Theory of d-Vector of in Spin-Triplet Superconductor Sr_2RuO_4

K. Miyake   KISOKO, Osaka University

Acknowledgements

Y. Yoshioka   JPSJ **78** (2009) 074701.

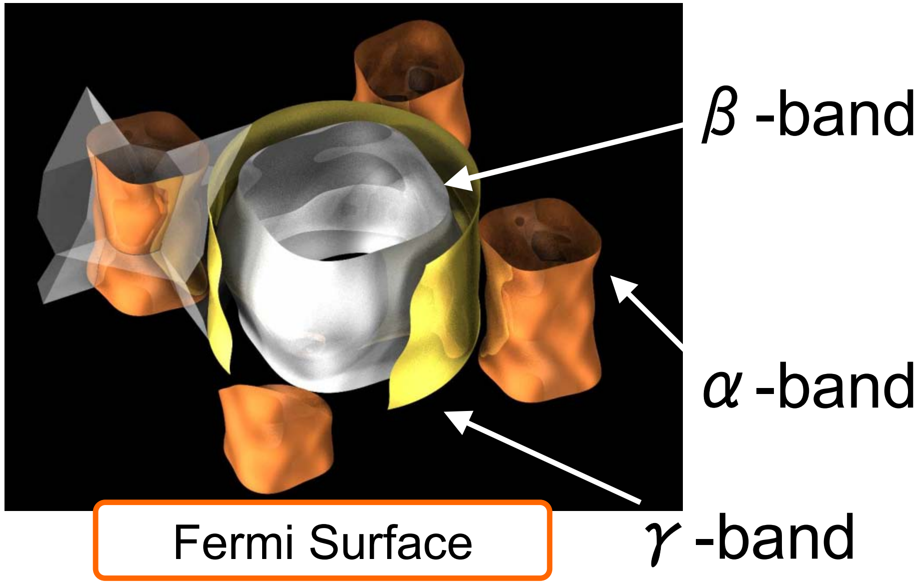
K. Hoshihara JPSJ **74** 2679 (2005) 2679.

K. Ishida, H. Kohno Discussions

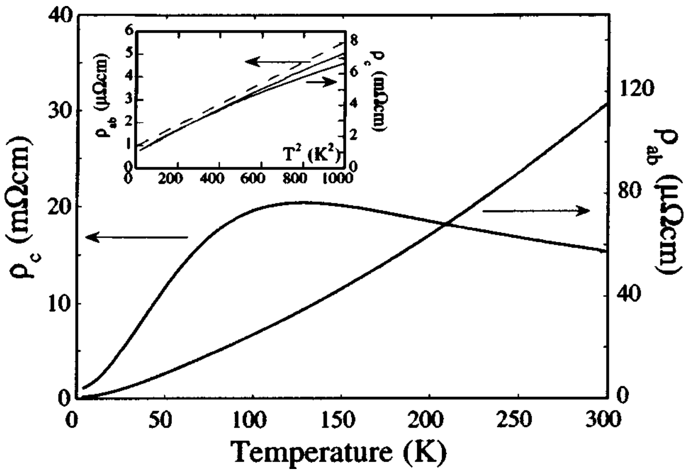
% Prologue

% Microscopic theory of d-vector on d-p model

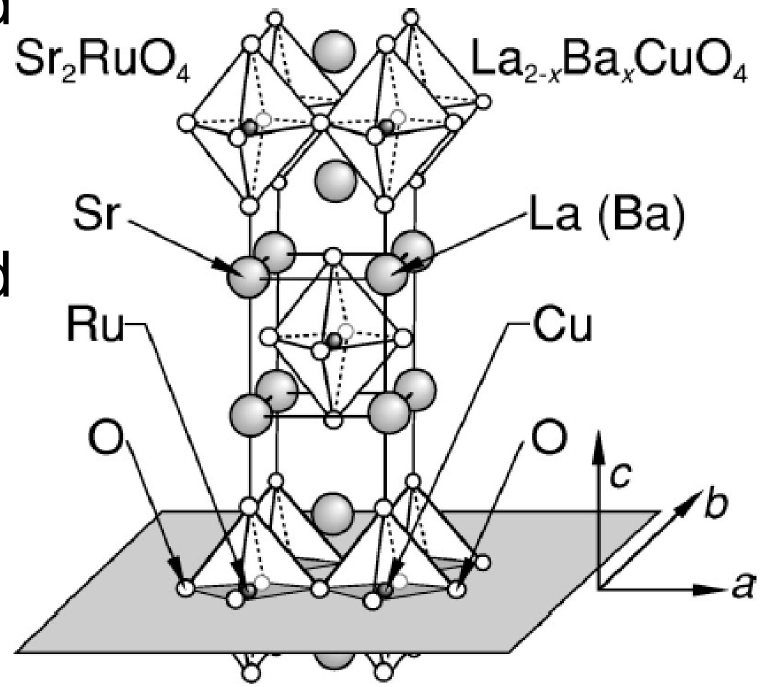
% Anomalous NQR relaxation rate by internal Josephson effect due to pair spin-orbit interaction



Fermi Surface



Two-dimensional



A. P. Mackenzie and Y. Maeno: Rev. Mod. Phys. 75 (2003) 657.

Layered Perovskite

NMR(Knight-shift, T_1), specific heat, impurity effect, μsR, etc …

p-wave chiral spin-triplet SC

%Prologue: anisotropy of *d*-vector by Knight shift

The first round

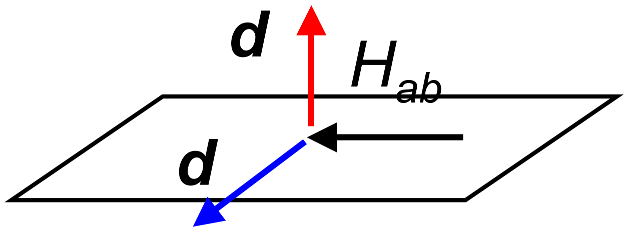
Knight shift (H ⊥ c) does not change below T_C

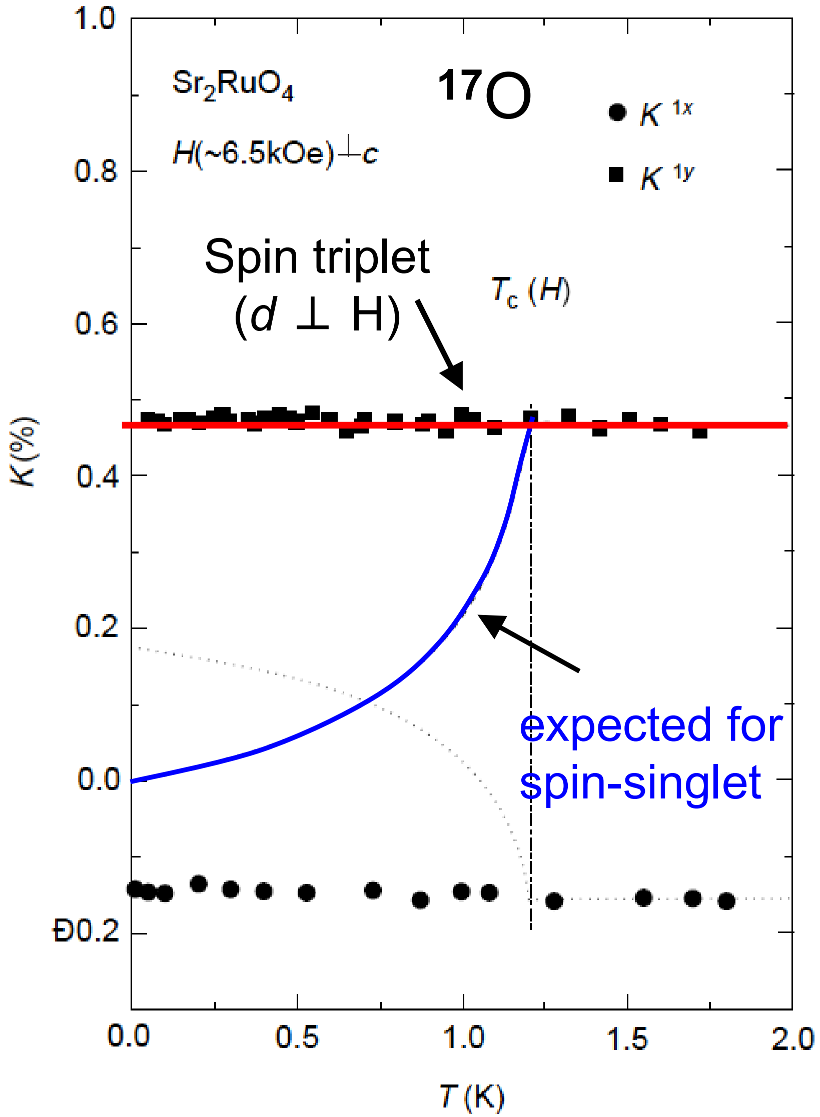
↓

Spin of Cooper pair ⊥ *c*

↓

d-vector || *c* ?





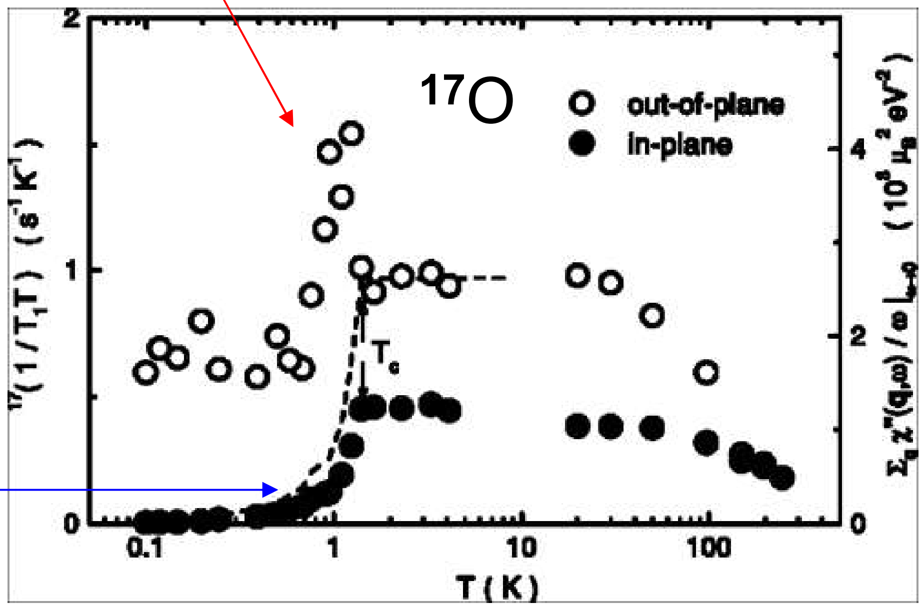
Ishida et al: Nature **396** (1998) 658

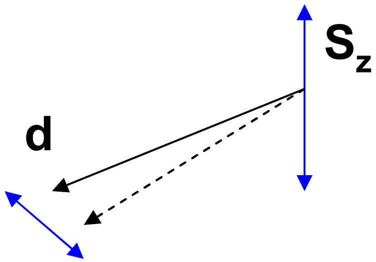
Crucial experiment: NQR relaxation

$\sum_{\mathbf{q}} \mathrm{Im}\chi_{zz}(\mathbf{q},\omega)/\omega|_{\omega=\omega_{\mathrm{NQR}}}$

To give an explanation for the anomalous NQR relaxation, ***d*-vector is necessary to be in the ab-plane**（Miyake & Kohno, STSR2004 ）

$\sum_{\mathbf{q}} \mathrm{Im}\chi_{xx}(\mathbf{q},\omega)/\omega|_{\omega=\omega_{\mathrm{NQR}}}$





Anomalous ^{17}O-NQR relaxation

Mukuda, Ishida et al: Phys. Rev. B **65** (2002) 132507

Also by NMR H// ab, Ishida P119

cf. Internal Josephson oscillations: Leggett (1973)

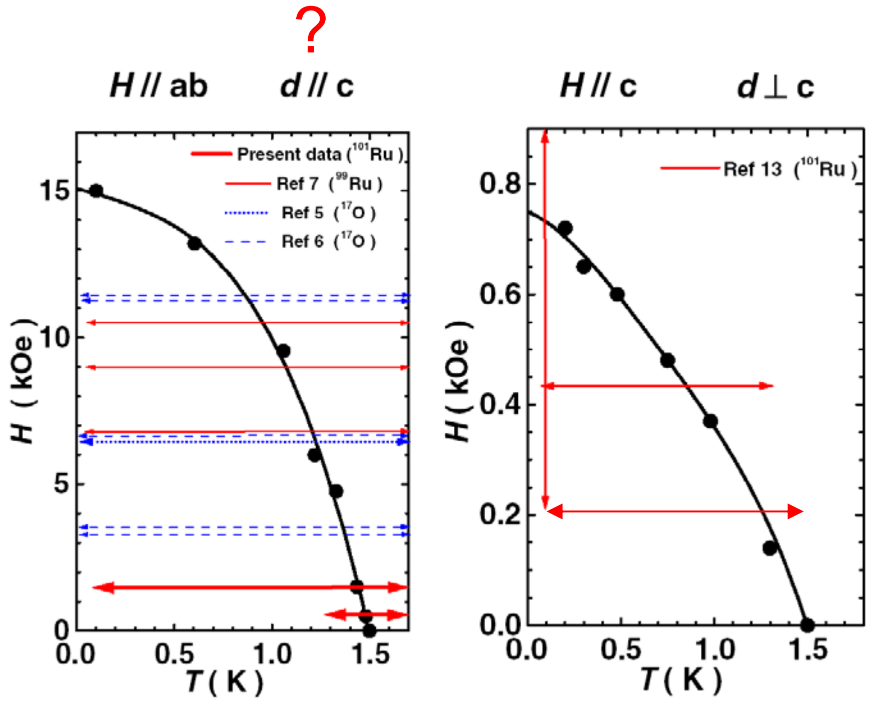
Experiment of Knight shift

The second round

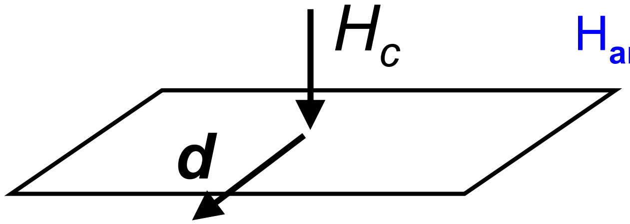
Murakawa, Ishida et al:

Phys. Rev. Lett. **93** (2004) 167004

The Knight-shift (H || c) **remains unchanged** across the T_c, as well as H || ab, even with a small magnetic field of **0.02[T]**.

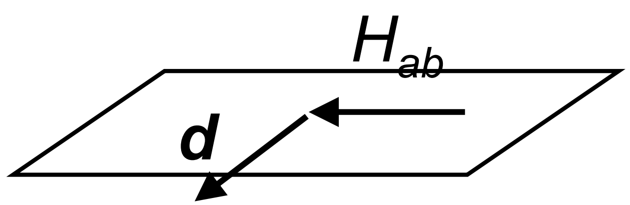


d-vector ⊥ c ?



H_{aniso} < 0.02[T]

or



%Microscopic theory of d-vector on d-p model

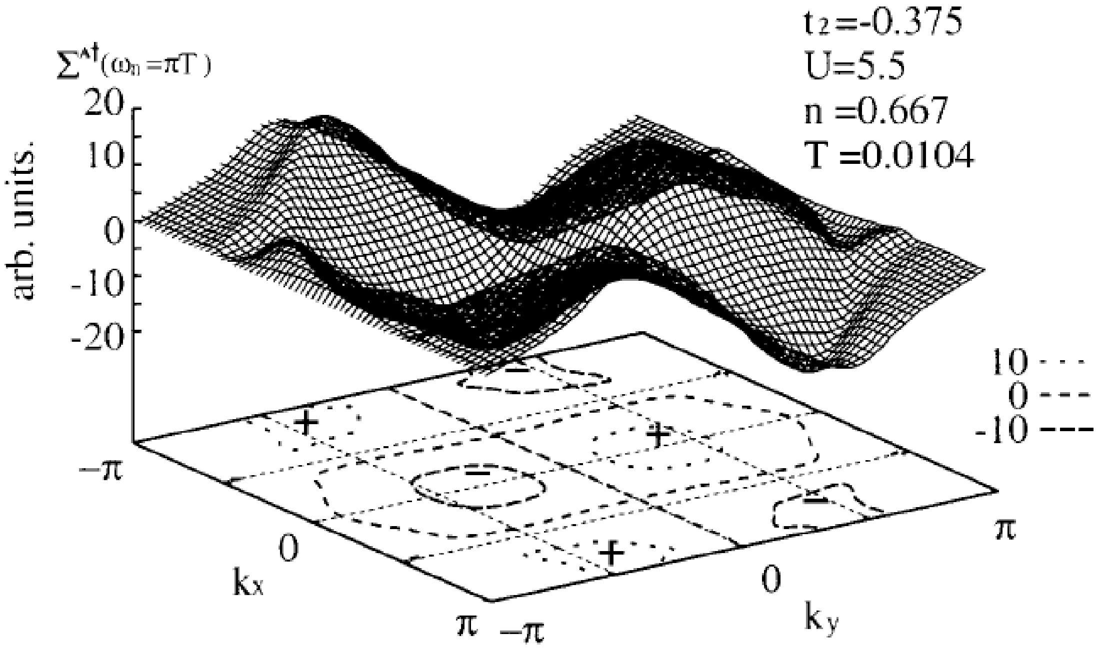
- Brief and incomplete history
  - *d*-vector issue and theory
- Calculation of T_c based on *d*-*p* model
- Anisotropy of *d*-vector
  - *d*-*p* model + spin-orbit interaction

Y. Yoshioka and KM: J. Phys. Soc. Jpn. **78**, 074701 (2009)

Hubbard model calculation

T. Nomura & K. Yamada: J. Phys. Soc. Jpn. **71** (2002) 404

The spin-singlet is more stable than the spin-triplet, within the second order perturbation theory (SOPT).



Third order perturbation terms stabilize the spin-triplet superconductivity

T-dependence of C and $1/T_1$ well explained

$$\Delta_{\mathbf{k}} \sim \sin k_y \cos k_x$$

For γ-band

Anisotropy of *d*-vector (Theory)

•Hubbard model + Atomic Spin-Orbit & Hund coupling
Yanase & Ogata :J. Phys. Soc. Jpn. **72** (2003)673

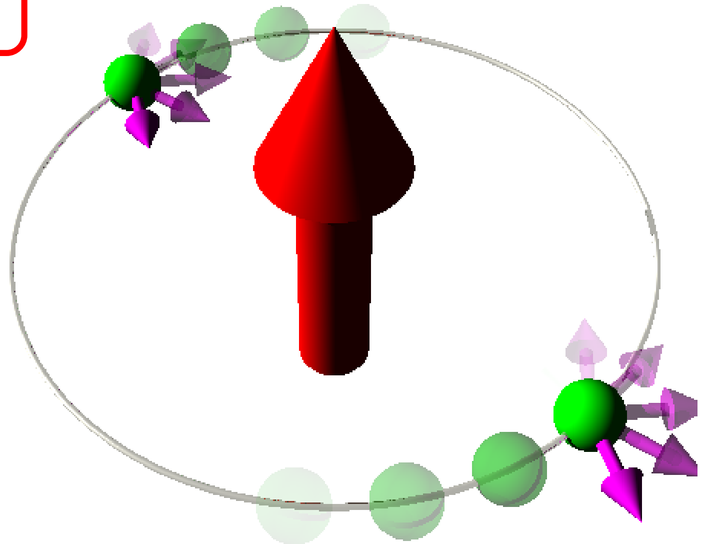
atomic spin-orbit interaction on Ru site
pin *d*-vector to c-axis $H_a \sim 0.015$[T]

▪Dipole-dipole interaction of Cooper pairs
Y. Hasegawa: J. Phys. Soc. Jpn. **72**(2003) 2456

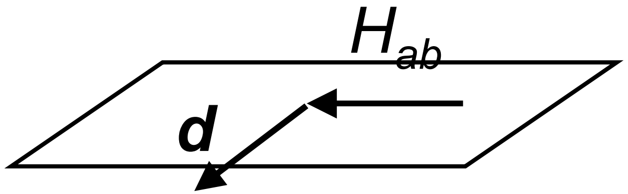
pin *d*-vector to c-axis $H_a \sim 0.019$[T]

0.015 + 0.019 = 0.034 [T]

The Knight shift for an external magnetic field (H || c) less than 0.034[T] should decrease across the T_C if the d-vector were fixed to the c-axis.



What is the mechanism which pins the *d*-vector in the *ab*-plane

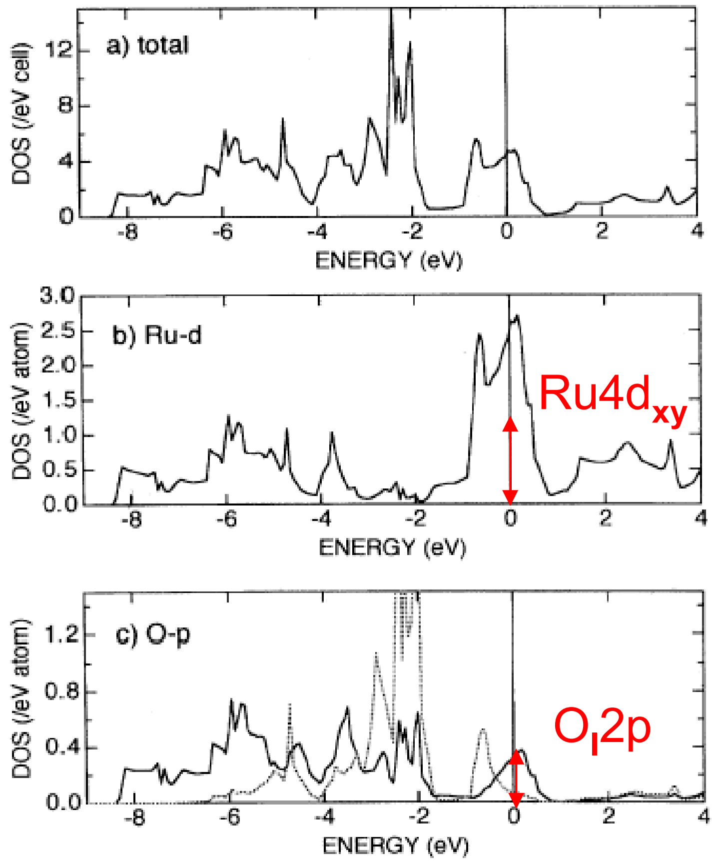


→ Calculation based on the *d*-*p* model

- We first discuss the microscopic mechanism of the superconductivity in Sr_2RuO_4 on the basis of the *d*-*p* model.
- We also calculate the effect of the atomic spin-orbit interaction on the *d*-vector starting from the *d*-*p* model.

Specialty of Sr_2RuO_4 based 4d electrons

Band structure calculation



T. Oguchi: PRB 51 (1995) 1385.

Appreciable weight of 2p-component remaining at Fermi level

$$\frac{N_{\mathrm{F}}(\mathrm{O_I}2p)}{N_{\mathrm{F}}(\mathrm{Ru}4d)} \simeq \boxed{0.17}$$

$$\frac{N_{\mathrm{F}}(\mathrm{O_I}2p)}{N_{\mathrm{F}}(\mathrm{Ru}4d_{xy})} \simeq \boxed{0.34}$$

Roles of oxygen cannot be eliminated

Necessity of d-p model beyond Hubbard model

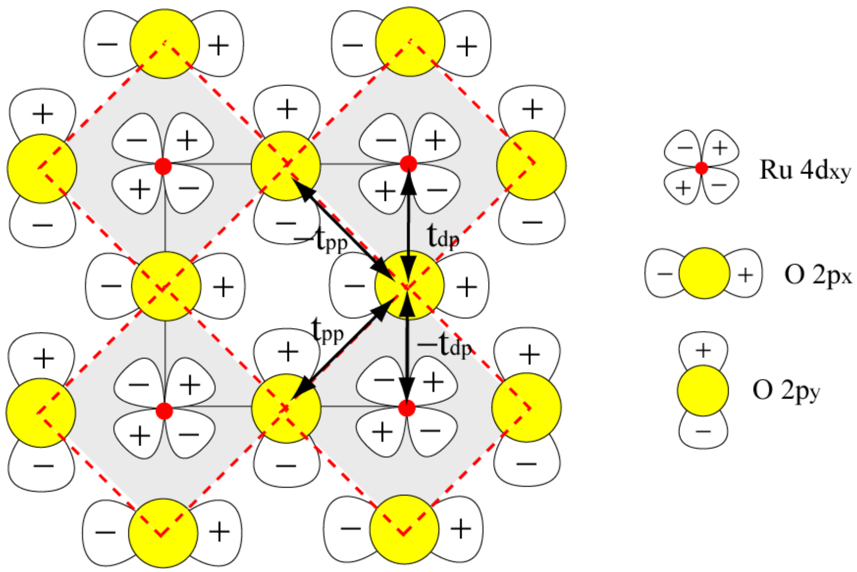
What kind of roles expected ?

d-p model

Hoshihara & Miyake:J. Phys. Soc. Jpn. **74**(2005)2679

2nd order perturbation calculation

$$H_{dp} = \sum_{<i,j>\sigma} (t_{dp} d^{+}_{i\sigma} p_{j\sigma} + h.c.) + \sum_{<i,j>\sigma} (t_{pp} p^{+}_{i\sigma} p_{j\sigma} + h.c.) + U_{dd} \sum_{i} d^{+}_{i\uparrow} d^{+}_{i\downarrow} d_{i\downarrow} d_{i\uparrow} + U_{pp} \sum_{i} p^{+}_{i\uparrow} p^{+}_{i\downarrow} p_{i\downarrow} p_{i\uparrow}$$



U_{pp} cannot be reduced by correlation among 4d electrons (on-site correlation)

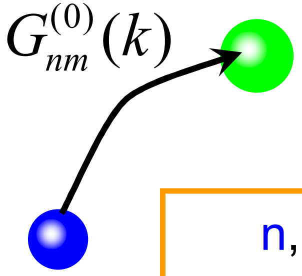
Interaction between (γ -band) quasi-particles

$$\mathcal{H}_{\rm int} = \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \tilde{J}_{\mathbf{k},\mathbf{k}';\mathbf{q}} a^{\dagger}_{\mathbf{k}+\mathbf{q}\uparrow} a^{\dagger}_{\mathbf{k}'-\mathbf{q}\downarrow} a_{\mathbf{k}'\downarrow} a_{\mathbf{k}\uparrow}$$

$\tilde{J}_{\mathbf{k},\mathbf{k}';\mathbf{q}}$: interaction intricately depends on wave vectors.

$$\tilde{J}_{\mathbf{k},\mathbf{k}';\mathbf{q}} = U_{\mathbf{k},\mathbf{k}';\mathbf{q}} + J_{\mathbf{k},\mathbf{k}';\mathbf{q}} + J_{\mathbf{k}',\mathbf{k};\mathbf{k}-\mathbf{k}'+\mathbf{q}}$$

➡ Fast Fourier Transformation (FFT) method is not available



$n,m = d_{xy}, p_x, p_y$

a,b = quasi particle

$$
\begin{aligned}
G_{nm}^{(0)}(k) &= -T_\tau \langle c_{nk\sigma} c_{mk\sigma}^\dagger \rangle \\
&= \sum_{ab} -T_\tau \langle a_{ak\sigma} a_{bk\sigma}^\dagger \rangle U_{na}(\mathbf{k}) U_{mb}^*(\mathbf{k}) \\
&= \sum_{a} U_{na}(\mathbf{k}) U_{ma}^*(\mathbf{k}) G_a^{(0)}(k)
\end{aligned}
$$

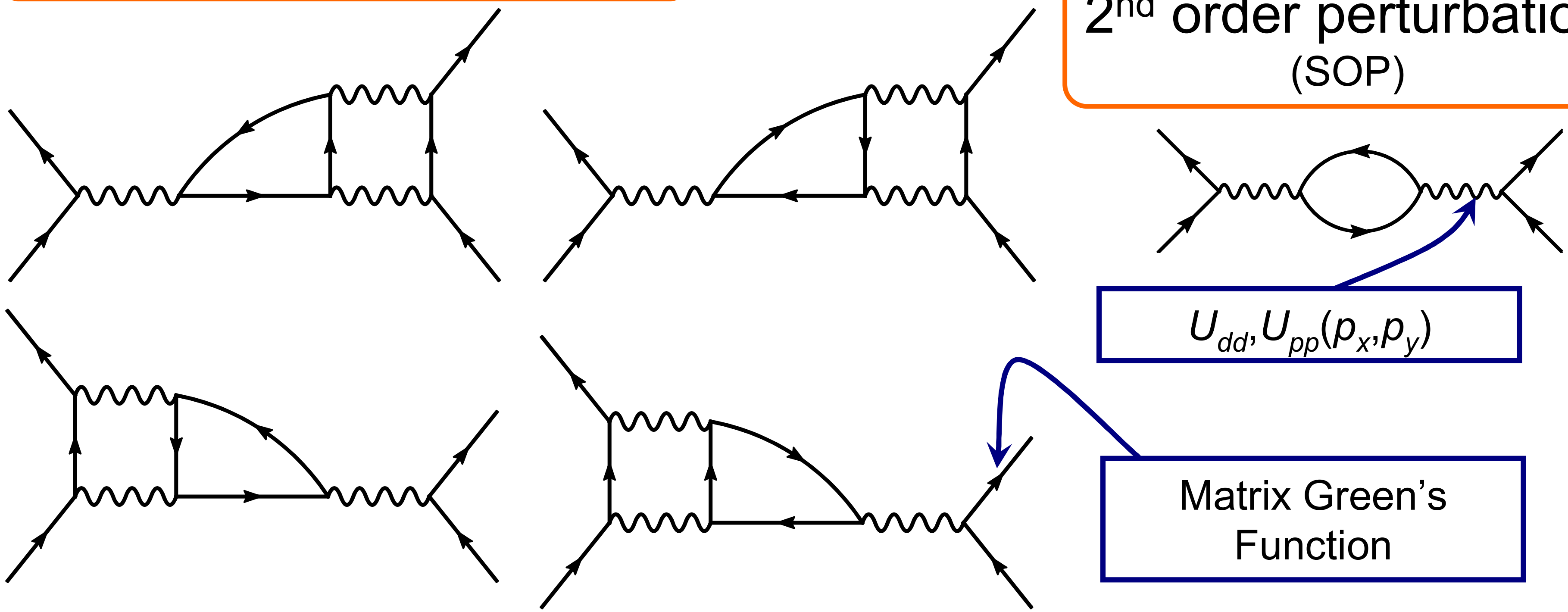
➡ Matrix Green function enables us to use FFT method.

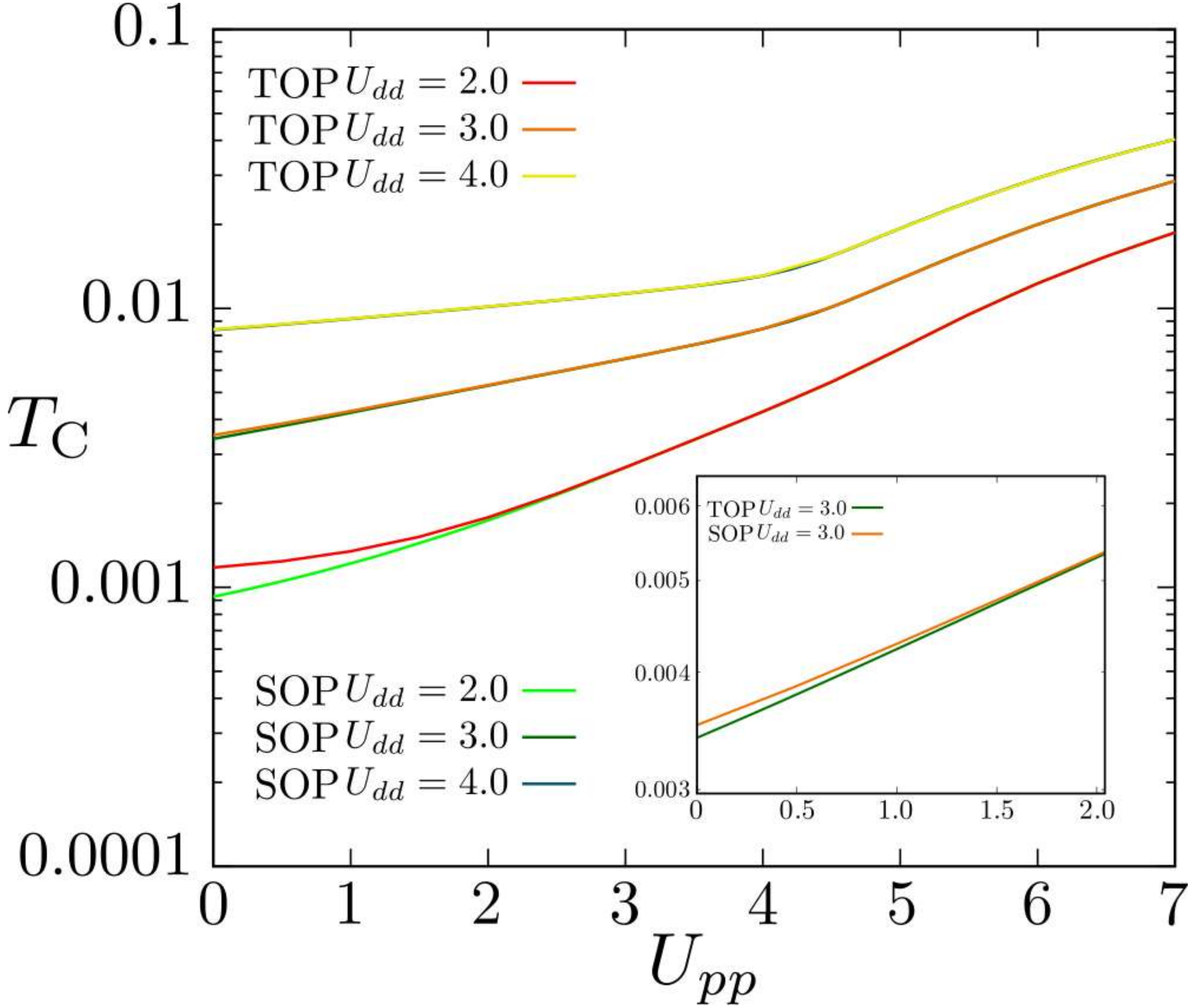
Interaction between equal-spin electrons

cf. Nomura &Yamada : J. Phys. Soc. Jpn. **69**(2000)3678

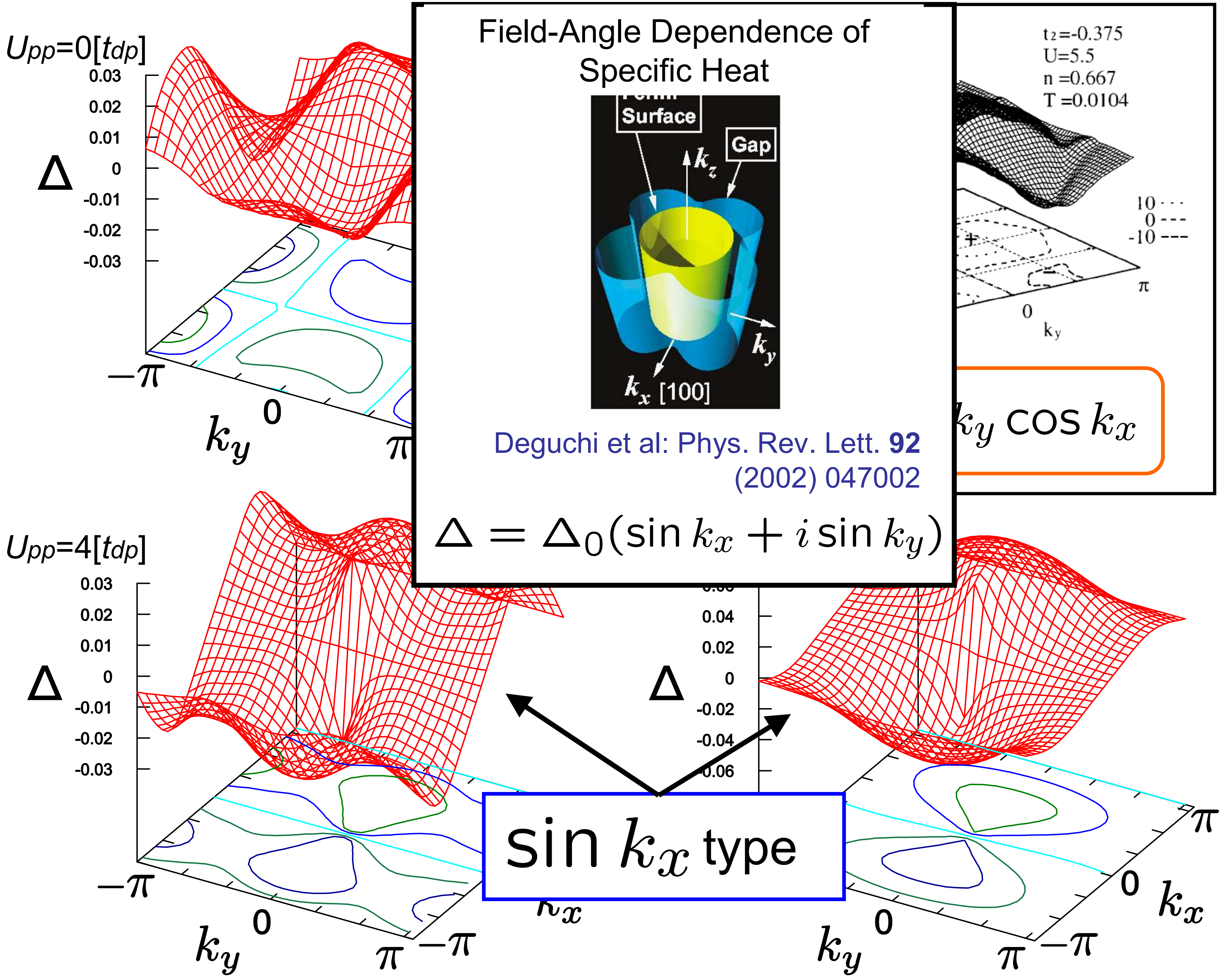
3rd order perturbation (TOP)

2nd order perturbation (SOP)





- Spin-triplet state is stabilized even within 2nd order perturbation (SOP), and we could not obtain sufficient $T_{\rm C}$ for spin-singlet state.
- $T_{\rm C}$ increases monotonically as U_{pp} increases.



Field-Angle Dependence of Specific Heat
Fermi Surface
Gap
k_z
k_y
k_x [100]
Deguchi et al: Phys. Rev. Lett. **92** (2002) 047002
$\Delta = \Delta_0(\sin k_x + i \sin k_y)$
U_{pp}=0[t_{dp}]
U_{pp}=4[t_{dp}]
Δ
0.03
0.02
0.01
0
-0.01
-0.02
-0.03
0.04
-0.04
-0.06
$-\pi$
0
π
k_y
k_x
t2=-0.375
U=5.5
n =0.667
T =0.0104
10
0
-10
$k_y \cos k_x$
$\sin k_x$ type

Anisotropy of d-vector due to atomic spin-orbit and Hund's rule coupling

To violate SU(2) symmetry in the spin space, namely to make a difference between $V_{\uparrow\uparrow}$ and $V_{\uparrow\downarrow}$, we introduce the atomic spin-orbit interaction λ up to second order and Hund-coupling J_H up to first order.

$$V_{\uparrow\uparrow} < V_{\uparrow\downarrow} \qquad\qquad V_{\uparrow\uparrow} > V_{\uparrow\downarrow}$$

d* || *c   ***d* ⊥ c**

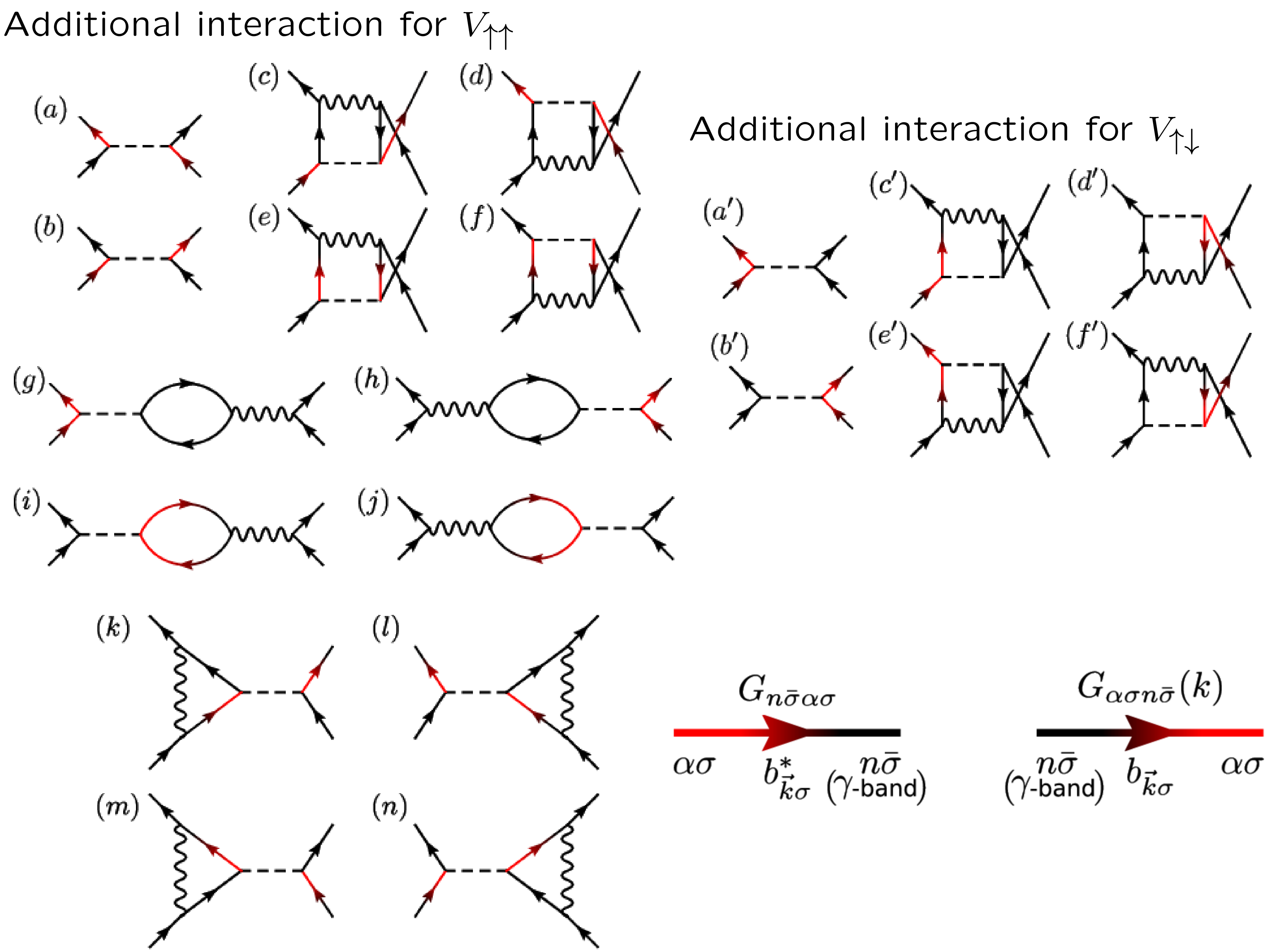
M. Ogata: J. Phys. Chem. Solids **63** (2002) 1329
K. K. Ng and M. Sigrist: Europhys. Lett. **49** (2000) 473

Hamiltonian at Ru site

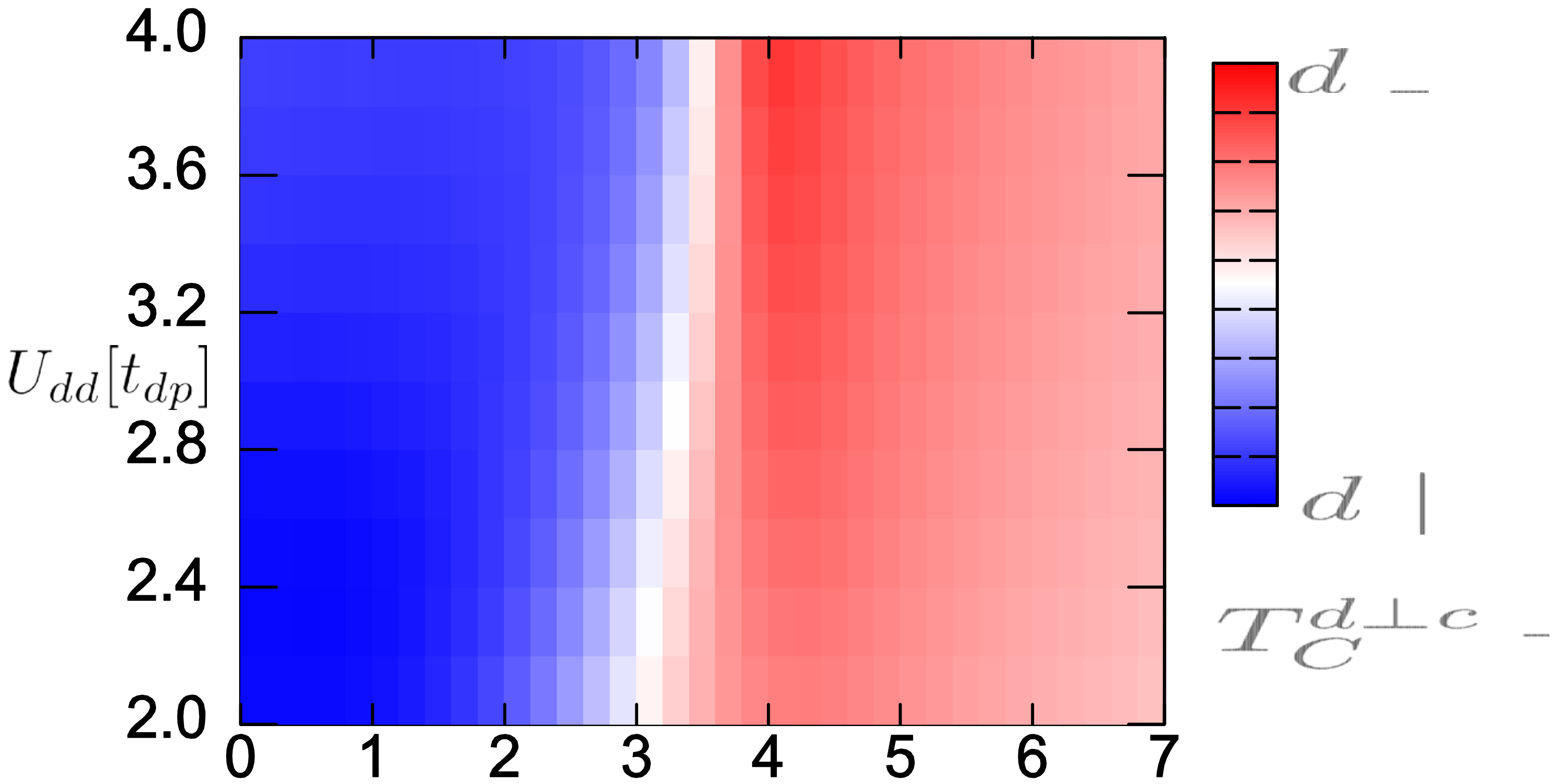
$$H_{4d} = \begin{pmatrix} c^{\dagger}_{k\alpha\sigma} & c^{\dagger}_{k\beta\sigma} & c^{\dagger}_{k\gamma-\sigma} \end{pmatrix} \begin{pmatrix} \varepsilon_{\alpha} & -i\sigma\frac{\lambda}{2} & b_{k\sigma} \\ i\sigma\frac{\lambda}{2} & \varepsilon_{\beta} & i\sigma b_{k\sigma} \\ b^{*}_{k\sigma} & -i\sigma b^{*}_{k\sigma} & \varepsilon_{\gamma} \end{pmatrix} \begin{pmatrix} c_{k\alpha\sigma} \\ c_{k\beta\sigma} \\ c_{k\gamma-\sigma} \end{pmatrix}$$

Green function containing α - and β -bands

e.g. $G_{\alpha\uparrow\gamma\downarrow}(k) = b_{k\uparrow} G_{\alpha}(k) G_{\gamma}(k)$



Additional interaction for $V_{\uparrow\uparrow}$
(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
(i)
(j)
(k)
(l)
(m)
(n)
Additional interaction for $V_{\uparrow\downarrow}$
(a′)
(b′)
(c′)
(d′)
(e′)
(f′)
$G_{n\bar{\sigma}\alpha\sigma}$
$\alpha\sigma$
$b^*_{\vec{k}\sigma}$
$n\bar{\sigma}$
(γ-band)
$G_{\alpha\sigma n\bar{\sigma}}(k)$
$n\bar{\sigma}$
(γ-band)
$b_{\vec{k}\sigma}$
$\alpha\sigma$



In agreement with recent experiment of Knight shift

d $\perp$ **c** in large U_{pp} region.
strength of anisotropy H_a ~ 0.01T~ 0.05T

cf. anisotropy due to dipole interaction H_a ~ 0.019T

Conclusion 1

- On d-p model with Upp, we calculated pairing interaction up to the 3rd order perturbation and the T_C of the superconductivity.
  - In contrast to the Hubbard model
    - The spin-triplet state is stable even within SOPT
    - sin k_x type gap structure is obtained
- Introducing the spin-orbit interaction and Hund coupling to the *d-p* model, we obtained the result that the *d*-vector can be perpendicular to the *c*-axis, in consistent with the recent Knight shift measurements.

% Anomalous NQR Relaxation by internal Josephson effect due to pair spin-orbit interaction

K. Miyake: JPSJ **79** (2010) 024714.

Spin-orbit interaction due to relative motion of quasiparticles near Fermi level

$$H_{\rm so} = -\frac{\mu_{\rm B}^2}{\hbar}\frac{m_{\rm band}}{m^*}\sum_i\sum_{j\neq i}\frac{1}{r_{ij}^3}\vec{\sigma}_i\cdot[\vec{r}_{ij}\times[(2\bar{g}-1)\vec{p}_i-2\bar{g}\vec{p}_j]]$$

Two Ward-Pitaevskii idenities:

$$-\frac{m_{\rm band}}{m^* a}(\mathrm{i}\vec{\nabla}_p\times\mathbf{p}) = -(\mathrm{i}\vec{\nabla}_p\times\mathbf{p})+\frac{\mathrm{i}}{2}\int\frac{\mathrm{d}^4q}{(2\pi)^4}\Gamma^k_{\alpha\beta,\alpha\beta}(p,q)\{G(q)(\mathrm{i}\vec{\nabla}_q\times\mathbf{q})G(q)\}_k$$

$$\frac{1}{a}\sigma_{\alpha\beta} = \sigma_{\alpha\beta} - \mathrm{i}\int\frac{d^4q}{(2\pi)^4}\sigma_{\xi\eta}\{G_\xi(q)G_\eta(q)\}_\omega\Gamma^\omega_{\eta\xi,\beta\alpha}(q,p)$$

2nd quantization representation:

$$H_{\rm so} = -\frac{\mu_{\rm B}^2}{\hbar}\frac{m_{\rm band}}{m^*}\int\int\mathrm{d}\mathbf{r}_1\mathrm{d}\mathbf{r}_2\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|^3}\psi^\dagger_\alpha(\mathbf{r}_1)\psi^\dagger_\gamma(\mathbf{r}_2)\vec{\sigma}_{\alpha\beta}\delta_{\gamma\delta} \cdot\left[(\vec{r}_1-\vec{r}_2)\times(-\mathrm{i}\hbar)\left((2\bar{g}-1)\vec{\nabla}_1-2\bar{g}\vec{\nabla}_2\right)\right]\psi_\delta(\mathbf{r}_2)\psi_\beta(\mathbf{r}_1)$$

$$H_{\rm so} = -\frac{\mu_{\rm B}^2}{\hbar}\frac{m_{\rm band}}{m^*}\int\int\mathrm{d}\mathbf{R}\mathrm{d}\mathbf{r}\frac{1}{r^3}\psi^\dagger_\alpha(\mathbf{R}+\mathbf{r}/2)\psi^\dagger_\gamma(\mathbf{R}-\mathbf{r}/2)\vec{\sigma}_{\alpha\beta}\delta_{\gamma\delta} \cdot\left[\vec{r}\times(-\mathrm{i}\hbar)\left((4\bar{g}-1)\vec{\nabla}_r-\frac{1}{2}\vec{\nabla}_R\right)\right]\psi_\delta(\mathbf{R}-\mathbf{r}/2)\psi_\beta(\mathbf{R}+\mathbf{r}/2)$$

Mean-field type decoupling approximation

$$\begin{aligned}&\langle\psi^\dagger_\alpha(\mathbf{R}+\mathbf{r}/2)\psi^\dagger_\gamma(\mathbf{R}-\mathbf{r}/2)\psi_\delta(\mathbf{R}-\mathbf{r}/2)\psi_\beta(\mathbf{R}+\mathbf{r}/2)\rangle\\ &\quad\simeq\langle\psi^\dagger_\alpha(\mathbf{R}+\mathbf{r}/2)\psi^\dagger_\gamma(\mathbf{R}-\mathbf{r}/2)\rangle\langle\psi_\delta(\mathbf{R}-\mathbf{r}/2)\psi_\beta(\mathbf{R}+\mathbf{r}/2)\rangle\\ &\quad=\langle\psi^\dagger_\alpha(\mathbf{r}/2)\psi^\dagger_\gamma(-\mathbf{r}/2)\rangle\langle\psi_\delta(-\mathbf{r}/2)\psi_\beta(\mathbf{r}/2)\rangle.\end{aligned}$$

Free energy for pair spin-orbit interaction

$$F_{\rm so}\equiv\langle H_{\rm so}\rangle=-\frac{\mu_{\rm B}^2}{\hbar}\frac{m_{\rm band}}{m^*}(4\bar{g}-1)V\int{\rm d}\mathbf{r}\frac{1}{r^3}\vec{\sigma}_{\alpha\beta}\delta_{\gamma\delta}\cdot F^*_{\gamma\alpha}(\mathbf{r})[\vec{r}\times(-{\rm i}\hbar)\vec{\nabla}_r)]F_{\delta\beta}(\mathbf{r})$$

$$F_{\delta\beta}(\mathbf{r})\equiv\langle\psi_\delta(\mathbf{r}/2)\psi_\beta(-\mathbf{r}/2)\rangle={\rm i}(\vec{\sigma}\sigma_2)_{\alpha\beta}\cdot\vec{F}(\mathbf{r})$$

$$\boxed{F_{\rm so}=-g_{\rm so}({\rm i}\vec{d}\times\vec{d}^*)\cdot\vec{L}}\qquad g_{\rm so}=\mu_{\rm B}^2\frac{m_{\rm band}}{m^*}(4\bar{g}-1)4\pi\Psi^2V$$

Free energy for dipole-dipole interaction

$$F_{\rm d}=-\frac{3c}{4a\pi}g_{\rm d}\left[(\vec{d}\cdot\vec{L})^2-\frac{1}{3}\right]\qquad a(=3.87\text{Å})\ \text{and}\ c(=6.37\text{Å})$$

$$g_{\rm d}=\frac{\pi}{2}\mu_{\rm eff}^2\Psi^2=\frac{\pi}{2}\bar{g}^2\mu_{\rm B}^2\Psi^2$$

Hasegawa: JPSJ **72** (2003) 2456

Condensation energy in GL region

$$F_{\mathrm{GL}} = \frac{1}{2}\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)\left[-\left(1-\frac{T}{T_{\mathrm{c}}}\right)\frac{\Delta_\uparrow^2+\Delta_\downarrow^2}{2} + \frac{7\zeta(3)}{16}\frac{\kappa}{(\pi k_{\mathrm{B}}T_{\mathrm{c}})^2}\frac{\Delta_\uparrow^4+\Delta_\downarrow^4}{2}\right]$$

$$F_{\mathrm{cond}}^{\mathrm{unit}} = -\frac{1}{4}\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)\frac{8}{7\zeta(3)}\frac{1}{\kappa}(\pi k_{\mathrm{B}}T_{\mathrm{c}})^2\left(1-\frac{T}{T_{\mathrm{c}}}\right)^2$$

Spin-orbit coupling in GL region

$$g_{\mathrm{d}} = \frac{\pi}{8}\mu_{\mathrm{eff}}^2\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)^2\frac{8}{7\zeta(3)}\frac{1}{\kappa}(\pi k_{\mathrm{B}}T_{\mathrm{c}})^2\left[\ln(1.14\beta_{\mathrm{c}}\epsilon_{\mathrm{c}})\right]^2\left(1-\frac{T}{T_{\mathrm{c}}}\right)$$

$$\frac{g_{\mathrm{so}}}{|F_{\mathrm{cond}}^{\mathrm{unit}}|} = \frac{m_{\mathrm{band}}}{m^*}\frac{(4\bar{g}-1)}{\bar{g}^2}4\pi\mu_{\mathrm{B}}^2\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)\left[\ln(1.14\beta_{\mathrm{c}}\epsilon_{\mathrm{c}})\right]^2\left(1-\frac{T}{T_{\mathrm{c}}}\right)^{-1}$$

Gap structure in equilibrium

$$\hat{\Delta} = \frac{\Delta_0}{\sqrt{1+\eta^2}}\begin{pmatrix}-1-\eta & 0\\ 0 & 1-\eta\end{pmatrix}$$

$$d_{0x} = \frac{1}{\sqrt{1+\eta^2}} \quad d_{0y} = \mathrm{i}\frac{\eta}{\sqrt{1+\eta^2}}$$

$$d_{0z} = 0$$

weakly non-unitary

Total free energy in the GL region

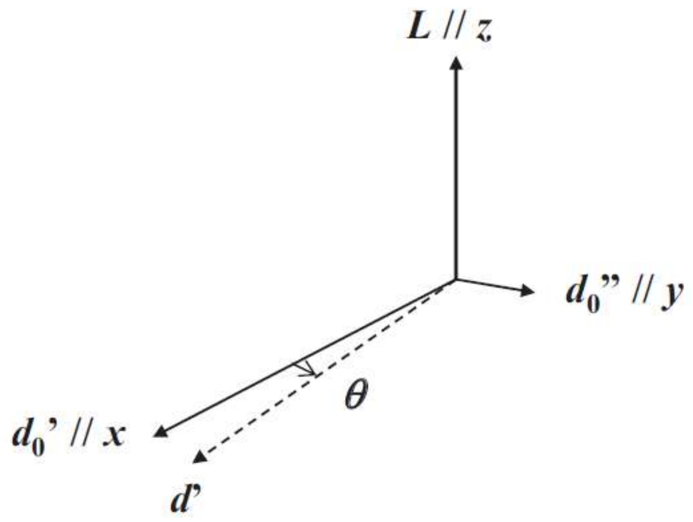
$$F(\eta) = -g_{\mathrm{so}}\frac{2\eta}{1+\eta^2} + |F_{\mathrm{cond}}^{\mathrm{unit}}|\frac{4\eta^2}{(1+\eta^2)^2}$$

$$\Delta F_{\mathrm{cond}} = |F_{\mathrm{cond}}^{\mathrm{unit}}|\frac{4\eta^2}{(1+\eta^2)^2}$$

$$F_{\mathrm{so}} = -g_{\mathrm{so}}\frac{2\eta}{1+\eta^2}$$

Internal Josephson Oscillations

$$\hat{\Delta} = \Delta_0 \begin{pmatrix} (-1-\eta)e^{-i\theta} & 0 \\ 0 & (1+\eta)e^{i\theta} \end{pmatrix}$$



$$F_{\rm so}(\theta) = -g_{\rm so}(2\eta)\cos\theta$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(N_\uparrow - N_\downarrow) = -\frac{1}{\hbar}\frac{\partial F_{\rm so}}{\partial(2\theta)} = -\frac{g_{\rm so}\eta}{\hbar}\sin\theta$$

$$\frac{\mathrm{d}}{\mathrm{d}t}(2\theta) = 2\Delta\mu = \frac{2\mu_{\rm B}^2/\hbar}{\chi_z}(N_\uparrow - N_\downarrow)$$

$$\Omega^2 = \frac{g_{\rm so}(\mu_{\rm B}/\hbar)^2}{\chi_z}\eta = \frac{g_{\rm so}(\mu_{\rm B}/\hbar)^2}{\chi_z}\frac{g_{\rm so}}{4|F_{\rm cond}|}$$

$$g_{\rm so} = \frac{m_{\rm band}}{m^*} 8 \frac{(4\bar{g}-1)}{\bar{g}^2}\frac{\pi}{8}\mu_{\rm B}^2\left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)^2 \frac{8}{7\zeta(3)}\frac{1}{\kappa}(\pi k_{\rm B}T_{\rm c})^2\left[\ln(1.14\beta_{\rm c}\epsilon_{\rm c})\right]^2\left(1-\frac{T}{T_{\rm c}}\right)$$

$$\chi_z = (1+F_0^a)^{-1}\mu_{\rm B}^2(\mathrm{d}n/\mathrm{d}\epsilon)$$

$$\Omega \simeq 4.3\times 10^7\sqrt{(1+F_0^a)/\kappa}\,T_{\rm c}\frac{m_{\rm band}}{m} \quad [\mathrm{sec}^{-1}]$$

Energy due to magnetic field

$$\Delta F_{\rm magn} = \frac{1}{\kappa}\frac{1-\frac{T}{T_{\rm c}}}{1+F_0^{\rm a}}\chi_z H^2$$

$$= \frac{1}{\kappa}\frac{1-\frac{T}{T_{\rm c}}}{(1+F_0^{\rm a})^2}\mu_{\rm B}^2\left(\frac{{\rm d}n}{{\rm d}\epsilon}\right)H^2$$

Energy due to pair spin-orbit coupling

$$F_{\rm so} = -g_{\rm so}\frac{2\eta}{1+\eta^2}$$

$$g_{\rm so} = \frac{m_{\rm band}}{m^*}8\frac{(4\bar{g}-1)}{\bar{g}^2}\frac{\pi}{8}\mu_{\rm B}^2\left(\frac{{\rm d}n}{{\rm d}\epsilon}\right)^2\frac{8}{7\zeta(3)}\frac{1}{\kappa}(\pi k_{\rm B}T_{\rm c})^2\left[\ln(1.14\beta_{\rm c}\epsilon_{\rm c})\right]^2\left(1-\frac{T}{T_{\rm c}}\right)$$

$$H_{\rm a}^{\rm so(2)} \simeq 1.2\times 10\left(1-\frac{T}{T_{\rm c}}\right)^{-1/2} \quad [\text{gauss}]$$

d ⊥c

In the limit of $T \to T_{\rm c}$

$$H_{\rm a}^{\rm so(2)} \simeq 6.4\times 10^2 \quad [\text{gauss}]$$

Energy due to dipole-dipole interaction

$$\frac{(3c/4a\pi)g_{\rm d}}{\Delta F_{\rm magn}} \simeq 0.39\times 10^4\frac{1}{H^2}(1+F_0^a)^2\frac{m^*}{m}T_{\rm c}^2 \simeq 3.6\times 10^4\frac{1}{H^2} \quad [\text{gauss}^{-2}]$$

$$H_{\rm a}^{\rm dd} \simeq 1.9\times 10^2 \quad [\text{gauss}]$$

d // c

Anisotropy field due to one-body spin-orbit coupling can win dipole-dipole term

NQR relaxation rate due to internal Josephson oscillations

$$\chi_z(\omega) = -\frac{\Omega^2 \chi_z}{\omega^2 - \Omega^2 + \mathrm{i}\Gamma\omega}$$

Leggett & Takagi: Ann. Phys. **106** (1977) 79

$$\Gamma = \gamma_0 \tau \Omega^2$$

$$\gamma_0 \equiv [1 - Y(T)]^{-1} Y(T) \frac{\chi_z}{\mu_\mathrm{B}^2 \left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right)}$$

$$\frac{1}{T_1 T} = \frac{A}{\mu_\mathrm{B}^2} \sum_{q<q_c} \frac{\mathrm{Im}\chi_z(q,\omega)}{\omega}$$

$$q_c^* \sim r(\pi/\xi_0)$$

$$\frac{\mathrm{Im}\chi_z(\omega)}{\omega} = \chi_z \frac{\gamma_0 \tau}{\left[\left(\frac{\omega}{\Omega}\right)^2 - 1\right]^2 + (\gamma_0 \omega \tau)^2}$$

$$\tau = b\frac{\hbar T_\mathrm{F}}{k_\mathrm{B} T^2} = 7.6 \times 10^{-12} b \frac{T_\mathrm{F}}{T^2}$$

$$\left(\frac{1}{T_1 T}\right)_{\mathrm{S(J)}} \simeq \frac{A}{\mu_\mathrm{B}^2} \chi_z \frac{\pi}{4} n_\mathrm{L} c r^2 \left(\frac{a}{\xi_0}\right)^2 \frac{\gamma_0 \tau}{1 + (\gamma_0 \omega \tau)^2}.$$

$$\frac{\xi_0}{a} = 1.1 \times 10^{-1} \frac{T_\mathrm{F}}{T_\mathrm{c}} \qquad \frac{T_\mathrm{F}}{T_\mathrm{c}} \simeq 2.5 \times 10^3 \qquad \left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right) \simeq \frac{1}{c} \frac{n_{2d}}{k_\mathrm{B} T_\mathrm{F}}$$

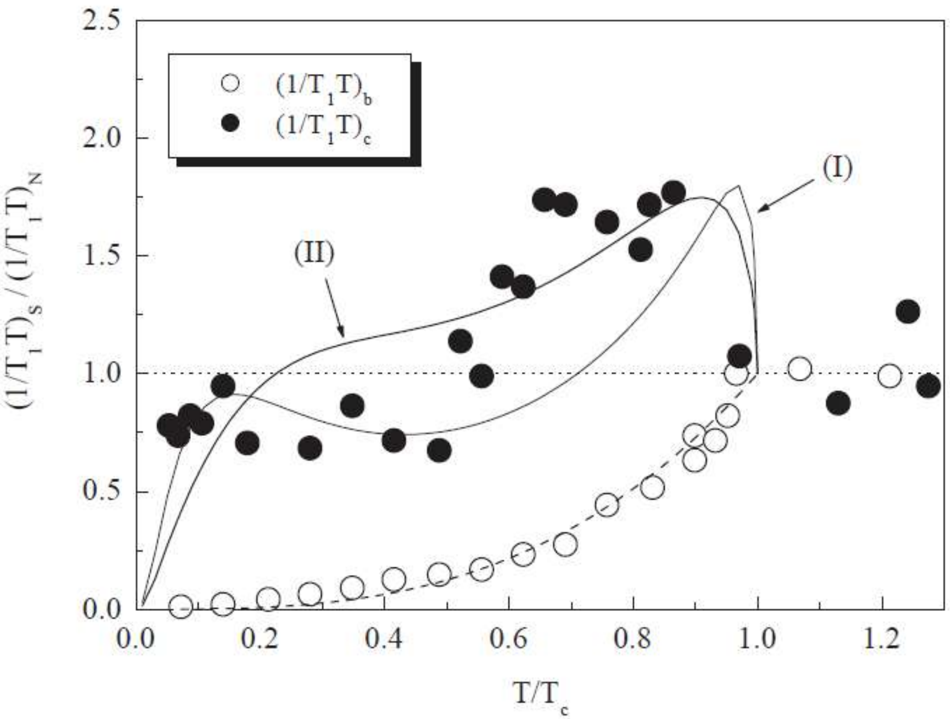
$$\left(\frac{1}{T_1 T}\right)_{\mathrm{S(J)}} = 6.5 \times 10 \frac{A}{\mu_\mathrm{B}^2} \frac{n_\mathrm{L} c^2}{n_{2d}} b r^2 \chi_z \hbar \left(\frac{\mathrm{d}n}{\mathrm{d}\epsilon}\right) \left(\frac{T_\mathrm{c}}{T}\right)^2 \frac{\gamma_0}{1 + (\gamma_0 \omega \tau)^2}$$

NQR relaxation rate in normal state

$$\left(\frac{1}{T_1 T}\right)_{\rm N} = A\frac{1}{4}\frac{\chi_z}{\mu_{\rm B}^2}\frac{\hbar\left(\frac{{\rm d}n}{{\rm d}\epsilon}\right)}{1+F_0^{\rm a}}\frac{q_{\rm c}}{k_{\rm F}}n_{\rm L}c^2a^2$$

$$\frac{(1/T_1T)_{\rm S(J)}}{(1/T_1T)_{\rm N}} = \frac{6.5\times 10}{(q_{\rm c}/k_{\rm F})a^2 n_{2d}}br^2 4(1+F_0^a)\left(\frac{T_{\rm c}}{T}\right)^2\frac{\gamma_0}{1+(\gamma_0\omega\tau)^2}$$

Two independent parameters $C \equiv \frac{6.5\times 10}{(q_{\rm c}/k_{\rm F})a^2 n_{2d}}br^2 \quad D \equiv 0.39\frac{b}{T_{\rm c}}$



$$(1/T_1T)_{\rm S} = (1/T_1T)_{\rm S(J)} + (1/T_1T)_{\rm S(Q)}$$

(I) $C = 0.2,\ D = 0.44$

(II) $C = 0.55,\ D = 1.0$

Mukuda, Ishida et al:

Phys. Rev. B **65** (2002) 132507

Conclusion 2

- It is shown that the SO coupling works only in the equal-spin pairing (ESP) state to make the pair angular momentum **L** and the pair spin angular momentum i **dxd*** parallel with each other.

- The SO coupling gives rise to the internal Josephson effect in a chiral ESP state as in superfluid A-phase of ^{3}He with a help of an additional anisotropy arising from SO coupling of atomic origin which works to direct the d-vector into ab-plane.

- This resolves the problem of the anomalous relaxation of ^{17}O-NQR and the structure of d-vector in Sr_2RuO_4.

Meaning of spin-orbit coupling for Cooper pairing

Gap structure of spin triplet state

$$\hat{\Delta}(k) = i\left(\sum_{\mu} d^{\mu}(k)\hat{\sigma}_{\mu}\right)\hat{\sigma}_y = \begin{bmatrix} -d_x(k)+id_y(k) & d_z(k) \\ d_z(k) & d_x(k)+id_y(k) \end{bmatrix}$$

Γ	J, J_z	$d(k)$
Γ_1^-	0, 0	$\hat{x}k_x + \hat{y}k_y$
Γ_2^-	1, 0	$\hat{x}k_y - \hat{y}k_x$
Γ_3^-	2, ±2	$\hat{x}k_x - \hat{y}k_y$
Γ_4^-	2, ±2	$\hat{x}k_y + \hat{y}k_x$
Γ_5^-	1, ±1	$\hat{z}(k_x \pm ik_y)$

Broken time reversal by μSR measurement

Rice & Sigrist: J. Phys.: Condens. Matter **7** (1995) L643

Fundamental assumption of group theoretical argument in the case of strong "pair" spin-orbit interaction – orbital and spin space are transformed simultaneously

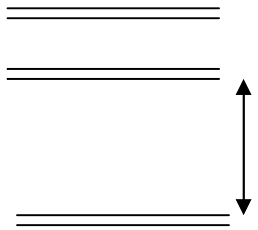
$$[\hat{R}\mathbf{d}(\mathbf{k})]_i = \sum_j R_{ij} d_j(\hat{R}\mathbf{k})$$

$\hat{R}$: crystal group transformation

This assumption is apparently broken if the "pair" spin-orbit coupling is negligibly small. Then, a question is what the condition of "pair" spin-orbit is strong enough to assure the above assumption is.

Point: strong **one-body** spin-orbit coupling does not necessarily imply strong **"pair"** spin-orbit coupling.

cf. In Ce-based heavy fermion systems with CEF of order 100K, one-body atomic spin-orbit coupling has already been used to form quasiparticles which are specified by the label of Kramers doublet of CEF ground state. Relevant "pair" spin-orbit coupling is estimated to be negligibly small: K. Miyake, Springer Series in Solid State Sciences 62, p.256



$\Delta \sim 100\mathrm{K} \gg E_{\mathrm{F}}^{*} \sim 10\mathrm{K} \gg T_{\mathrm{C}} \sim 1\mathrm{K}$

Group theoretical arguments:

Anderson, Volovik & Gorkov, Ueda & Rice, Blount (1984)

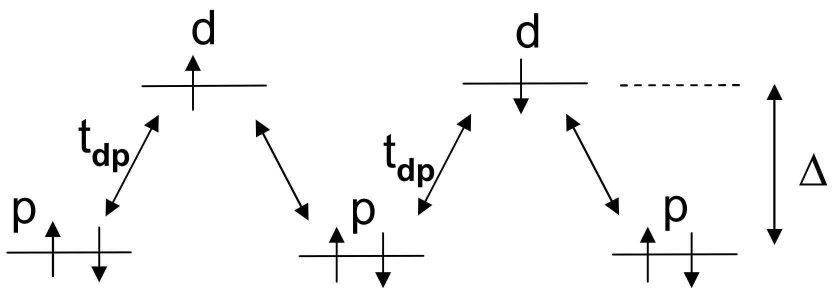
In any odd parity state, gap can vanish only at point(s) if the "pair" spin-orbit interaction is strong enough.

Counter example: UPt_3

Tou et al: PRL **77** (1996) 1374.
PRL **80** (1998) 3129.

Relation between d-p & Hubbard model

d-p model



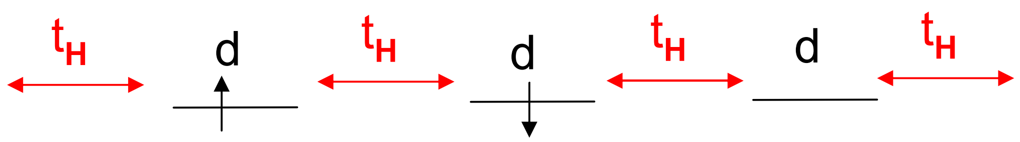
$t_{dp} << \Delta$

condition for p-degrees of freedom to be eliminated

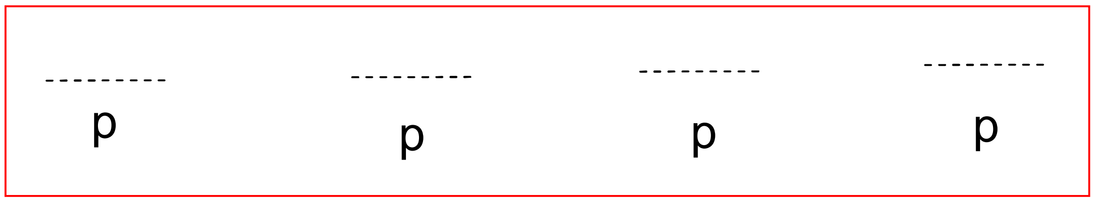
Hubbard model

$t_H = t_{dp}^2/\Delta$

Effective transfer in Hubbard model

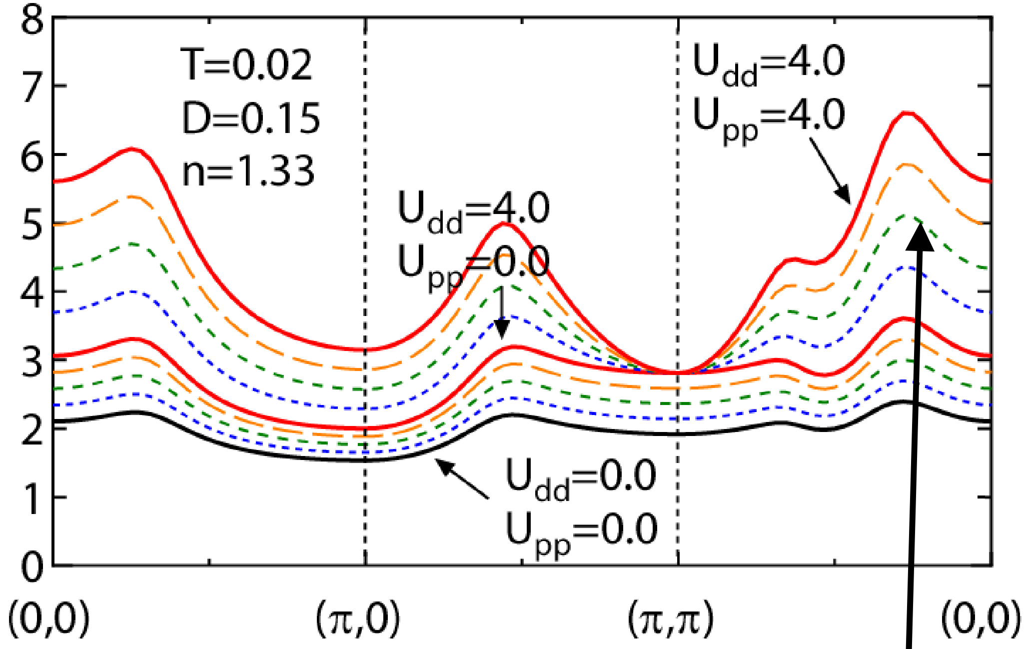


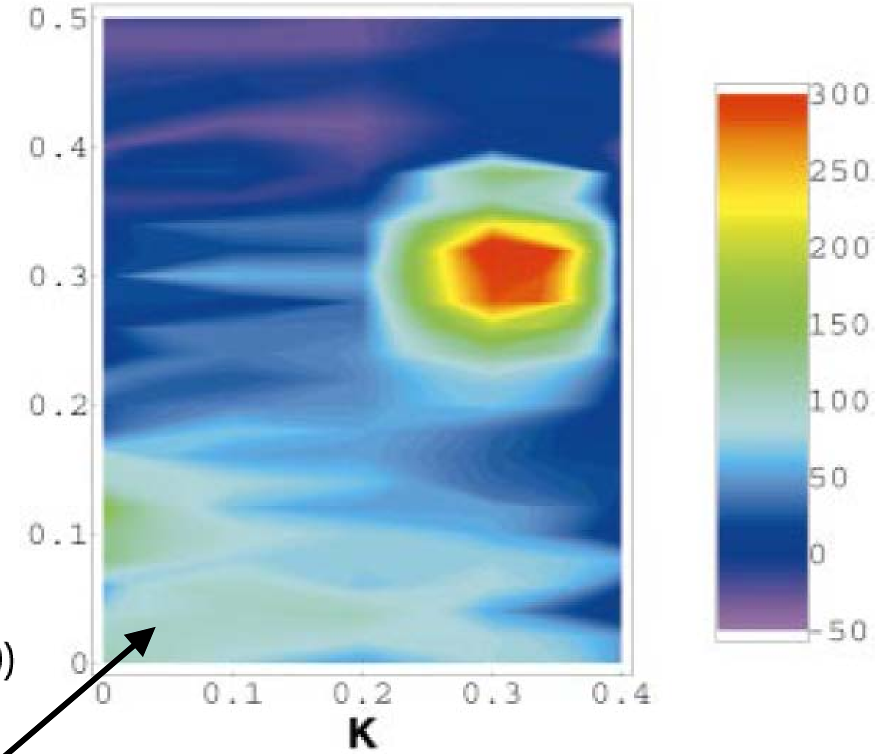
weight of p-orbital at Fermi level
$\sim t_{dp}/\Delta << 1$



"p-degrees of freedom eliminated"

$\chi_\perp(\mathbf{q},0)$ 1st order in U_{dd} and U_{pp}





Broad peak at q=(0,0)

M. Braden et al: Phys. Rev. B **66**, 064522 (2002)