Aspects of microscopic theories of superconductivity in Sr_2RuO_4

Srinivas Raghu

Stanford University

References

PRL **105,** 136401 (2010) PHYSICAL REVIEW LETTERS week ending 24 SEPTEMBER 2010

Hidden Quasi-One-Dimensional Superconductivity in Sr_2RuO_4

S. Raghu, A. Kapitulnik, and S. A. Kivelson

Theory of 'hidden' quasi-1D superconductivity in Sr_2RuO_4

S Raghu, Suk Bum Chung and Samuel Lederer

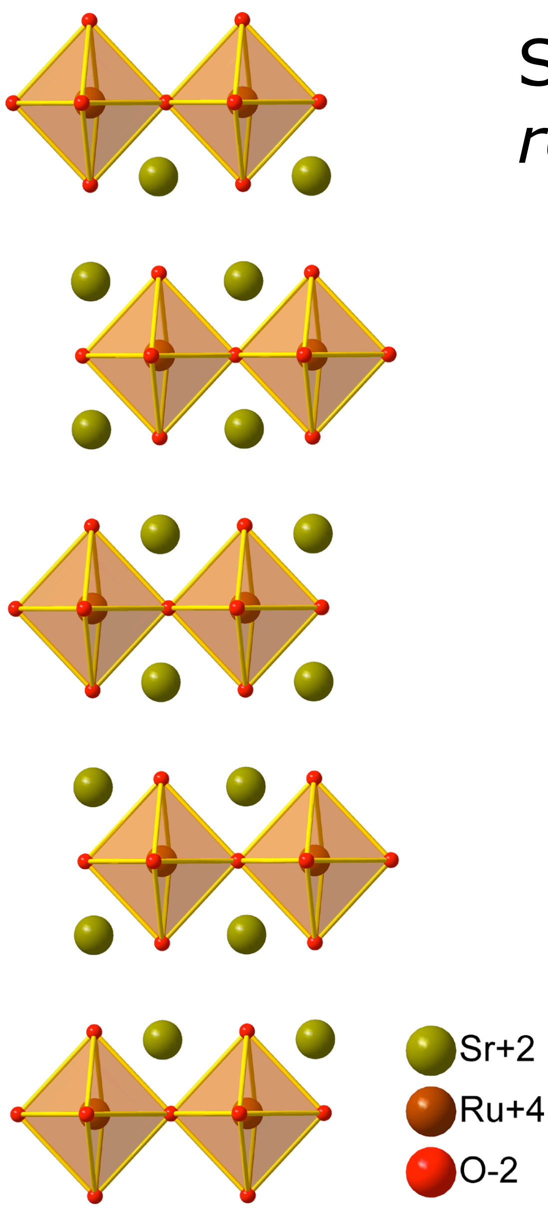
arXiv:1208.6344 (M2S proceeding)

Sam Lederer and SR, manuscript in preparation

Introduction and experimental overview

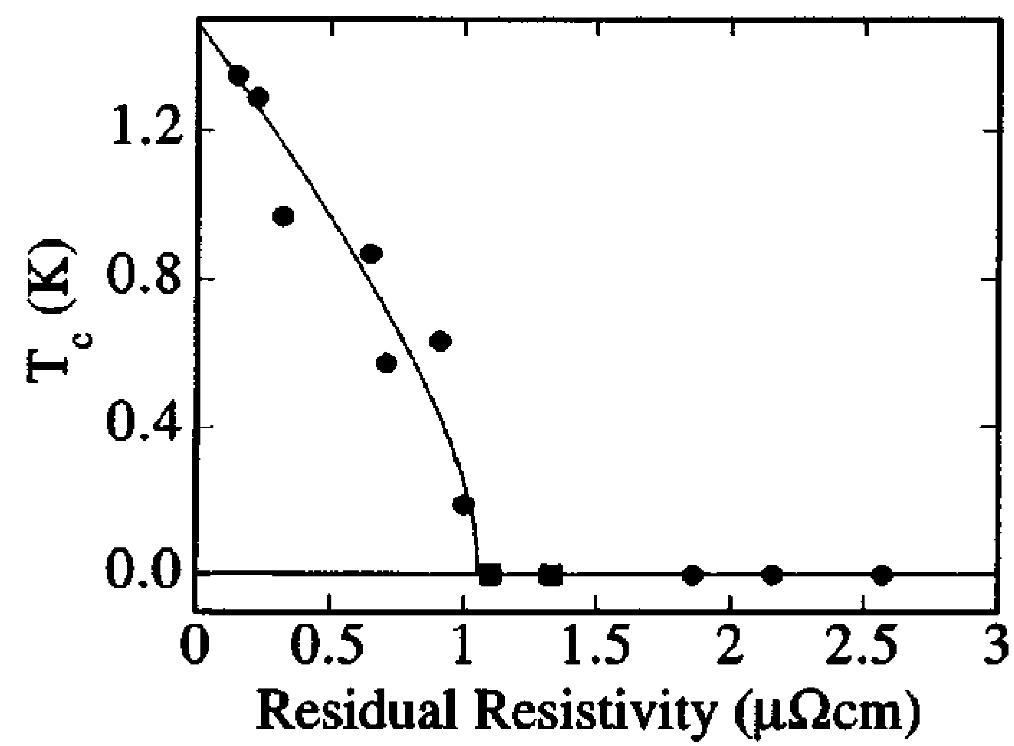
The Unconventional superconductor Sr_2RuO_4

Sr_2RuO_4 (T_c = 1.5 K) is an archetypal unconventional superconductor.



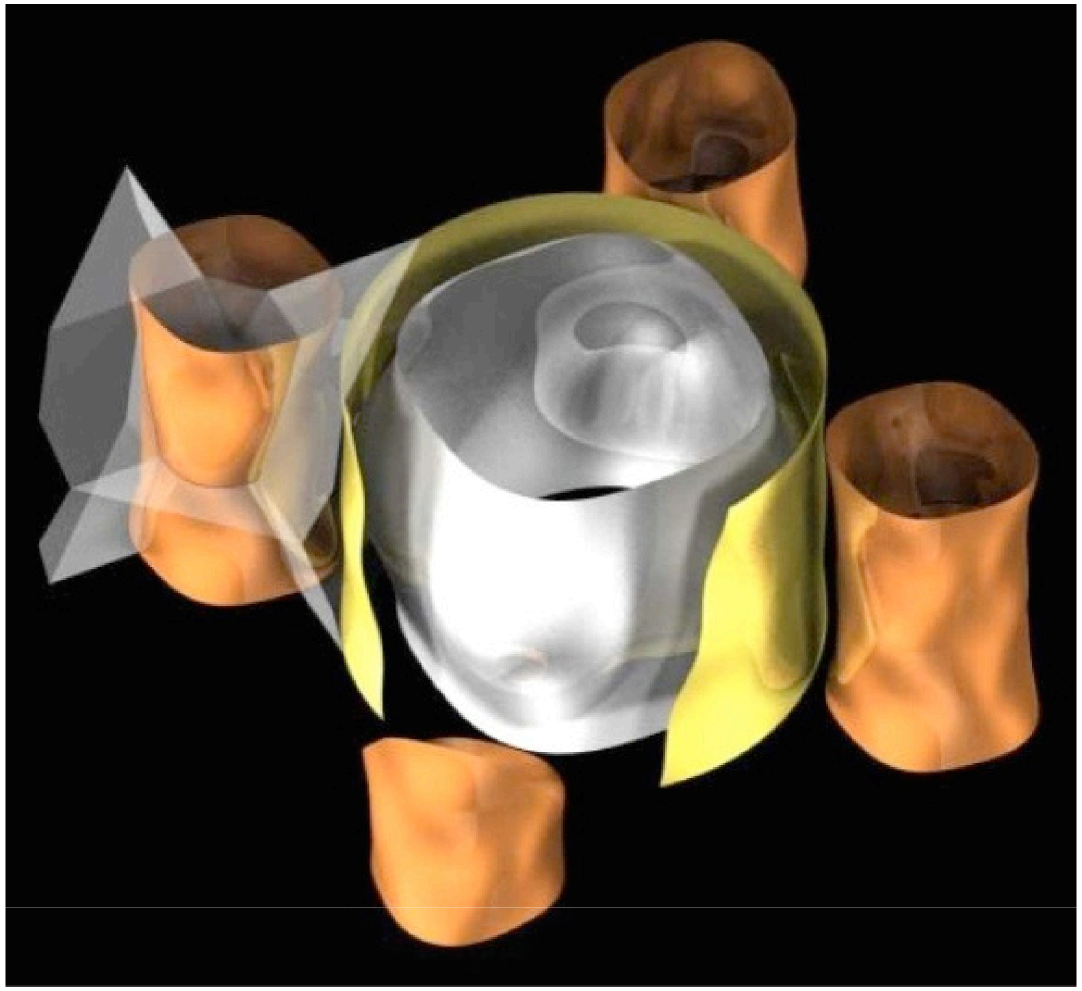
Spin triplet superconductivity arises directly from *repulsive* electron-electron interactions.

Sensitivity to disorder



Mackenzie *et al.*, 1998

The Unconventional superconductor Sr_2RuO_4



The normal state is a pristine quasi 2d Fermi liquid ($T_c<T<25K$).

There is excellent agreement between ARPES and quantum oscillations: long-lived, dressed quasiparticle excitations above T_c.

Electronic structure is very simple.

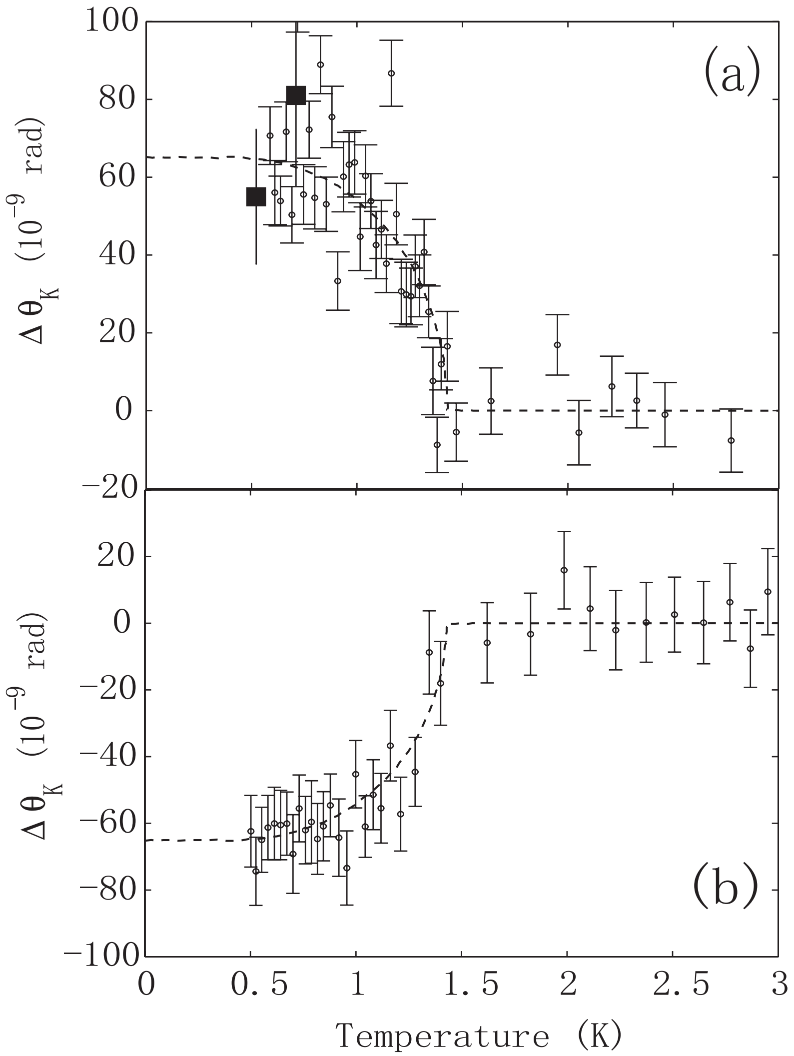
Controlled, microscopic theory of superconductivity should be feasible.

Mackenzie and Maeno, RMP 2003

Properties of the superconducting state: T_c = 1.5 K

Phase-sensitive measurements have confirmed that SrRuO has odd-parity in the superconducting state. (K.D. Nelson *et al.*, 2004)

mu-SR, Kerr effect experiments have confirmed that SrRuO breaks time-reversal symmetry in the superconducting state. (Xia *et al.* 2006, G. Luke *et al.* 1998).



Odd-Parity superconductivity

$$\Psi_{\alpha\beta}(\vec{k}) = \langle c_{\vec{k}\alpha} c_{-\vec{k}\beta} \rangle$$ Pair wave-function

$$\Psi_{\alpha\beta}(\vec{k}) = -\Psi_{\alpha\beta}(-\vec{k})$$ Odd parity

$$\Psi_{\alpha\beta}(\vec{k}) = -\Psi_{\beta\alpha}(-\vec{k})$$ Pauli Principle

$$\boxed{\Psi_{\alpha\beta}(\vec{k}) = \Psi_{\beta\alpha}(\vec{k})}$$ spin-triplet pairing

Odd-parity = (pseudo)spin-triplet superconductivity

Spin-triplet superconductivity

$$\Psi_{\alpha\beta}(\vec{k}) = \langle c_{\vec{k}\alpha} c_{-\vec{k}\beta} \rangle$$

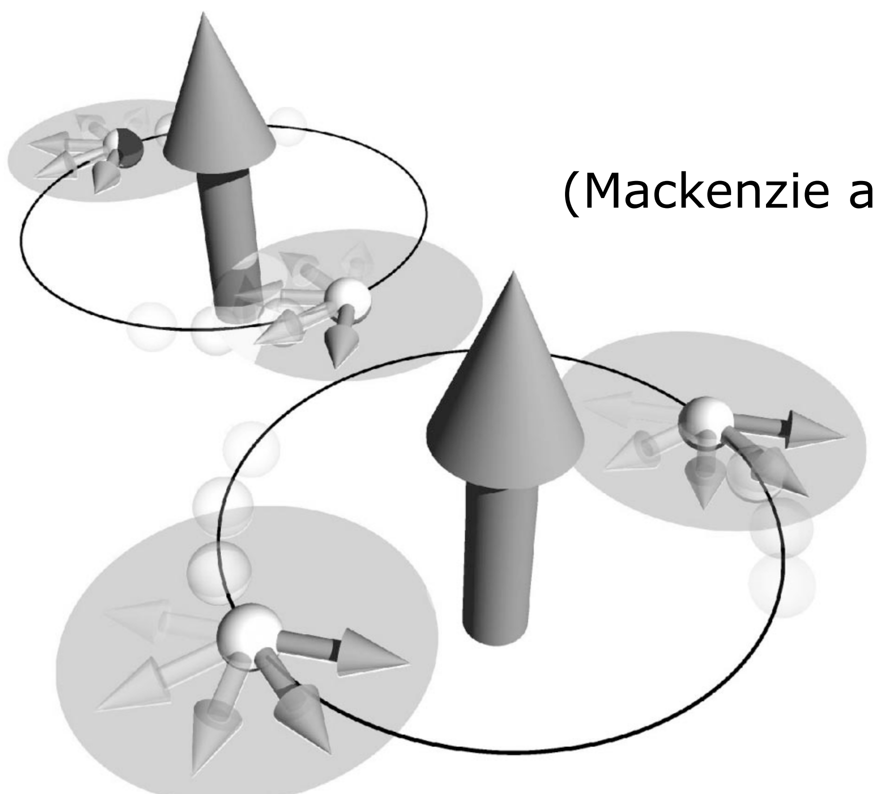
$$\hat{\Psi}_{\alpha\beta} = \begin{pmatrix} \Psi_{\uparrow\uparrow} & \Psi_{\uparrow\downarrow} \\ \Psi_{\downarrow\uparrow} & \Psi_{\downarrow\downarrow} \end{pmatrix} = \begin{pmatrix} -d_x + i d_y & d_z \\ d_z & d_x + i d_y \end{pmatrix}$$

$$\Psi_{\alpha\beta}(\vec{k}) = i \left(\vec{d}(\vec{k}) \cdot \vec{\sigma} \sigma^y \right)_{\alpha\beta}$$

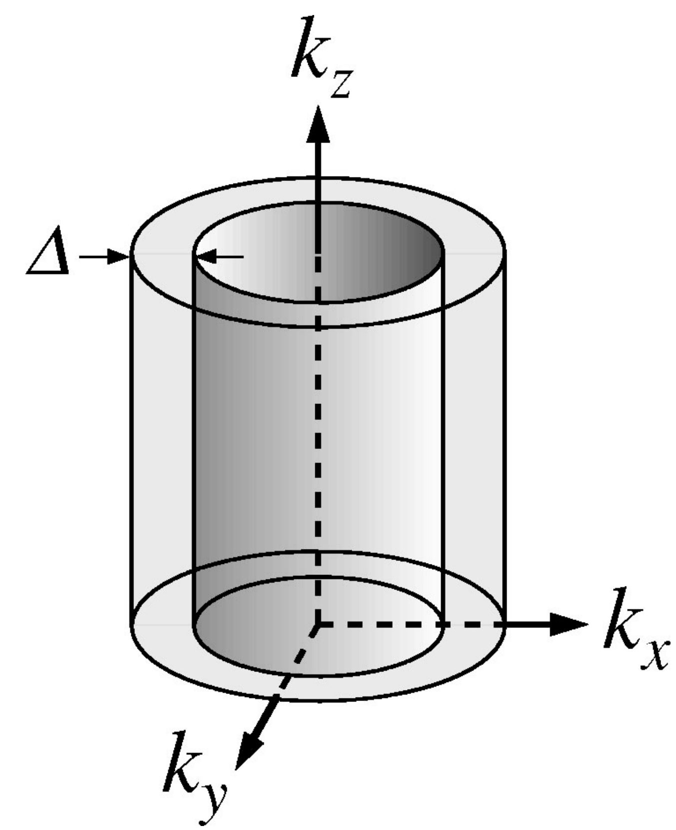
Order parameter is described by a vector in spin-space.

Knight shift experiments have confirmed the spin-1 nature of the order parameter (Ishida *et al.* 1998, Murakawa *et al.* 2004).

2D triplet states with broken T



(Mackenzie and Maeno, RMP 2003)



Simplest state of a quasi-2d system that breaks T: the chiral p-wave state:

$$\vec{d}(\vec{k}) \sim (k_x \pm i k_y)\hat{z}$$

in 2d, such a state is fully gapped and “topologically ordered”.

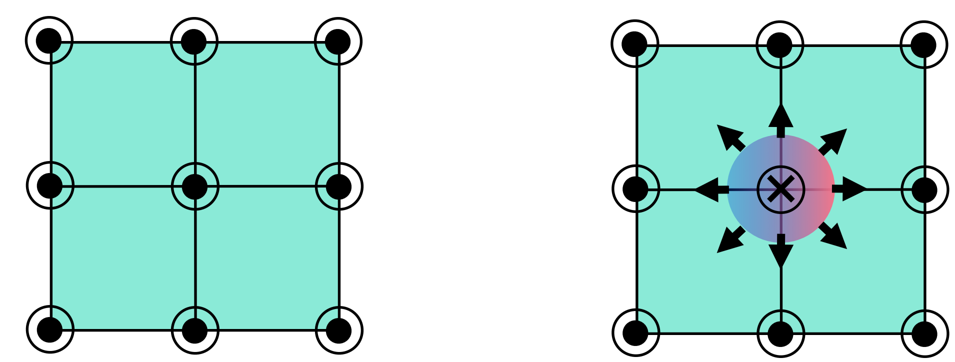
Topological properties of the chiral state

$$H = \vec{\delta}(\vec{k}) \cdot \vec{\tau}$$ Anderson pseudospin representation of BCS

$$\delta(\vec{k}) = (\mathrm{Re}(\Delta(\vec{k})), \mathrm{Im}(\Delta(\vec{k})), \epsilon(\vec{k}) - \mu)$$

$$N = \frac{1}{4\pi} \int d^2k \hat{\delta} \cdot \left(\partial_x \hat{\delta} \times \partial_y \hat{\delta} \right)$$

$\mu < 0$ $\mu > 0$



Strong pairing (trivial) weak pairing (skyrmion)

Single-band system

N = number of net forward
moving Majorana edge modes at a s.c/normal interface.

These quasiparticle edge modes contribute to electrical
currents which are experimentally detectable.

Experimental Puzzles

Low temperature power laws are observed in specific heat and NMR. This is evidence against a simple chiral superconductor.

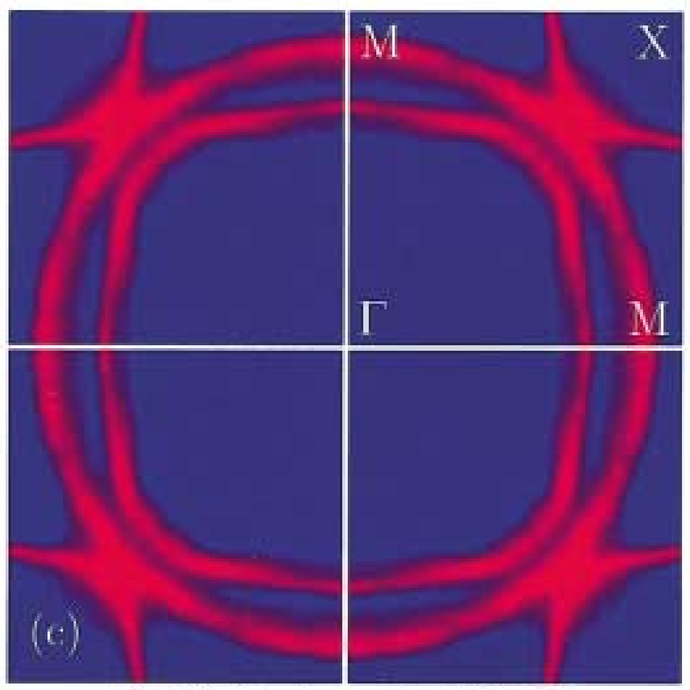
Edge currents are several orders of magnitude smaller than theoretical expectations based on the simple chiral state.

Only a single phase transition in an in-plane magnetic field near T_c.

These findings are inconsistent with a simple chiral state

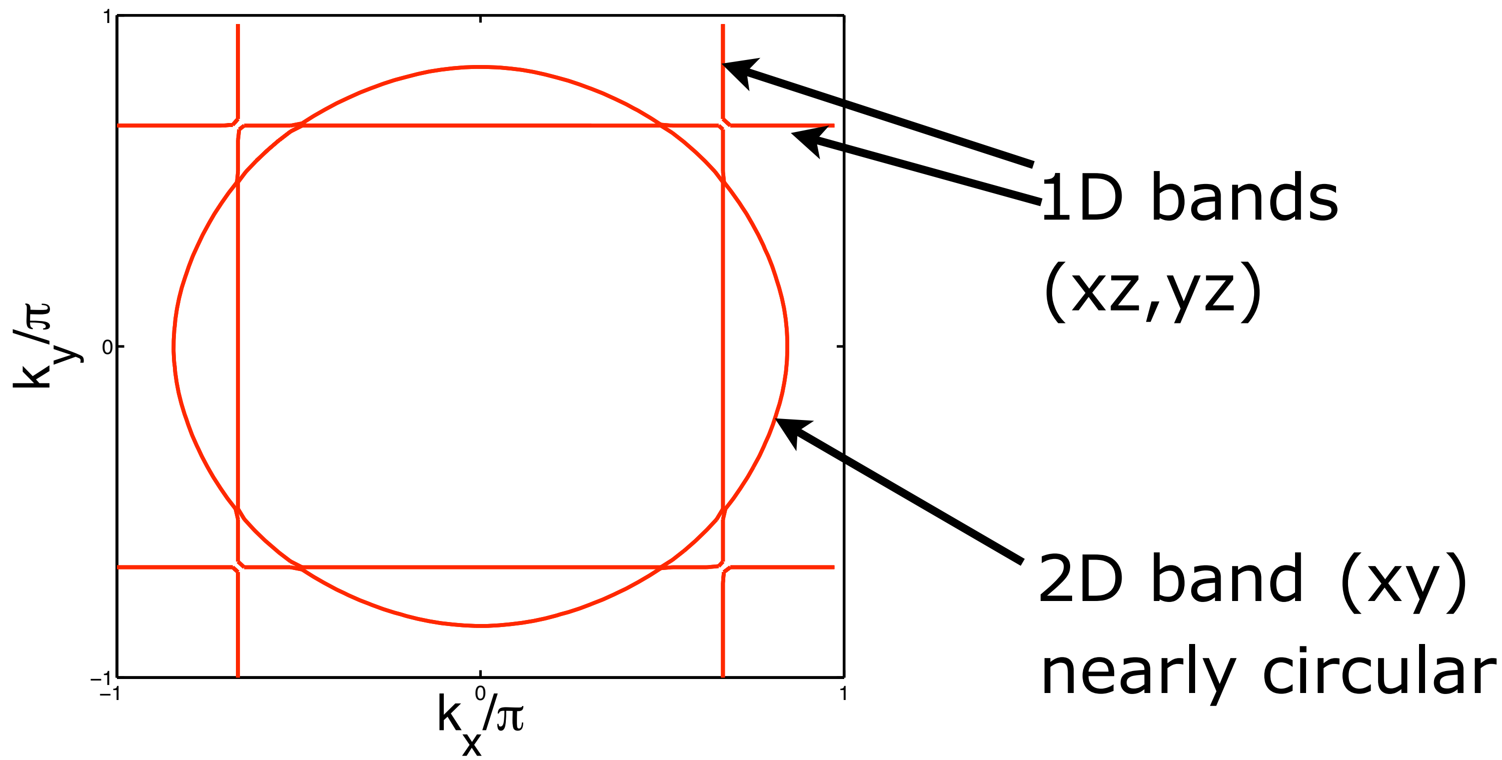
Electronic structure of Sr_2RuO_4

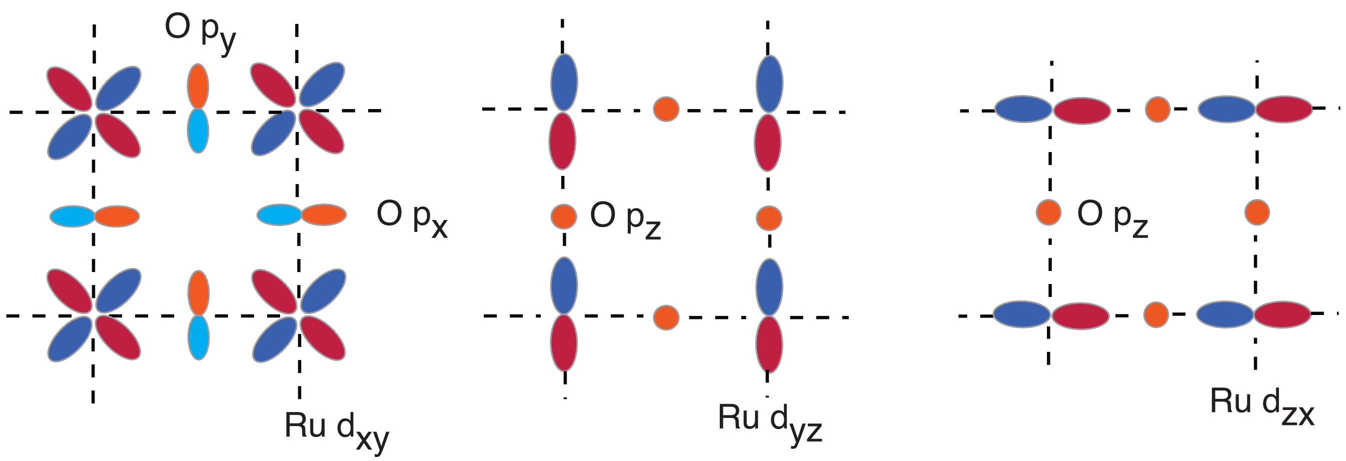
A. Damascelli *et al.*



Sr_2RuO_4 cleaved at 180 K
T= 10 K hν=28 eV

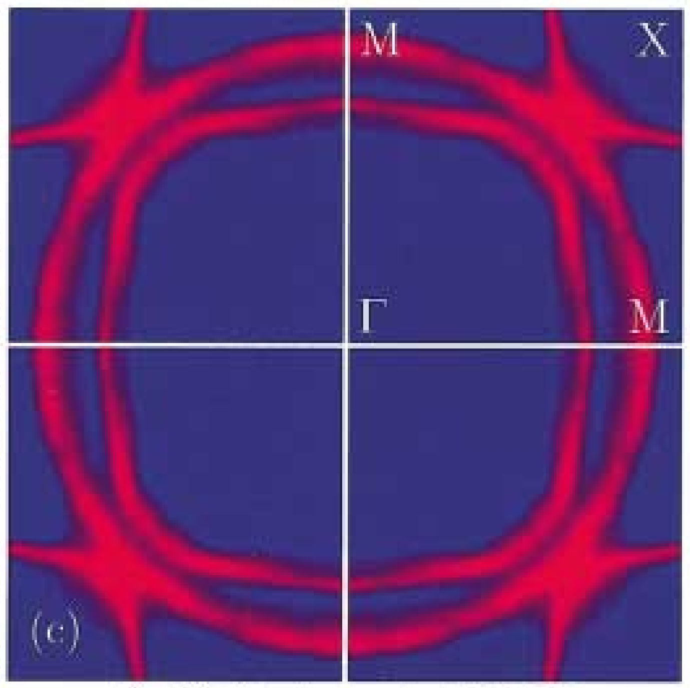
≈





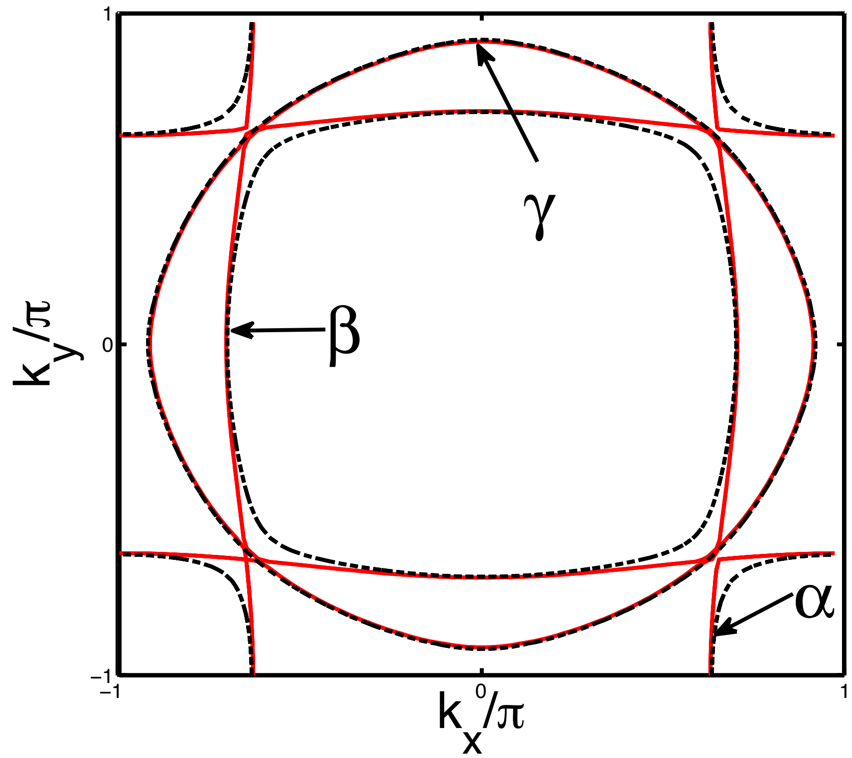
Electronic structure of Sr_2RuO_4

A. Damascelli *et al.*



Sr_2RuO_4 cleaved at 180 K
T= 10 K   hν=28 eV

$\approx$



$\{\alpha, \beta\}$:

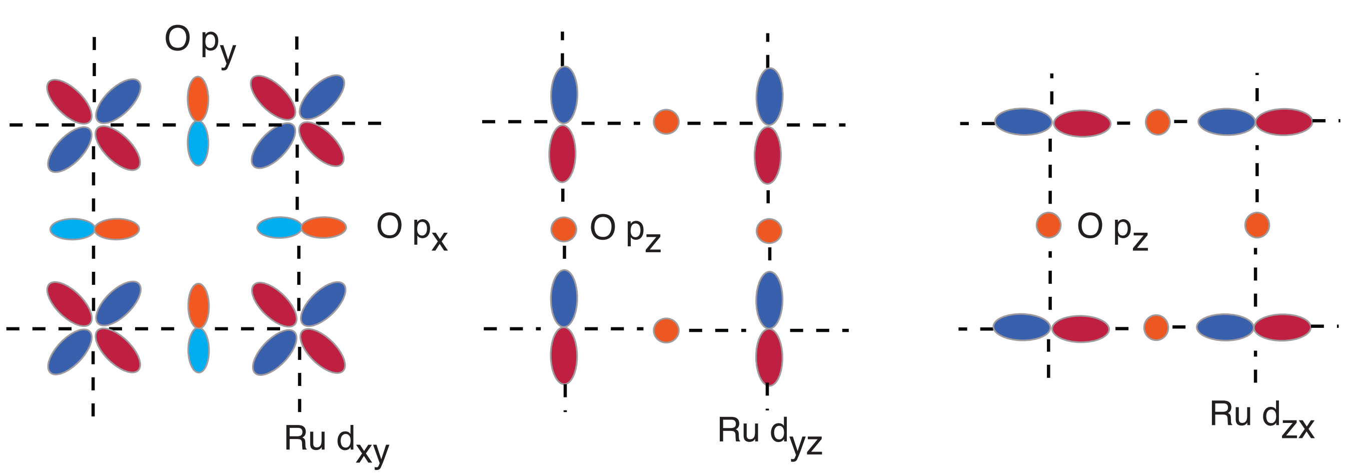
primarily d_{xz},d_{yz}

quasi-1d bands

γ :

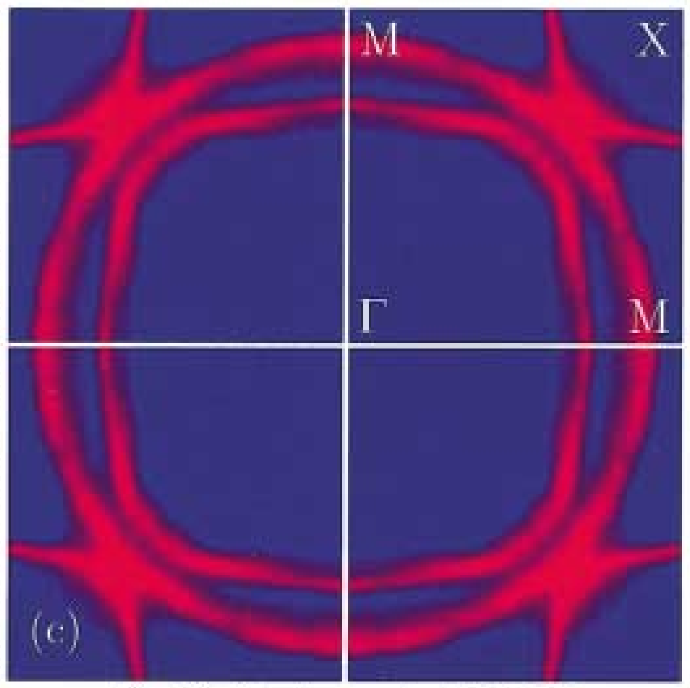
primarily d_{xy}

quasi-2d bands



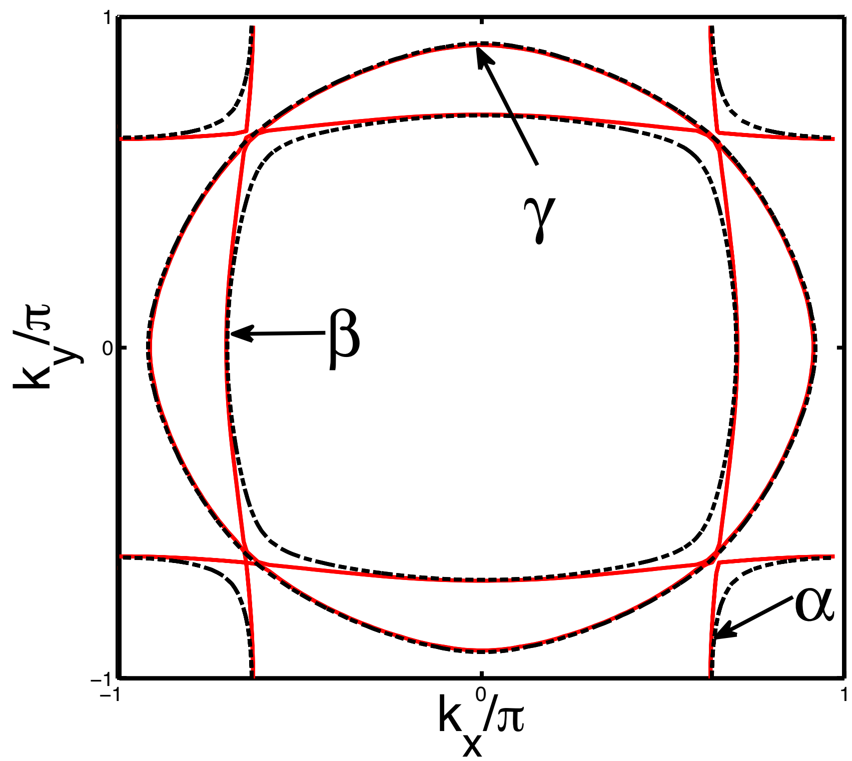
Electronic structure of Sr_2RuO_4

A. Damascelli *et al.*



Sr_2RuO_4 cleaved at 180 K
T= 10 K   hν=28 eV

$\approx$



$\{\alpha, \beta\}$:

primarily d_{xz},d_{yz}

quasi-1d bands

γ :

primarily d_{xy}

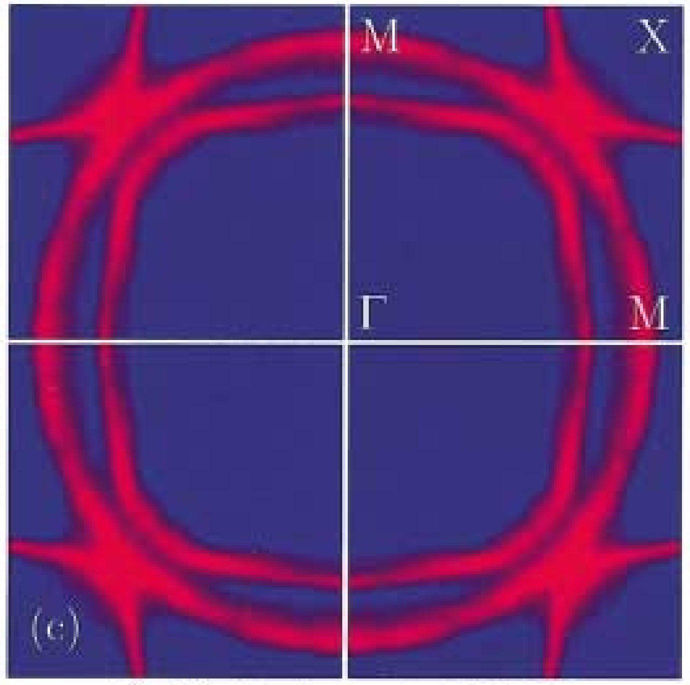
quasi-2d bands

Tetragonal symmetry: $\{\alpha, \beta\}$ and γ have very different orbital character.

Superconductivity is likely derived primarily from either subset - "active" band(s).

Superconductivity is induced via a proximity effect in the remaining "passive" band(s). See D.F. Agterberg *et al.*, PRL **78** 3374 (1998).

Orbital-dependent superconductivity



Sr_2RuO_4 cleaved at 180 K
T= 10 K hν=28 eV

A popular "assumption": γ is the "active" band.

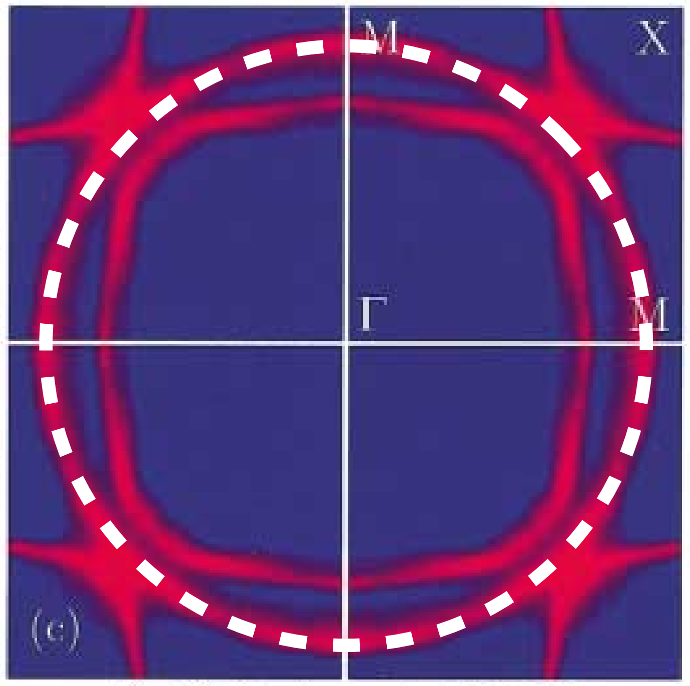
Several good reasons for this viewpoint:

1) γ has the largest mass enhancement.

2) Its proximity to a van Hove singularity - enhances Ferromagnetic fluctuations.

These features are reminiscent of ^{3}He.

Orbital-dependent superconductivity



Sr_2RuO_4 cleaved at 180 K
T= 10 K hν=28 eV

A popular "assumption": γ is the "active" band.

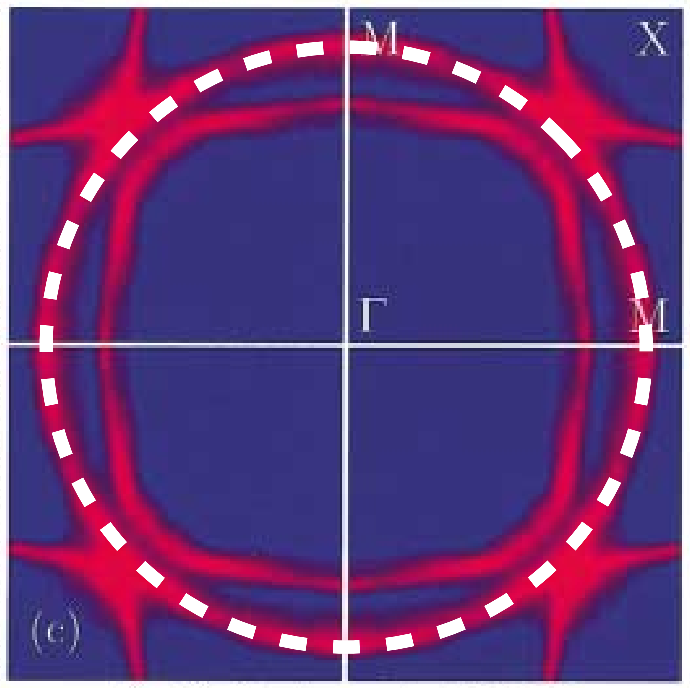
Several good reasons for this viewpoint:

1) γ has the largest mass enhancement.

2) Its proximity to a van Hove singularity - enhances Ferromagnetic fluctuations.

These features are reminiscent of ^{3}He.

Orbital-dependent superconductivity



Sr_2RuO_4 cleaved at 180 K
T= 10 K   hν=28 eV

A popular "assumption": γ is the "active" band.

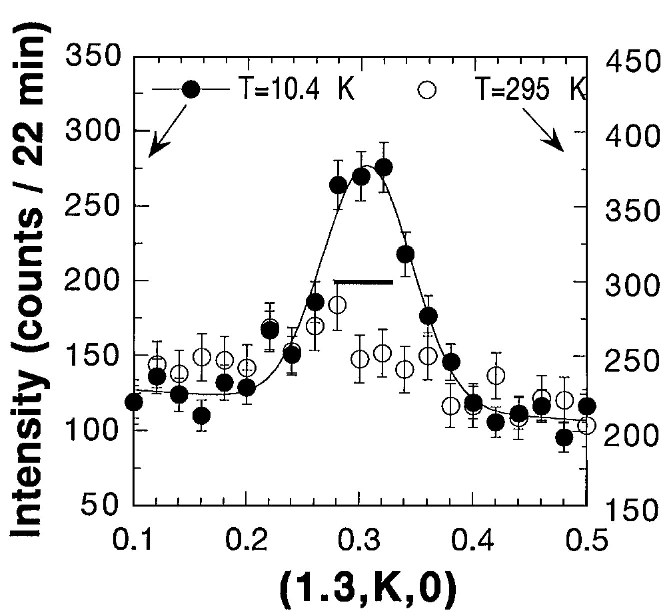
Several good reasons for this viewpoint:

1) γ has the largest mass enhancement.

2) Its proximity to a van Hove singularity - enhances Ferromagnetic fluctuations.

These features are reminiscent of ^{3}He.

Sidis *et al.*, PRL 1999



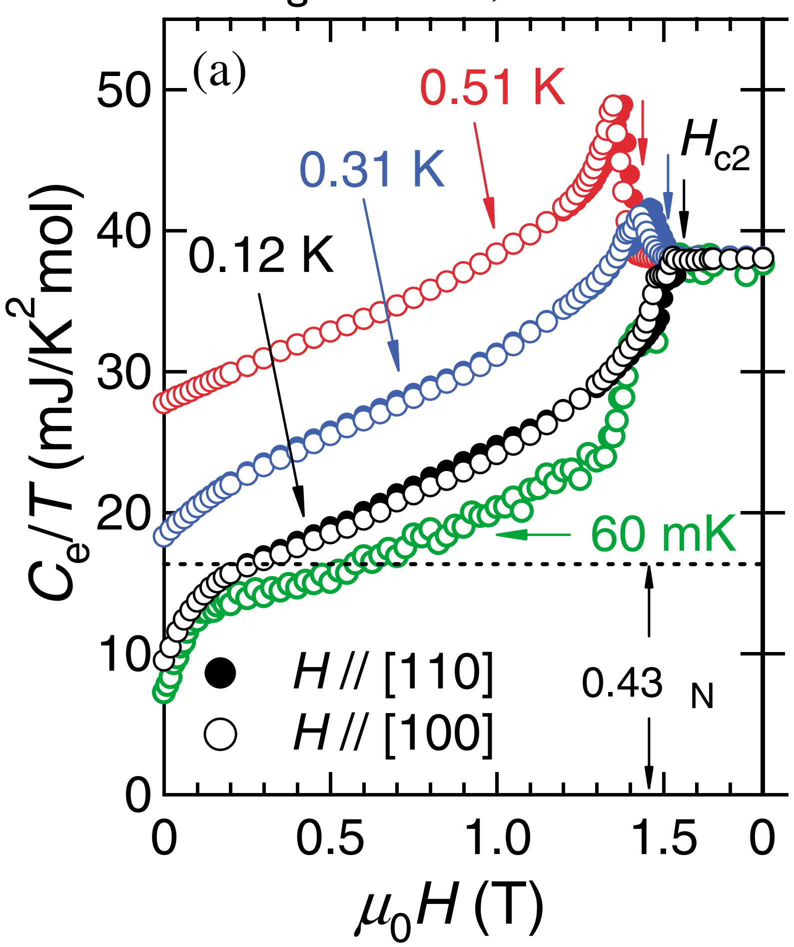
However, the dominant magnetic excitations are at **q** = ($2k_F$,$2k_F$): strong nesting among 1d bands.

Triplet pairing from primarily *large* momentum particle-hole fluctuations?

(See Scalapino, RMP 2012).

Heat capacity measurements

Deguchi *et al.*, PRL 2004



Cited as evidence in favor of γ as active band.

Contribution to total normal state DOS(E_F):

$$\{\alpha, \beta\} : 43\%$$

$$\gamma : 57\%$$

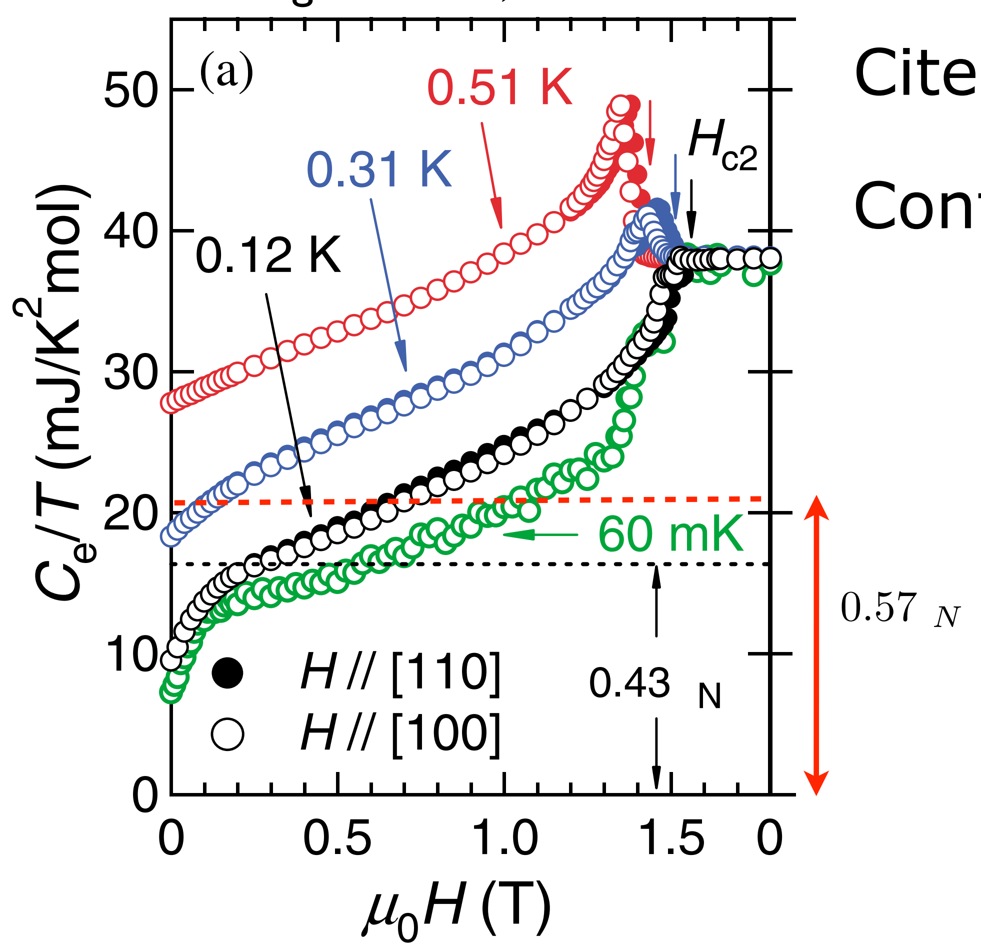
$$\left.\frac{C}{T}\right|_{T_c} = 32\ \mathrm{mJ/K^2 mol}$$

from dH-vA

Actual C/T: 38 mJ/K^2 mol
(15% disagreement with dH-vA).

Heat capacity measurements

Deguchi et al., PRL 2004



Cited as evidence in favor of γ as active band.

Contribution to total normal state DOS(E_F):

$$\{\alpha, \beta\} : 43\%$$

$$\gamma : 57\%$$

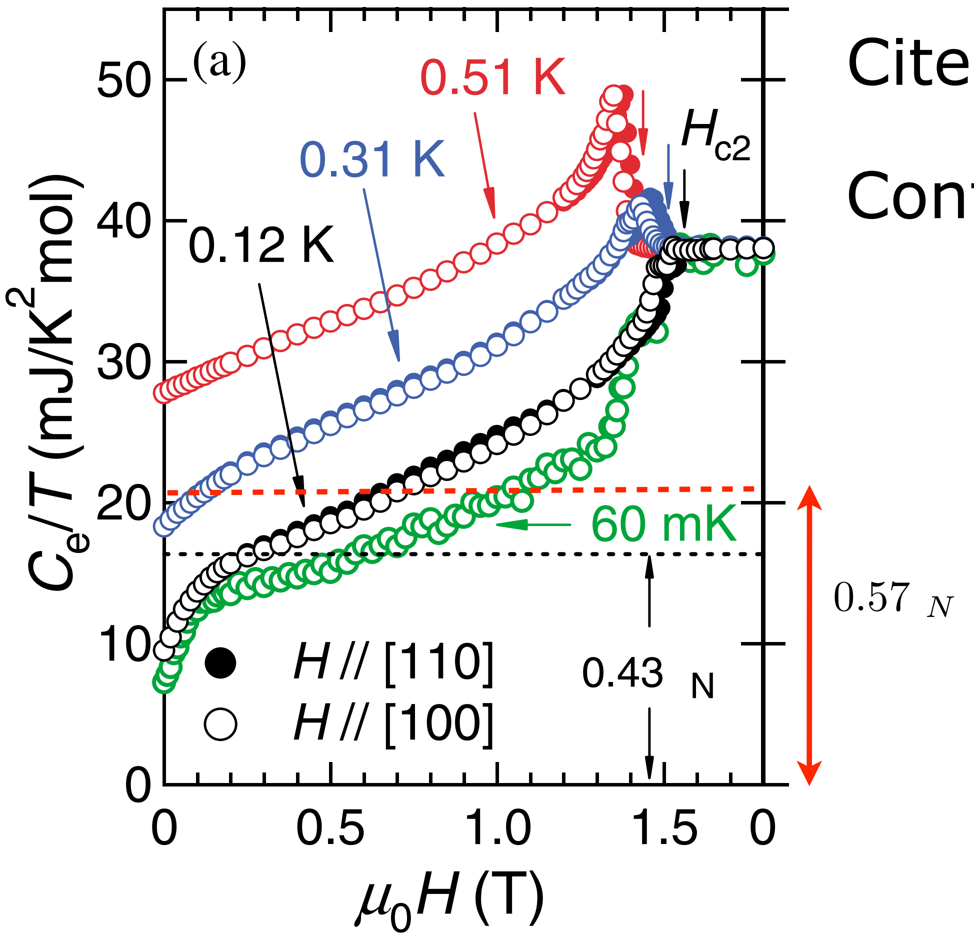
$$\left.\frac{C}{T}\right|_{T_c} = 32 \text{ mJ/K}^2\text{mol}$$

from dH-vA

Actual C/T: 38 mJ/K^2 mol
(15% disagreement with dH-vA).

Heat capacity measurements

Deguchi et al., PRL 2004



Cited as evidence in favor of γ as active band.

Contribution to total normal state DOS(E_F):

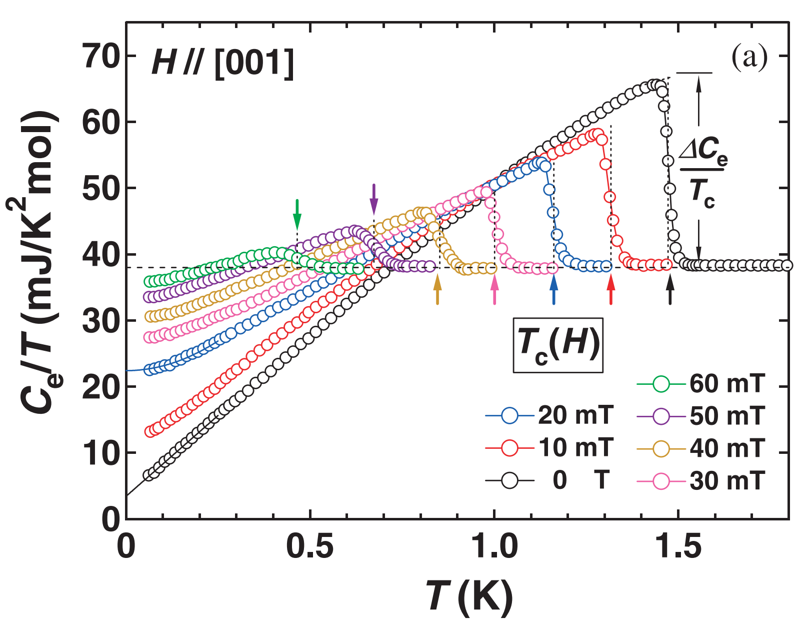
$$\{\alpha, \beta\} : 43\%$$

$$\gamma : 57\%$$

$$\left.\frac{C}{T}\right|_{T_c} = 32\ \mathrm{mJ/K^2 mol}$$

from dH-vA

Actual C/T: 38 mJ/K² mol
(15% disagreement with dH-vA).



Temperature dependence of heat capacity does not show two gaps.

The data does not point towards either scenario for “active” bands.

Microscopic model and superconductivity

Microscopic Model

$$H = H_{kin} + U \sum_{i,\alpha} n_{i\alpha\uparrow} n_{i\alpha\downarrow} + \frac{V}{2} \sum_{i\alpha\neq\alpha'} n_{i\alpha} n_{i\alpha'} + \delta H$$

strongest hybridizations among all 3 t_{2g} orbitals

Intra-orbital repulsion

Inter-orbital repulsion

We consider the simplest multi-orbital model which contains the essential physics.

Start by neglecting δH:band mixings and couple distinct orbitals only with V.

We will treat effect of band mixing phenomenologically as a small perturbation.

Weak-coupling solution

We follow the asymptotically exact weak-coupling method described in the following work:

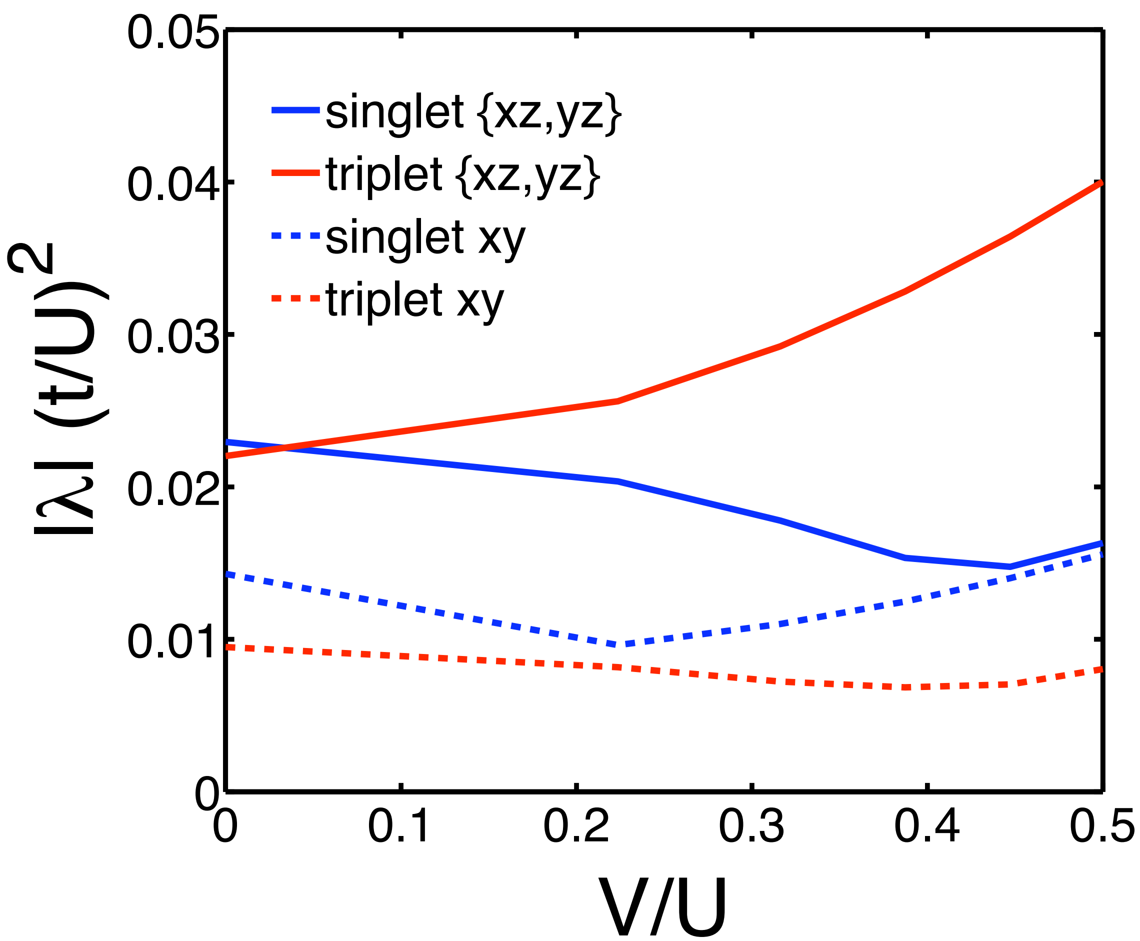
S.R., S. A. Kivelson and D. J. Scalapino, PRB **81**, 224505 (2010).

Strategy:

1) Integrate out states above an artificial initial cutoff.
2) Study the RG flow of the resulting effective action.
3) Determine scale at which RG flows in the Cooper channel break down. This is the pairing scale.

Prescription is based on R. Shankar and J. Polchinsky's RG treatment of the Fermi liquid.

Weak-coupling solution



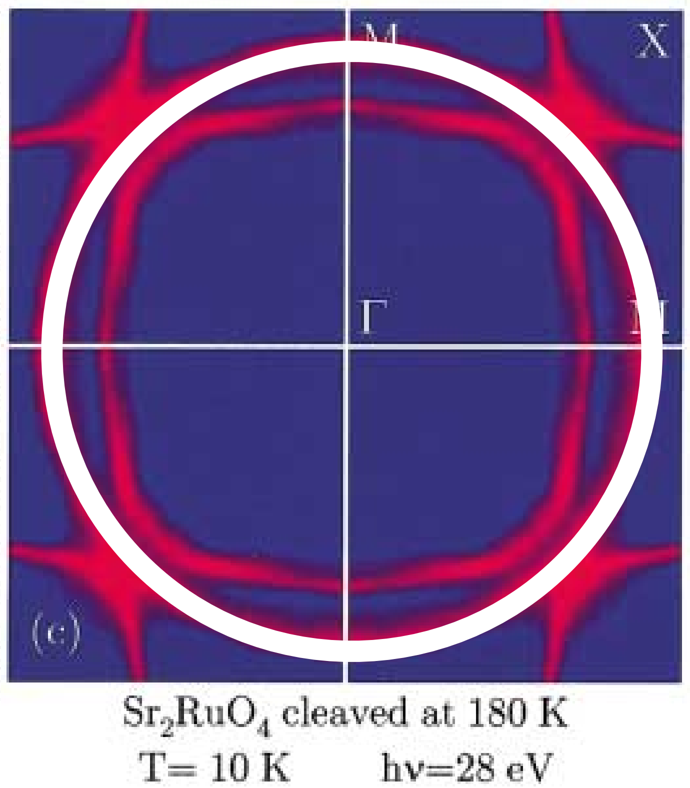
Superconductivity in the weak coupling limit is dominant on the xz,yz orbitals. The xy orbital has an exponentially lower pairing strength.

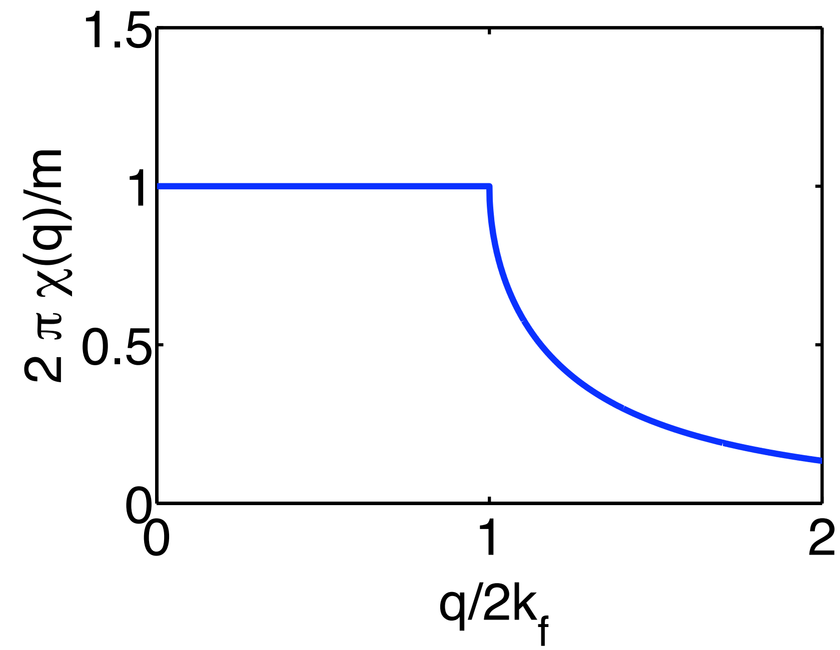
There is a near-degeneracy between singlet and triplet pairing on the xz,yz orbitals for small V.

For V finite: triplet pairing is dominant. All other solutions have exponentially smaller T_c.

Weak-coupling limit: pairing occurs primarily among {xz,yz} electrons.

Weak-coupling solution



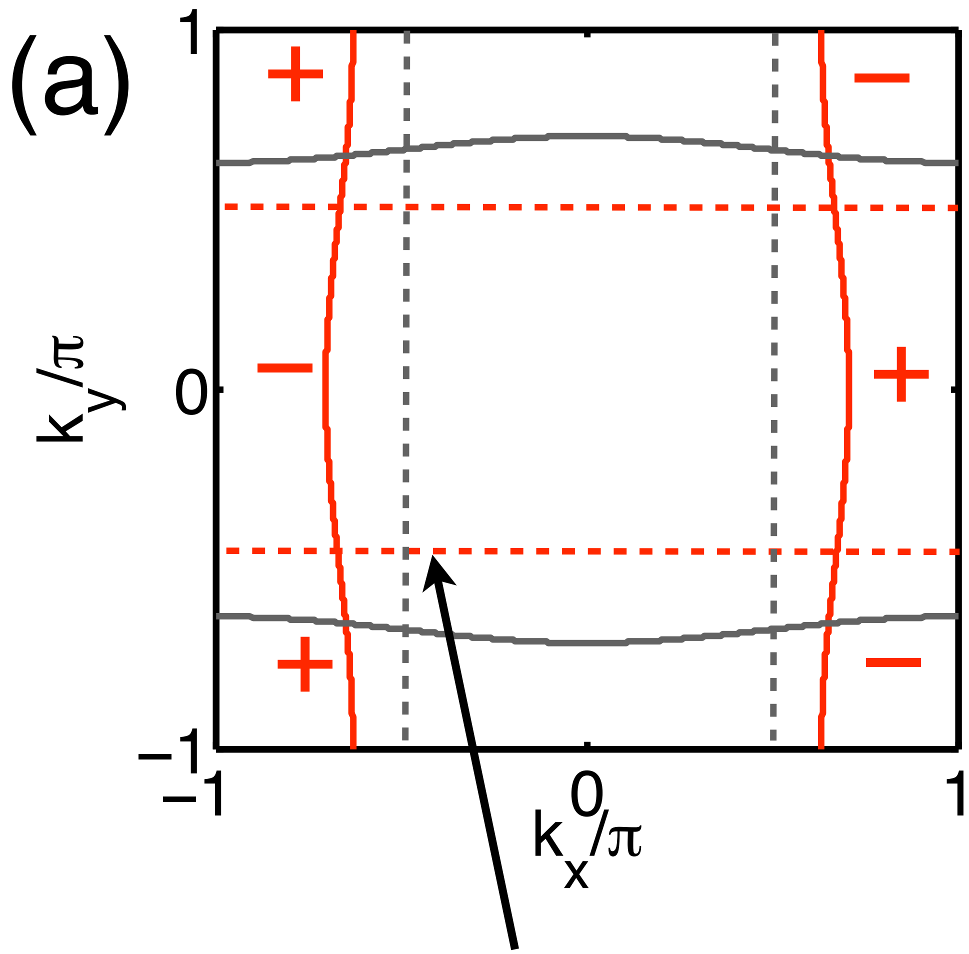


The γ Fermi surface is nearly perfectly circular.

$\chi(\hat{k} \pm \hat{q})$ is a constant for any two points on the Fermi surface.

The pairing interaction depends on the susceptibility and is weak for a circular Fermi surface, independent of the mass enhancement.

Weak-coupling solution



nodal line: pair wave function changes sign.

$$\vec{d}_{xz}(\vec{k}) \approx e^{i\phi_x} \sin k_x \cos k_y \hat{\Omega}_x$$

$$\vec{d}_{yz}(\vec{k}) \approx e^{i\phi_y} \sin k_y \cos k_x \hat{\Omega}_y$$

In the absence of band mixings between xz,yz,

$$\phi_x, \phi_y, \hat{\Omega}_x, \hat{\Omega}_y$$

are completely arbitrary.

This state is similar to the quasi-1D organic superconductors.

They are determined by small perturbations of the electronic structure which mix xz,yz bands.

Effect of small perturbations

Near T_c, the effect of small perturbations (spin-orbit coupling λ and longer range inter-orbital hopping t'') is to introduce a binary choice for the orientation of the d-vector.

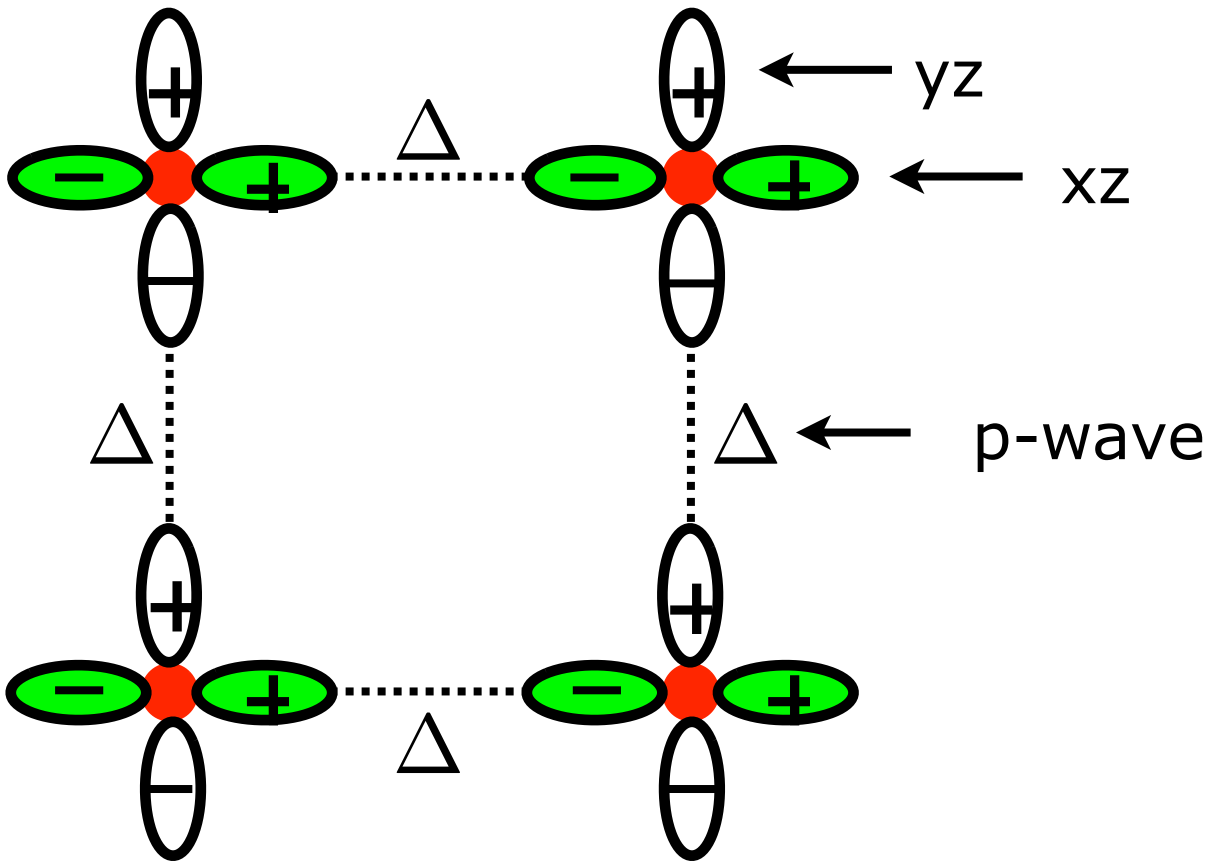
$$\mathcal{F} = r\left(|\vec{d}_{xz}|^2 + |\vec{d}_{yz}|^2\right) + r_1\left(|d^z_{xz}|^2 + |d^z_{yz}|^2\right) + r_2\left(|d^x_{xz}|^2 + |d^y_{yz}|^2\right)$$

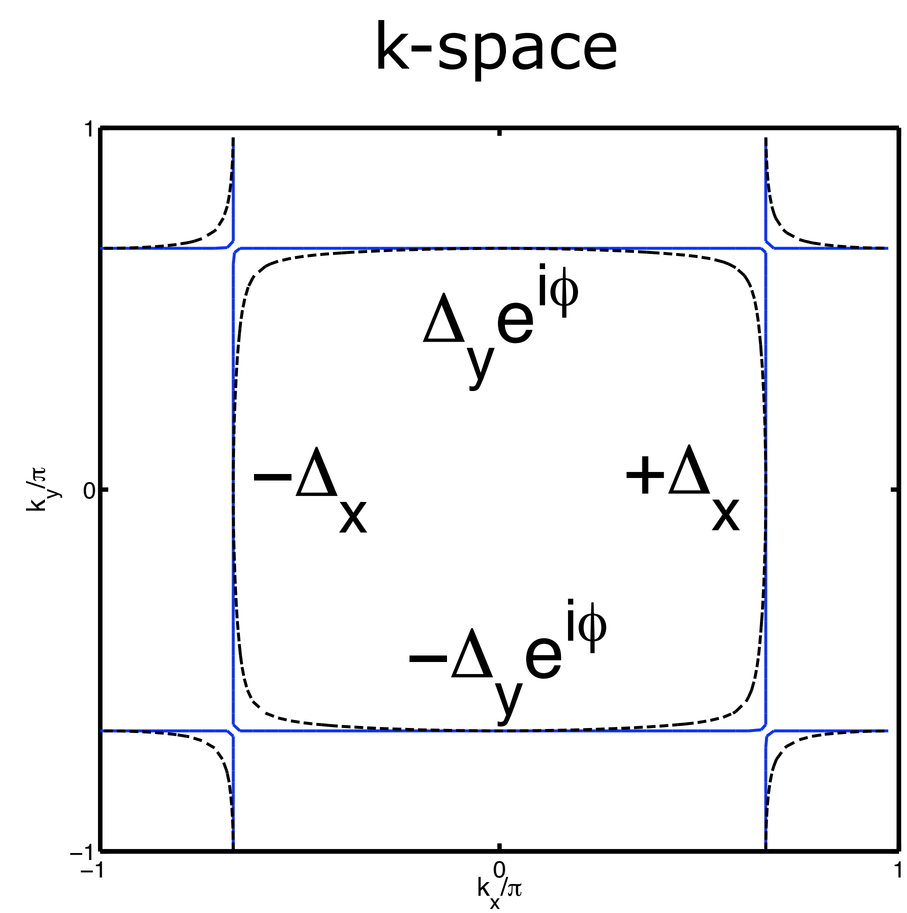
$r_1 < \mathrm{Min}[0, r_2]$ Both d-vectors are perpendicular to the xy plane.

$r_2 < \mathrm{Min}[0, r_1]$ Both d-vectors lie in the xy plane.

Formation of the Chiral p-wave state

$\vec{d} \propto \hat{z}$





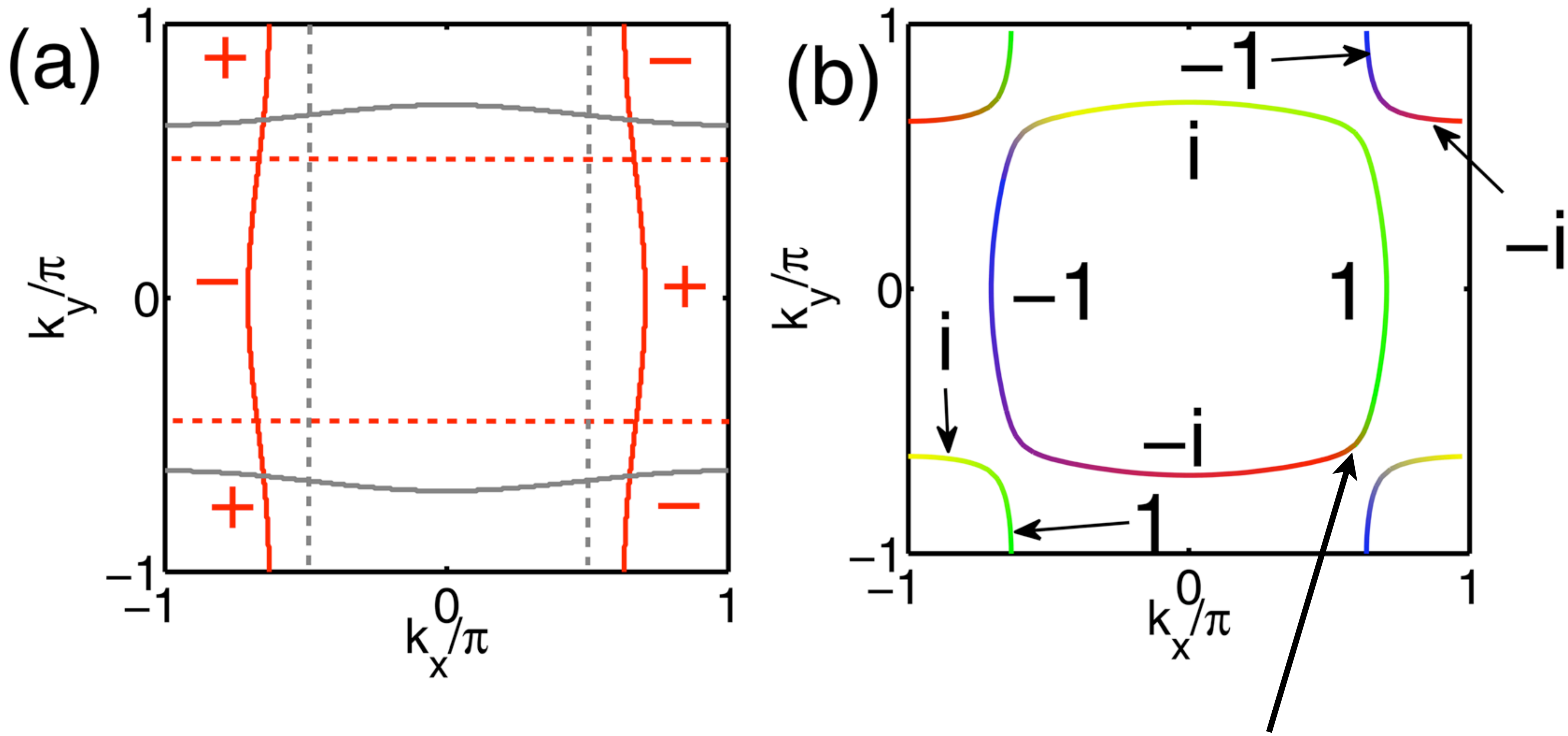
ϕ is arbitrary for nearly decoupled xz,yz orbitals.

hybridization of orbitals just below Tc: $\cos\phi = 0$

i.e. px+ipy or px-ipy

System spontaneously breaks T to maximize condensation energy.

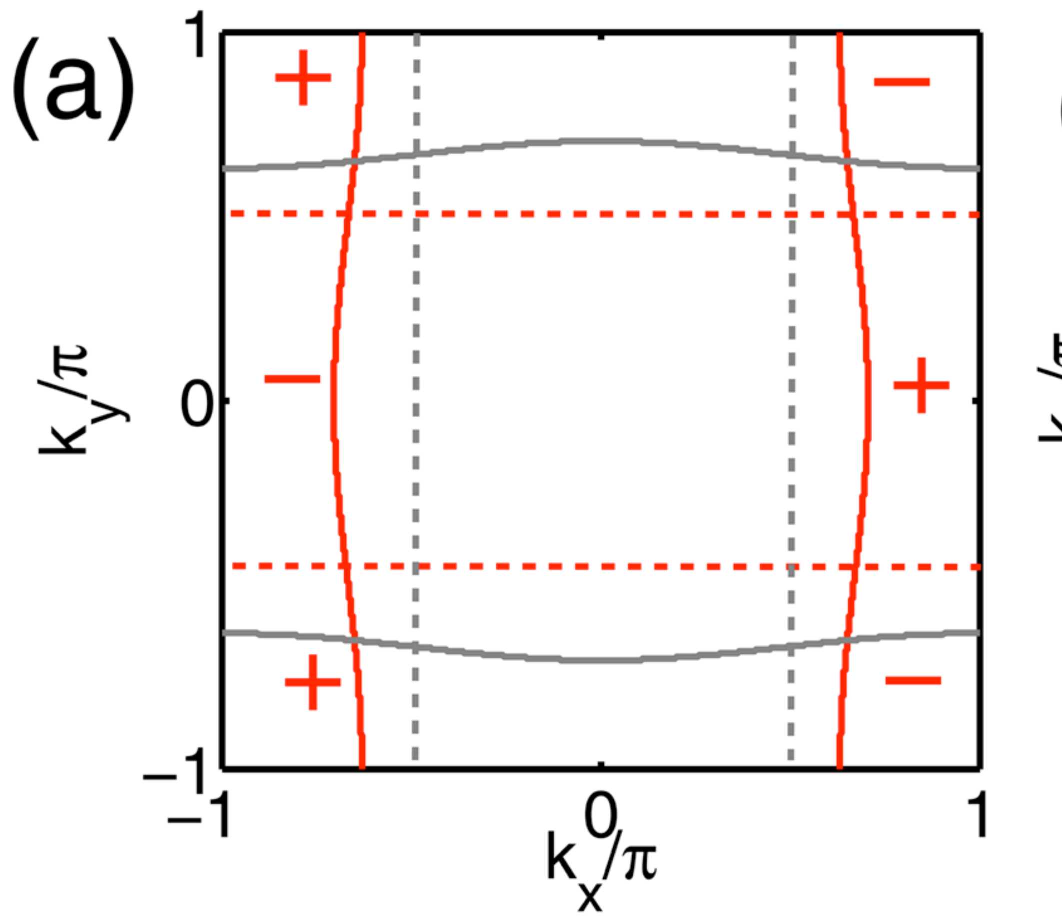
Structure of the Chiral p-wave state

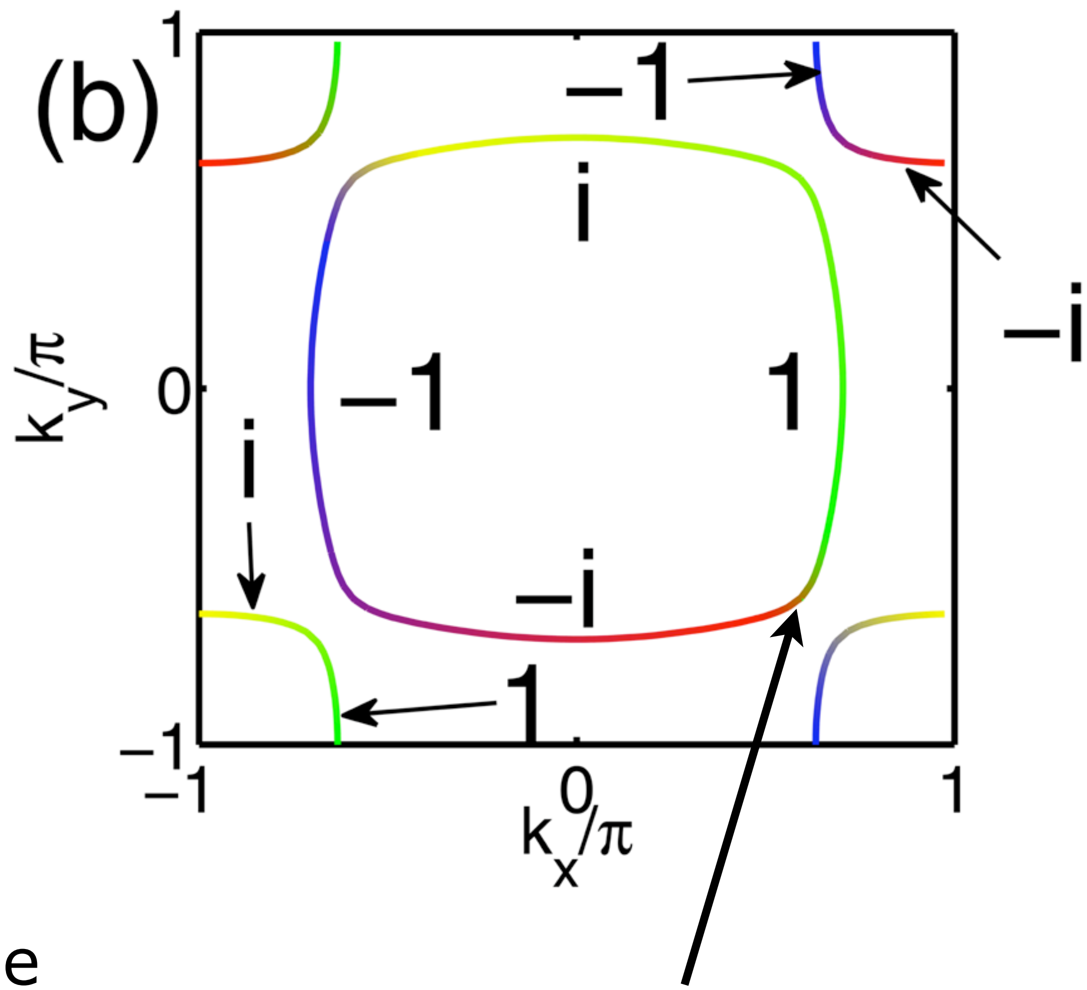


Sharp gap minima ~ $(t''/t)^2 T_c$

$p_x + ip_y$ state on both quasi-1D Fermi surfaces -> Multiband state.

Structure of the Chiral p-wave state



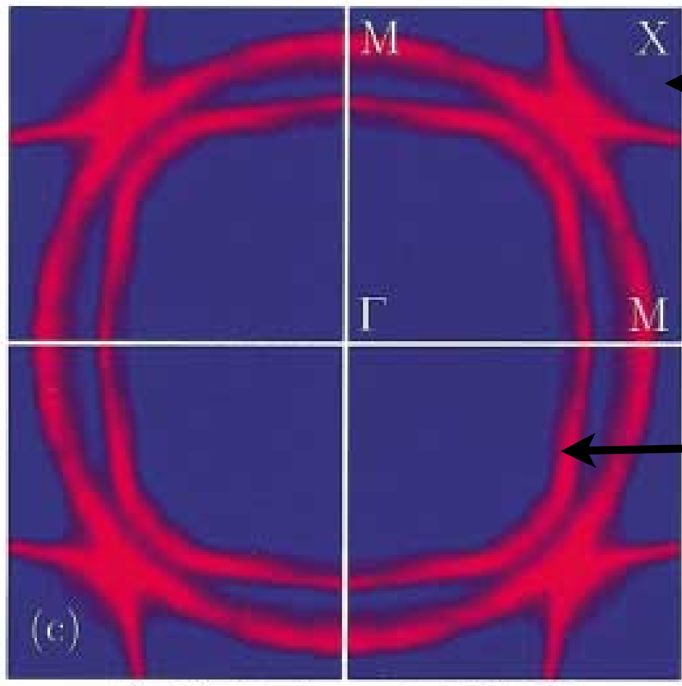


Similar to the high field phase of quasi-1D organic superconductors?

Sharp gap minima ~ $(t''/t)^2 T_c$

p_x+ip_y state on both quasi-1D Fermi surfaces -> Multiband state.

Properties of the quasi-1D superconductor



Sr_2RuO_4 cleaved at 180 K
T= 10 K hν=28 eV

hole pocket

electron pocket

$$N = \frac{1}{4\pi} \int d^2k \hat{\delta} \cdot \left(\partial_x \hat{\delta} \times \partial_y \hat{\delta} \right)$$

Two ways to change sgn(N):

1) flip chirality: p+ip -> p-ip
2) electron-pocket -> hole pocket

p+ip pairing on both q1D Fermi surfaces: net skyrmion number = 0.

No chiral edge modes (2 counter-propagating edge channels), no quantized thermal Hall effect. (All of these are present for a p+ip superconductor on the 2D sheet).

Can this naturally explain the absence of edge *currents*?

Edge currents and Chern invariants

Our original intuition: chern number = 0 on d_{xz},d_{yz} bands. Therefore, Majorana edge modes can be localized, leading to small edge currents.

However, this isn't quite right. Consider explicit example: electrons on a bipartite lattice.

$$H = \sum_{\langle i,j \rangle} (c_i^\dagger c_j + c_j^\dagger c_i) - \mu \sum_i c_i^\dagger c_i + H_{pair}$$

Couple to gauge field: $c_i \to c_i e^{-iA_{r,i}}, \ A_{r,i} = \frac{e}{hc} \int_r^i \vec{A} \cdot d\vec{l}$

Particle-hole transformation: $c_i e^{-iA_{r,i}} \to (-1)^i e^{iA_{r,i}}$

Changes sign of Chern number, but the current operator is left invariant:

$$\mathcal{J}_{ij} = -i(c_j^\dagger c_i - c_i^\dagger c_j)$$

Reason for small edge currents

$$
\begin{aligned}
F_{grad} = \beta_1 & \left[|D_x\psi_x|^2 + |D_y\psi_y|^2\right] \\
+\beta_2 & \left[|D_y\psi_x|^2 + |D_x\psi_y|^2\right] \\
+\beta_3 & \left[(D_x\psi_x)^*(D_y\psi_y) + c.c.\right] \\
+\beta_4 & \left[(D_x\psi_y)^*(D_y\psi_x) + c.c.\right]
\end{aligned}
$$

$\left.\begin{matrix}\beta_3 \\ \beta_4\end{matrix}\right\}$ Responsible for edge currents.

$$\beta_3, \beta_4 \propto \langle \psi_x(\hat{k}_F)\psi_y(\hat{k}_F)v_{F,x}v_{F,y}\rangle_{F.S.}$$

These Fermi surface averages are order-1 for theories based on the circular dxy band,

However, they are reduced by 2-3 orders of magnitude for the multi-band theory discussed here.

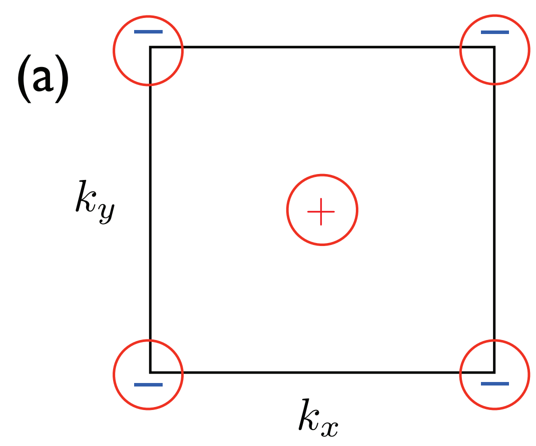
Currents are $\propto \beta_3$

and therefore substantially smaller for the multiband theory.

Criticism of the weak-coupling theory

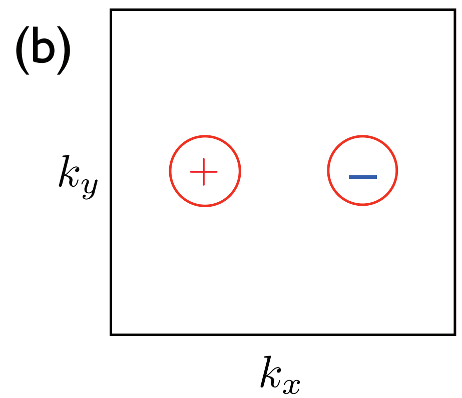
The γ band is close to the van Hove filling. It has enhanced ferromagnetic spin fluctuations, which are favorable for spin-triplet pairing. Our weak-coupling result seems contrary to this reasonable intuitive picture.

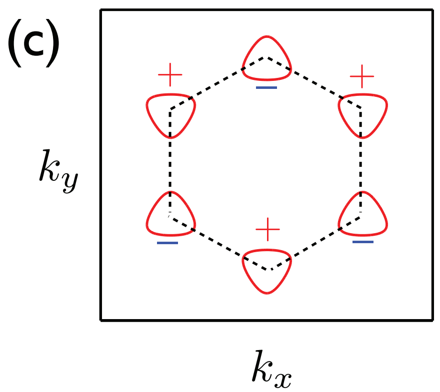
Consider a system with two pockets, with interactions peaked at large momentum transfer. Gap function changes sign but can be *either singlet or triplet* depending on lattice geometry.



sign-changing s-wave

p-wave





f-wave

Phenomenological consequences

The multi-band p+ip state we found has an intrinsic Kerr effect (Observerd first by E. Taylor and C. Kallin, PRL **108**, 157001 (2012)).

p+ip pairing on both q1D Fermi surfaces: 2 counter-propagating edge channels. Majorana fermion modes are not topologically protected. Their contribution to edge currents can vanish with disorder.

The p_x, p_y components "live" on different orbitals and are weakly coupled. The Cooper pair "angular momentum" is substantially lower than in a 1 band chiral superconductor - S. Lederer and SR, *in preparation*.

The weak-coupling between the p_x, p_y components allow for low energy collective mode excitations: relative phase and spin-orientation modes. S.-B. Chung, SR, A. Kapitulnik, S. Kivelson, PRB **86**, 064525 (2012).

Summary

1) Experiments do NOT point towards an unequivocal origin of the "active" band(s), where superconductivity originates in Sr_2RuO_4.

2) Asymptotically exact weak-coupling calculations involving all 3 bands point towards $\{\alpha, \beta\}$ as the "active" bands.

3) The results obtained in the weak-coupling limit have some phenomenological consequences: 1) *intrinsic* Kerr response, 2) reduced edge currents, 3) low energy collective and quasiparticle excitations.

4) The microscopic theory presented here unifies Sr_2RuO_4 with the cuprates, pnictides, and organic superconductors: all derive their pairing interaction mainly from large momentum particle-hole fluctuations, in contrast to Helium-3.