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Mechanism of the spin-triplet superconductivity of Sr_2RuO_4: Understanding by the Kohn-Luttinger effect.

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Points of the talk

What is the microscopic mechanism of the spin-triplet pairing in Sr_2RuO_4?

We show that the spin-triplet superconductivity in Sr_2RuO_4
can be understood by the Kohn-Luttinger mechanism
of anisotropic pairing in two dimensions.
The microscopic origin of triplet pairing will be naturally attributed
to the on-site Coulomb interaction between t2g electrons at Ru sites.

- Introduction: the Kohn-Luttinger(KL) theory of anisotropic pairing,
- KL mechanism in the two-dimensional isotropic space,
- Single-band calculation for the γ band of Sr_2RuO_4,
- Three-band calculation for Sr_2RuO_4,
- Most stable direction of *d*-vector: effect of spin-orbit coupling,
- Summary & Remarks.

Introduction: the Kohn-Luttinger effect

W. Kohn & J.M. Luttinger, Phys. Rev. Lett. 15, 154 (1965).
M.Y. Kagan & A.V. Chubukov, JETP Lett. 47 614 (1988).

3D Isotropic fermion system
with δ-function interaction *u*.

$$H = \sum_{\mathbf{p}\sigma} \frac{\mathbf{p}^2}{2m} c^+_{\mathbf{p}\sigma} c_{\mathbf{p}\sigma} + u \sum_{\mathbf{p}_i \mathbf{q}\sigma} c^+_{\mathbf{p}_1\uparrow} c^+_{\mathbf{p}_2\downarrow} c_{\mathbf{p}_2-\mathbf{q}\downarrow} c_{\mathbf{p}_1+\mathbf{q}\uparrow}$$

Condition of pairing instability:
Eliashberg equation (linearized)

$$\lambda(T)\cdot\Delta_{\sigma_1\sigma_2}(p) = -\sum_{p',\sigma_3\sigma_4} V_{\sigma_1\sigma_2,\sigma_4\sigma_3}(p,p')\,|G(p')|^2\,\Delta_{\sigma_3\sigma_4}(p')$$

$$\lambda(T_c) = 1$$

Effective interaction is expanded in *u*:

$$V(p,p') = u + V^{(2)}(p,p')u^2 + V^{(3)}(p,p')u^3 + V^{(4)}(p,p')u^4 + \dots$$

Kohn & Luttinger concluded
within 2nd order calc. :
one of anisotropic (i.e., $\ell \neq 0$) pairing states can occur at low temperatures due to the non–trivial *p*- and *p*'-dependence of *V*(*p*, *p*'), even when *u* is positive (i.e., repulsive in *s*-wave).

Contribution to *V*(*p*,*p*') up to 2nd order in *u*:

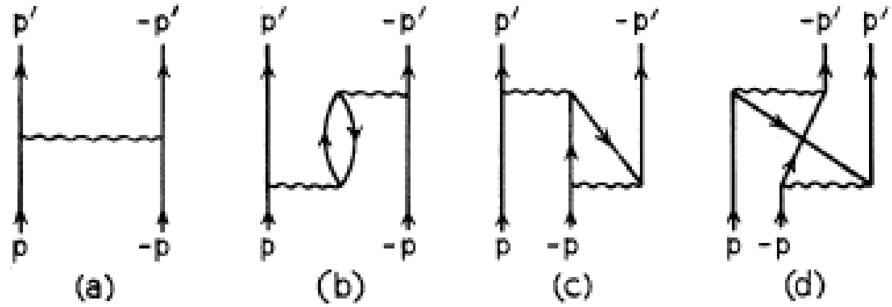


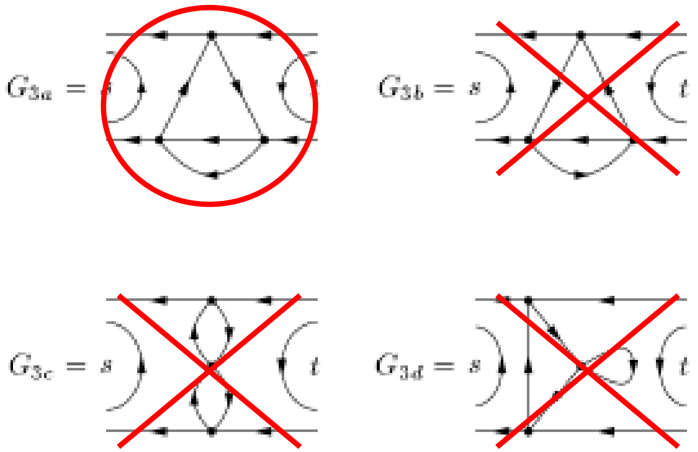
FIG. 1. Types of particle-particle interaction diagrams up to the second order which contribute to the irreducible scattering vertex.

Kagan & Chubukov showed that the ℓ=1 (triplet *p*-wave) state is the most probable among all ℓ's.

Kohn-Luttinger effect in 2D isotropic space

J. Feldman et al., Helv. Phys. Acta 70, 154 (1997).
A.V. Chubukov, Phys. Rev. B 48 1097 (1993).

How is it in 2D? In 2D the second order contribution is trivial (constant for |*p*|,|*p*'|=k_F), which is neither attractive nor repulsive for anisotropic pairing.
Necessary to proceed to 3rd order:



Theorem II.7 *Let $s_0 = t_0 = 0$ and $|\mathbf{s}|, |\mathbf{t}| = k_F$. Denote by $2\theta \in [0,\pi]$ the angle between* **s** *and* **t**. *Then, for sufficiently large ultraviolet cutoff $\mathfrak{C}$,*

a) there are constants $B_\mathfrak{C}, B'_\mathfrak{C}$ depending on $\mathfrak{C}$ such that

$$G_{3a}(s,t) = B'_\mathfrak{C} + \frac{m^2}{4\pi^2}\theta\frac{\cos\theta}{\sin\theta} + O(1/\mathfrak{C})$$
$$= B_\mathfrak{C} - \tfrac{1}{2}\sum_{\ell=1}^{\infty}(-1)^\ell \alpha_\ell \cos(2\ell\theta) + O(1/\mathfrak{C})$$

where

$$a_\ell = \frac{m^2}{\pi^2}\left[\frac{1}{2\ell} - \left(\frac{1}{\ell+1} - \frac{1}{\ell+2} + \frac{1}{\ell+3} - \frac{1}{\ell+4} \pm \cdots\right)\right]$$

b)

$$G_{3b}(s,t) = \frac{m^2}{(2\pi)^2}(1 - \ln 2) + O(1/\mathfrak{C}) \longrightarrow \times$$

c)

$$G_{3c}(s,t) = \frac{m^2}{(2\pi)^2} \longrightarrow \times$$

Corollary II.8 *Let $s_0 = t_0 = 0$ and $|\mathbf{s}|, |\mathbf{t}| = k_F$. Denote by $2\theta \in [0,\pi]$ the angle between* **s** *and* **t** *and let*

$$K^{(3)}(s,t) = \frac{\alpha_0}{2} + \sum_{\ell=1}^{\infty}\alpha_\ell\cos(2\ell\theta)$$

be the Fourier series expansion of $K^{(3)}$. Then,

$$\alpha_\ell = -\frac{m^2}{\pi^2}\left[\frac{1}{2\ell} - \left(\frac{1}{\ell+1} - \frac{1}{\ell+2} + \frac{1}{\ell+3} - \frac{1}{\ell+4} \pm \cdots\right)\right] + O(1/\mathfrak{C})$$

with the error $O(1/\mathfrak{C})$ uniform in ℓ. In particular,

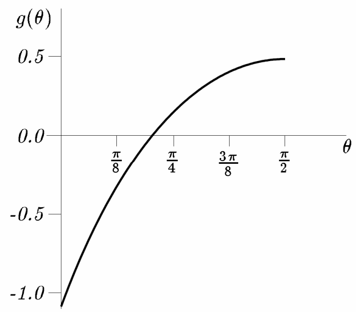
$$\alpha_1 = -\tfrac{m^2}{\pi^2}\left(\ln 2 - \tfrac{1}{2}\right) + O(1/\mathfrak{C})$$

and for all $\ell \geq 2$ and sufficiently large $\mathfrak{C}$

$$\alpha_1 < \alpha_\ell < 0 \longrightarrow \ell=1,\ p\text{-wave}$$

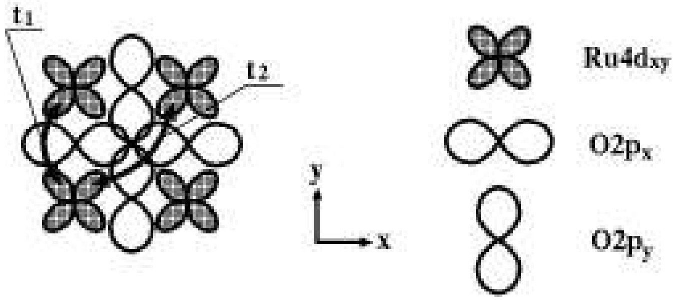
There is a constant $B''_\mathfrak{C}$ such that

$$K^{(3)}(s,t) = \frac{m^2}{4\pi^2}(\pi - 2\theta)\frac{\sin\theta}{\cos\theta} + B''_\mathfrak{C} + O(1/\mathfrak{C})$$



Single-band Hubbard model for the γ band of Sr_2RuO_4

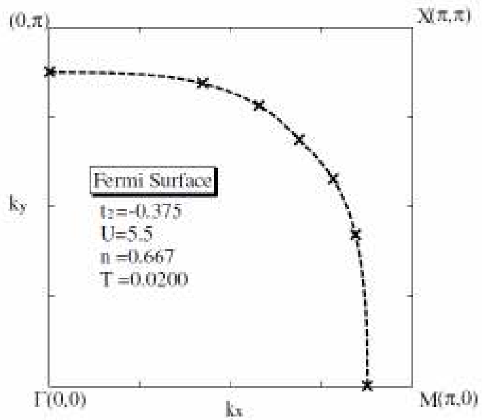
T. N. and K. Yamada, J. Phys. Soc. Jpn. 69, 3678 (2000).



$$H = -\sum_{\mathbf{xx}',\sigma} t_{\mathbf{xx}'} c^{+}_{\mathbf{x}\sigma} c_{\mathbf{x}'\sigma} + U \sum_{\mathbf{x}} c^{+}_{\mathbf{x}\uparrow} c^{+}_{\mathbf{x}\downarrow} c_{\mathbf{x}\downarrow} c_{\mathbf{x}\uparrow}$$

$$t_1 = 1.00$$

$$t_2 = 0.375$$

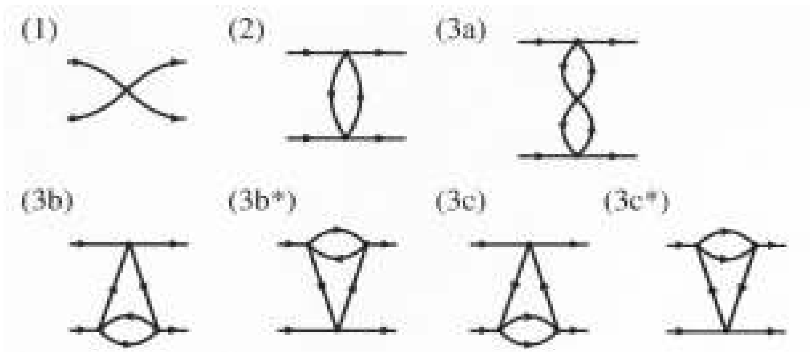


U is the Coulomb repulsion between $\mathrm{Ru4d}_{xy}$ electrons at Ru sites

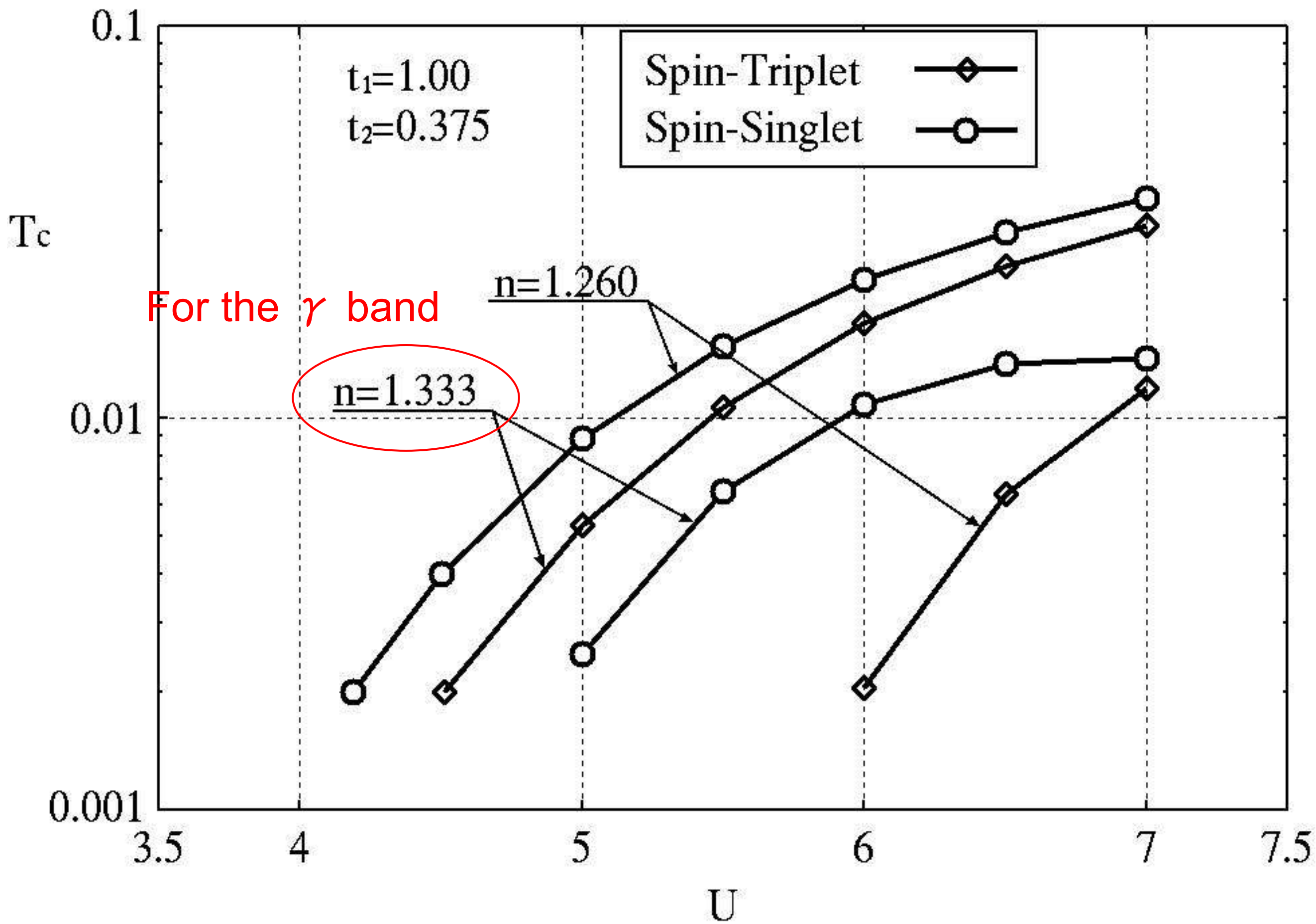
◆ Eliashberg equation: $\lambda(T) \cdot \Delta_{\sigma_1\sigma_2}(k) = -\sum_{k',\sigma_3\sigma_4} V_{\sigma_1\sigma_2,\sigma_4\sigma_3}(k,k') \,|\, G(k') \,|^2\, \Delta_{\sigma_3\sigma_4}(k')$

$\lambda(T_c) = 1$ determines the T_c.

◆ Effective pairing interaction *V(k,k')* (Particle-particle irreducible vertex function) is perturbatively expanded to 3rd order in *U.*



T_c as a function of U : p-wave state vs. $d_{x^2-y^2}$-wave state



Real T_c will be ~ 0.0003.

- Triplet p-wave is the most probable pairing symmetry for the γ band.

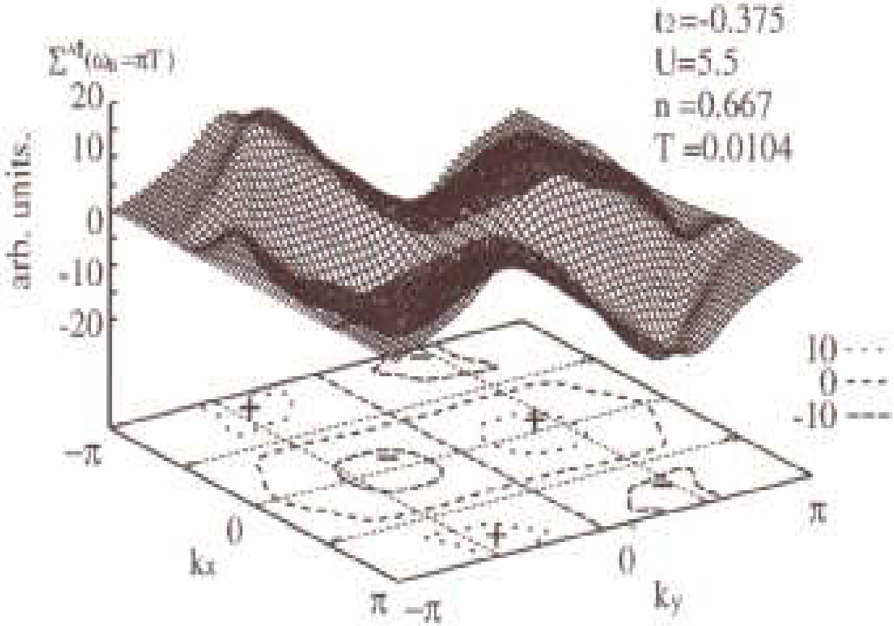
Anomalous self-energy $\Delta(k)$ and anomalous Green's function $F(k)$ (for k_y-symmetry)

◆ The obtained momentum dependence is *p*-wave like (not f-wave).

Anomalous self-energy

$\Delta(k) \sim \cos k_x \sin k_y$ (~ p_{x+y} –wave like)

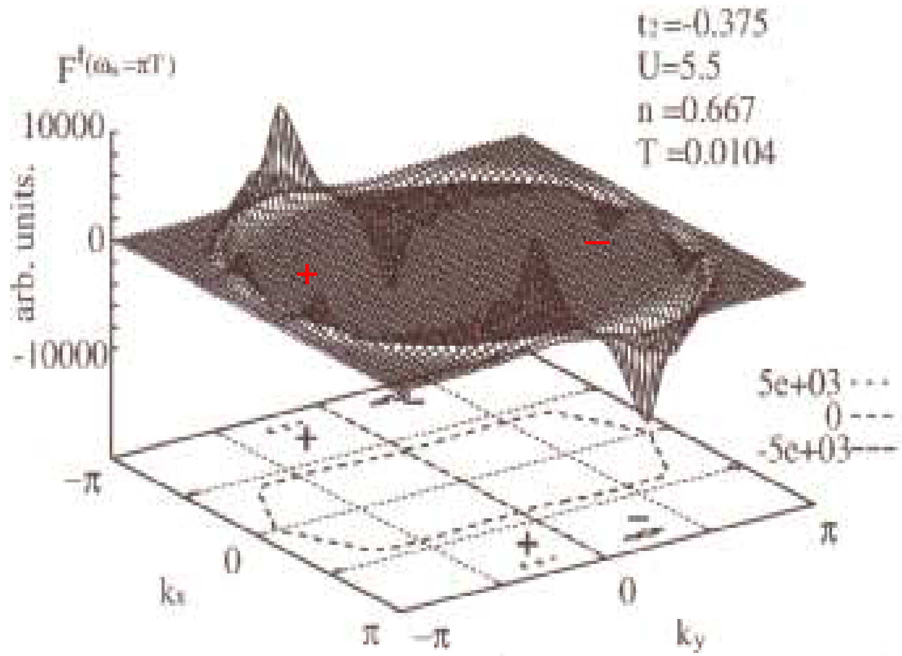
cf. $\sin(k_x + k_y) = \sin k_x \cos k_y + \cos k_x \sin k_y$



Anomalous Green's function

$F(k) = |G(k)|^2 \Delta(k)$

(~ p_y – (or p_x-)wave like just on FS)

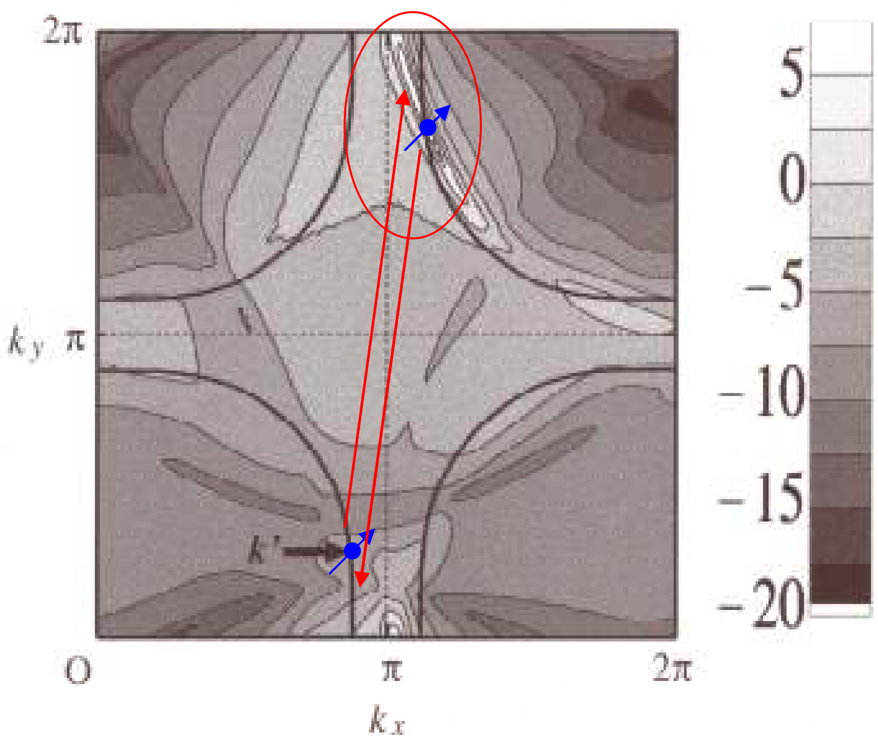


Remarks: k_x-like solution also exists, degenerating with this.

Effective pairing interaction $V(k,k')$ in single-band Hubbard model for the γ band

T. N. and K. Yamada, J. Phys. Soc. Jpn. 69, 3678 (2000).

◆ Amplitude $V_{\sigma\sigma,\sigma\sigma}(k,k')$ for parallel-spin-pair scattering $(k'\sigma, -k'\sigma) \Rightarrow (k\sigma, -k\sigma)$ is shown as a function of k for fixed k'



Enhancement around $k = -k'$.

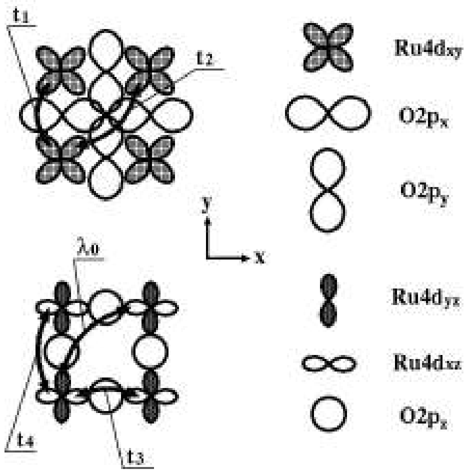
$\Rightarrow$ $\Delta_{\text{triplet}}(k)$ takes favorably opposite sign between k and $-k$ (due to the front factor -1 in Eliashberg equation).

$\Rightarrow$ Odd parity *p*-wave pairing.

Remark: The same vertex corrected terms are important as in the case of repulsive fermions in 2D isotropic space.

Three-band calculation for Sr_2RuO_4

T. N. and K. Yamada, J. Phys. Soc. Jpn. 71, 1993 (2002).

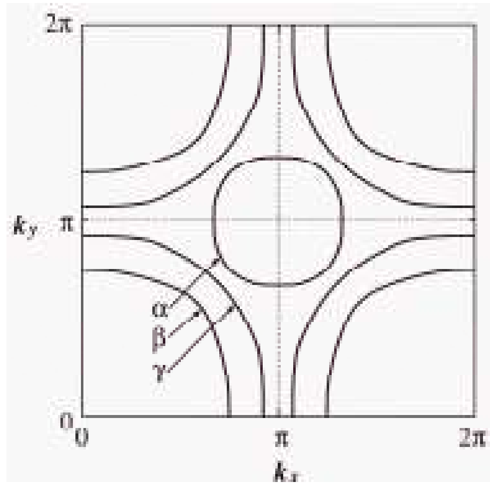


$$H = H_0 + H'$$

$$H_0 = -\sum_{xx'\ell\ell'\sigma} t_{x\ell,x'\ell'} c^{+}_{x\ell\sigma} c_{x'\ell'\sigma} \qquad \ell,\ell' = xy,\ yz,\ xz$$

$$H' = \frac{U}{2}\sum_{x\ell\sigma\neq\sigma'} c^{+}_{x\ell\sigma} c^{+}_{x\ell\sigma'} c_{x\ell\sigma'} c_{x\ell\sigma} + \frac{U'}{2}\sum_{x\ell\neq\ell'\sigma\sigma'} c^{+}_{x\ell\sigma} c^{+}_{x\ell'\sigma'} c_{x\ell'\sigma'} c_{x\ell\sigma}$$

$$+ \frac{J}{2}\sum_{x\ell\neq\ell'\sigma\sigma'} c^{+}_{x\ell\sigma} c^{+}_{x\ell'\sigma'} c_{x\ell\sigma'} c_{x\ell'\sigma} + \frac{J'}{2}\sum_{x\ell\neq\ell'\sigma\neq\sigma'} c^{+}_{x\ell\sigma} c^{+}_{x\ell\sigma'} c_{x\ell'\sigma'} c_{x\ell'\sigma}$$

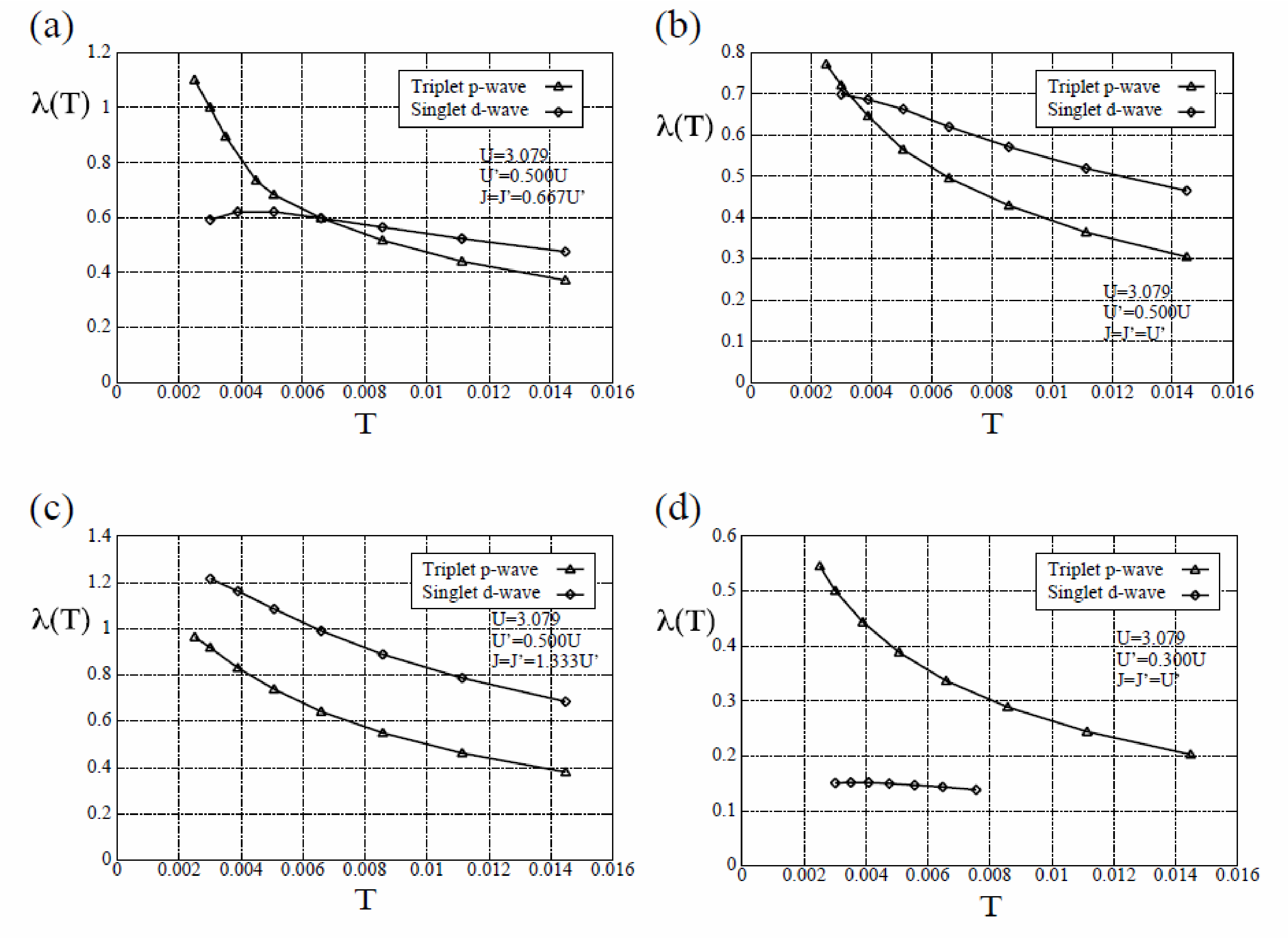


◆ Effective pairing interaction $V(k,k')$ expanded to third order in H'

Linearized Eliashberg equation:

$$\lambda(T)\cdot\Delta_{a\sigma_1\sigma_2}(k) = -\sum_{\substack{k',\sigma_3\sigma_4 \\ a'=\alpha,\beta,\gamma}} V_{a\sigma_1\sigma_2,a'\sigma_4\sigma_3}(k,k')\,|G_{a'}(k')|^2\,\Delta_{a'\sigma_3\sigma_4}(k')$$

Eigenvalues of Eliashberg equation for three-band case: p-wave state vs. $d_{x^2-y^2}$-wave state



U=3.079

a) $U' = 0.5U$
$J=J'=0.667U'$
⇒ $p>d$

b) $U' = 0.5U$
$J=J'=U'$
⇒ $p>d$

c) $U'=0.5U$
$J=J'=1.333U'$
⇒ $p<d$

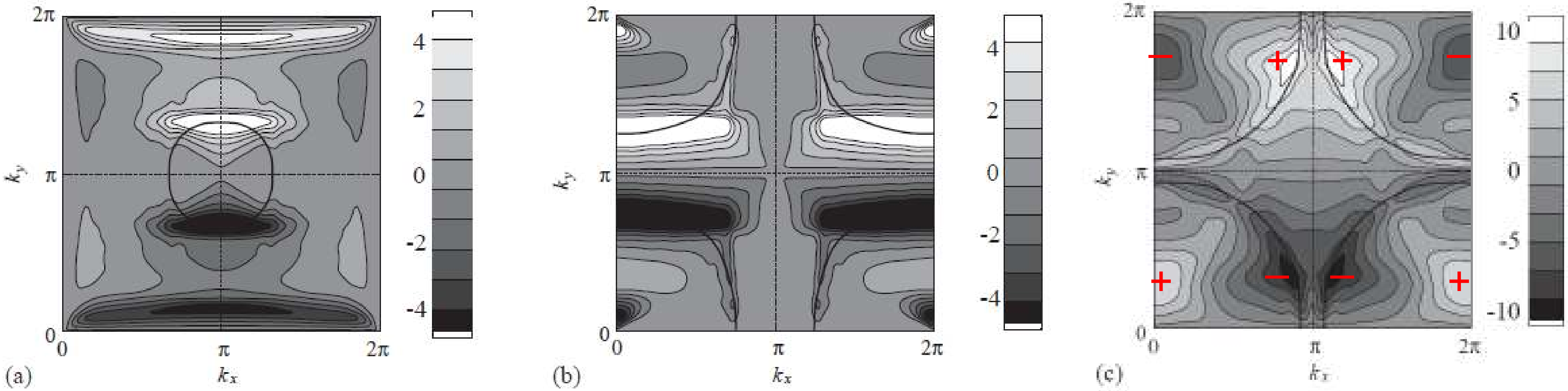
d) $U' = 0.3U$
$J=J'=U'$
⇒ $p>d$

◆ The probable pairing symmetry is *p*-wave for reasonable strength of inter-orbital couplings.

Momentum dependence of superconducting order parameter
(only for k_y-like symmetry solution)

$\Delta_\alpha(k), \Delta_\beta(k), \Delta_\gamma(k)$ for the most probable pairing state:

(α) (β) (γ)



T. N. and K. Yamada, J. Phys. Soc. Jpn. 71, 1993 (2002).

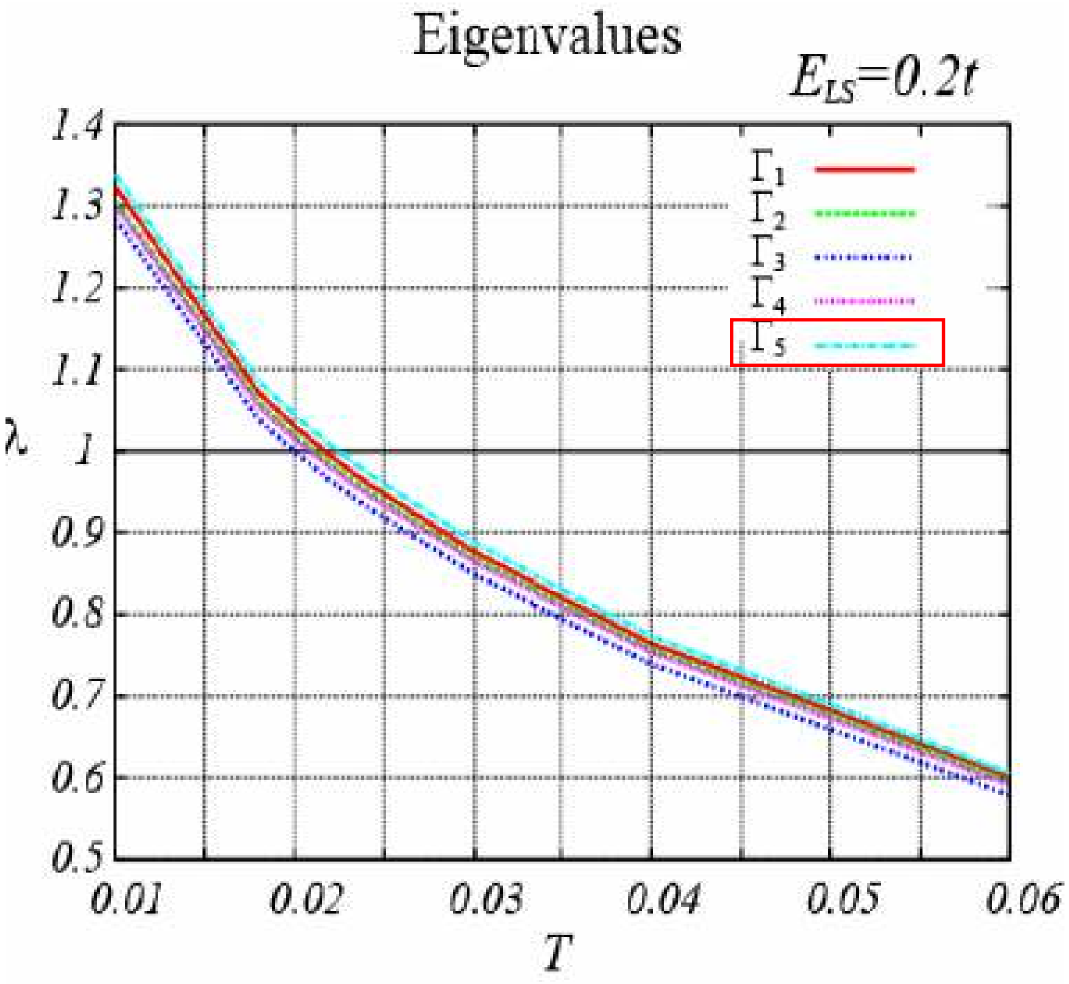
- Robust dominance of the γ band (D.F. Agterberg et al. (1997)) .
  "Orbital Dependent Superconductivity"
- *p*–wave-like on the γ band:

$$\Delta_\gamma(k) \sim \sin k_y - 15.8 \times \cos k_x \sin k_y + \cdots$$

☺ R. P. Kaur et al. (2005),
" $\Delta(k) \sim \sin k_y - 12 \times \cos k_x \sin k_y$ "
explains the double transition
in low-*T* and high-*H* region !

Spin-orbit coupling removes the degeneracy

Y. Yanase & M. Ogata, 2003,
H. Ikeda.



Spin-Orbit Coupling for t2g orbitals:

$$H_{so} = i\xi \sum_{lmn} \varepsilon_{lmn} \sum_{\mathbf{k}\sigma\sigma'} c^{+}_{\mathbf{k}l\sigma} c_{\mathbf{k}m\sigma'} (s_n)_{\sigma\sigma'}$$

Γ_1 $p_x\mathbf{x}+p_y\mathbf{y}$

Γ_2 $p_y\mathbf{x}-p_x\mathbf{y}$

Γ_3 $p_x\mathbf{x}-p_y\mathbf{y}$

Γ_4 $p_y\mathbf{y}+p_x\mathbf{y}$

Γ_5 $(p_x+ip_y)\mathbf{z}$

(*U*=5*t* *U'*=*J*=*J'*=0.3*U*)

$\Delta T_c/T_c \sim 0.01$

Remark: Chiral state $(k_x \pm ik_y)\hat{z}$ (Γ_5) is the most stable by LS coupling.
Next stable one is $k_x\hat{x} + k_y\hat{y}$ (Γ_1) .

Summary & Remarks

The mechanism of triplet pairing in Sr_2RuO_4 has been discussed by the KL effect in 2D:

- The most probable pairing symmetry is *p*-wave-like
  (not f-wave, and not singlet),
  but could not be described only by one or a few harmonics. :
  roughly $\sin k_x \cos k_y$–wave like on the γ band, but more complex.
- The attractive momentum dependence of effective interaction originates from the vertex corrected terms:
  The physical picture that the attraction originates from exchange processes of some kind of bosonic excitations (spin fluctuation or paramagnon, charge fluctuation and others) will *not* be appropriate,
  consistent with the absence of enhanced FM fluctuations in Sr_2RuO_4.

Orbital Dependent Superconductivity is microscopically derived.:

- The γ band dominates the superconducting transition.

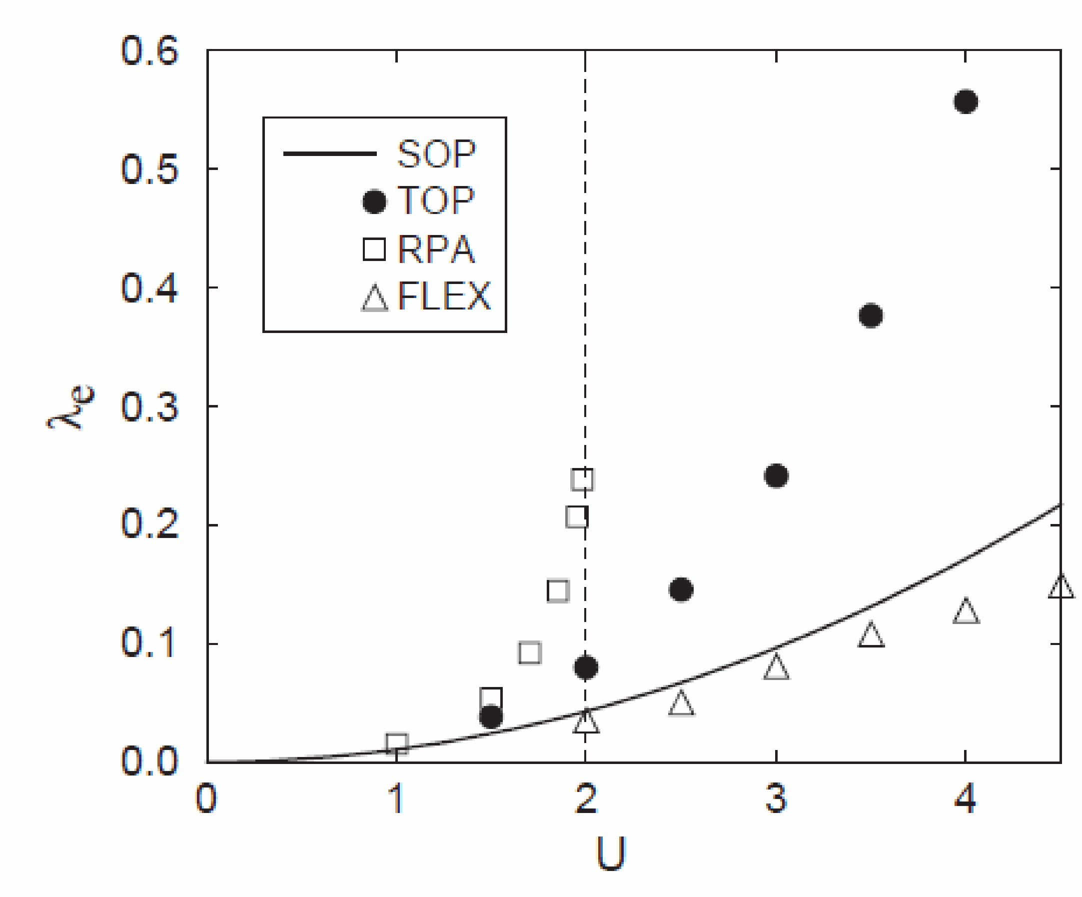
Spin-orbit coupling stabilizes *d*-vector perpendicular to the basal plane.

- Chiral *p*-wave-like state is microscopically derived.
  But the energy for stabilization will be small. $\Delta T_c/T_c \sim 0.01$.

Additional remark on the gap structure: preliminary calc. (not shown here) by 3D model for the γ band suggests that the horizontal line node is almost impossible (ruled out) within our framework.

Eigenvalues by various methods

Y. Yanase, T. Jujo, T. Nomura, H. Ikeda, T. Hotta, K. Yamada,
Phys. Reports 387, 1-149 (2003).



T=0.005t

(without normal self-energy corr.)