Interplay of valence and magnetic fluctuations in heavy fermions

3d

or

Super-exchange ferromagnetic correlations in Ruthenate

– Origin of triplet superconductivity in Sr2RuO4 –

2d

YKIS 2007

"Interaction and Nanostructural Effects
in Low-Dimensional Systems"

Microscopic Model for Spin-Triplet Superconductor Sr_2RuO_4

- Crucial Role of Oxygen -

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In Collaboration with

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K. Hoshihara Japan Self-Defense Navy

OUTLINE

1) Introduction for Sr_2RuO_4

2) Role of oxygen in Sr_2RuO_4

  2-a) Specialty of Sr_2RuO_4 based 4d electrons

  2-b) Coulomb repulsion U_{pp} at oxygen site

  2-c) Effect of p-orbitals on q-dependent spin susceptibility

3) Issue on anisotropy of d-vector of Sr_2RuO_4

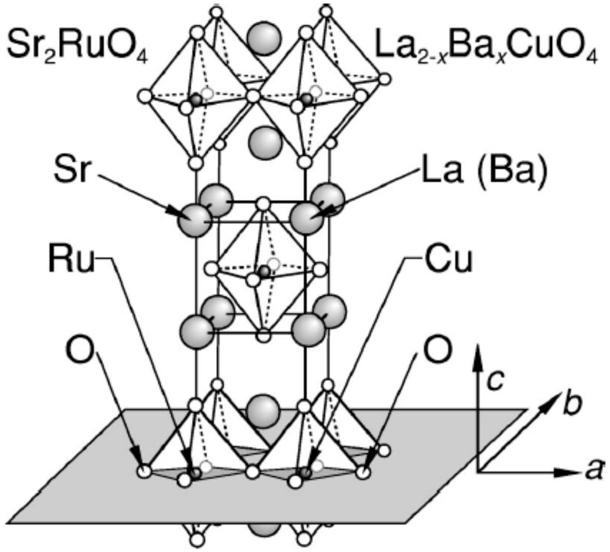
  3-a) Knight shift & anomalous relaxation in superconducting state

  3-b) Microscopic calculation

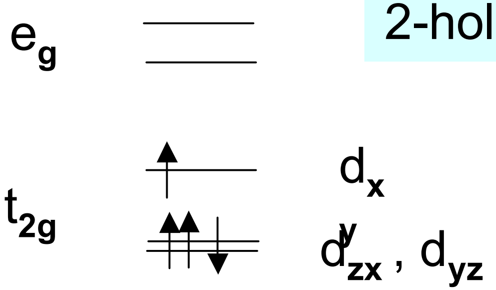
1) Introduction for Sr_2RuO_4

Crystal structure

– Isomorphic to high-Tc cuprate



CEF level scheme of Ru^{4+}



e_g

t_{2g}

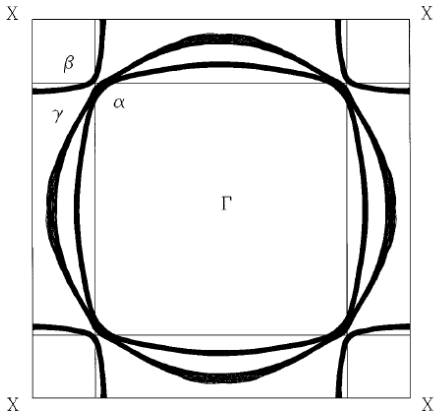
d_{xy}

d_{zx} , d_{yz}

2-holes in t_{2g}

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

Quasi-2d Fermi surface



I. I. Mazin and D. J. Singh:
PRL **79** (1997) 733.

γ - band : $d_{xy} + p_x + p_y$

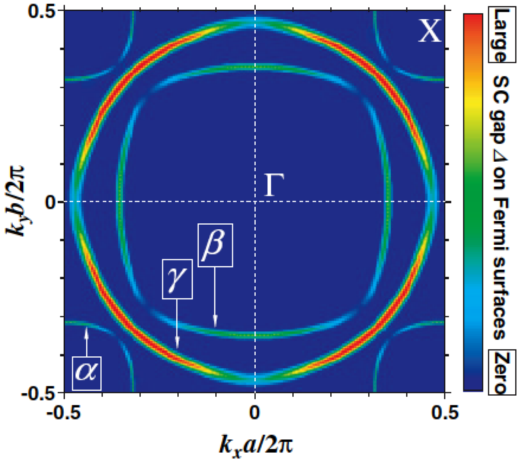
α, β - band : $d_{zx} + p_z + p_x$

& $d_{yz} + p_y + p_x$

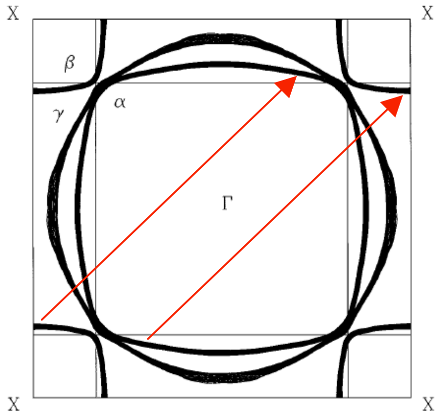
Spin-triplet superconductivity with Tc ～1.5K

Gap structure (specific heat measurement)

Order parameter: $\mathbf{d}(\mathbf{k}) = \hat{z}\Delta_0(\sin k_x \pm \mathrm{i}\sin k_y)$

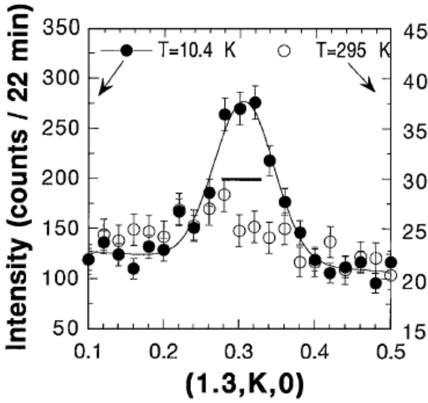


K. Deguchi et al.:
J. Phys. Soc. Jpn. **73** (2004) 1313.



I. I. Mazin and D. J. Singh:
PRL **79** (1997) 733.

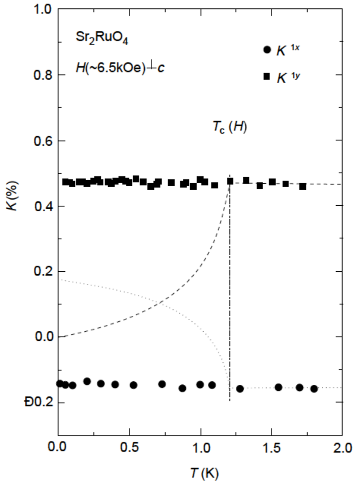
Incommensurate spin fluctuation (inelastic neutron scattering)



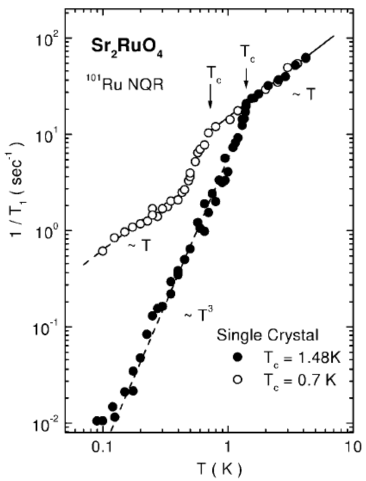
Y. Sidis et al.: PRL **83** (1999) 3320.

magnetic instability at
$\mathbf{q}_0 = (\pm 0.6\pi, \pm 0.6\pi)$

Triplet-pairing and line node gap (NMR and NQR)

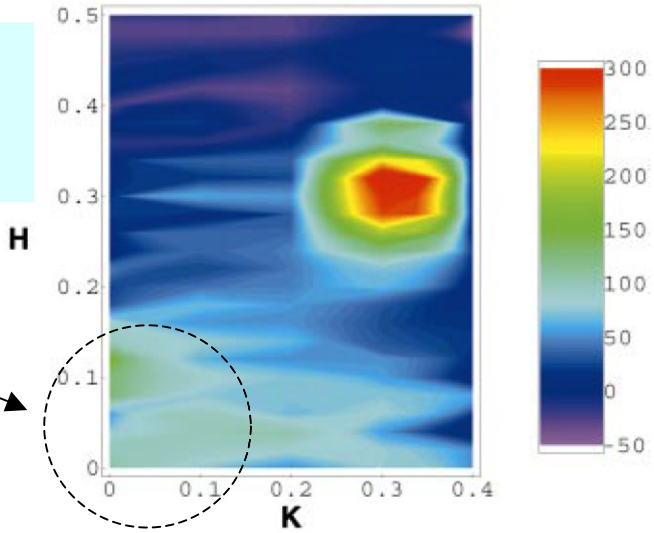


K. Ishida et al.:
Nature **396** (1998) 658.



K. Ishida et al.:
PRL **84** (2000) 5387.

Short-range
Ferromagnetic
correlation

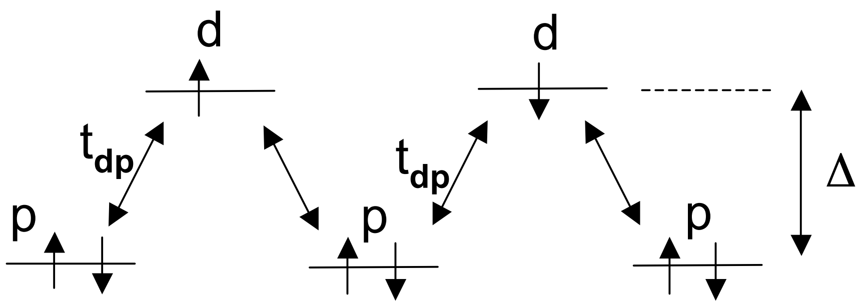


Braden et al: PRB (2002)

2) Roles of oxygen in Sr_2RuO_4

Relation between d-p & Hubbard model

d-p model



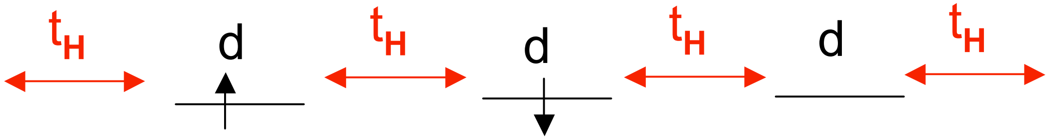
$t_{dp} << \Delta$

condition for p-degrees of freedom to be eliminated

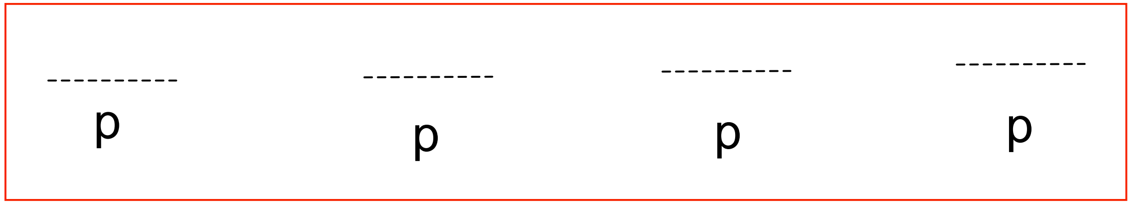
Hubbard model

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

Effective transfer
in Hubbard model



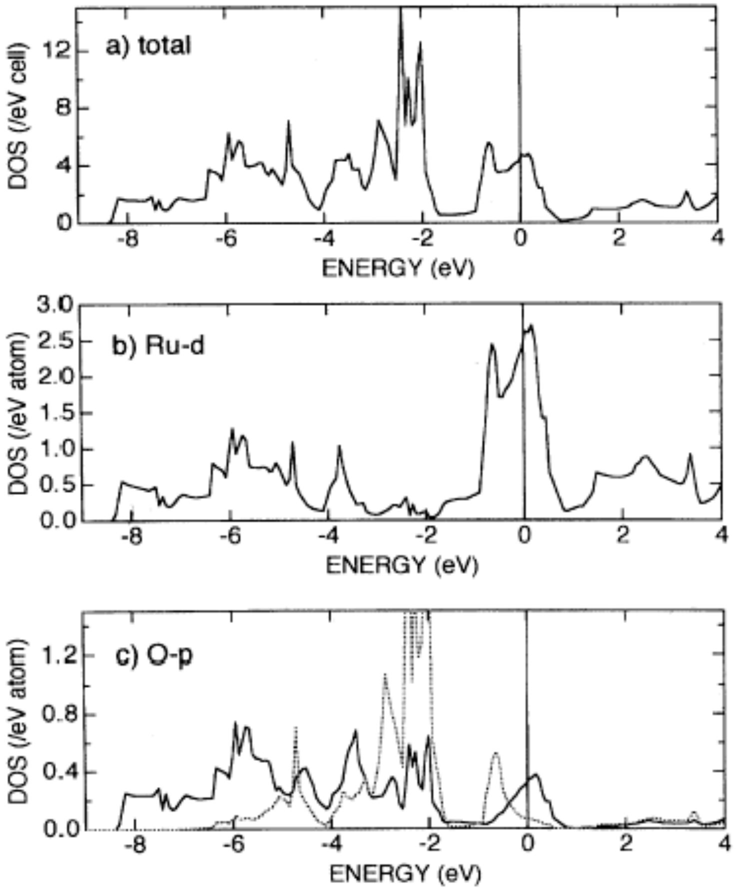
weight of p-orbital at Fermi level
$\sim t_{dp}/\Delta << 1$



**"p-degrees of freedom
Eliminated"**

2-a) 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 ?

2-b) Coulomb repulsion U_{pp} at oxygen site

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

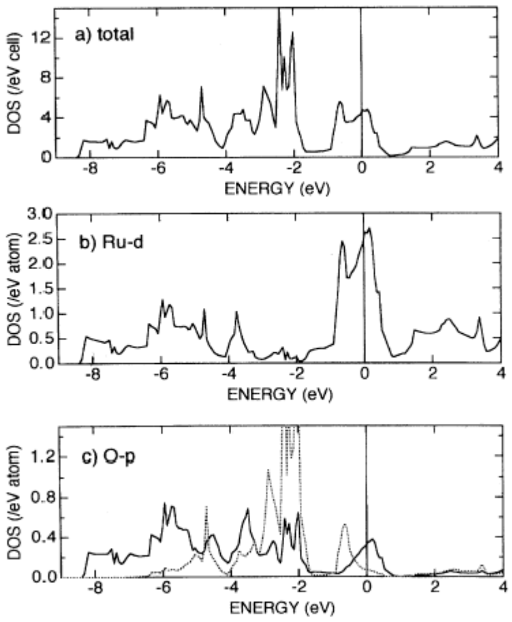
Microscopic Model: Coulomb repulsion at O site

In usual transition metal oxides, the Coulomb interaction at O site play only minor role because the weight of d-electron molecular orbital at O site small as in high-T_c cuprates.

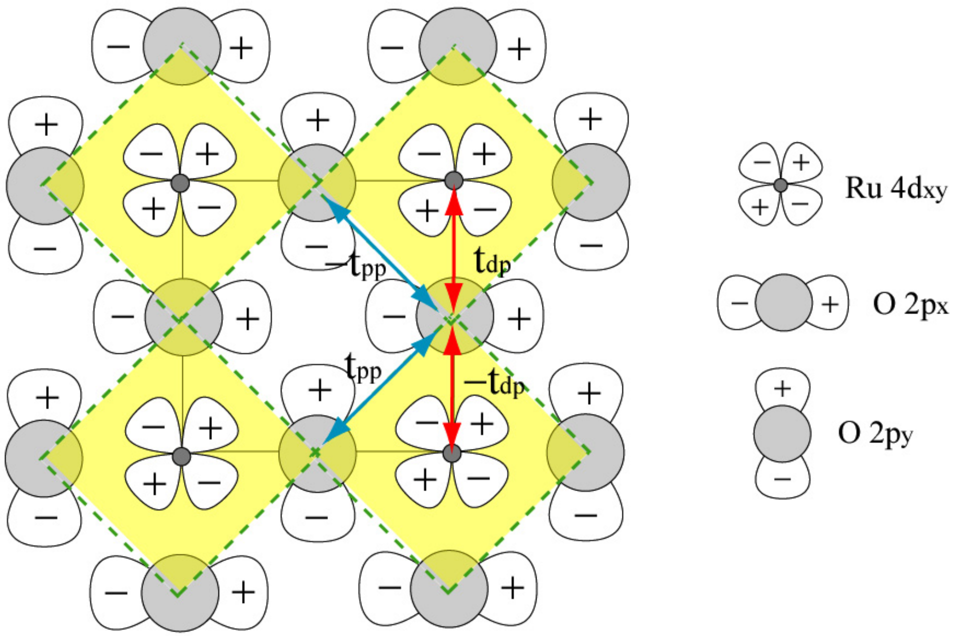
On the other hand, in Sr_2RuO_4, there seems to be a moderately strong hybridization between the wave functions of 4d-electron in Ru and 2p-electron in O, making the “d-electron”.

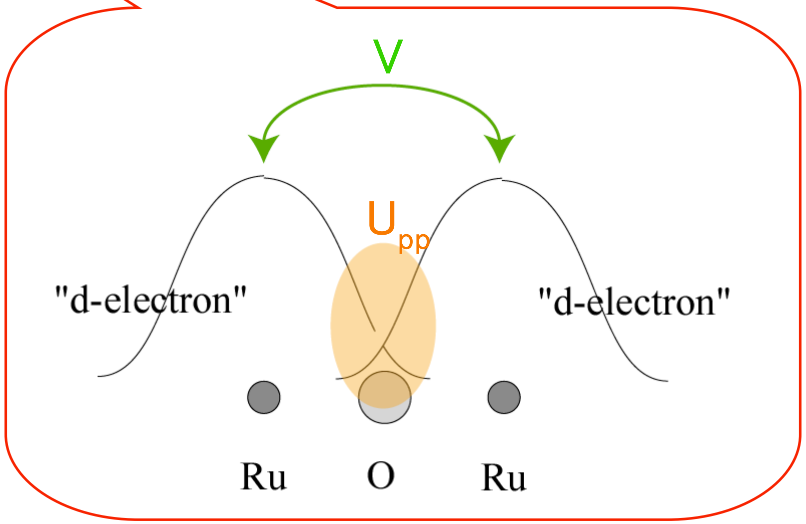
The Coulomb interaction U_{pp} at O site may not be neglected, while the direct Coulomb interaction V at the nearest-neighbor Ru sites would be negligibly small.

Band structure calculation



T. Oguchi: PRB **51** (1995) 1385.





Origin of the inter−site exchange interaction on the d−p model

Non−interacting d−p model

$$\mathcal{H}^{(0)}_{dp} = \sum_{\mathbf{k},\sigma} \left(d^\dagger_{\mathbf{k}\sigma}\ p^\dagger_{x\mathbf{k}\sigma}\ p^\dagger_{y\mathbf{k}\sigma}\right) \begin{pmatrix} \varepsilon_d & V^*_{y\mathbf{k}} & V^*_{x\mathbf{k}} \\ V_{y\mathbf{k}} & \varepsilon_p & W_\mathbf{k} \\ V_{x\mathbf{k}} & W_\mathbf{k} & \varepsilon_p \end{pmatrix} \begin{pmatrix} d_{\mathbf{k}\sigma} \\ p_{x\mathbf{k}\sigma} \\ p_{y\mathbf{k}\sigma} \end{pmatrix}$$

$$V_{m\mathbf{k}} = 2it_{dp}\sin(\tfrac{k_m}{2})$$

$$W_\mathbf{k} = 4t_{pp}\sin(\tfrac{k_x}{2})\sin(\tfrac{k_y}{2})$$

Unitary transformation

eigen−value : $\varepsilon_{i\mathbf{k}}$ eigen−vector : $\vec{u_{i\mathbf{k}}}$

$$\hat{U}_\mathbf{k} = (\vec{u}_{1\mathbf{k}}\ \vec{u}_{2\mathbf{k}}\ \vec{u}_{3\mathbf{k}}) \qquad \begin{pmatrix} d_{\mathbf{k}\sigma} \\ p_{x\mathbf{k}\sigma} \\ p_{y\mathbf{k}\sigma} \end{pmatrix} = U_\mathbf{k} \begin{pmatrix} a_{1\mathbf{k}\sigma} \\ a_{2\mathbf{k}\sigma} \\ a_{3\mathbf{k}\sigma} \end{pmatrix}$$

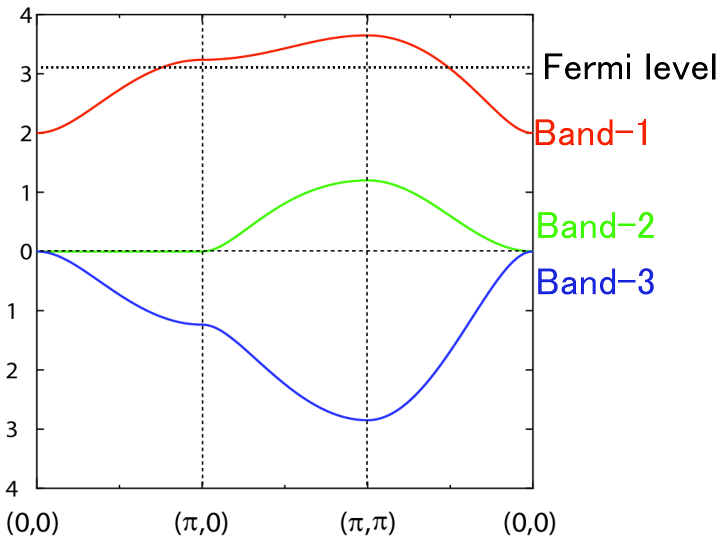
Diagonalization

$$\mathcal{H}^{(0)}_{dp} = \sum_{\mathbf{k},\sigma} \left(a^\dagger_{1\mathbf{k}\sigma}\ a^\dagger_{2\mathbf{k}\sigma}\ a^\dagger_{3\mathbf{k}\sigma}\right) \begin{pmatrix} \varepsilon_{1\mathbf{k}} & 0 & 0 \\ 0 & \varepsilon_{2\mathbf{k}} & 0 \\ 0 & 0 & \varepsilon_{3\mathbf{k}} \end{pmatrix} \begin{pmatrix} a_{1\mathbf{k}\sigma} \\ a_{2\mathbf{k}\sigma} \\ a_{3\mathbf{k}\sigma} \end{pmatrix}$$

Band−1 forms the Fermi surface.

$$a_{1\mathbf{k}\sigma}\ ,\ \varepsilon_{1\mathbf{k}}\ ,\ D_{1\mathbf{k}} \longrightarrow a_{\mathbf{k}\sigma}\ ,\ \varepsilon_\mathbf{k}\ ,\ D_\mathbf{k}$$

We restrict our discussion within the γ−band. Namely, we consider only d_{xy}−electrons.



$$d_{\mathbf{k}\sigma} = \frac{\varepsilon_{1\mathbf{k}}}{D_{1\mathbf{k}}}a_{1\mathbf{k}\sigma} + \frac{\varepsilon_{2\mathbf{k}}}{D_{2\mathbf{k}}}a_{2\mathbf{k}\sigma} + \frac{\varepsilon_{3\mathbf{k}}}{D_{3\mathbf{k}}}a_{3\mathbf{k}\sigma}$$

$$p_{x\mathbf{k}\sigma} = \frac{V_{y\mathbf{k}}}{D_{1\mathbf{k}}}a_{1\mathbf{k}\sigma} + \frac{V_{y\mathbf{k}}}{D_{2\mathbf{k}}}a_{2\mathbf{k}\sigma} + \frac{V_{y\mathbf{k}}}{D_{3\mathbf{k}}}a_{3\mathbf{k}\sigma}$$

$$p_{y\mathbf{k}\sigma} = \frac{V_{x\mathbf{k}}}{D_{1\mathbf{k}}}a_{1\mathbf{k}\sigma} + \frac{V_{x\mathbf{k}}}{D_{2\mathbf{k}}}a_{2\mathbf{k}\sigma} + \frac{V_{x\mathbf{k}}}{D_{3\mathbf{k}}}a_{3\mathbf{k}\sigma}$$

$$D_{i\mathbf{k}} = (|V_{x\mathbf{k}}|^2 + |V_{y\mathbf{k}}|^2 + \varepsilon^2_{i\mathbf{k}})^{1/2}$$

Interaction terms

$$\mathcal{H}_U = U_{dd}\sum_i d^\dagger_{i\uparrow}d_{i\uparrow}d^\dagger_{i\downarrow}d_{i\downarrow} = -\frac{U_{dd}}{6}\sum_i\sum_{\alpha\beta\gamma\delta} d^\dagger_{i\alpha}d^\dagger_{i\gamma}d_{i\delta}d_{i\beta}(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta})$$

$$\mathcal{H}_{\rm ex} = U_{pp}\sum_{m,i} p^\dagger_{mi\uparrow}p_{mi\uparrow}p^\dagger_{mi\downarrow}p_{mi\downarrow} = -\frac{U_{pp}}{6}\sum_{m,i}\sum_{\alpha\beta\gamma\delta} p^\dagger_{mi\alpha}p^\dagger_{mi\gamma}p_{mi\delta}p_{mi\beta}(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta})$$

$a_{\mathbf{k}\sigma}$: The operator for the “d–electron”

$$\mathcal{H}^{(x)}_{\rm ex} = -\frac{U_{pp}}{6}\sum_{\mathbf{kk'q}}\sum_{\alpha\beta\gamma\delta}\frac{V_{x\mathbf{k+q}}V_{x\mathbf{k'-q}}V_{x\mathbf{k'}}V_{x\mathbf{k}}}{D_{\mathbf{k+q}}D_{\mathbf{k'-q}}D_{\mathbf{k'}}D_{\mathbf{k}}}a^\dagger_{\mathbf{k+q}\alpha}a^\dagger_{\mathbf{k'-q}\gamma}a_{\mathbf{k'}\delta}a_{\mathbf{k}\beta}(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta})$$

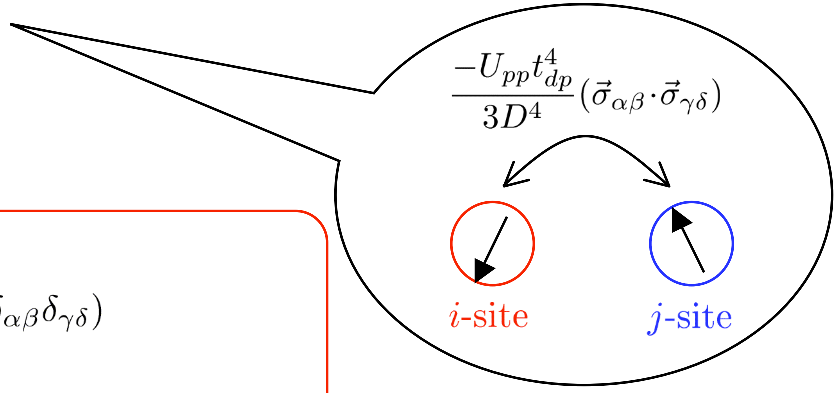
$$V_{x\mathbf{k+q}}V_{x\mathbf{k'-q}}V_{x\mathbf{k'}}V_{x\mathbf{k}}/(2{\rm i}t_{dp})^4 = \frac{1}{8}\Big\{1+\cos q_x+\cos(k_x-k'_x+q_x)+\cos(k_x+k'_x)-\cos k_x-\cos k'_x-\cos(k_x+q_x)-\cos(k'_x-q_x)\Big\}$$

Fourier transformation (k to x)

$$D_{\mathbf{k+q}}D_{\mathbf{k'-q}}D_{\mathbf{k'}}D_{\mathbf{k}} \equiv D^4 = {\rm const.}$$

$$\mathcal{H}_{\rm ex} = \frac{-U_{pp}t^4_{dp}}{3D^4}\sum_{\langle i,j\rangle}\sum_{\alpha\beta\gamma\delta}\Big\{(i,i,i,i)+(i,j,j,i)+(i,j,i,j)+(i,i,j,j)-(i,i,i,j)-(i,i,j,i)-(j,i,i,i)-(i,j,i,i)\Big\}(\vec{\sigma}_{\alpha\beta}\vec{\sigma}_{\gamma\delta})$$

$$(i,j,j,i) \equiv a^\dagger_{i\alpha}a^\dagger_{j\gamma}a_{j\delta}a_{i\beta}$$



Fourier transformation (x to k)

Effective inter–site interaction

$$\mathcal{H}_{\rm ex} = -\frac{1}{4}\sum_{\mathbf{kk'q}}\sum_{\alpha\beta\gamma\delta}J_{\mathbf{k},\mathbf{k'};\mathbf{q}}a^\dagger_{\mathbf{k+q}\alpha}a^\dagger_{\mathbf{k'-q}\gamma}a_{\mathbf{k'}\delta}a_{\mathbf{k}\beta}(\vec{\sigma}_{\alpha\beta}\cdot\vec{\sigma}_{\gamma\delta}-\delta_{\alpha\beta}\delta_{\gamma\delta})$$

$$J_{\mathbf{k},\mathbf{k'};\mathbf{q}} = \frac{2U_{pp}t^4_{dp}}{D_{\mathbf{k+q}}D_{\mathbf{k'-q}}D_{\mathbf{k'}}D_{\mathbf{k}}}\sum_m\Big\{\frac{1}{2}+\cos q_m-\cos k_m-\cos k'_m+\frac{1}{2}\cos(k_m+k'_m)\Big\}$$

In order that H_{ex} plays an important role, the ratio t_{dp}/D should not be too small.

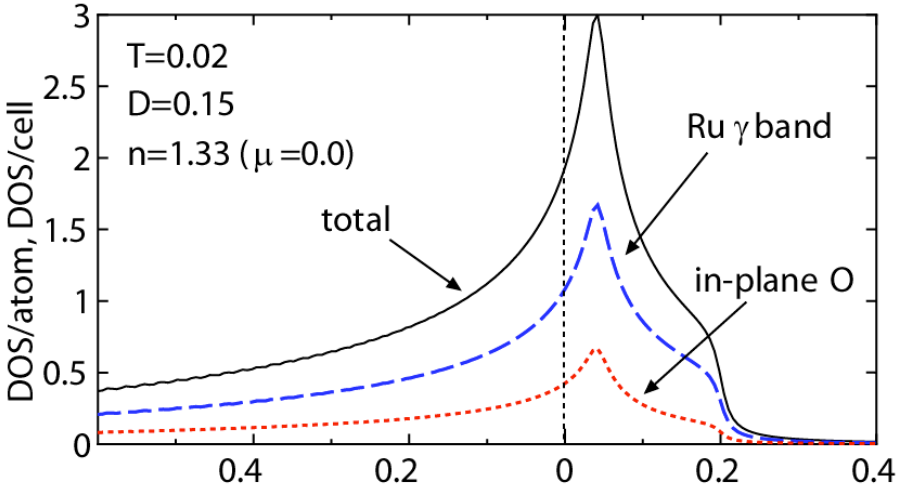
Such a condition is expected to be fulfilled in Ru−oxide, because the energy level of 4d−electron in Ru is deeper than that of 3d−electron in Fe or of 5d−electron in Os in general, and is located near that of 2p−electron in O.

This implies that there exists a moderately strong hybridization between electrons in Ru and O.

T. Oguchi: PRB **51** (1995) 1385., D. J. Singh: PRB **52** (1995) 1358.

Indeed, the partial DOS for $4d_{xy}$, $2p_x$ and $2p_y$ obtained by the band structure calculation can be reproduced in our calculation by taking **$D/t_{dp} = 0.15$ where $D = \varepsilon_d - \varepsilon_p$.**

$$t_{dp} = 1.0$$



The same procedure is applicable for H_U.

$$\mathcal{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} U_{\mathbf{k},\mathbf{k}';\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} a^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} a_{\mathbf{k}'\downarrow} a_{\mathbf{k}\uparrow} + \mathcal{H}_{\rm ex}$$

$$U_{\mathbf{k},\mathbf{k}';\mathbf{q}} = \frac{U_{dd} V_{\mathbf{k}+\mathbf{q}} V_{\mathbf{k}'-\mathbf{q}} V_{\mathbf{k}'} V_{\mathbf{k}}}{8 D_{\mathbf{k}+\mathbf{q}} D_{\mathbf{k}'-\mathbf{q}} D_{\mathbf{k}'} D_{\mathbf{k}}}$$

Complicated wave vector dependence

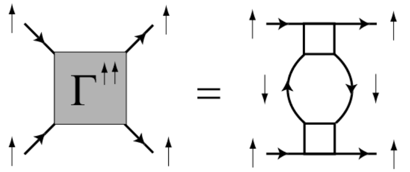
Effective Hamiltonian

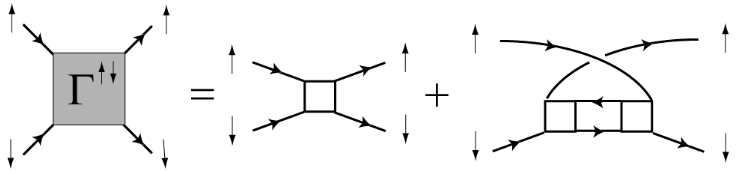
$$\mathcal{H} = \sum_{\mathbf{k},\sigma} (\varepsilon_{\mathbf{k}} - \mu) a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \widetilde{J}_{\mathbf{k},\mathbf{k}';\mathbf{q}} a^\dagger_{\mathbf{k}+\mathbf{q}\uparrow} a^\dagger_{\mathbf{k}'-\mathbf{q}\downarrow} a_{\mathbf{k}'\downarrow} a_{\mathbf{k}\uparrow}$$

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

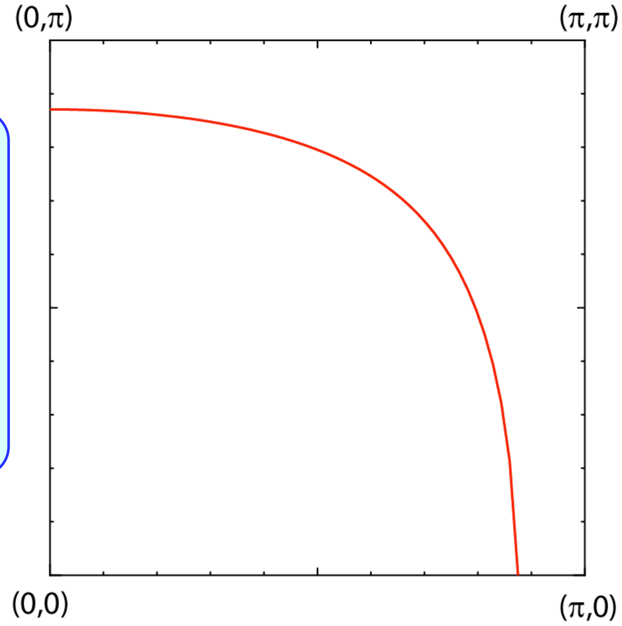
Pairing interaction up to the second order perturbation

cf. 3rd order perturbation is necessary for theory on multi-band Hubbard model
Nomura & Yamada : J. Phys. Soc. Jpn. **69** (2000) 3678





Fermi surface of the non-interacting d-p model (n=1.33)



$$\Gamma^{\uparrow\uparrow}_{\mathbf{k},\mathbf{k}'} = T\sum_{\varepsilon,\mathbf{p}} \widetilde{J}_{\mathbf{k},\mathbf{p};-\mathbf{k}+\mathbf{k}'}\widetilde{J}_{\mathbf{p}+\mathbf{k}-\mathbf{k}',-\mathbf{k};-\mathbf{k}+\mathbf{k}'}\mathcal{G}(\mathbf{p},\mathrm{i}\varepsilon)\mathcal{G}(\mathbf{p}+\mathbf{k}-\mathbf{k}',\mathrm{i}\varepsilon)$$

$$\Gamma^{\uparrow\downarrow}_{\mathbf{k},\mathbf{k}'} = \widetilde{J}_{\mathbf{k},-\mathbf{k};-\mathbf{k}+\mathbf{k}'} - T\sum_{\varepsilon,\mathbf{p}} \widetilde{J}_{\mathbf{k},\mathbf{p};\mathbf{p}+\mathbf{k}'}\widetilde{J}_{-\mathbf{k},\mathbf{p}+\mathbf{k}+\mathbf{k}';\mathbf{p}+\mathbf{k}}\mathcal{G}(\mathbf{p},\mathrm{i}\varepsilon)\mathcal{G}(\mathbf{p}+\mathbf{k}+\mathbf{k}',\mathrm{i}\varepsilon)$$

$$\mathcal{G}(\mathbf{p},\mathrm{i}\varepsilon) = \frac{1}{\mathrm{i}\varepsilon - \varepsilon_{\mathbf{p}}}$$

Pairing interaction

Spin Triplet

$$V^t_{\mathbf{k},\mathbf{k}'} = \frac{\Gamma^{\uparrow\uparrow}_{\mathbf{k},\mathbf{k}'} - \Gamma^{\uparrow\uparrow}_{\mathbf{k},-\mathbf{k}'}}{2}$$

Spin Singlet

$$V^s_{\mathbf{k},\mathbf{k}'} = \frac{\Gamma^{\uparrow\downarrow}_{\mathbf{k},\mathbf{k}'} + \Gamma^{\uparrow\downarrow}_{\mathbf{k},-\mathbf{k}'}}{2}$$

Of course, SU(2) symmetry is preserved, namely: $V^t_{\mathbf{k},\mathbf{k}'} = \frac{\Gamma^{\uparrow\uparrow}_{\mathbf{k},\mathbf{k}'} - \Gamma^{\uparrow\uparrow}_{\mathbf{k},-\mathbf{k}'}}{2} = \frac{\Gamma^{\uparrow\downarrow}_{\mathbf{k},\mathbf{k}'} - \Gamma^{\uparrow\downarrow}_{\mathbf{k},-\mathbf{k}'}}{2}$

Structure of the SC gap and transition temperature

Variational Solution

Linearized gap equation

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V^{t,s}_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{\xi_{\mathbf{k}'}} \tanh\left(\frac{\xi_{\mathbf{k}'}}{2T_c}\right)$$

Specified gaps Δ_{k} :

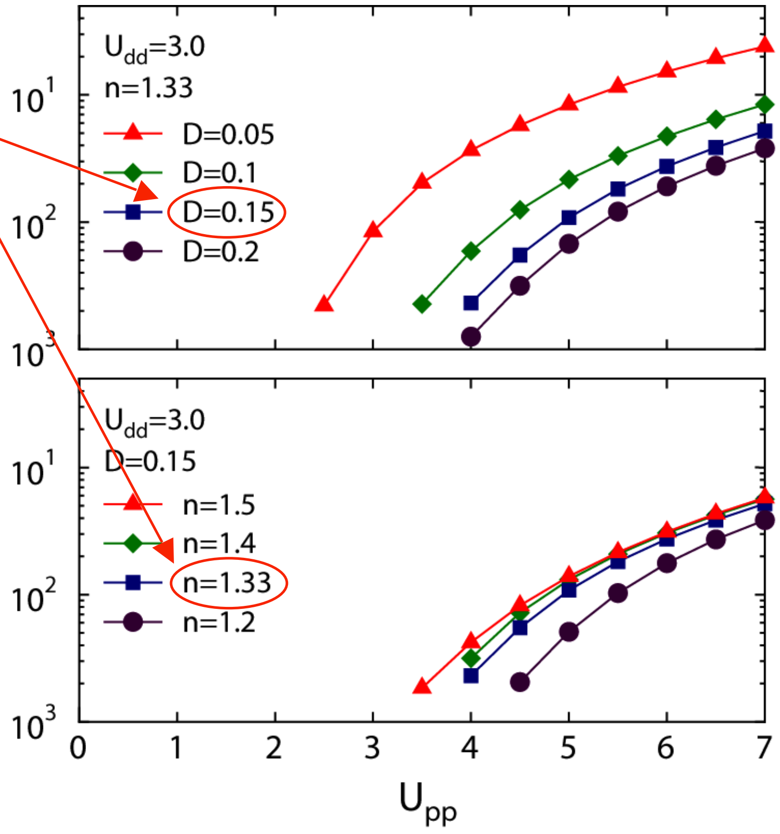
$$\boxed{\sqrt{2}\sin k_x \ \ (p_x\text{-pairing})}$$

$$\sqrt{2}\sin(k_x + k_y) \ \ (p_{x+y}\text{-pairing})$$

$$2\sin k_x \sin k_y \ \ (d_{xy}\text{-pairing})$$

$$\cos k_x - \cos k_y \ \ (d_{x^2-y^2}\text{-pairing})$$

Sr_2RuO_4 corresponds to the parameters, n=1.33, D=0.15 and a moderate value of U_{pp}.



T_c is enhanced as U_{pp} is applied and D becomes smaller.

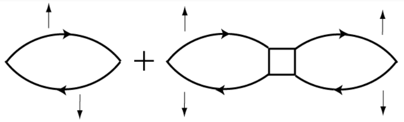
T_c is also enhanced when the system is located away from the half-filling (n=1.0).

It is noted that U_{dd} and U_{pp} are the renormalized interaction so that U_{pp}=4.0t_{dp} is not unrealistically large.

Short-range ferromagnetic correlations

Spin susceptibility including the vertex correction up to the first order perturbation

$\chi_\perp(\mathbf{q}\,,\, i\omega) =$

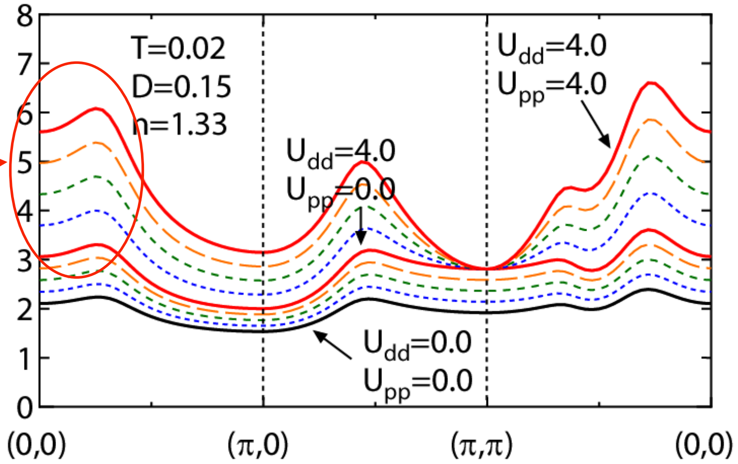


$$= -T\sum_{\varepsilon,\mathbf{p}}\Big\{1-T\sum_{\varepsilon',\mathbf{p}'}\widetilde{J}_{\mathbf{p}+\mathbf{q},\mathbf{p}';-\mathbf{p}+\mathbf{p}'}\mathcal{G}(\mathbf{p}'+\mathbf{q},i\varepsilon'+i\omega)\mathcal{G}(\mathbf{p}',i\varepsilon)\Big\}\mathcal{G}(\mathbf{p}+\mathbf{q},i\varepsilon+i\omega)\mathcal{G}(\mathbf{p},i\varepsilon)$$

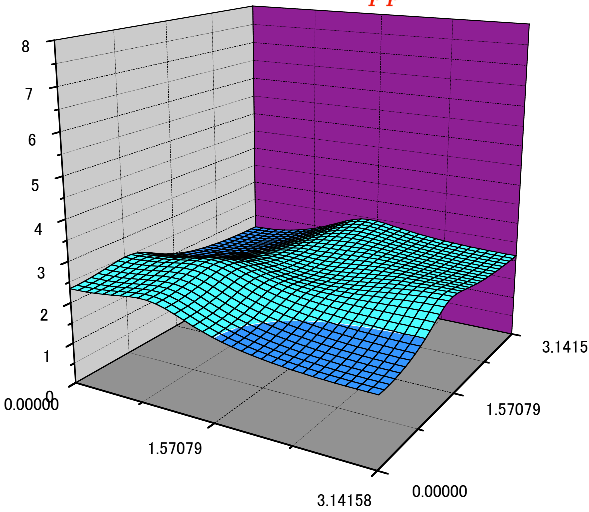
The effect of U_{dd} is to enhance the static spin susceptibility in the entire **q**-space.

Short-range ferromagnetic correlations are much enhanced by applying U_{pp}.

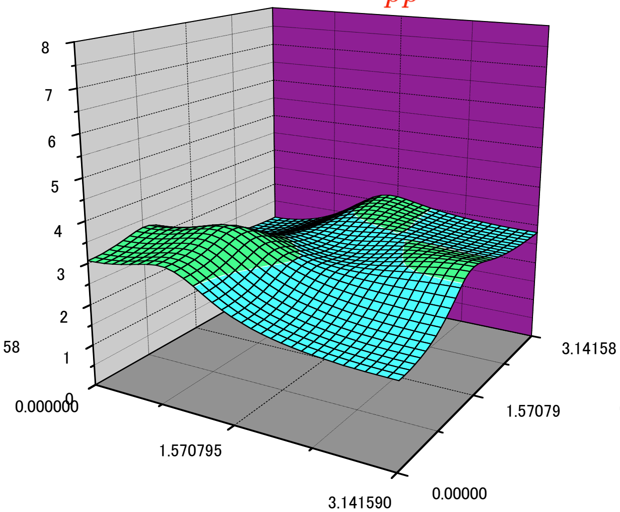
As for the results of the different electron filling, the more electrons are doped, the more the peak structure around **q**=(0,0) is enhanced.



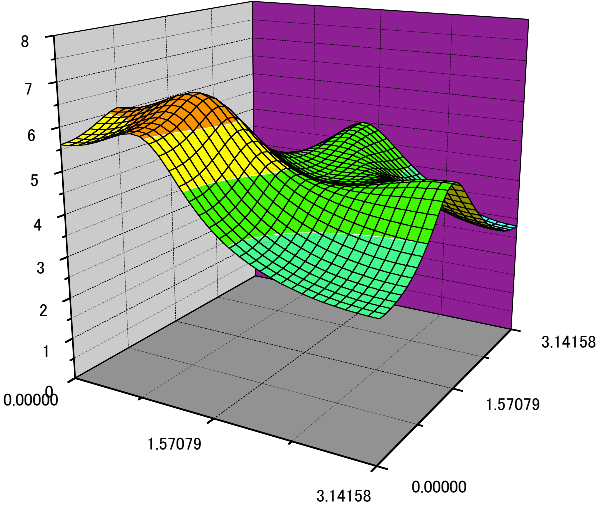
$U_{dd} = 0.0$
$U_{pp} = 0.0$

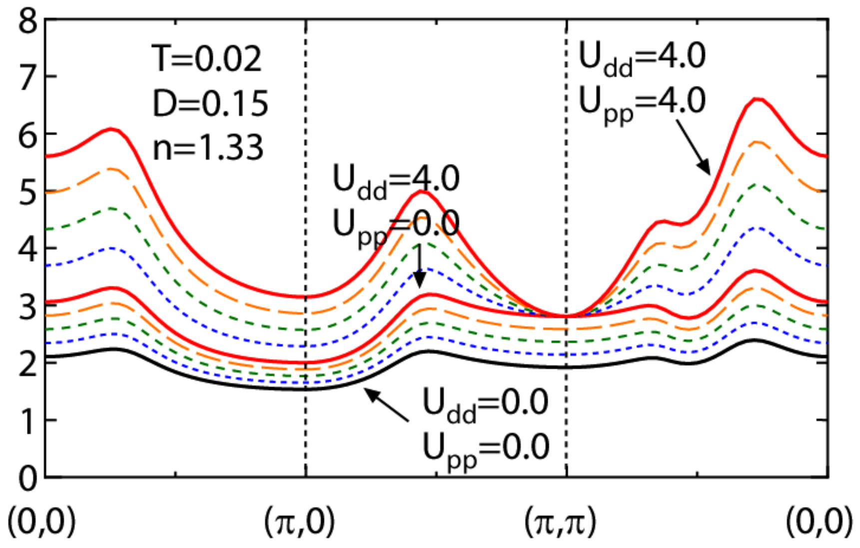


$U_{dd} = 4.0$
$U_{pp} = 0.0$



$U_{dd} = 4.0$
$U_{pp} = 4.0$



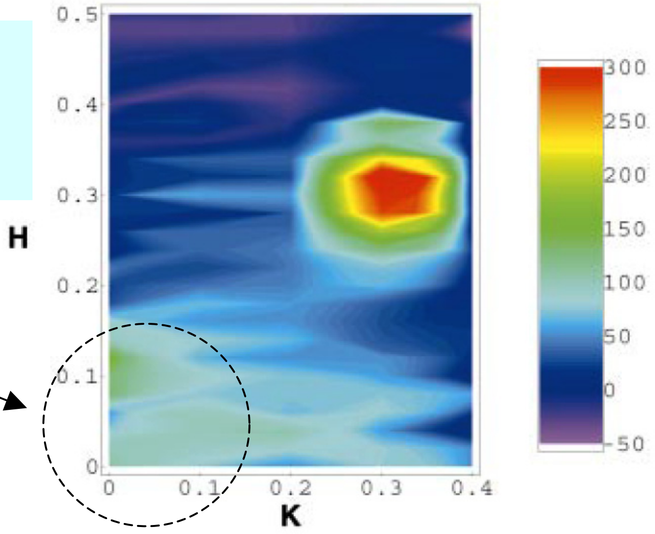


Theory

Good Agreement ?

As far as short-range ferromagnetic correlations are concerned

Short-range Ferromagnetic correlation



Braden et al: PRB (2002)

Experiment of Neutron Scattering

Conclusions of 2-b)

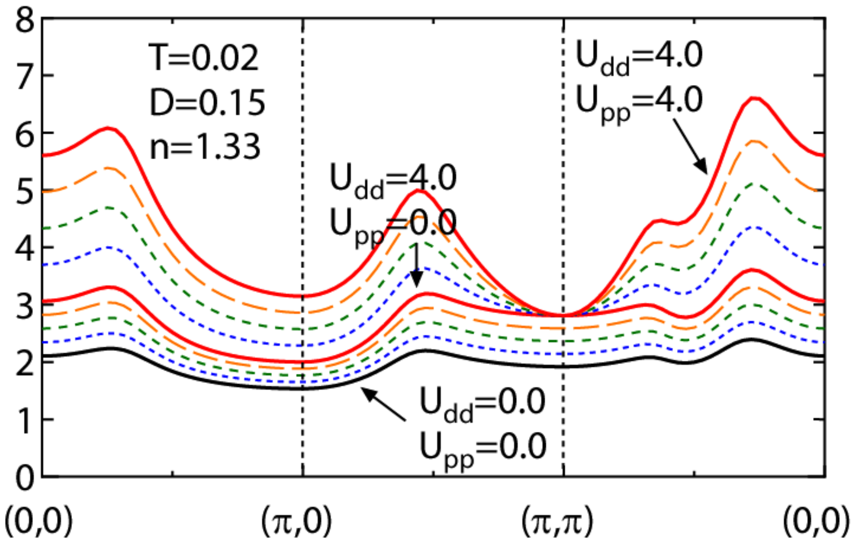
- We have derived from the so-called d-p model the effective inter-site interaction H_{ex}, whose origin is the on-site Coulomb interaction at O site.

- Unlike the Cuprates, H_{ex} is important in Sr_2RuO_4 due to a moderately strong hybridization between electrons in Ru and O.

- Short-range ferromagnetic correlations were induced by H_{ex}.

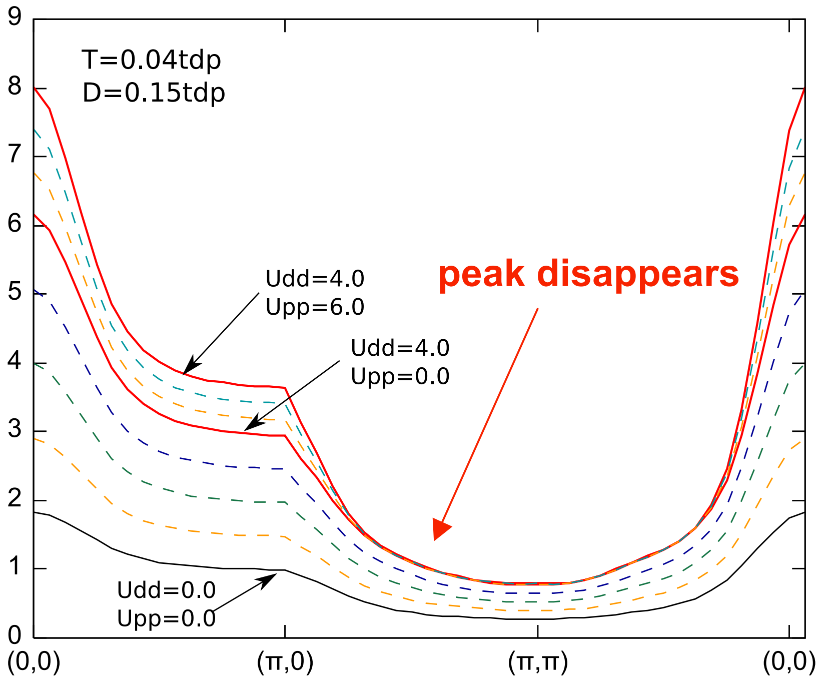
- Within the second order perturbation theory, we have shown that the triplet superconducting state of $(\sin p_x + i \sin p_y)$-type is promoted as applying U_{pp}.

2-c) Effect of p-orbitals on q-dependent spin susceptibility



$$\chi_\perp^{(0)}(q,0) \equiv -T\sum_{\epsilon_n}\sum_{\mathbf{k}} G_\gamma^{(0)}(\mathbf{k}, i\epsilon_n) \times G_\gamma^{(0)}(\mathbf{k}+\mathbf{q}, i\epsilon_n)$$

Hoshihara & KM



peak disappears

$$\chi_\perp^{(0)}(q,0) \equiv -T\sum_{\epsilon_n}\sum_{\mathbf{k}}\sum_{n,m} G_{nm}^{(0)}(\mathbf{k}, i\epsilon_n) \times G_{mn}^{(0)}(\mathbf{k}+\mathbf{q}, i\epsilon_n)$$

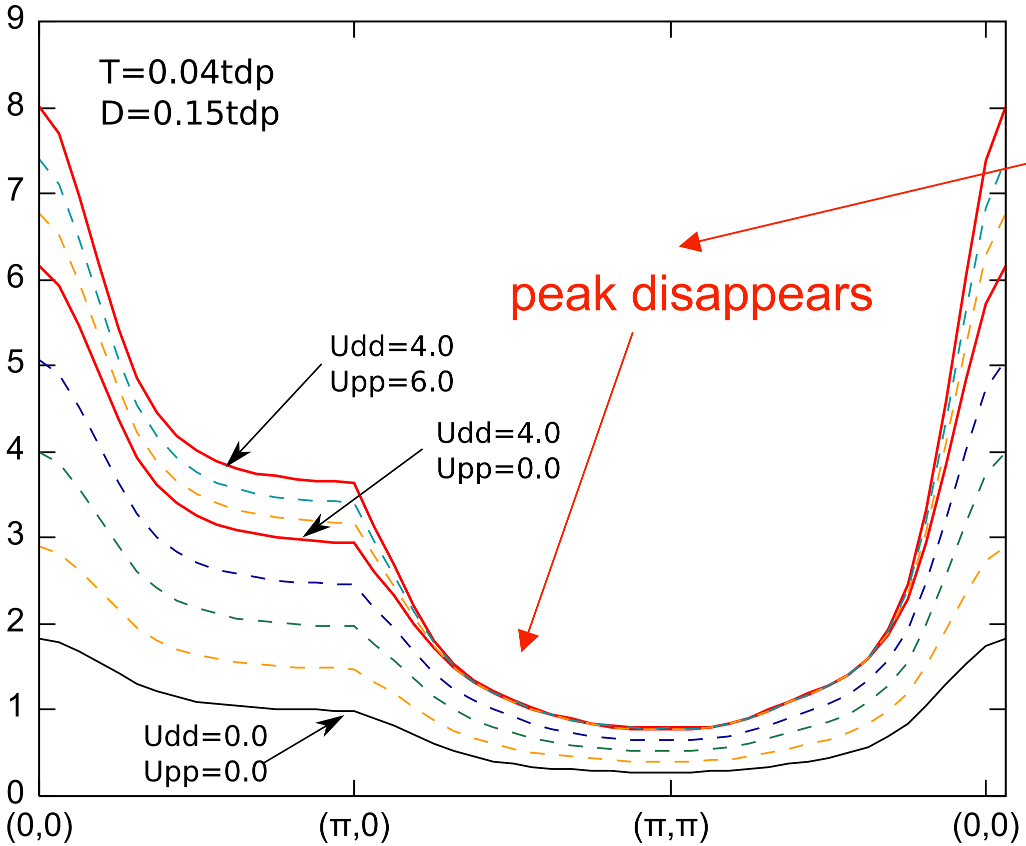
$$(\, n, m \;=\; p_x,\, p_y,\, d_{xy} \,)$$

$$G_{nm}^{(0)}(k) = \sum_a U_{na}(\mathbf{k})U_{ma}^*(\mathbf{k})G_a^{(0)}(k)$$

$$(\, a \;=\; \gamma,\, \tilde{p}_1,\, \tilde{p}_2 \,)$$

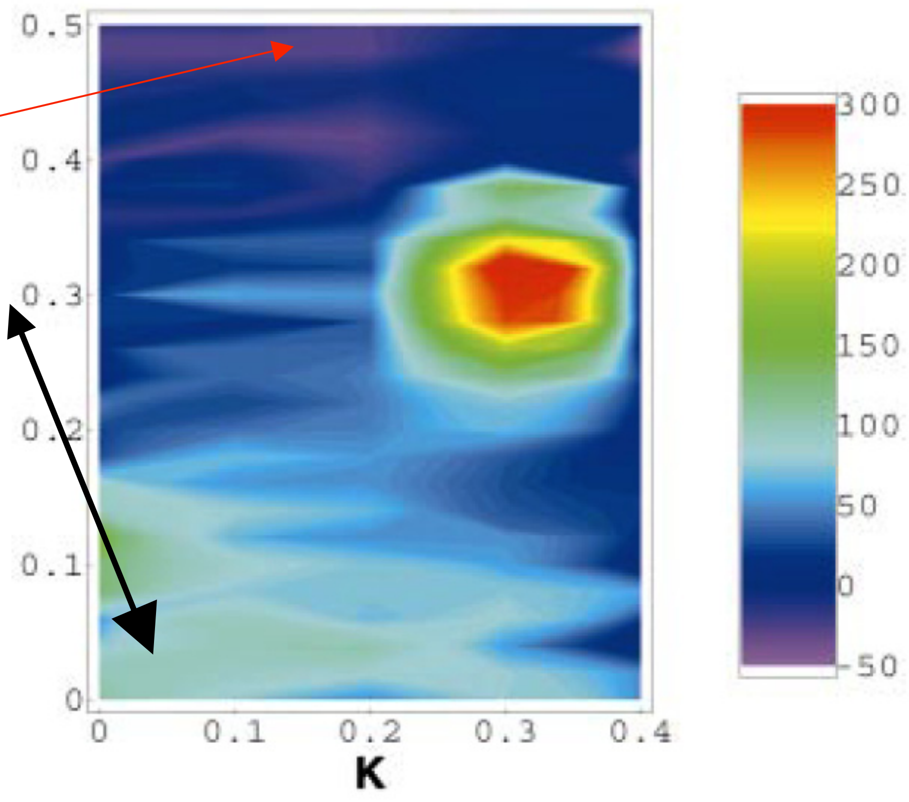
Yoshioka & KM

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



Broad peak around q=(0,0)

Experiment of neutron scattering



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

Agreement between experiment and theory greatly improved

Role of p-orbitals cannot be neglected even for non-interacting case

$$\mathcal{H}_{dp}^{(0)} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} d^\dagger_{\mathbf{k}\sigma} & p^\dagger_{x\mathbf{k}\sigma} & p^\dagger_{y\mathbf{k}\sigma}\end{pmatrix} \begin{pmatrix} \varepsilon_d & V^*_{y\mathbf{k}} & V^*_{x\mathbf{k}} \\ V_{y\mathbf{k}} & \varepsilon_p & W_\mathbf{k} \\ V_{x\mathbf{k}} & W_\mathbf{k} & \varepsilon_p\end{pmatrix}\begin{pmatrix} d_{\mathbf{k}\sigma}\\ p_{x\mathbf{k}\sigma}\\ p_{y\mathbf{k}\sigma}\end{pmatrix}$$

Unitary transformation

$$\begin{pmatrix} a_{1\mathbf{k}\sigma}\\ a_{2\mathbf{k}\sigma}\\ a_{3\mathbf{k}\sigma}\end{pmatrix} = U^{-1}(\mathbf{k})\begin{pmatrix} d_{\mathbf{k}\sigma}\\ p_{x\mathbf{k}\sigma}\\ p_{y\mathbf{k}\sigma}\end{pmatrix}$$

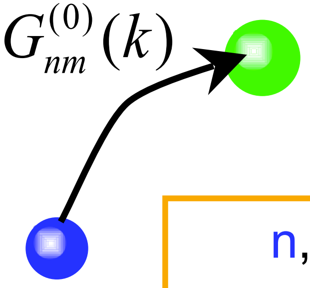
$$\mathcal{H}_{dp}^{(0)} = \sum_{\mathbf{k}\sigma} \begin{pmatrix} a^\dagger_{1\mathbf{k}\sigma} & a^\dagger_{2\mathbf{k}\sigma} & a^\dagger_{3\mathbf{k}\sigma}\end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3\end{pmatrix}\begin{pmatrix} a_{1\mathbf{k}\sigma}\\ a_{2\mathbf{k}\sigma}\\ a_{3\mathbf{k}\sigma}\end{pmatrix}$$

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

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

$\tilde{J}_{\mathbf{k},\mathbf{k}';\mathbf{q}}$: dependence on k & k’

➡ FFT is unavailable



$G_{nm}^{(0)}(k)$

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

a, b = quasi particle

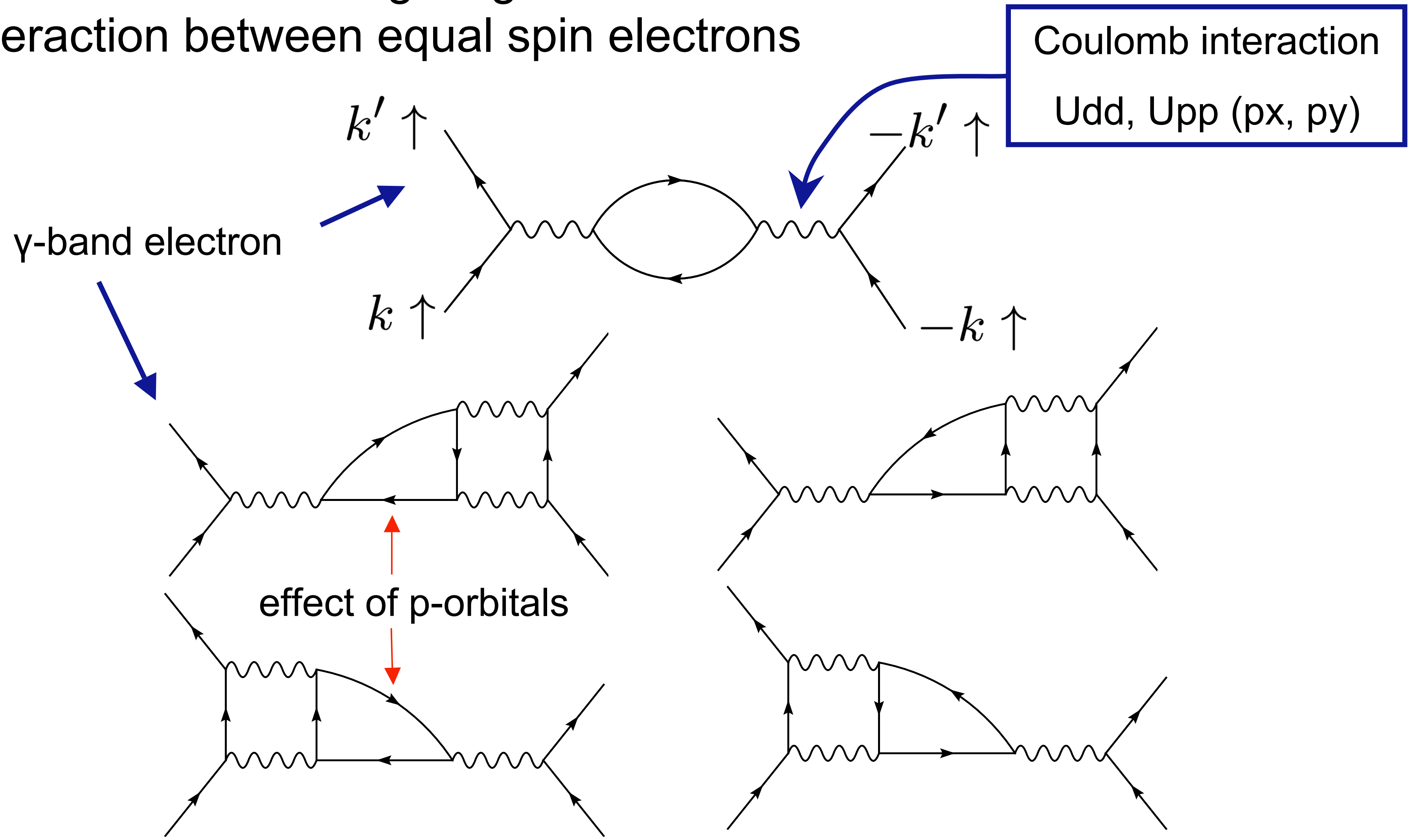
$$\begin{aligned} G_{nm}^{(0)}(k) &= -T_\tau\langle c_{nk\sigma}c^\dagger_{mk\sigma}\rangle \\ &= \sum_{ab} -T_\tau\langle a_{ak\sigma}a^\dagger_{bk\sigma}\rangle U_{na}(\mathbf{k})U^*_{mb}(\mathbf{k}) \\ &= \sum_{a} U_{na}(\mathbf{k})U^*_{ma}(\mathbf{k})G_a^{(0)}(k) \end{aligned}$$

➡ Matrix Green’s function enables us to use FFT method.

3^{rd} order perturbation for pairing interaction

(Yoshioka & KM)

We consider following diagrams as interaction between equal spin electrons



Coulomb interaction

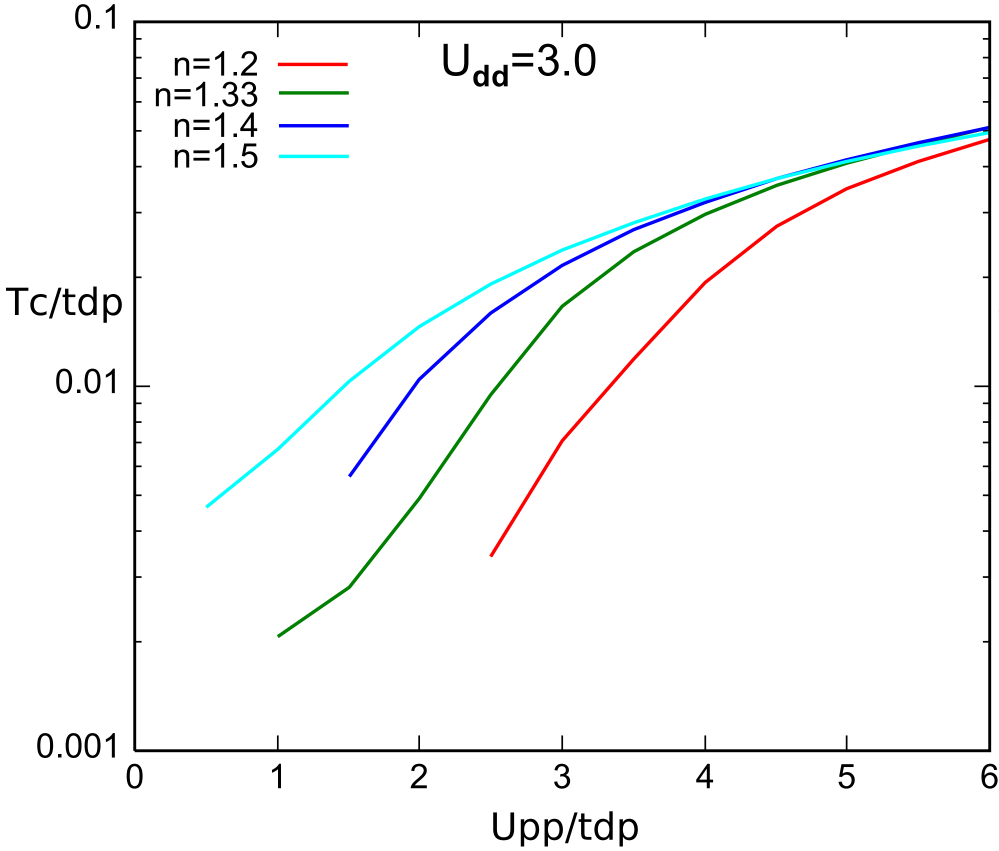
Udd, Upp (px, py)

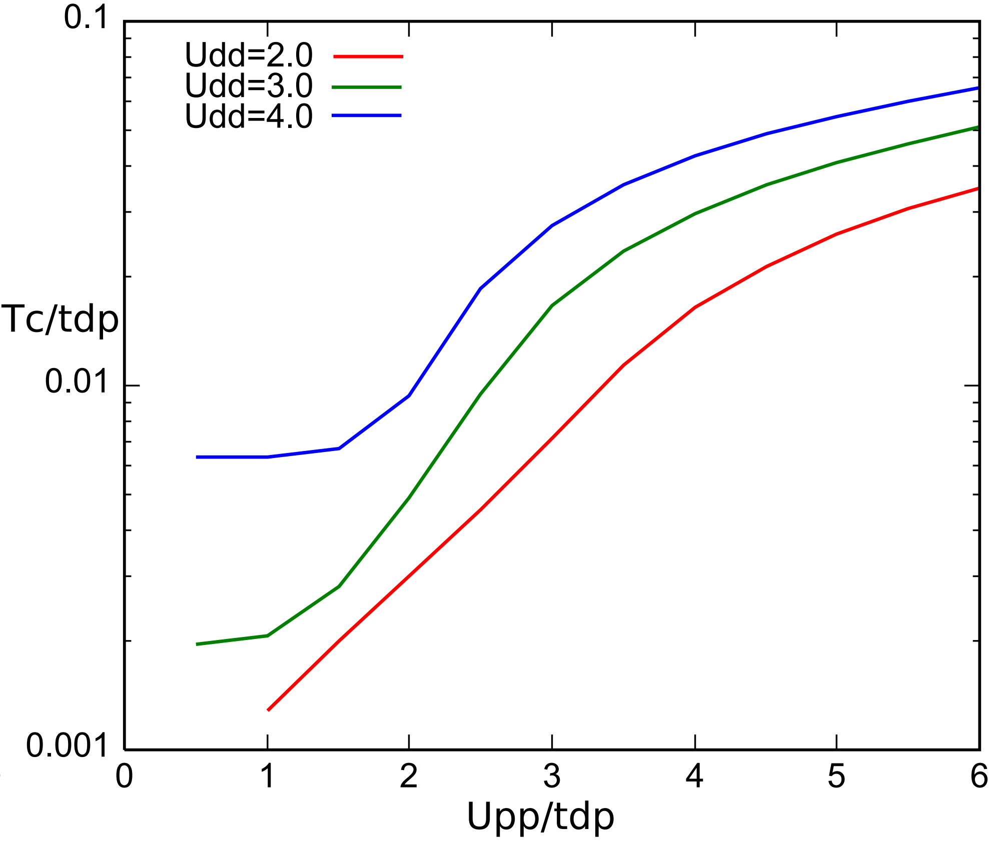
γ-band electron

effect of p-orbitals

cf. Nomura & Yamada, J. Phys. Soc. Jpn. **69** (2000) 3678
J. Phys. Soc. Jpn. **71** (2002) 1993

Results of T_c on 3rd order perturbation





- Tc monotonically increases with U_{pp}, indicating the importance of U_{pp} for spin-triplet superconductivity.
- It is noted that U_{dd} and U_{pp} are the renormalized interaction so that $U_{pp} \sim U_{dd}$ is not unrealistic.

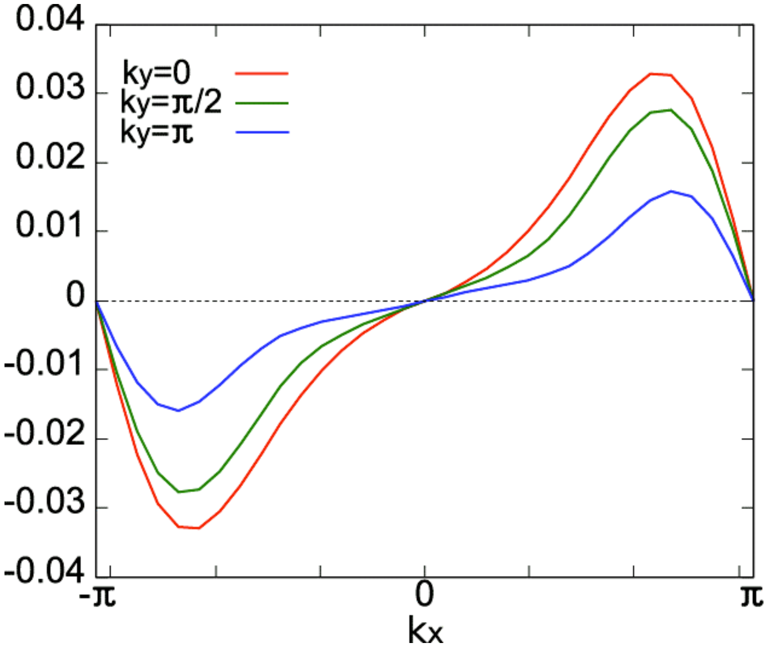
Effect of 3rd order perturbation is very small: vertex correction is not important

In contrast to the case of Nomura & Yamada for Hubbard model

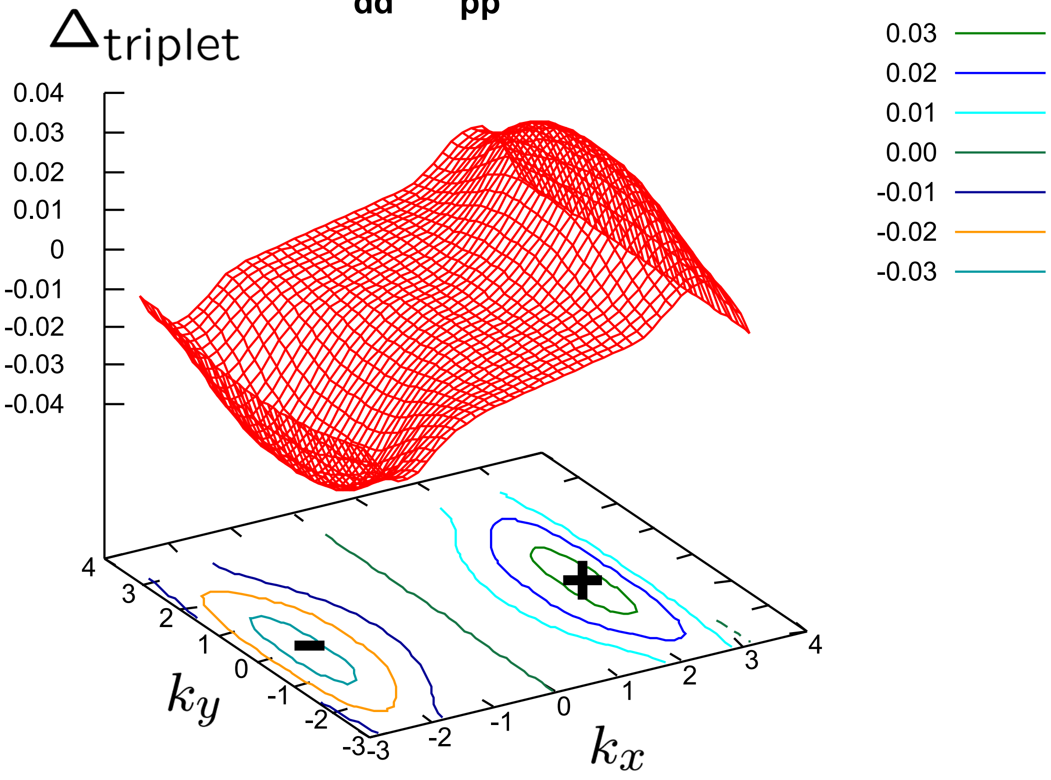
Gap function on 3rd order perturbation

Since only spin-triplet pairing appears within 2nd order perturbation, we solve the Eliashberg equation for spin-triplet channel.

Right figure shows the resulting gap function, which has nearly sin-wave structure.



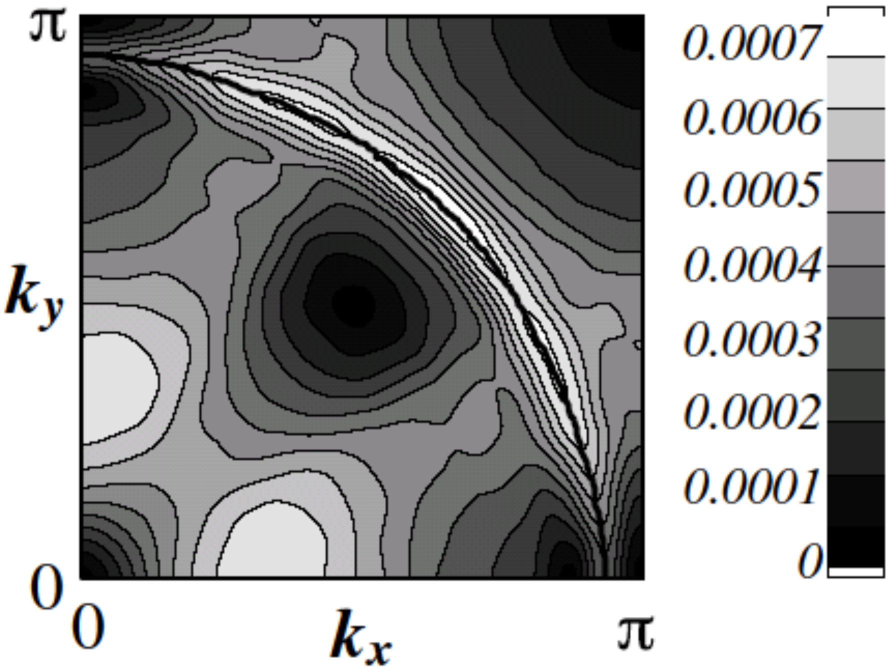
$U_{dd}=U_{pp}=3.0 \quad n=1.33$



$$\Delta \simeq \sin k_x \ (\sin k_y)$$

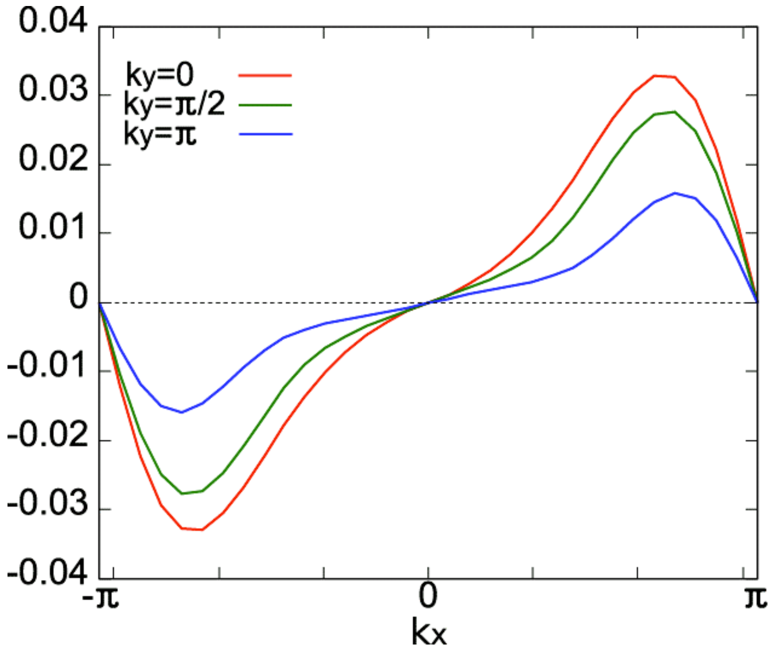
$$T < T_c$$

$$\Delta \simeq \Delta_0(\sin k_x + i \sin k_y)$$



Nomura & Yamada

J. Phys. Soc. Jpn. **71** (2002) 404



Yoshioka & KM

Conclusions of 2–c)

- Effect of p-orbitals is very crucial for q-dependence of spin–susceptibility, and leads to better agreement between experiment. So obtained short-range ferromagnetic correlations promote the spin-triplet pairing.

- Tc is calculated on the d-p model within the 3rd order perturbation, leading to essentially the same value calculated within 2nd order perturbation in which effect of U_{pp} is crucial .

- The resultant superconducting state is

  $$(\sin p_x + i \sin p_y)$$

  which is promoted by U_{pp}.

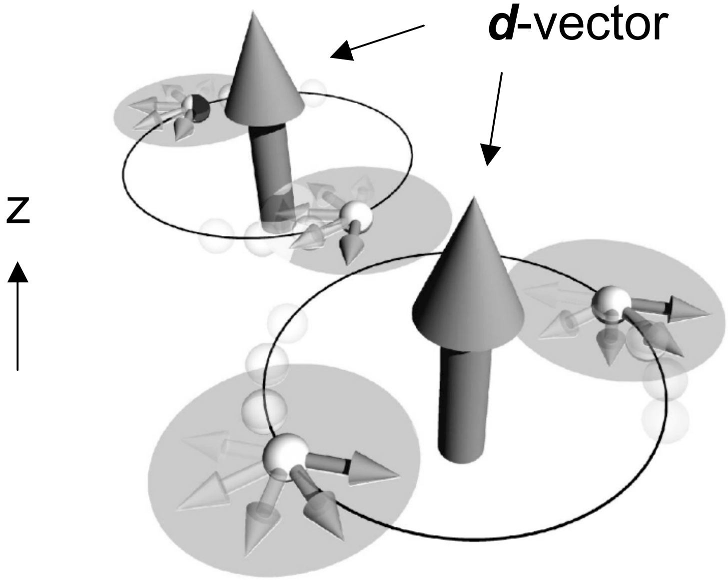
3) Issue on anisotropy of d-vector of Sr_2RuO_4

d-vector of spin-triplet pairing

$$\hat{\Delta}_{\mathbf{k}} = \begin{array}{ccc} \uparrow & \downarrow & \\ -d_x(\mathbf{k}) + id_y(\mathbf{k}) & d_z(\mathbf{k}) & \uparrow \\ d_z(\mathbf{k}) & d_x(\mathbf{k}) + id_y(\mathbf{k}) & \downarrow \end{array}$$

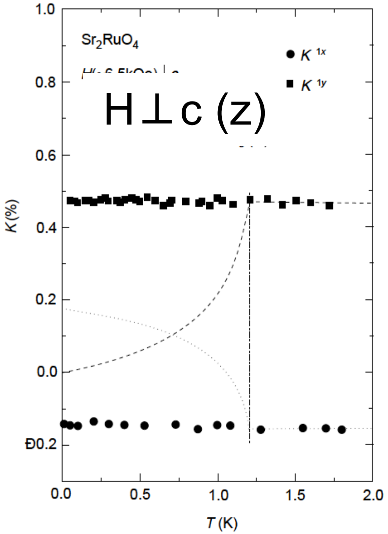
d-vector ⊥ spin of pairs
(magnetic field)

First guess

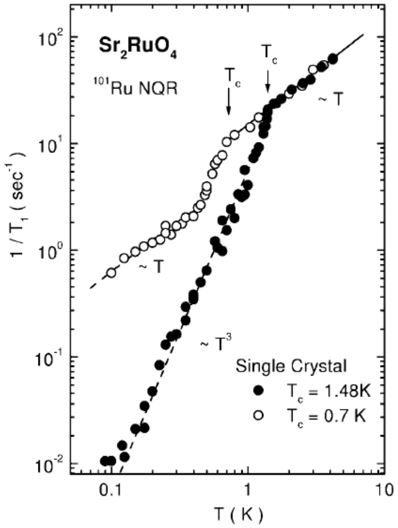


0.05T < H < 1.1T ***d*** // c (z)

Triplet–pairing and line node gap (NMR and NQR)



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



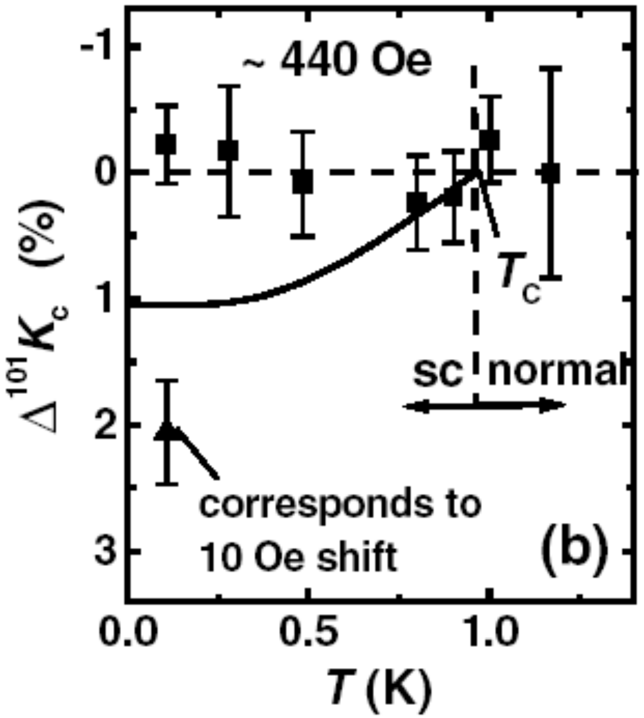
K. Ishida et al.:
PRL **84** (2000) 5387.

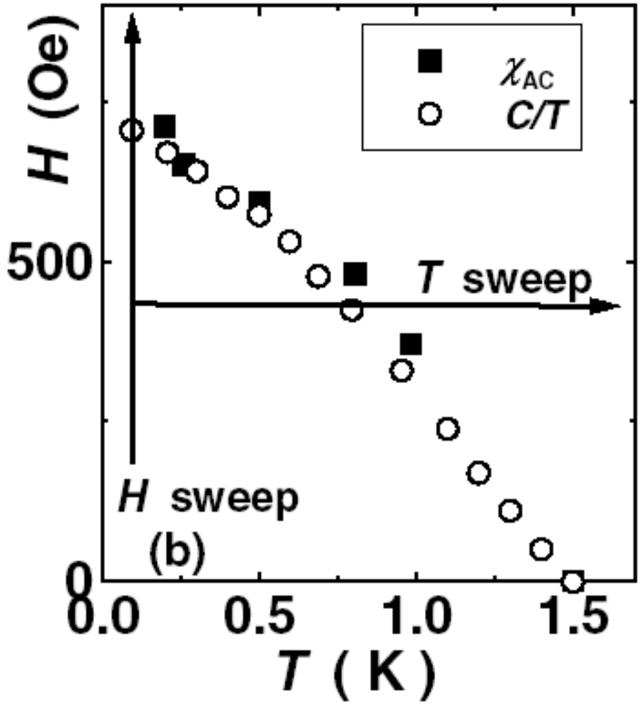
$$\mathbf{d}(\mathbf{k}) = \hat{z}\Delta_0(\sin k_x \pm \mathrm{i}\sin k_y)$$

Recent development of Knight shift measurements

Knight Shift for H // c (z)

Murakawa et al: Phys. Rev. Lett. **93** (2004) 167004
J. Phys. Soc. Jpn. **76** (2007) 024716





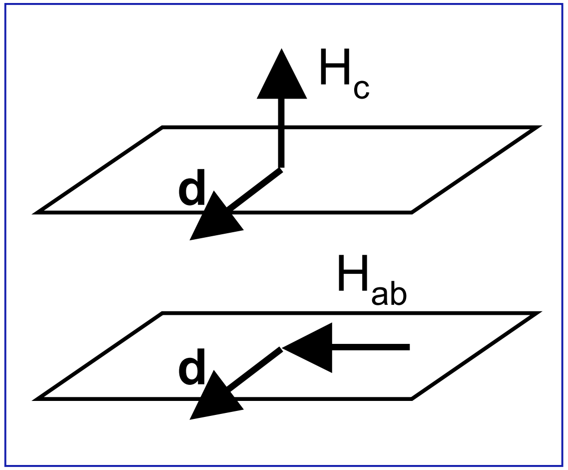
0.02T < H < 0.8T

d ⊥ c (z)

Summary of d-vector under magnetic field H

$H \perp c$ (z) : $0.05T < H < 1.1T$ ***d*** // c (z)

H // c (z) : $0.02T < H < 0.8T$ ***d*** $\perp$ c (z)



expected picture

Pinning force of d-vector expressed by anisotropy field H_a

Dipole-dipole interaction : ***d*** // c (z)

$H_a \sim 0.05T$ Hasegawa: JPSJ 72 (2003) 2456 cf. 3He-A (Leggett)

Spin-orbit interaction of atomic origin : ***d*** // c (z)

$H_a \sim 0.015T$ Yanase & Ogata: JPSJ 72 (2003) 673

Multiband Hubbard model (3rd order purturbation)
+ atomic spin-orbit + Hund coupling

These pinning forces cannot explain Knight shift measurements under magnetic field H

d $\perp$ c (z) may be intrinsic direction of ***d*** -vector
and there exists a missing pinning force

d-vector (2nd order perturbation theory)

To violate SU(2) symmetry in the spin space, namely to make difference between $V_{\uparrow\uparrow}$ and $V_{\uparrow\downarrow}$, we introduce 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 // ab**

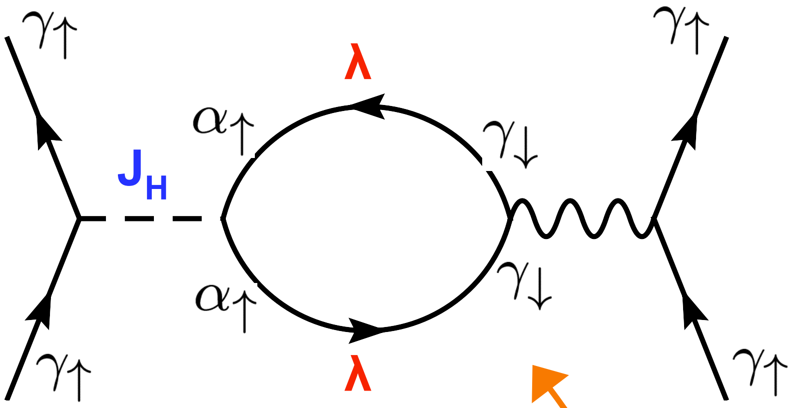
Green's function containing α- and β-band

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

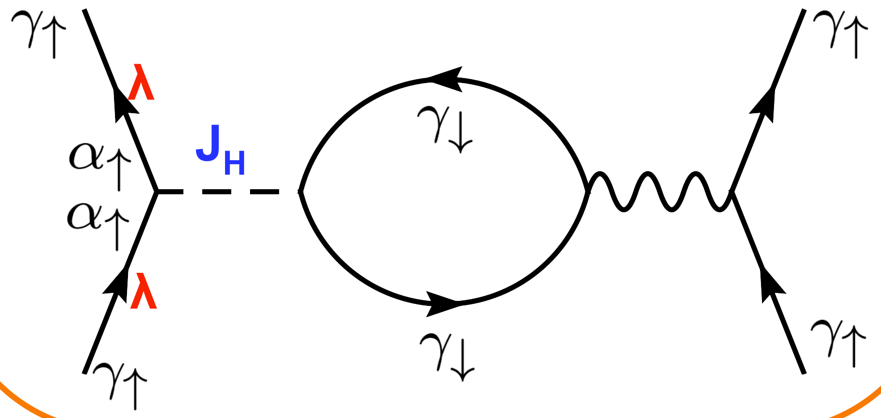
$$H_{SO} = \begin{pmatrix} c^\dagger_{k\alpha\sigma} & c^\dagger_{k\beta\sigma} & c^\dagger_{k\gamma-\sigma} \end{pmatrix} \begin{pmatrix} \varepsilon_\alpha & -i\sigma\frac{\lambda}{2} & b_{k\sigma} \\ i\sigma\frac{\lambda}{2} & \varepsilon_\beta & i\sigma b_{k\sigma} \\ b^*_{k\sigma} & -i\sigma b^*_{k\sigma}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

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

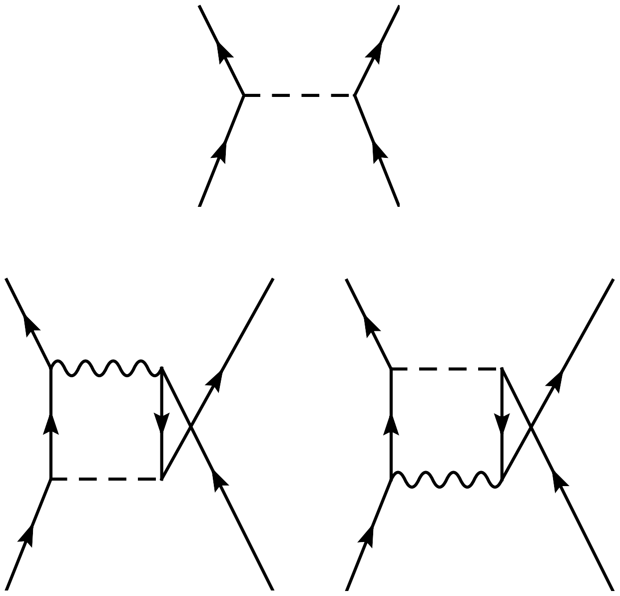
equal spin pairing



The main contribution
comes from this diagram.



anti-parallel spin pairing



λ: spin-orbit interaction

J_H: Hund coupling

$U_{dd}=U_{pp}=3.0$ n=1.33

$$\Delta T_c = T_c(\uparrow\uparrow) - T_c(\uparrow\downarrow) \sim 0.03 T_c$$

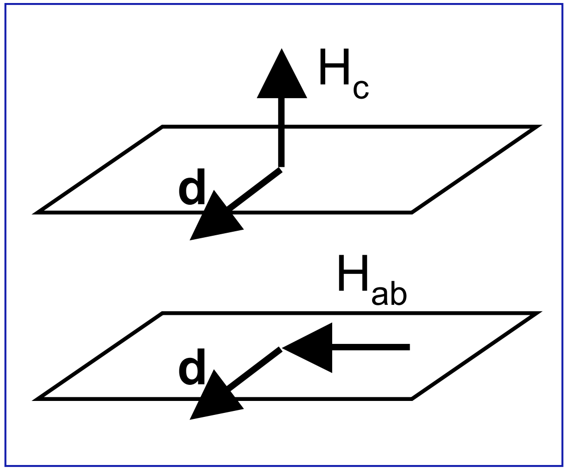
d // ab ∼750Oe

Conclusion of 3)

Paring interaction on d-p model together with the atomic spin-orbit coupling of Ru site and the Hund-rule coupling stabilizes the d-vector perpendicular to the c-axis.

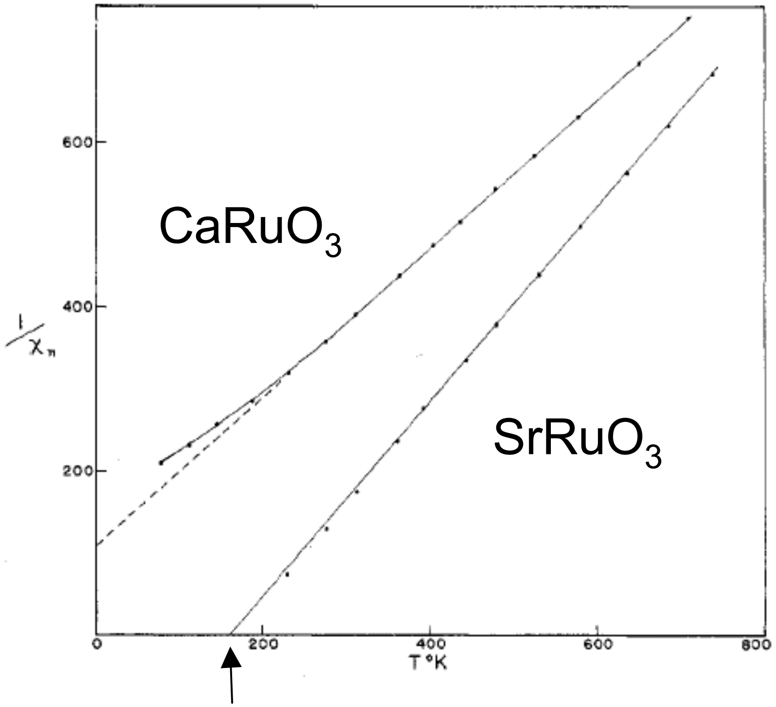
In contrast to previous theories on the basis of multi-band Hubbard model

In agreement with recent experiment of Knight shift



At H=0, d // ab

Ferromagnetic transition of $SrRuO_3$ (3d perovskite)



T_c=160 K

Callagham et al :
Inorg Chem **5** (1966) 1572

Open question for origin of FM

Super-exchange FM interaction via Coulomb correlation at O-site as a possible origin

Band structure calculation

Allen et al : PRB **53** (1996) 4393

		DOS [states/(Ry cell)]			
		Sr	Ru	O_3	Total
Paramagnetic		12	246	67	325
Magnetic	Up	5	84	25	114
	Down	4	55	17	76
	Total	9	139	42	190

Appreciable weight of p-component at FS

$$\frac{N_F(O2p)}{N_F(Ru4d)} \simeq \boxed{0.27}$$

cf. 0.17 (Sr_2RuO_4)

Effect of Spin-Orbit Interaction in Spin-Triplet Superconductor: Structure of d-vector and Anomalous O^{17}-NQR Relaxation in Sr_2RuO_4

K. Miyake and H. Kohno

Free energy F_{so} for SO coupling:

$$F_{so} = - g_{so}(\mathrm{i}\boldsymbol{d}\times \boldsymbol{d}^*)\cdot \boldsymbol{L}$$

$$g_{so} = 24(m/m^*)\, g_d$$

cf. Dipole coupling

$$F_{so} \sim - g_d (\boldsymbol{d} \cdot \boldsymbol{L})^2$$

Estimation of g_{so} in GL region:

$$g_{so} = | F_{cond} | \mu_B^2 (m/m^*) 12\pi N_F \times \times[\ln(1.14\beta_c\varepsilon_c)]^2 (1 - T/T_c)^{-1}$$

F_{cond}: condensation energy

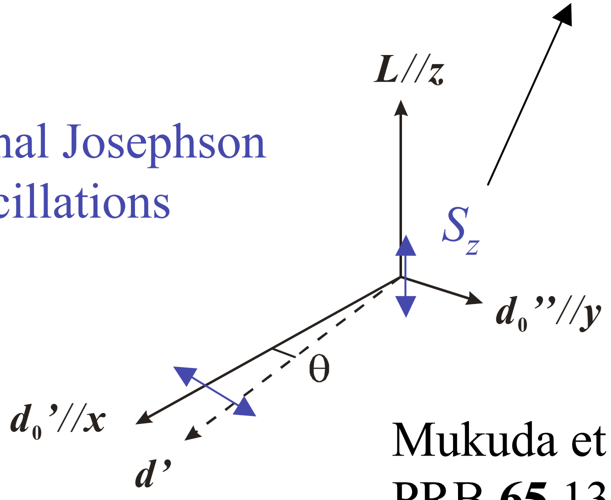
d -vector $\boldsymbol{d}_0$ in equilibrium state:

$$d_{0x}= (1+\eta^2)^{-1/2},\ d_{0y}=\mathrm{i}\eta(1+\eta^2)^{-1/2},\ d_{0z}=0$$

$\eta = g_{so} / 4| F_{cond} |$: weakly non-unitary

Anomalous relaxation of NQR in z-direction

Internal Josephson oscillations



Leggett-Takagi (1977)

Mukuda et al 2002
PRB **65** 132507