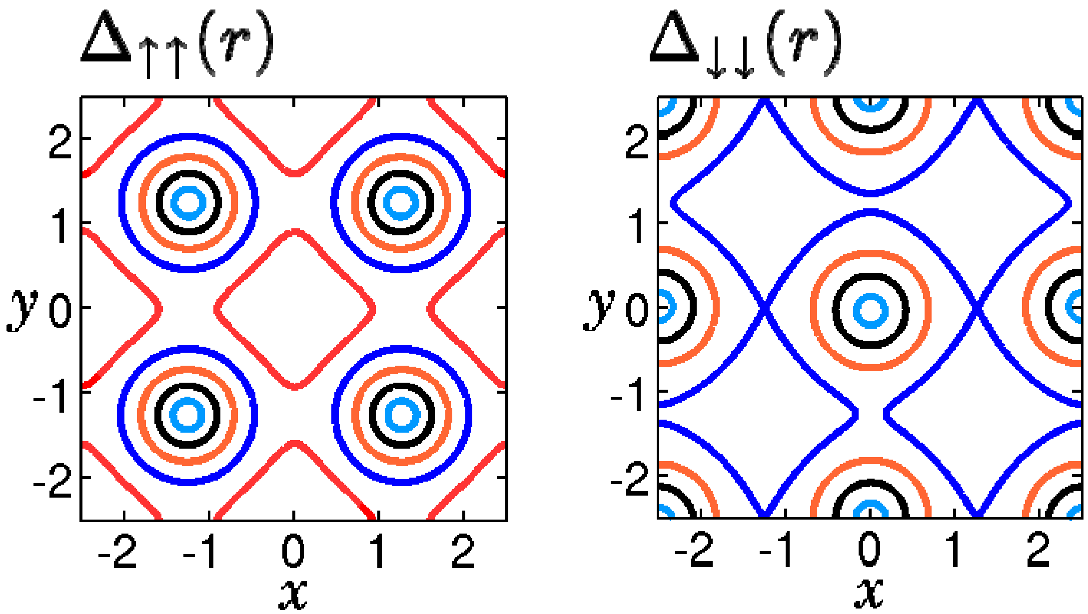
Fractional vortex

Pseudo spin

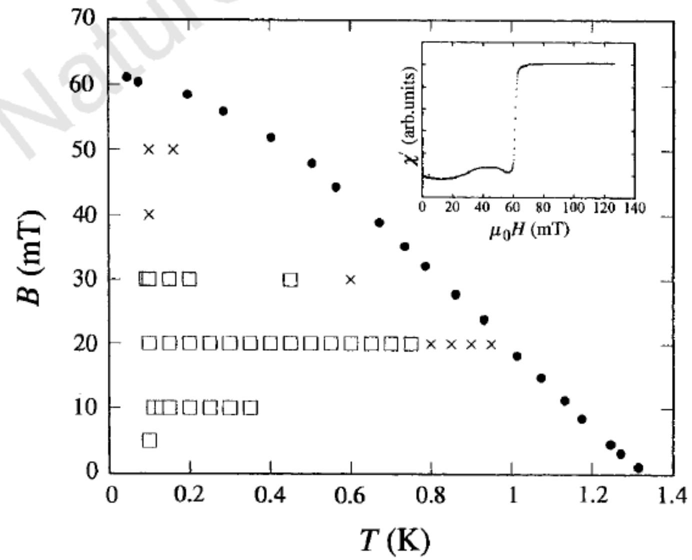
$$\vec{S}(r) = C^\dagger(r)\vec{\sigma}C(r)$$

$$C^\dagger(r) = (\Delta^*_{\uparrow\uparrow}(r), \Delta^*_{\downarrow\downarrow}(r))$$

Fractional vortex lattice in chiral-II phase



Small angle neutron scattering
Riseman, *et al*., Nature.(1998)



Why spin-active ?

Non-chiral spin-triplet SC (UCoGe etc...)

Spin degree of freedom is quenched by the spin-orbit coupling.

S. B. Chung, *et al*. New. J. Phys.(2009)

$$\Delta F = \delta_{\mathrm{so}}\left[\Delta^*_{\uparrow\uparrow}\Delta_{\downarrow\downarrow} + c.c.\right]$$

⇔

Chiral spin-triplet SC

Linear spin-orbit coupling vanishes due to chirality of Cooper pairs.

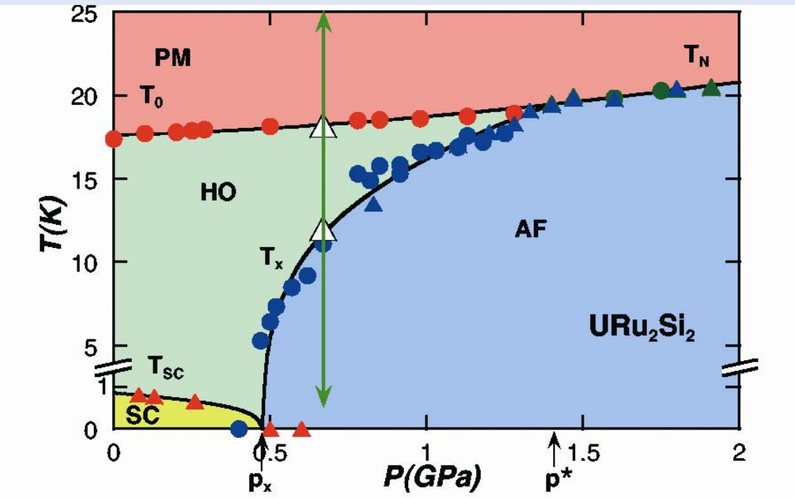
“Hidden order” and chiral SC in URu_2Si_2

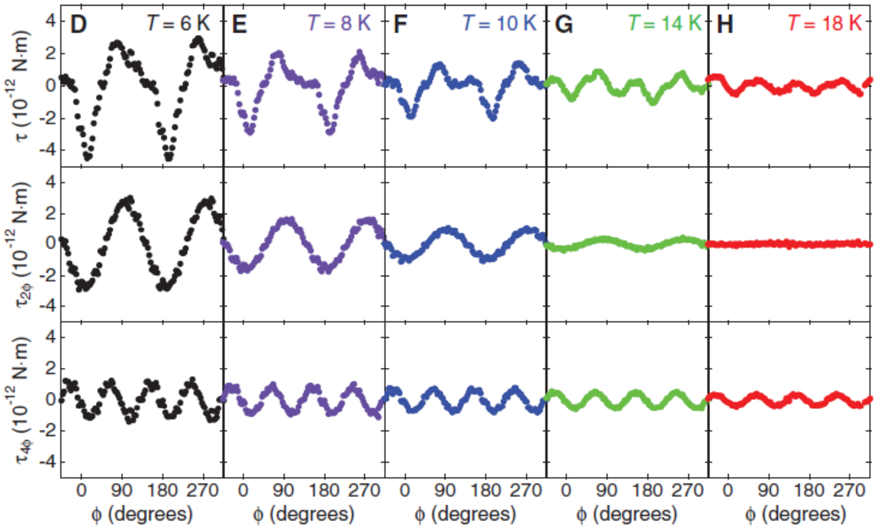
Mystery of "hidden order" in URu_2Si_2

$T < T_{HO}$ "Hidden order" The order parameter has not been identified.

Theory

- Multipole order ?
- Hybridization wave ?
- Spin nematic order ?
- ....





Broken 4-fold rotation symmetry in HO state

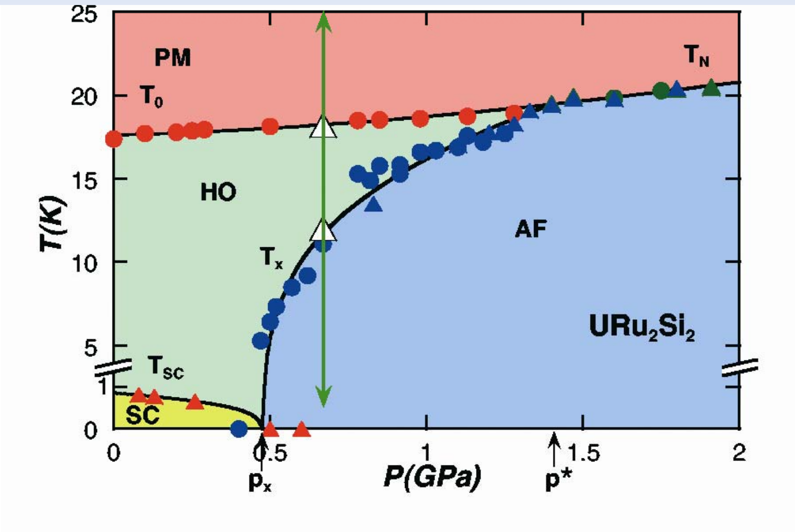
- Magnetic torque
  R. Okazaki et al., Science (2011)
- Cyclotoron resonance
  S. Tonegawa *et al.*, PRL (2012)
- NMR
  S. Kambe *et al.*, PRL (2013)
- X-ray scattering
  S. Tonegawa *et al.*, Nature commun. (2014)

4-fold rotation symmetry in HO state

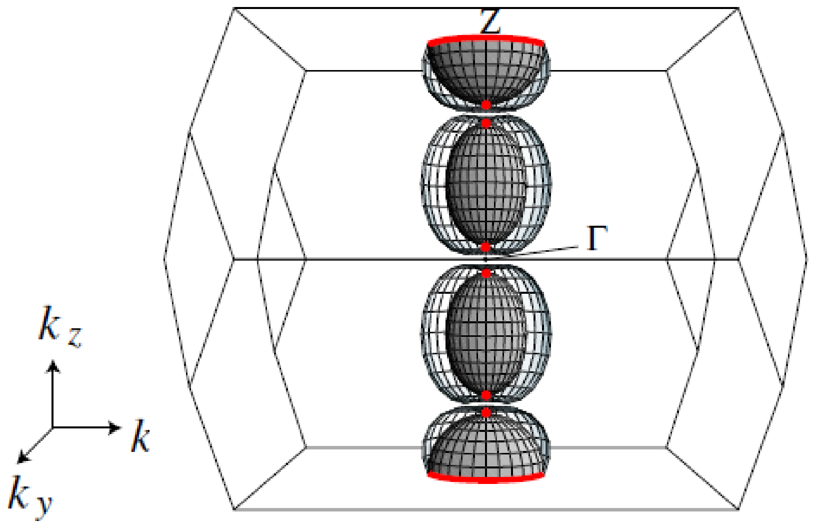
- Neutron scattering: P. G. Niklowiz *et al.*, PRL (2010)
- X-ray scattering: H. C. Walker *et al.*, PRB (2011), C. Tabata *et al.*, (2013)

Chiral d-wave superconductivity in URu_2Si_2

$T < T_C$ Superconductivity coexists with HO.



Schematic gap structure



Thermal conductivity:

Y. Kasahara *et al*., New J. Phys. (2009)

Specific heat:

K. Yano *et al*., PRL (2008)

Chiral $d_{xz} \pm id_{yz}$ -wave SC

Our message: Chiral d-wave SC is sensitive to the broken rotation symmetry.

2-component Ginzburg-Landau model

- GL free energy of the E_g representation in the D_{4h} symmetry
  M. Sigrist and K. Ueda: Rev. Mod. Phys. (1991)

$$
\begin{aligned}
f_0 =& (T/T_c^0 - 1)\left(|\Delta_x|^2 + |\Delta_y|^2\right) + \left(|\Delta_x|^2 + |\Delta_y|^2\right)^2/2 \\
&+ \beta_2 (\Delta_x \Delta_y^* - \text{c.c.})^2/2 + (3\beta_2 - 1)|\Delta_x|^2|\Delta_y|^2 \\
&+ \left[|D_x\Delta_x|^2 + |D_y\Delta_y|^2\right] + \kappa_2\left[|D_x\Delta_y|^2 + |D_y\Delta_x|^2\right] \\
&+ \kappa_3\left[(D_x\Delta_x)(D_y\Delta_y)^* + (D_x\Delta_y)(D_y\Delta_x)^* + \text{c.c.}\right]
\end{aligned}
$$

- Agterberg model [D. F. Agterberg; Phys. Rev. Lett. **58** (1998) 14484]
  for chiral p-wave SC in Sr_2RuO_4

$$
\kappa_2 = \kappa_3 = \beta_2 = \frac{\langle v_x^2 v_y^2 \rangle_{FS}}{\langle v_x^4 \rangle_{FS}} = \frac{1+\nu}{3-\nu}
$$

Anisotropy of Fermi surface

$-1 < \nu < 1 \ (0 < \kappa_2 < 1)$

For an istropic Fermi surface,

$\nu = 0 \ (\kappa_2 = 1/3)$

- **Symmetry breaking term** $f_h = g(\Delta_x \Delta_y^* + \text{c.c.})$

Variational method with use of Landau level expansion

- Chirality basis $\begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -\mathrm{i} \\ 1 & \mathrm{i} \end{pmatrix} \begin{pmatrix} \Delta_x \\ \Delta_y \end{pmatrix}$

- Linearized GL equation

$$\begin{pmatrix} 1 + 2\Pi_+\Pi_- & e^{-2\mathrm{i}\theta}\Pi_-^2 - \nu e^{2\mathrm{i}\theta}\Pi_+^2 \\ e^{2\mathrm{i}\theta}\Pi_+^2 - \nu e^{-2\mathrm{i}\theta}\Pi_-^2 & 1 + 2\Pi_-\Pi_- \end{pmatrix} \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix} = \lambda \begin{pmatrix} \Delta_1 \\ \Delta_2 \end{pmatrix}$$

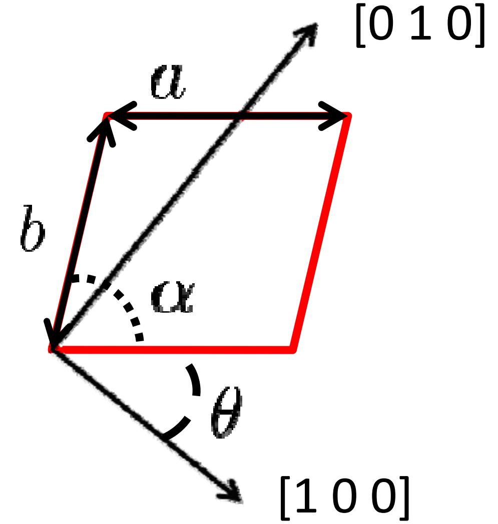
$$\begin{pmatrix} \psi_{1+}(\boldsymbol{r}) \\ \psi_{2+}(\boldsymbol{r}) \end{pmatrix} = \sum_{n\geq 0} \begin{pmatrix} a_{4n}(\theta)\phi_{4n}(\boldsymbol{r}; b/a, \alpha) \\ a_{4n+2}(\theta)\phi_{4n+2}(\boldsymbol{r}; b/a, \alpha) \end{pmatrix}, \quad \begin{pmatrix} \psi_{1-}(\boldsymbol{r}) \\ \psi_{2-}(\boldsymbol{r}) \end{pmatrix} = \sum_{n\geq 0} \begin{pmatrix} b_{4n+2}(\theta)\phi_{4n+2}(\boldsymbol{r}; b/a, \alpha) \\ b_{4n}(\theta)\phi_{4n}(\boldsymbol{r}; b/a, \alpha) \end{pmatrix}$$

Chirality +　　　　Chirality −

- Variational wave function

$$\begin{pmatrix} \Delta_1(\boldsymbol{r}) \\ \Delta_2(\boldsymbol{r}) \end{pmatrix} = C_1 \begin{pmatrix} \psi_{1+}(\boldsymbol{r}) \\ \psi_{2+}(\boldsymbol{r}) \end{pmatrix} + C_2 \begin{pmatrix} \psi_{1-}(\boldsymbol{r}) \\ \psi_{2-}(\boldsymbol{r}) \end{pmatrix}$$

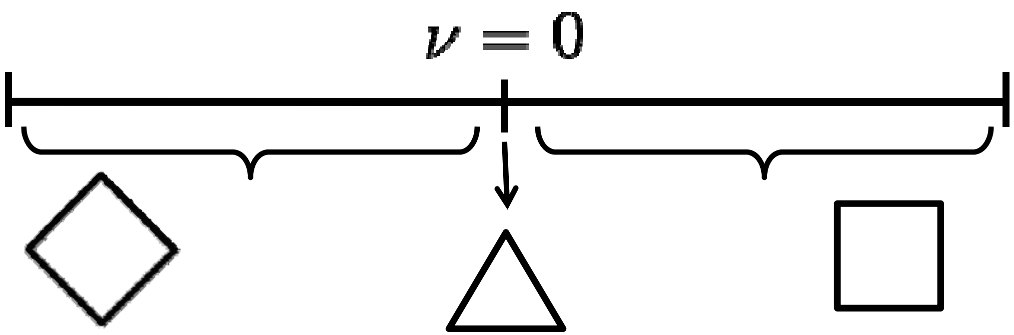
- Variational parameters $(C_1, C_2, b/a, \alpha, \theta)$



Vortex lattice structure in chiral SC

Conventional SC: Triangular lattice

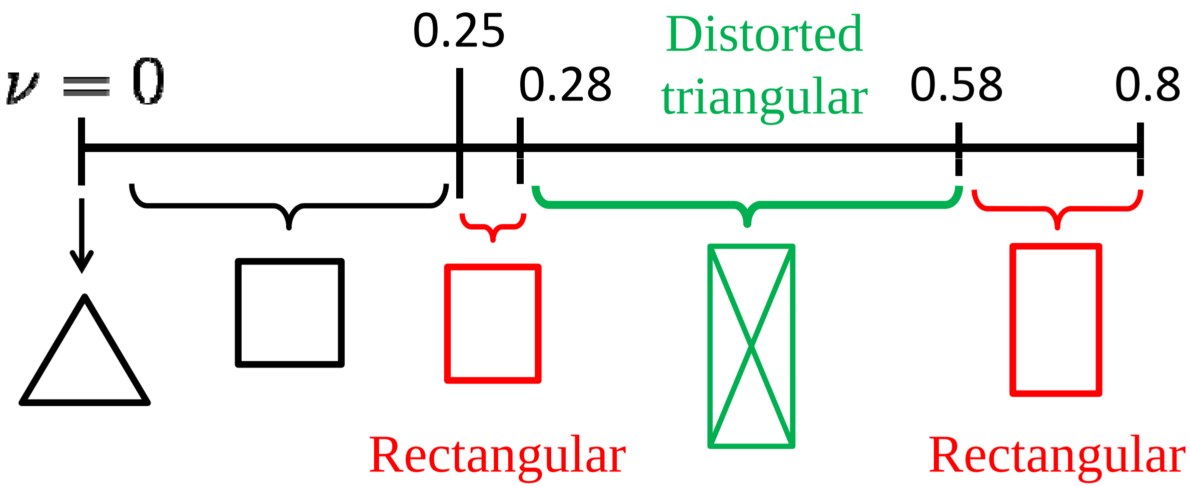
D. F. Agterberg: PRL **58** (1998) 14484, PRB **80** (1998) 5184. $(\kappa = \lambda/\xi \to \infty)$



Square lattice:

$|\nu| > 0.011$

Our results



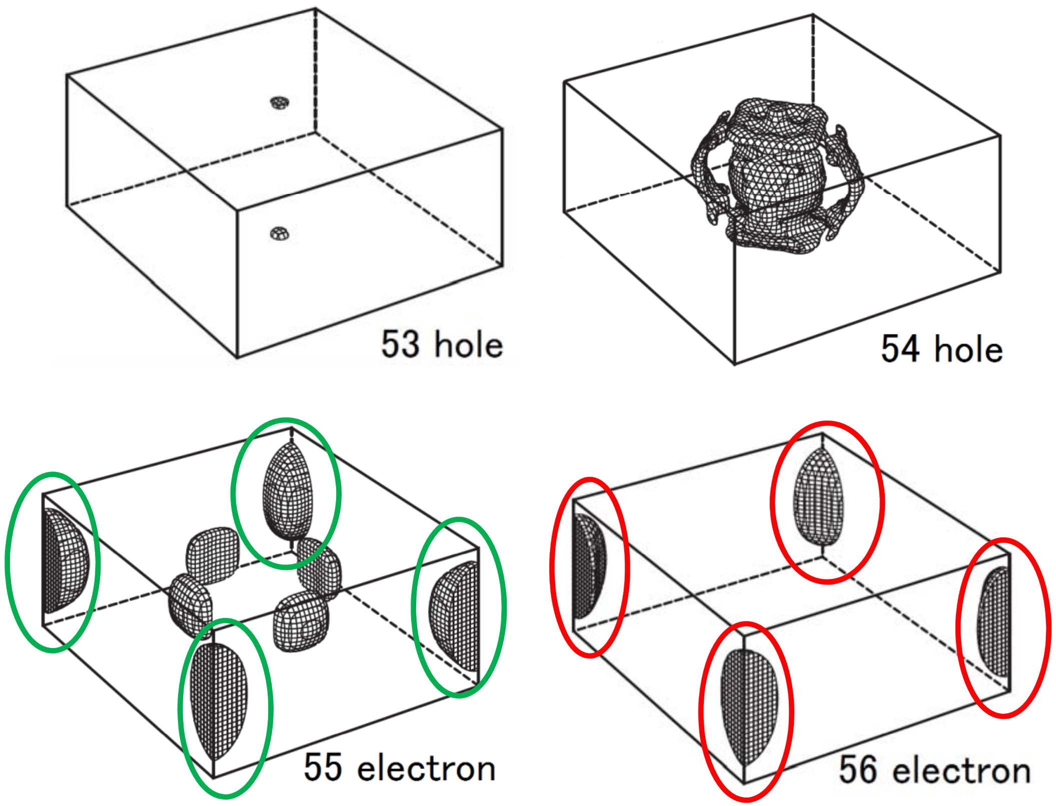
Estimation of GL parameters: Fermi surfaces

LDA band structure calculation by Harima

(1) Large DOS of 55 and 55 bands

(2) SdH measurement

55 and 56 electron pockets are mainly superconducting.



Estimation of GL parameters: 2-band Agterberg model

Agterberg model for
2-band Chiral d-wave SC

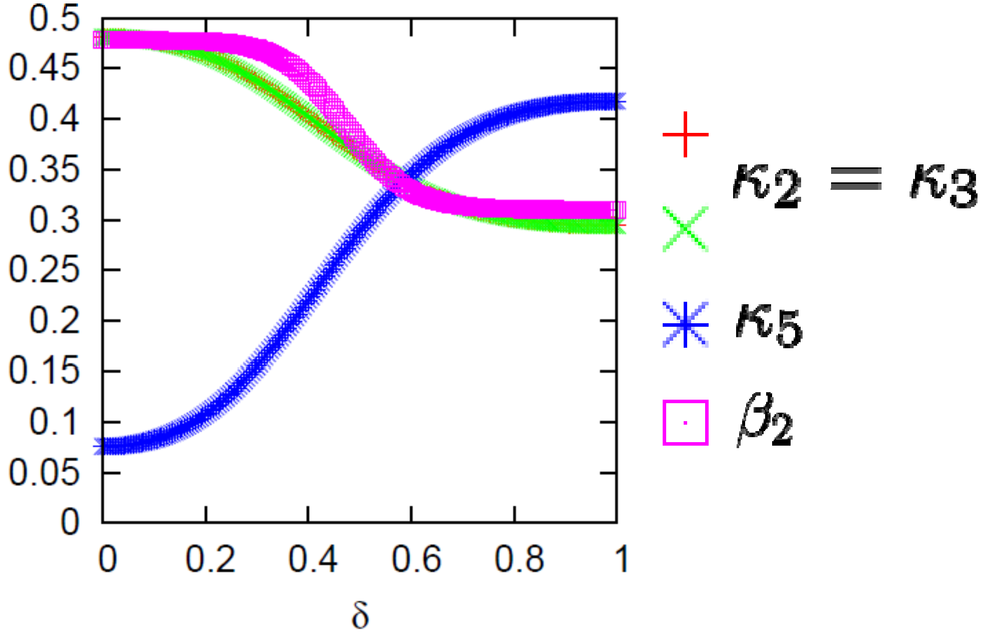
$$\phi_{\alpha,m}(\boldsymbol{k}) = \Delta_m v_{\alpha,m}(\boldsymbol{k}) \sin k_z$$

$$\langle F \rangle_{\rm FS} \equiv \frac{1}{\rho_0} \sum_{m=55,56} \sum_{\boldsymbol{k}} F_m(\boldsymbol{k}) \delta(E_m(\boldsymbol{k}))$$

$$\kappa_2 = \frac{\langle v_{\rm x}^2 \phi_{\rm y}^2 \rangle_{\rm FS}}{\langle v_{\rm x}^2 \phi_{\rm x}^2 \rangle_{\rm FS}}, \quad \kappa_3 = \frac{\langle v_{\rm x} v_{\rm y} \phi_{\rm x} \phi_{\rm y} \rangle_{\rm FS}}{\langle v_{\rm x}^2 \phi_{\rm x}^2 \rangle_{\rm FS}}$$

$$\beta_2 = \frac{\langle \phi_{\rm x}^2 \phi_{\rm y}^2 \rangle_{\rm FS}}{\langle \phi_{\rm x}^4 \rangle_{\rm FS}}$$

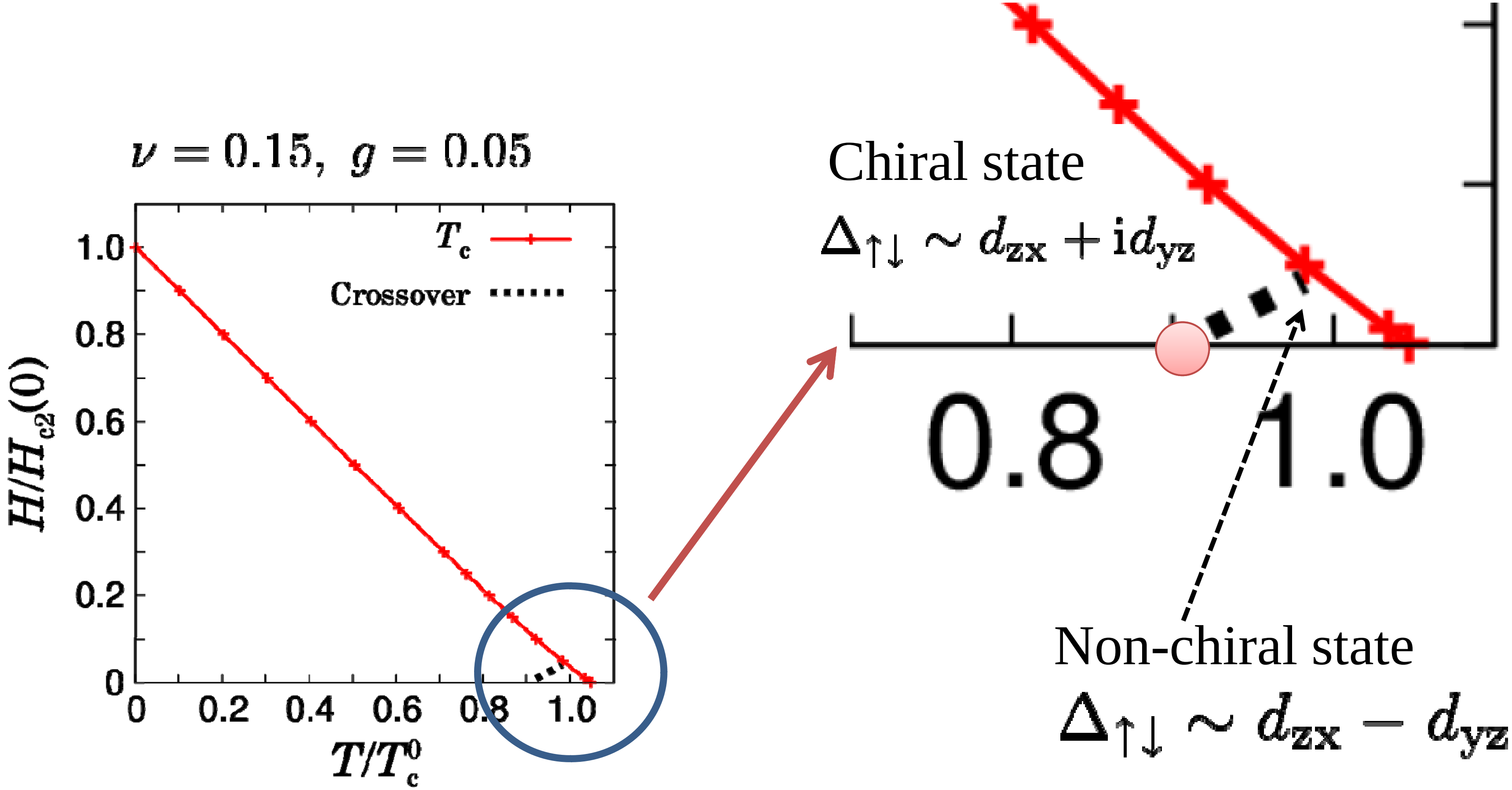
$$(\Delta_{55}, \Delta_{56}) = (\delta, 1-\delta)$$



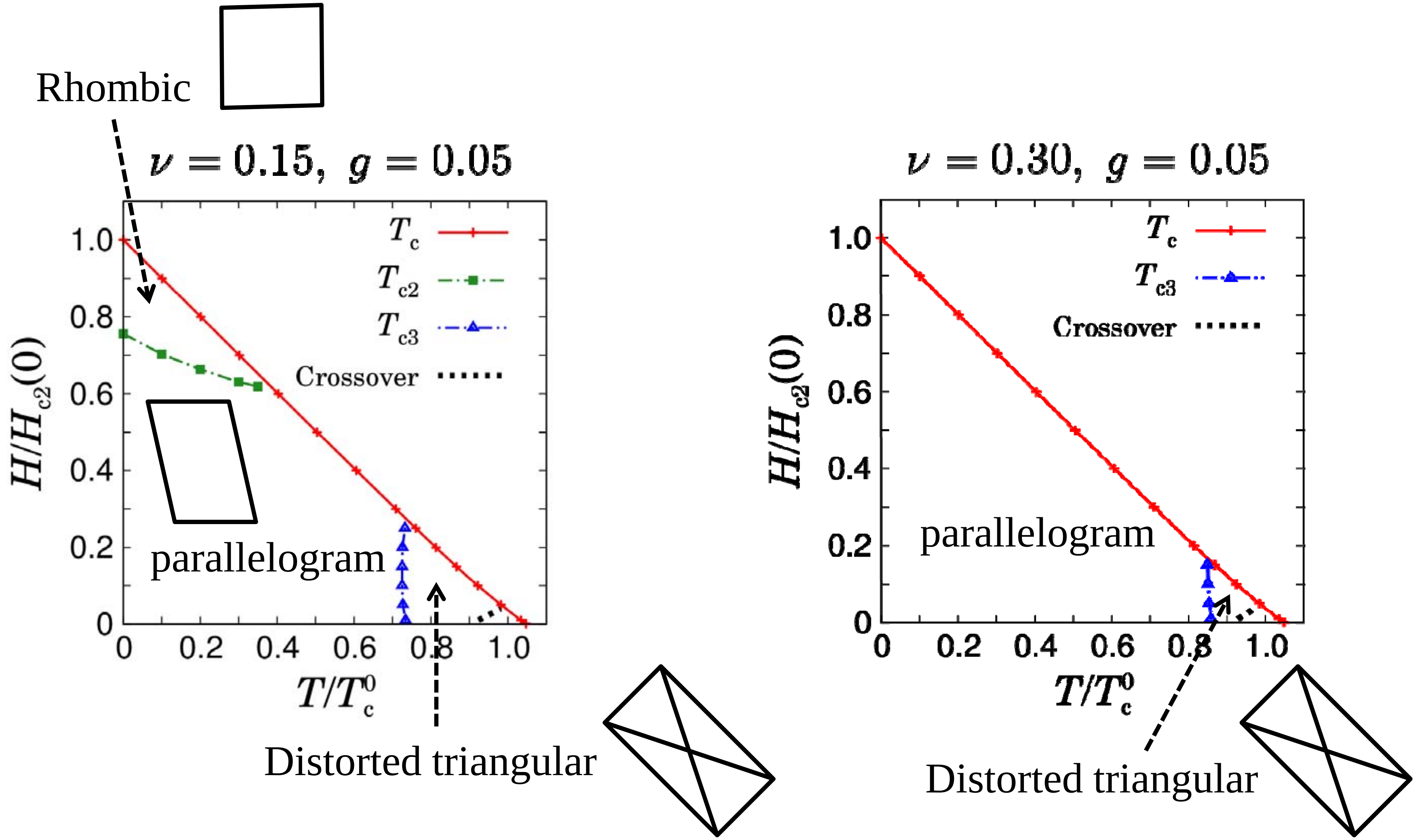
$$\nu = -0.076 \sim 0.30$$

Square lattice: $0.011 < |\nu| < 0.25$
(4-fold symmetric case)

Phase diagram (Broken 4-fold rotation symmetry)



Phase diagram (Broken 4-fold rotation symmetry)



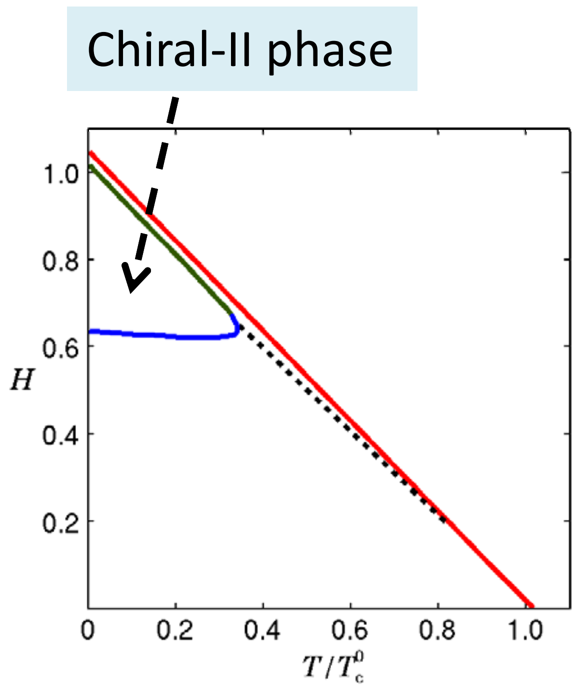
Vortex lattice structural transition (by small angle neutron scattering) will be a clear evidence for the broken rotation symmetry in the “hidden order” state.

Summary

Spin-active chiral superconductivity in Sr_2RuO_4

- Small but finite spin-orbit coupling ($\eta < 0.01$)
- Spin-active chiral-II phase

  (Fractional vortex lattice = Skyrmion lattice)



Chiral superconductivity coexisting with "hidden order " in URu_2Si_2

- Chiral to Non-chiral transition

  due to rotation symmetry breaking
- Vortex lattice structural transition