COFUS08 workshop

- Competing orders, Pairing Fluctuations, and Spin Orbit Effects in Novel Unconventional Superconductors
- 30 June -July 11   2008, MPI PKS, Dresden
- Organizers: JF Annett, D. Morr and I. Eremin

University of BRISTOL

Spin Orbit Effects and Pairing Symmetry in Sr_2RuO_4

James Annett and

Balazs Gyorffy (Bristol)

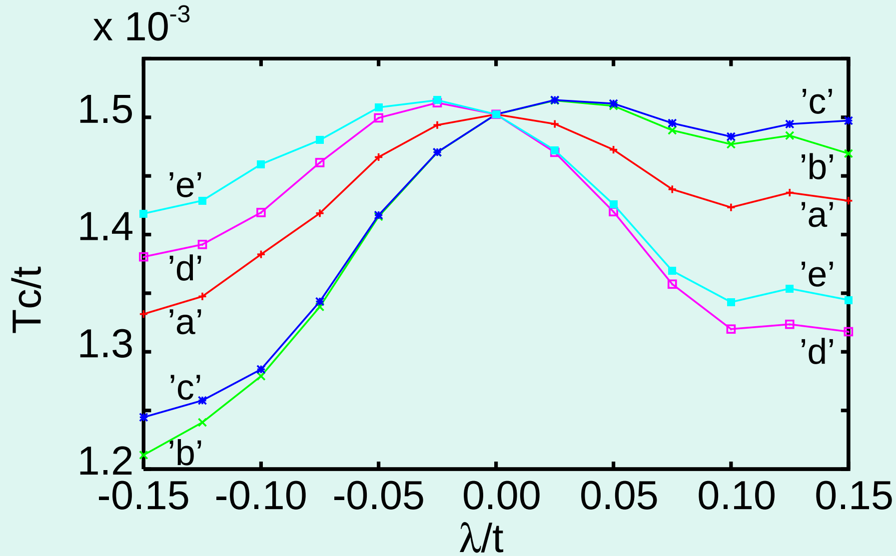
Karol Wysokinski and

Grzegorz Litak(Lublin)

PRB 2006, Physica C 2007, + unpublished

We find a surprising result!

T_c as a function of spin-orbit parameter λ



$(a) \quad \underline{\mathbf{d}}_{\mathbf{k}} \sim (0, 0, X + \mathrm{i}Y)$

$(b) \quad \underline{\mathbf{d}}_{\mathbf{k}} \sim (X, Y, 0)$

$(c) \quad \underline{\mathbf{d}}_{\mathbf{k}} \sim (Y, -X, 0)$

$(d) \quad \underline{\mathbf{d}}_{\mathbf{k}} \sim (X, -Y, 0)$

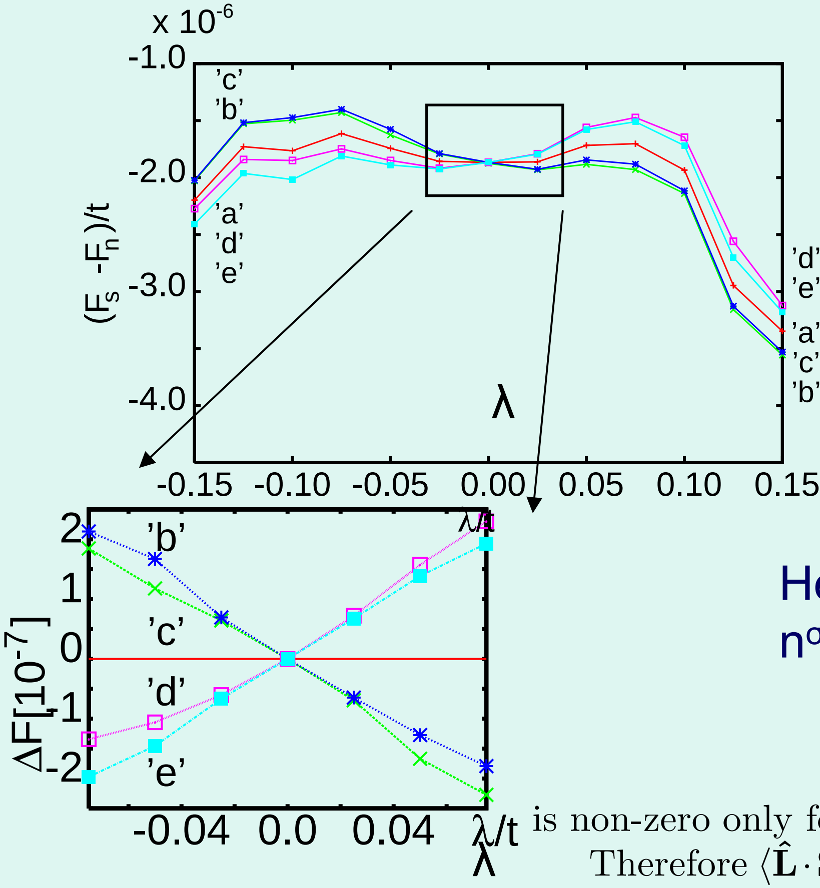
$(e) \quad \underline{\mathbf{d}}_{\mathbf{k}} \sim (Y, X, 0)$

X(**k**), Y(**k**) are basis functions in the 1st BZ transforming as k_x, k_y

For λ>0 b and c are most stable
For λ<0 e and d are most stable

Surprisingly the expected chiral (a) state is NEVER stable!

Simple perturbation theory in λ



$$\delta F = \frac{\lambda}{2}\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\rangle = \frac{\lambda}{2}\sum_{m,m'}\langle m|\hat{L}_z|m'\rangle n^{\uparrow\uparrow}_{mm'} + \frac{\lambda}{2}\sum_{m,m'}\langle m|\hat{L}_x - \mathrm{i}\hat{L}_y|m'\rangle n^{\uparrow\downarrow}_{mm'} + \frac{\lambda}{2}\sum_{m,m'}\langle m|\hat{L}_x + \mathrm{i}\hat{L}_y|m'\rangle n^{\downarrow\uparrow}_{mm'} - \frac{\lambda}{2}\sum_{m,m'}\langle m|\hat{L}_z|m'\rangle n^{\downarrow\downarrow}_{mm'},$$

Here |m › = |d xz ›, |d yz ›, |d xy › Ru orbitals
$n^{\sigma\sigma'}_{mm'}$ = ‹ $c^{+}_{m\sigma}\, c_{m'\sigma'}$ › relative to | p+ip BCS ›

$$\langle \hat{L}_z\rangle = n^{\uparrow\uparrow}_{ab} + n^{\downarrow\downarrow}_{ab} - \left(n^{\uparrow\uparrow}_{ba} + n^{\downarrow\downarrow}_{ba}\right),$$

is non-zero only for the chiral state.

Therefore $\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\rangle$ is non-zero for four states (b)–(e) which have $\langle \hat{\mathbf{S}}\rangle = \langle \hat{\mathbf{L}}\rangle = 0$ while the (a) state has $\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}\rangle = 0$, $\langle \hat{L}_z\rangle \neq 0$.

Spin-dependent pairing interaction?

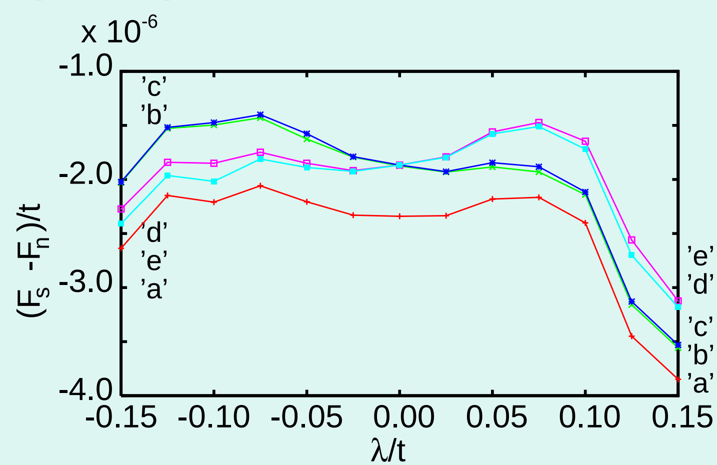
The chiral spin orientation of the Cooper pair must arise from another mechanism: such as spin-dependent pairing interactions.

We implicitly assumed $U^{\uparrow\uparrow}_{mm'}(ij) = U^{\uparrow\downarrow}_{mm'}(ij).$

But in general: $U^{\uparrow\uparrow}_{mm'}(ij) \neq U^{\uparrow\downarrow}_{mm'}(ij),$

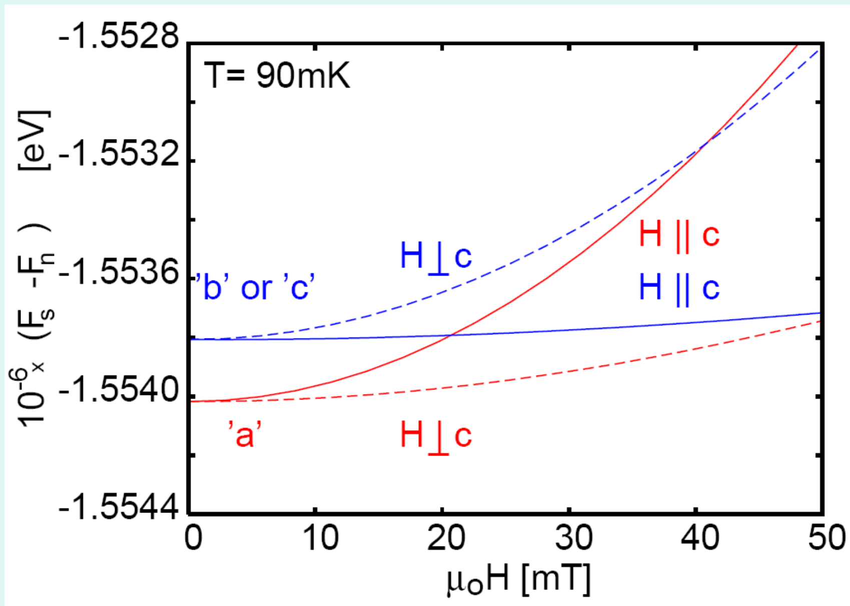
These can be different corresponding to the Fermi liquid parameters for parallel and opposite spin quasi-particles

Chiral state is $\uparrow\downarrow$ pairing only, while the others are $\uparrow\uparrow$ and $\downarrow\downarrow$ only



Effect of a c-axis magnetic field

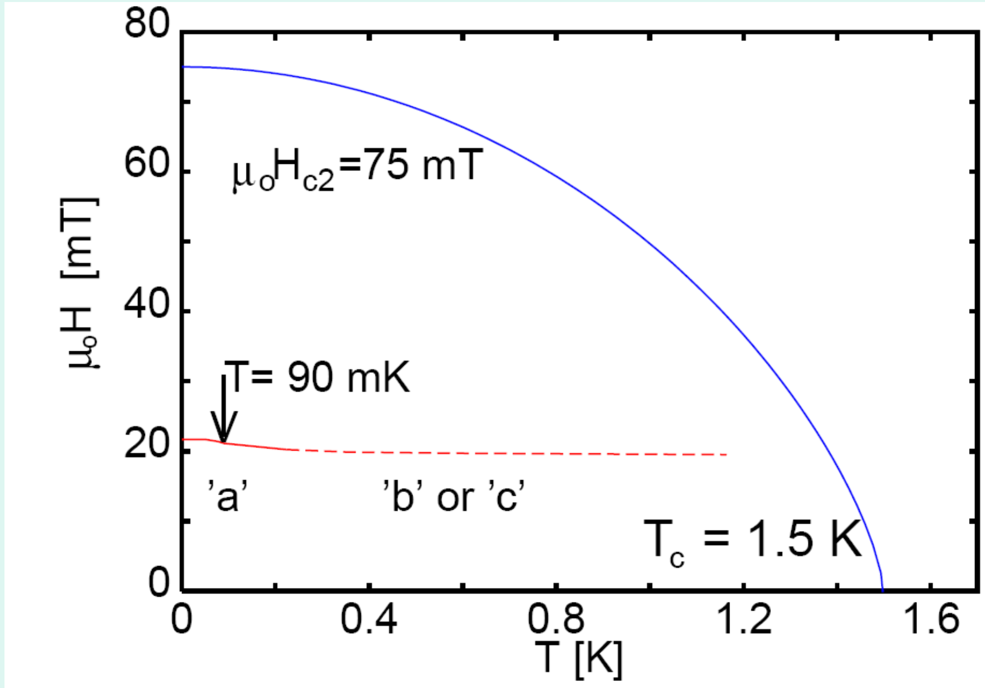
The d-vector cannot simply rotate. It must make a transition from (a) to one of the other phases b-e we saw earlier



This is what we find in our model. For c-axis fields (a) is stable for H=0, but there is a finite field transition to another phase, usually (b/c).

The parameters can be chosen to make the transition occur below 400G

Stability of phases in H-T plane



This transition has not been seen, but necessary to reconcile the Murukawa experiments with chiral pairing

-- 1st order but entropy change is tiny since $|d|^2$ identical in all phases

Location of boundary depends on combination of λ and U'/U

Size of the spin orbit term?

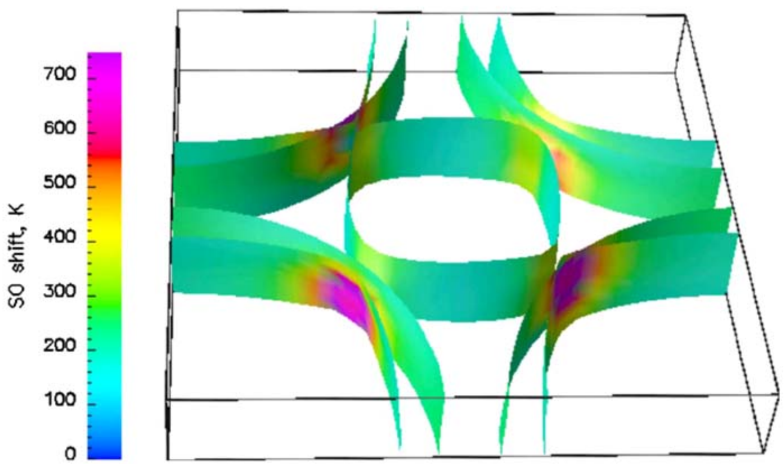
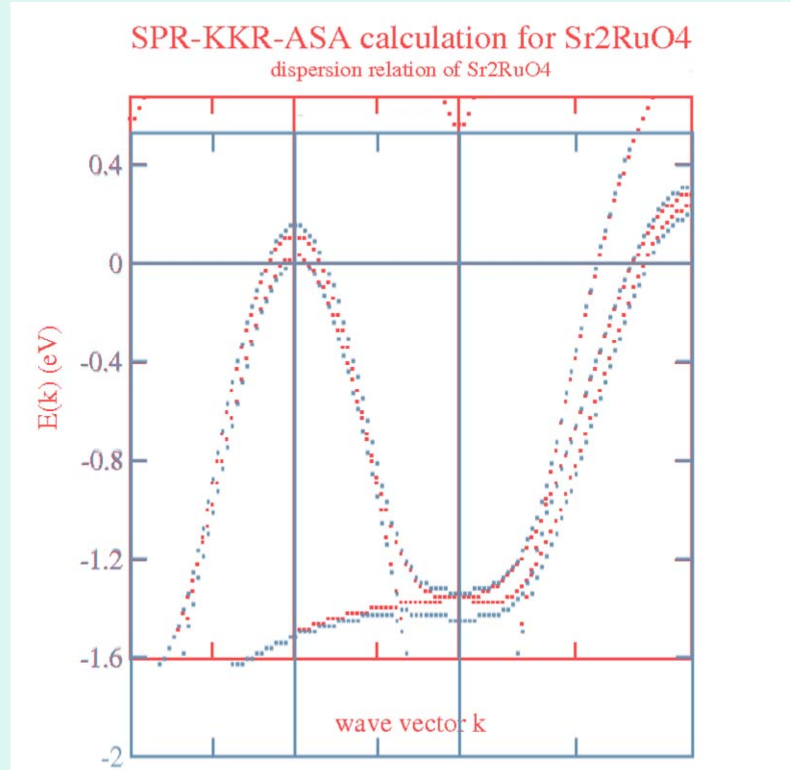


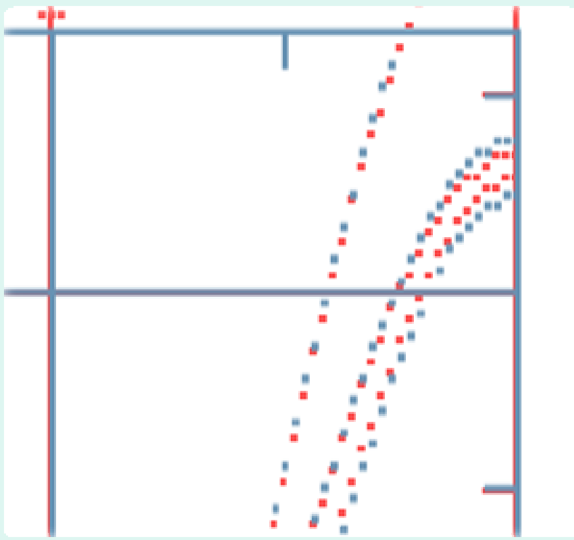
FIG. 3. (Color online) LAPW Fermi surface, painted according to the spin-orbit splitting at each point (see the color bar for the scale in the temperature units).

Mazin PRB2006, LAPW bands coloured by relativistic shift

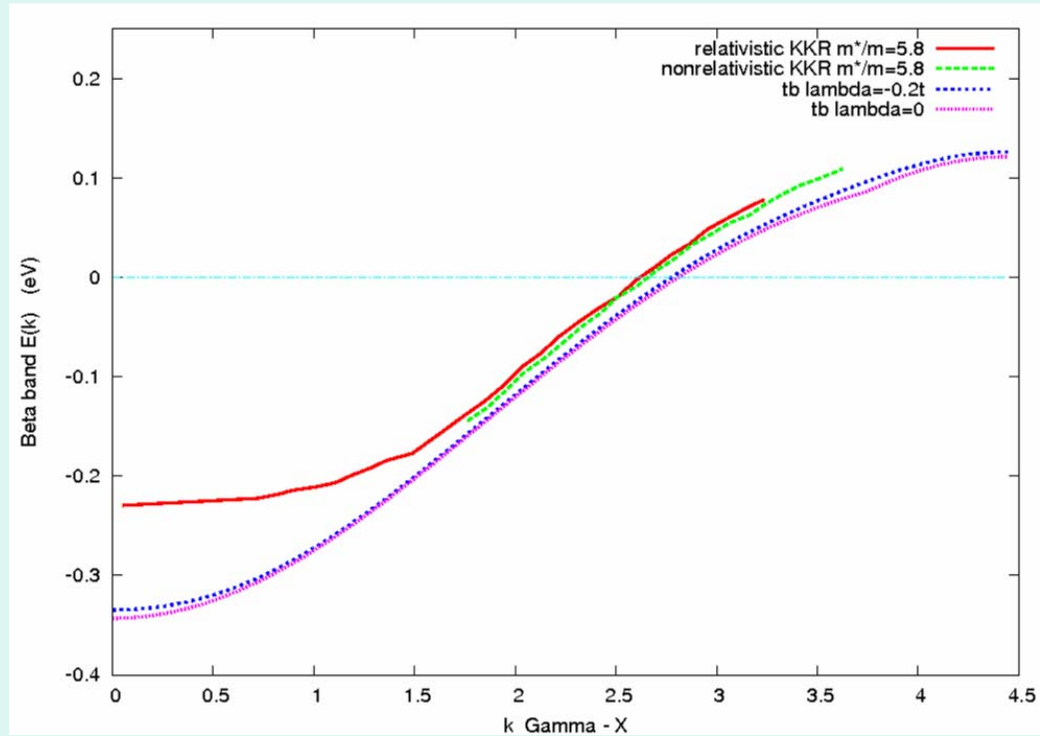


Our KKR bands,
Blue c=1x (fully relativistic)
Red c=100x (non-relativistic)

Strength of spin-orbit term?



KKR-bands close up near (π,π)
Blue c=1x
Red c=100x



Our tight-binding β sheet band from de Haas data, with $\lambda=0$ or $-0.2t$ compared to relativistic KKR bands (scaled by $m^*/m \approx 5$)

Pairing in tetragonal symmetry: (JF Annett, Adv Phys 1990)

TABLE I: Irreducible representations of even and odd parity in a tetragonal crystal. The symbols X, Y Z represent any functions transforming as x, y and z under crystal point group operations, while I represents any function which is invariant under all point group symmetries.

Rep.	symmetry	Rep.	symmetry
A_{1g}	I	A_{1u}	$XYZ(X^2-Y^2)$
A_{2g}	$XY(X^2-Y^2)$	A_{2u}	Z
B_{1g}	X^2-Y^2	B_{1u}	XYZ
B_{2g}	XY	B_{2u}	$Z(X^2-Y^2)$
E_g	$\{XZ,YZ\}$	E_u	$\{X,Y\}$

TABLE III: Basis functions $\gamma_i^\Gamma(\mathbf{k})$ for the odd parity irreducible representations of body-centred tetragonal crystals.

Rep.	in-plane	inter-plane
A_{1u}	-	-
A_{2u}	-	$\cos\frac{k_x}{2}\cos\frac{k_y}{2}\sin\frac{k_z c}{2}$
B_{1u}	-	$\sin\frac{k_x}{2}\sin\frac{k_y}{2}\sin\frac{k_z c}{2}$
B_{2u}	-	-
E_u	$\sin k_x$	$\sin\frac{k_x}{2}\cos\frac{k_y}{2}\cos\frac{k_z c}{2}$
	$\sin k_y$	$\cos\frac{k_x}{2}\sin\frac{k_y}{2}\cos\frac{k_z c}{2}$

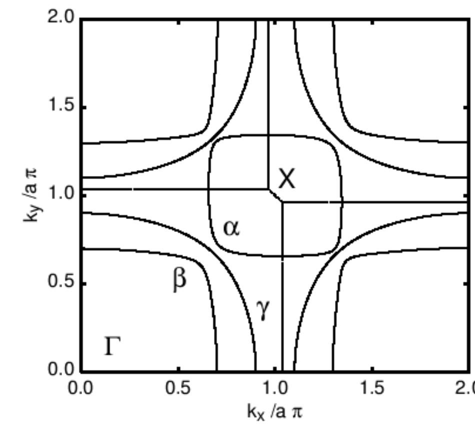
a

Here X(**k**), Y(**k**) and Z(**k**) are any basis functions in the 1st BZ transforming as x,y,z under point group operations (analogues of cubic harmonics)

Note: even within the E_u 'p-wave' symmetry class there are basis functions with or without line nodes

Simple effective Hamiltonian model

$$\hat{H} = \sum_{ijmm',\sigma} \left((\varepsilon_m - \mu)\delta_{ij}\delta_{mm'} - t_{mm'}(ij) \right) \hat{c}^{+}_{im\sigma} \hat{c}_{jm'} - \frac{1}{2} \sum_{ijmm'} U^{\alpha\beta,\gamma\delta}_{mm'}(ij) \hat{c}^{+}_{im\alpha} \hat{c}^{+}_{jm'\beta} \hat{c}_{jm'\gamma} \hat{c}_{im\delta},$$



$$H^{SO} = \mathrm{i}\frac{\lambda}{2} \sum_{i,\sigma\sigma'} \sum_{mm'} \varepsilon^{\kappa mm'} \sigma^{\kappa}_{\sigma\sigma'} c^{+}_{im\sigma} c_{im'\sigma'},$$

An effective 3 band Hamiltonian is constructed
Parameters fit to the 3d experimental Fermi surface

Hubbard interaction parameters U introduce attractive
Interactions between different sites (ij) and orbitals (mm')