Spin-Orbit Coupling and Electronic Correlations in Sr_2RuO_4

Jernej Mravlje

Hvar, 5. Oct 2017

IJS

Outline

- Intro:
  - unconventional superconductivity
  - Sr_2RuO_4 , a Fermi liquid with a small coherence scale
  - role of Hund's rule coupling : Sr_2RuO_4 is a "Hund's metal"; LDA+DMFT results (no SOC)
  - spin-orbit in Sr_2RuO_4 seen in LDA and srARPES: is this compatible with Hund's metal picture?
- Results
  - realistic DMFT results (with SOC)
  - impurity model NRG results with (SOC)
  - remarkably simple picture of SOC & correlations and quantitative understanding of srARPES

Spin-Orbit Coupling and Electronic Correlations in Sr_2RuO_4

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ArXiv:1707.02462 (2017)

PHYSICAL REVIEW B **96**, 085122 (2017)

Spin-orbit coupling in three-orbital Kanamori impurity model and its relevance for transition-metal oxides

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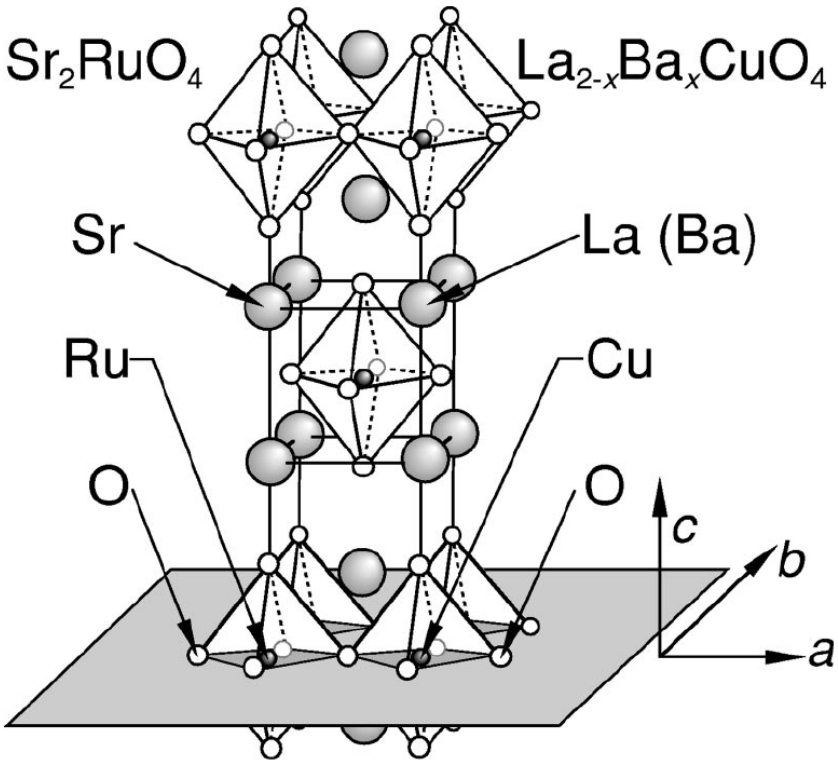
Sr_2RuO_4 properties



p-wave supercond.

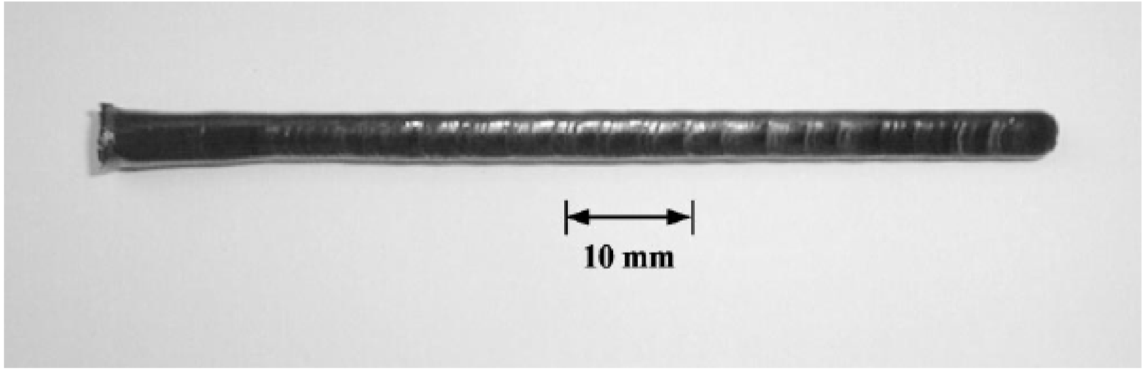
T_c ~2K

Maeno et al., Nature'94

Rice and Sigrist , J.Phys.CM'95

Correlated metal: Fermi liquid, (m*/m~4)

4 el. in Ru t_{2g} orbitals



- chiral p-wave state best? candidate

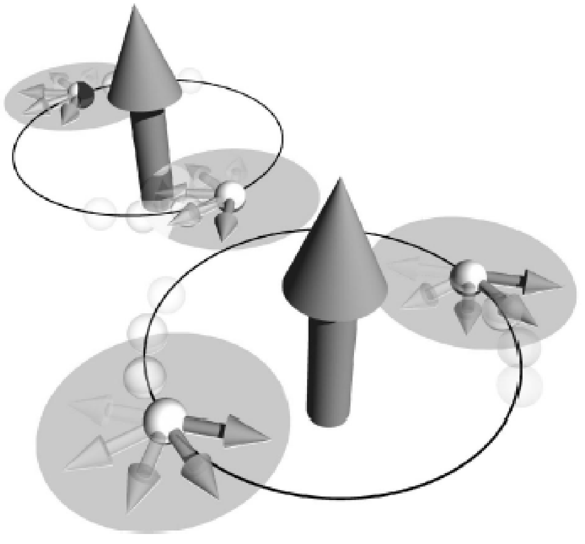


FIG. 20. Sketches of Cooper pair **S** and **L** vectors for the order parameter $\mathbf{d}=\Delta_0\hat{\mathbf{z}}(k_x \pm ik_y)$. The large arrows denote **L** and

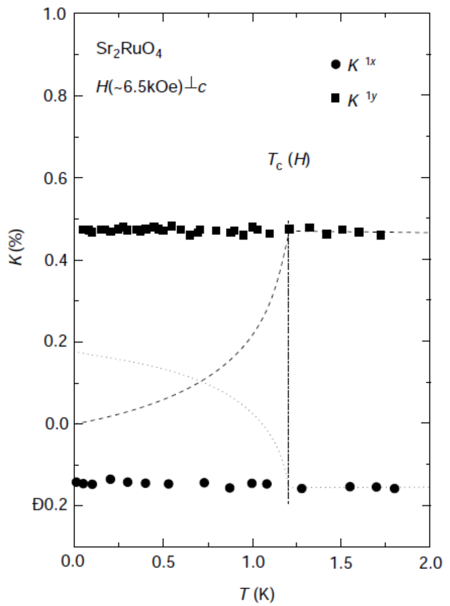
$$\mathbf{d}=\Delta_0\hat{\mathbf{z}}(k_x \pm ik_y)=\Delta_0\begin{bmatrix}0\\0\\k_x \pm ik_y\end{bmatrix}.$$

Mackenzie et al. RMP’03

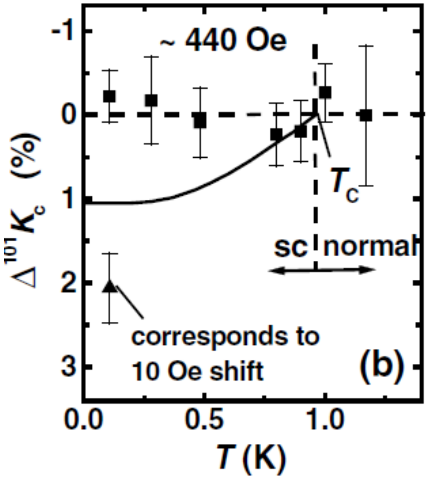
Rotating of order parameter with field? Demands weak enough SOC

- Knight shift field inplane

field out of ab-plane



Ishida et al., PRB 56 R505 (1997)
Ishida et al. Nature 396, 658 (1998).

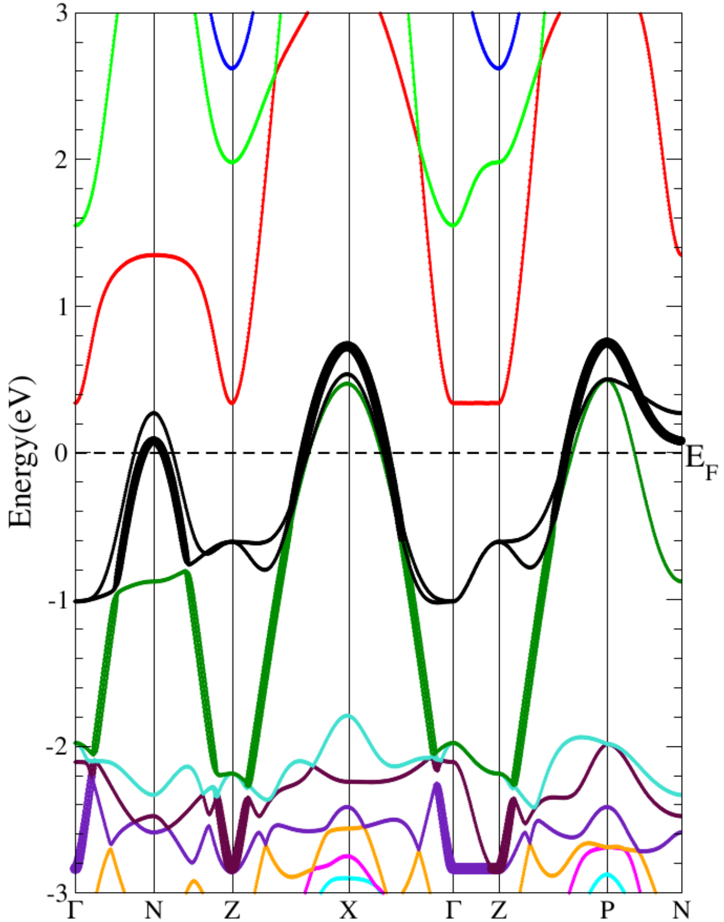


Murakawa et al., PRL 93, 167004 (2004).

For a recent discussion, see:
Kim,Khmelevskyi, Mazin, Agterberg, Franchini, npj Quantum Materials 2, 37 (2017) &
Mackenzie, Scaffidi, Hicks, Maeno, npj Quantum Materials 2, 40 (2017). (100 Oe =0.01 T)

Sr_2RuO_4: el. structure (without LS coupling)

Oguchi, PRB'95
Singh, PRB'95

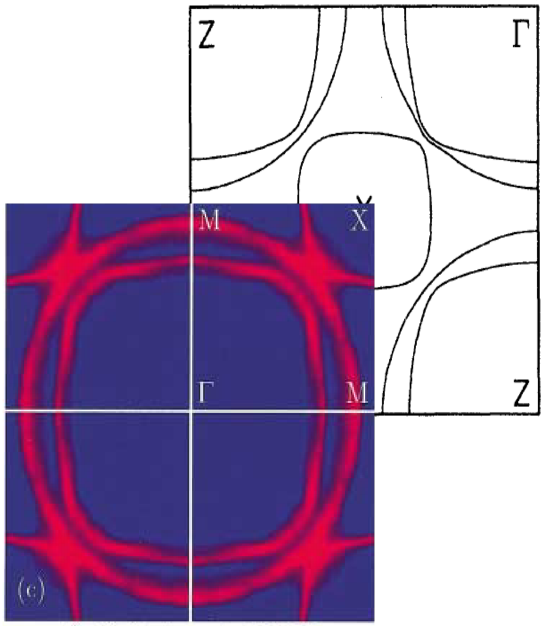


In ionic picture, 4 electrons on Ru; crystal field splitting → t_{2g} orbitals: xy and degenerate xz, yz

Wide xy band (ϒ sheet)

Fermi surfaces of DFT, quantum oscillations, ARPES **agree well.**

Mass enhancements with respect to DFT ~4.



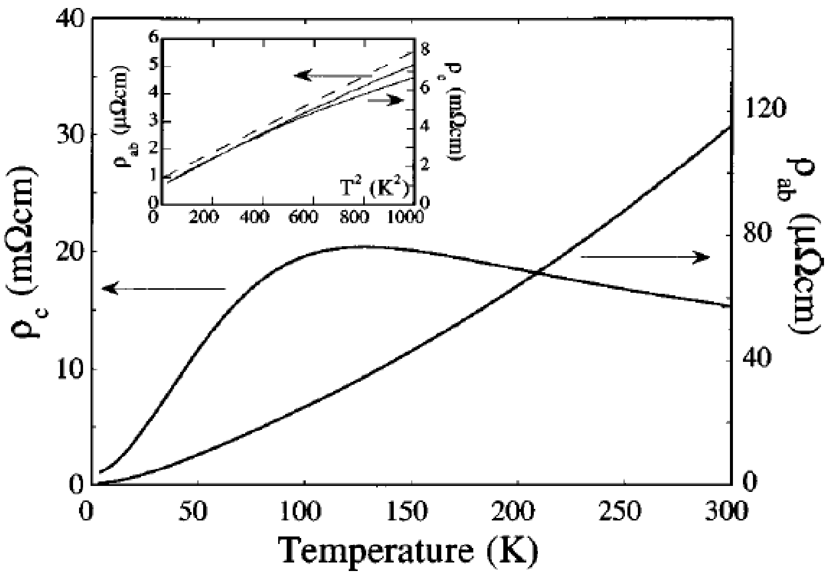
Damascelli, Shen et al., PRL'00

	α	β	γ
Frequency F (kT)	3.05	12.7	18.5
Average k_F (Å^{-1})	0.302	0.621	0.750
$\Delta k_F/k_F$ (%)	0.21	1.3	<0.9
Cyclotron mass (m_e)	3.4	6.6	12.0
Band calc. F (kT)	3.4	13.4	17.6
Band calc. $\Delta k_F/k_F$ (%)	1.3	1.1	0.34
Band mass (m_e)	1.1	2.0	2.9

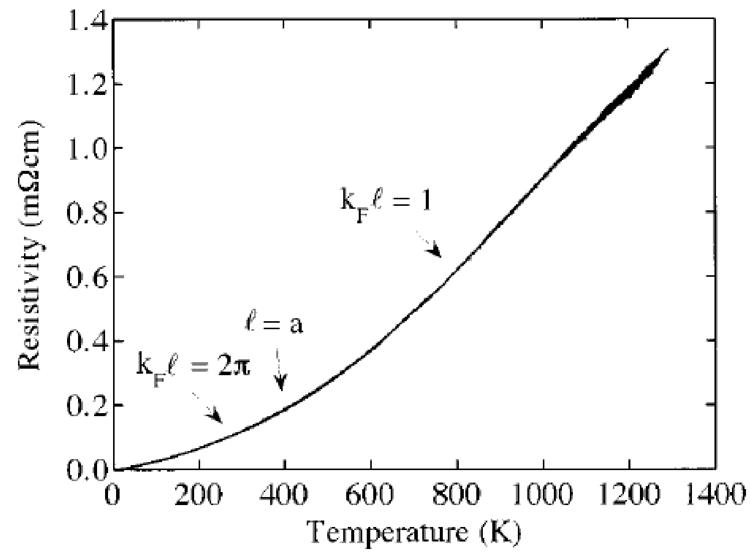
Mackenzie et al, PRL'96

Low coherence scale in transport

- 4d compound : U~2eV <W, yet strong correlations : large mass, coherence-incoherence crossover at low T <20K & bad metal behavior at high T

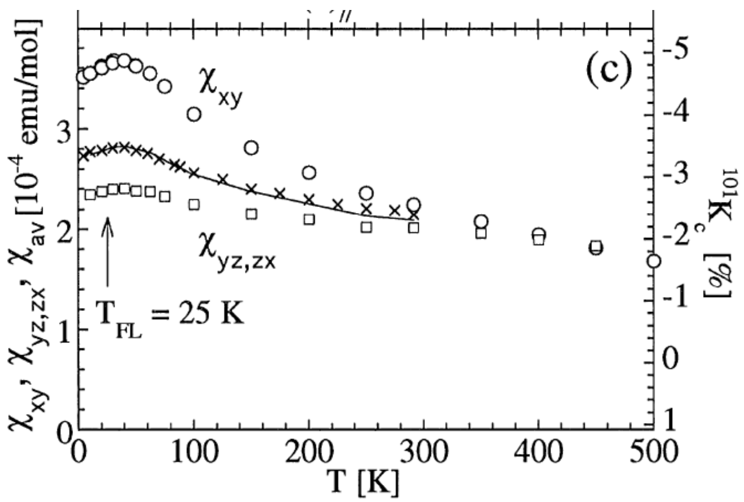


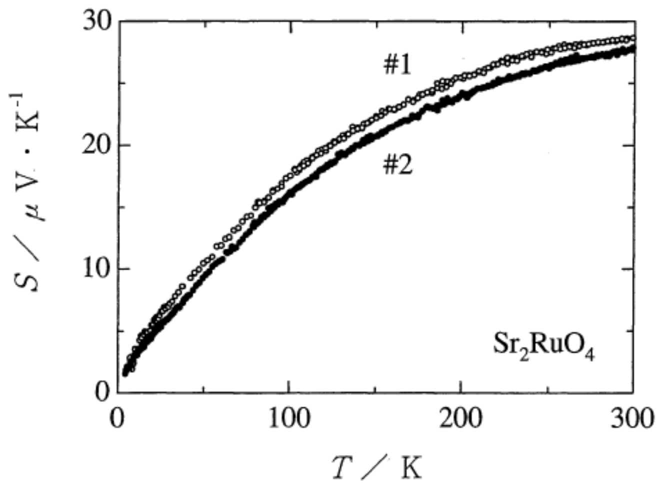
Hussey et al. PRB'98



Tyler et al. PRB'98

Low coherence scale in NMR, thermopower ...

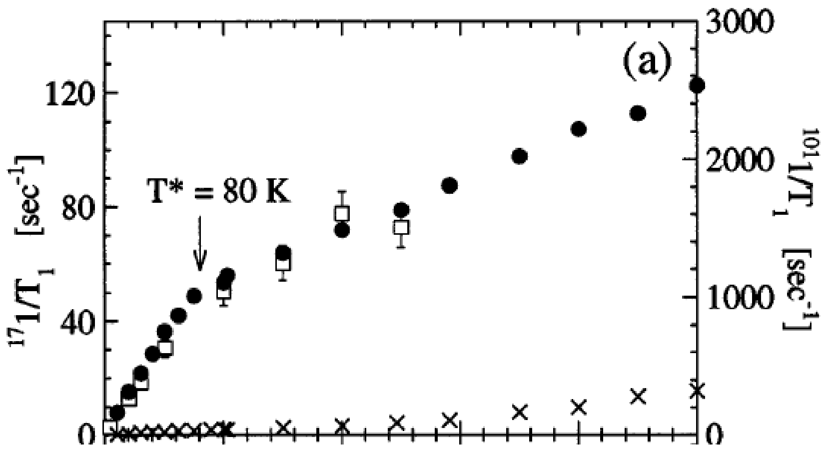




Yoshino et al. J.Phys. Soc. Jpn. 6 1548(1996).

Optical spectroscopy:
Stricker et al. PRL 113, 087404 (2014).

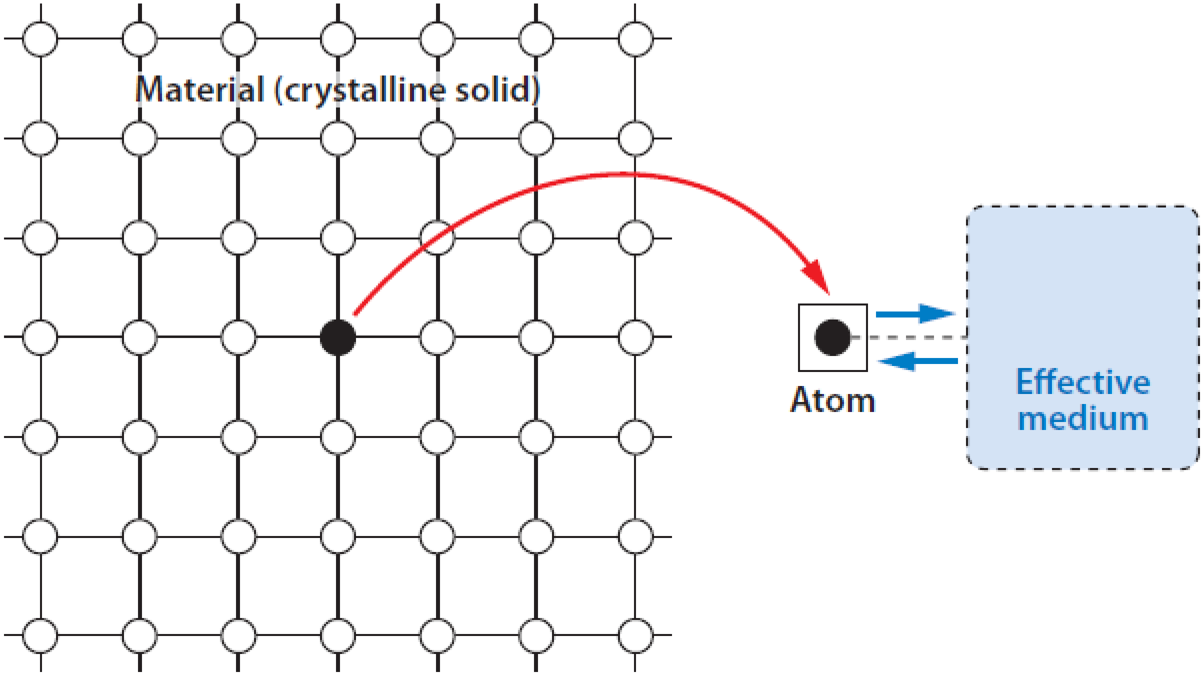
Photoemission: Wang et al. PRL 92 137002 (2004)



Imai et al. PRL 81, 3006(1998)

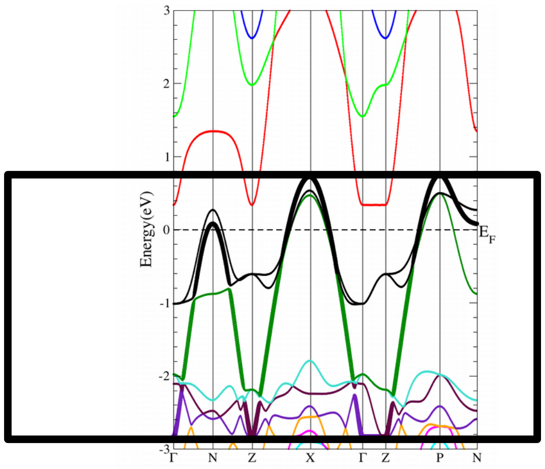
WHY IS COHERENCE SCALE LOW?

DMFT



Sr_2RuO_4 within LDA+DMFT

- Wannier function constructed out of t2g
- Full rotationaly invariant vertex is used
- Constrained RPA to calculate U(=2.3eV) & J
- Hybridization expansion CTQMC



$$H_I = U \sum_m n_{m\uparrow} n_{m\downarrow} + \sum_{m<n,\sigma} [U' n_{m\sigma} n_{n\bar{\sigma}} + (U'-J) n_{m\sigma} n_{n\sigma} - J c^\dagger_{m\sigma} c_{m\bar{\sigma}} c^\dagger_{n\bar{\sigma}} c_{n\sigma}] - J \sum_{m<n} [c^\dagger_{m\uparrow} c^\dagger_{m\downarrow} c_{n\uparrow} c_{n\downarrow} + h.c.]$$

$$H = (U - 3J) n(n-1)/2 - 2JS^2 - 1/2 J L^2$$

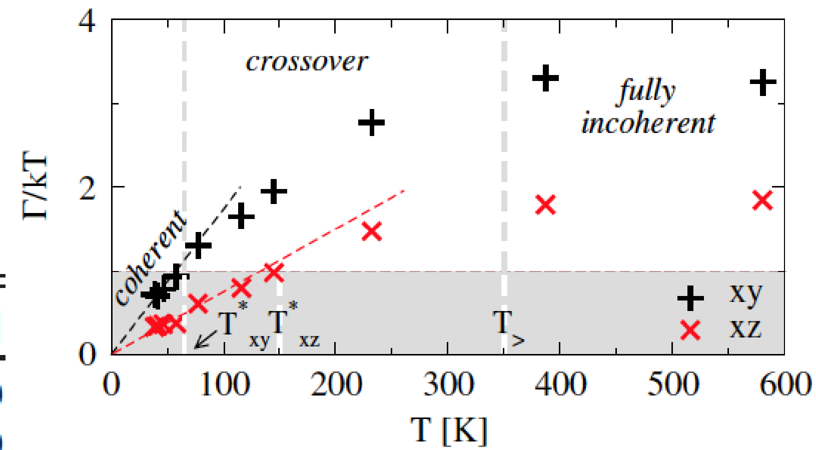
$$\vec{S} = 1/2 \sum_{m\sigma\sigma'} c^\dagger_{m\sigma} \vec{\tau} c_{m\sigma'}$$

$$L_m = i \sum_{\sigma m' m''} \epsilon_{m m' m''} c^\dagger_{\sigma m'} c_{\sigma m''}$$

Werner et al, PRL'06
Parcollet,Ferrero et al. TRIQS implementation

Coherence scale drops due to Hund's rule coupling J

- LDA+DMFT applied to Sr_2RuO_4
- T^* determined from T-dep of $\Gamma = -Z\, \mathrm{Im}\Sigma(0)$
- T^* suppresed by J !



Hund's rule coupling

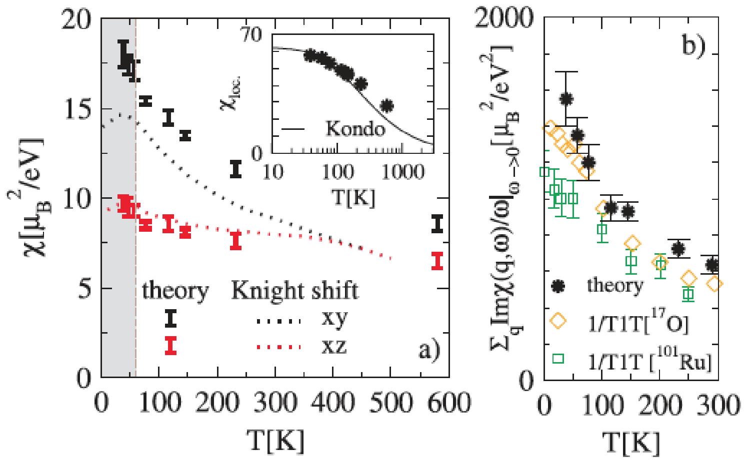
J [eV]	$m^*/m_{\mathrm{LDA}}\vert_{xy}$	$m^*/m_{\mathrm{LDA}}\vert_{xz}$	T^*_{xy} [K]	T^*_{xz} [K]	$T_>$ [K]
0.0, 0.1	1.7	1.7	>1000	>1000	>1000
0.2	2.3	2.0	300	800	>1000
0.3	3.2	2.4	100	300	500
0.4	4.5	3.3	60	150	350

Mravlje et al. PRL 106 096401 (2011).

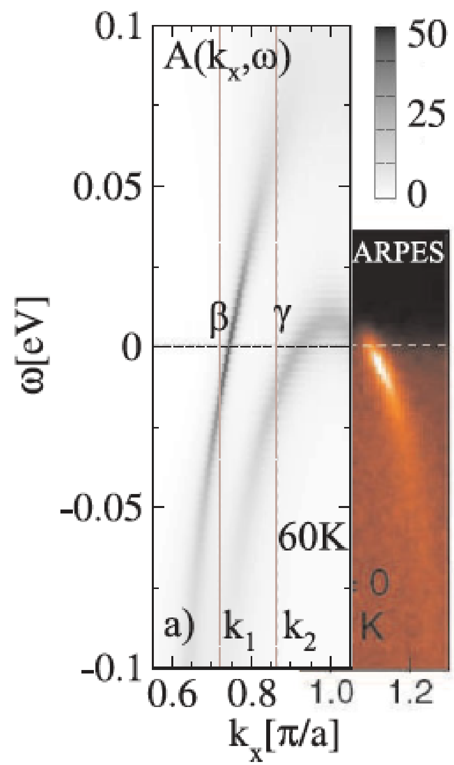
Masses in agreement with quantum oscillations & specific heat at physical value of J

Good agreement with experiment ; low coherence scale

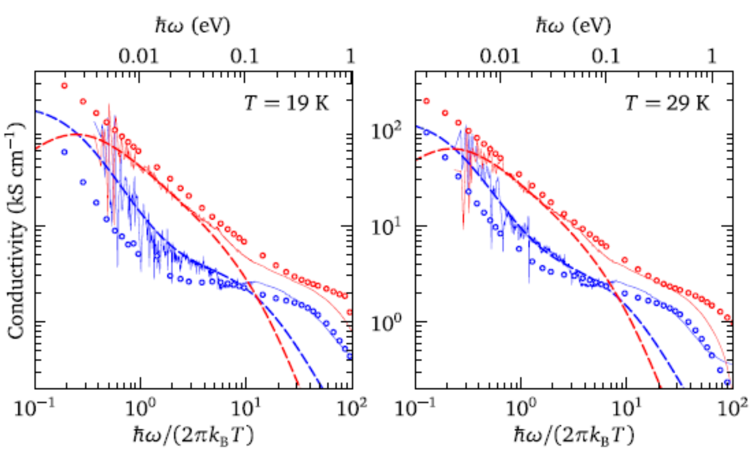
NMR



ARPES



Optics



R, ARPES, quantum oscillations Mravlje et al. PRL 106 096401(2011)
ics : Stricker et al. PRL 113 087404 (2014).
beck coefficient Mravlje, Georges, PRL 117 036401(2016).

DMFT : Hund's metals

- Hund’s metal: correlated metals far from a U-driven Mott transition

L. de'Medici, JM, A.Georges, PRL'11

Haule, Kotliar, NJP'09
Werner,Gull, Troyer,Millis PRL'08
Werner,Gull, Millis, PRB'09
Georges, de'Medici, Mravlje, Annu Rev CM'13
Yin, Haule, Kotliar,PRB'13
Aron, Kotliar PRB’15
de’Medici, Capone, …
Fanfarillo, Bascones PRB’15 ...

In corresponding Kondo model, suppressed spin-spin Kondo coupling

$$H_{\rm imp} = \frac{1}{2}(U-3J)N_d(N_d-1) - 2J\mathbf{S}^2 - \frac{J}{2}\mathbf{L}^2$$

- Schrieffer-Wolff

$$H_{\rm K} = -P_n H_{\rm hyb}\left(\sum_a \frac{P^a_{n+1}}{\Delta E^a_{n+1}} + \sum_b \frac{P^b_{n-1}}{\Delta E^b_{n-1}}\right) H_{\rm hyb} P_n$$

- result

$$H_K = J_p N_f + J_s \mathbf{S}\cdot\mathbf{s} + J_l \mathbf{L}\cdot\mathbf{l} + J_q \mathbf{Q}\cdot\mathbf{q} + J_{ls}(\mathbf{L}\otimes\mathbf{S})\cdot(\mathbf{l}\otimes\mathbf{s}) + J_{qs}(\mathbf{Q}\otimes\mathbf{S})\cdot(\mathbf{q}\otimes\mathbf{s})$$

For Nd=2 → S=1, L=1

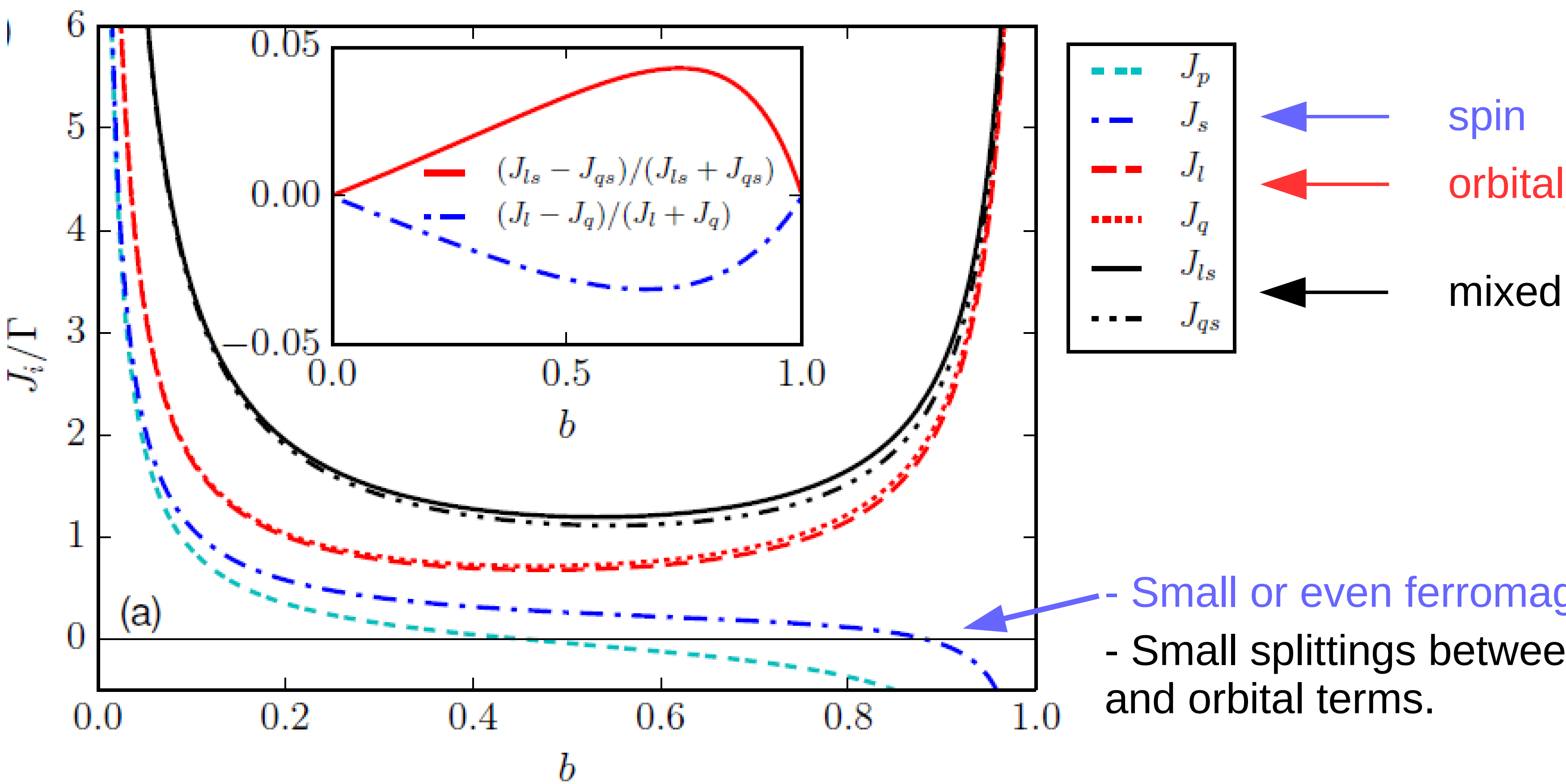
- Spin-spin, orbital-orbital, Q-Q, and mixed terms
- S-spin, L-orbit, Q- orbital quadrupole

$$Q^{bc}_{i,j} = \frac{1}{2}\left(L^b_{i,m}L^c_{m,j} + L^c_{i,m}L^b_{m,j}\right) - \frac{2}{3}\delta_{b,c}\delta_{i,j}$$

$$\mathrm{Tr}(Q^\alpha Q^\beta) = 2\delta_{\alpha,\beta}$$

Yin, Haule, Kotliar PRB'12
Aron, Kotliar PRB'15
Stadler et al. PRL'15
Horvat, Zitko, Mravlje PRB'16

Hund's rule coupling suppresses spin-spin Kondo coupling constants

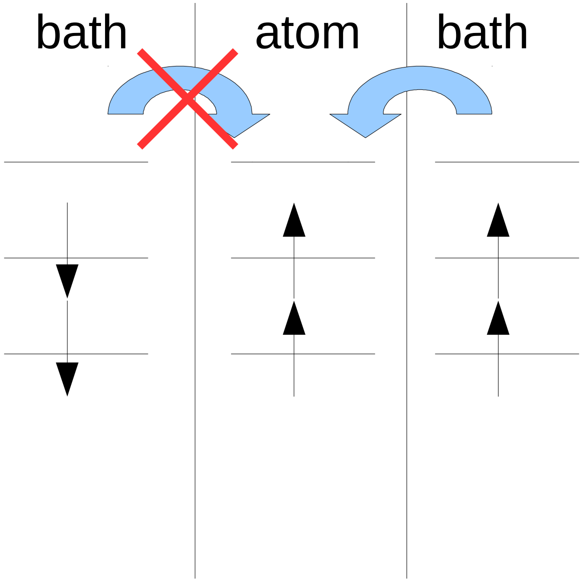


- Small or even ferromagnetic J_s !
- Small splittings between quadrupole and orbital terms.

b- local potential
→ 0 – charge fluctuations to N=1
→ 1 – charge fluctuations to N=3 (half-filling)

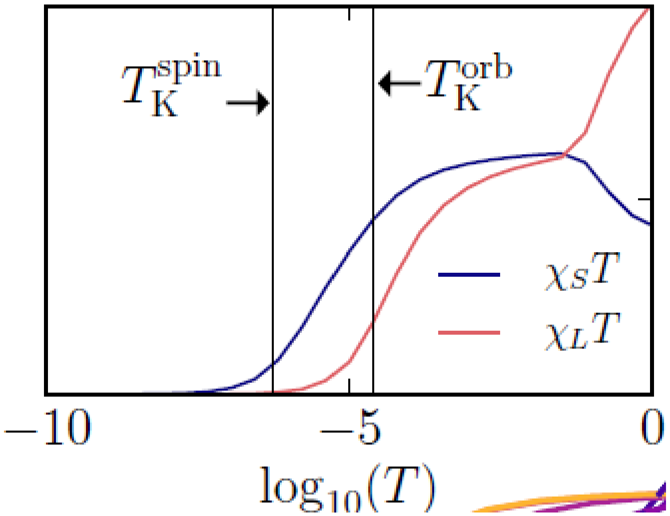
Yin, Haule, Kotliar PRB'12
Aron, Kotliar PRB'15
Stadler et al. PRL'15
Horvat, Zitko, Mravlje PRB'16

- Why ferromagnetic? Fluctuations to N=3 (half-filled) states prefer ferromagnetic arrangement [in contrast to single-orbital!]



Yin, Haule, Kotliar PRB’12
Aron, Kotliar PRB’15
Stadler et al. PRL’15
Horvat, Zitko, Mravlje PRB’16

Impurity model results

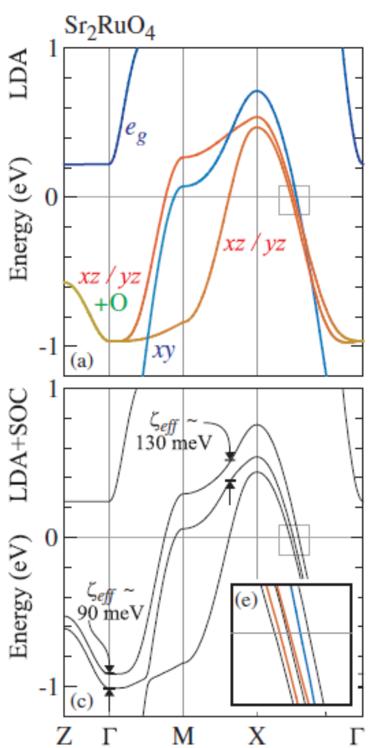


Horvat, Zitko, Mravlje, PRB 94 165140 (2011).

So: Sr_2RuO_4 a Hund's metal with different behavior of spin and orbital moments

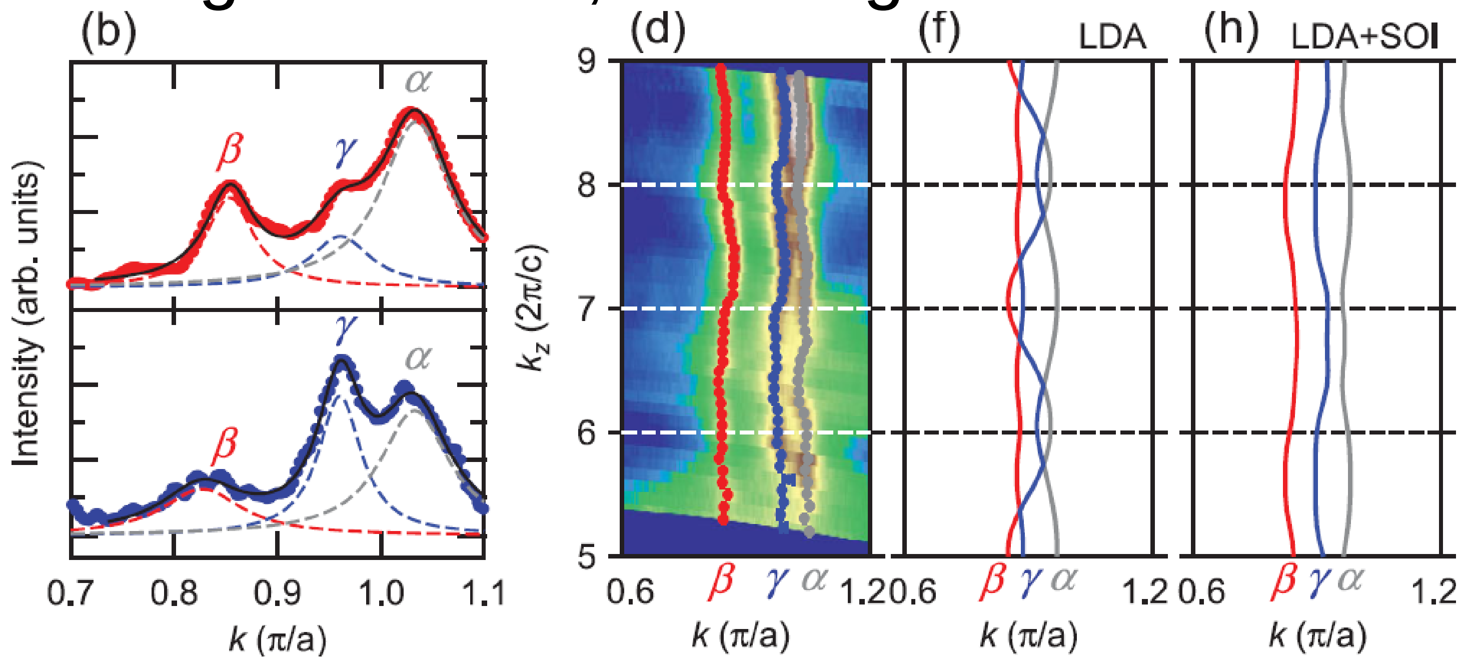
What about LS coupling?

- L-S coupling not small ~0.1eV
- certainly larger than Fermi liquid coherence scale
- What are its consequences?



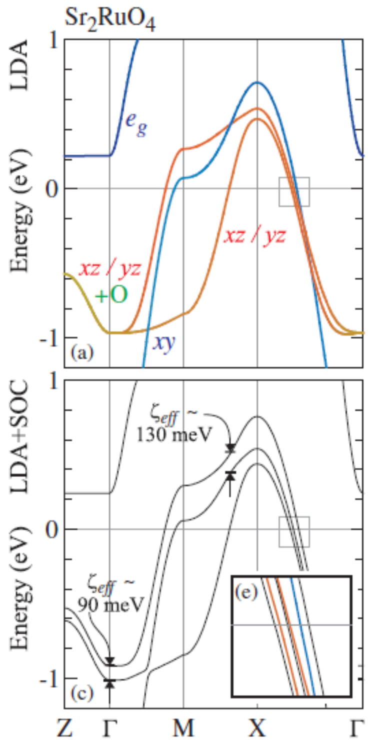
Earnshaw, Figgis, Lewis,Peacock, J. Chem. Soc., (1961).
Pavarini, Mazin, PRB 74, 035115 (2006).
Haverkort et al., PRL 101, 026406 (2008)

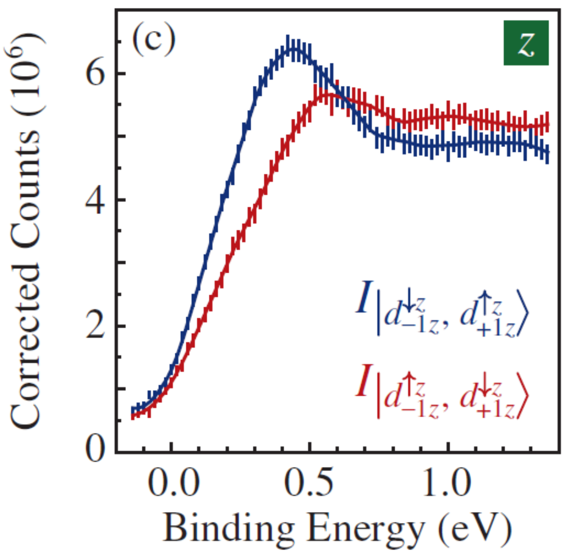
- spin anisotropy in NMR (3*) Ishida et al., PRB 64 R100501 (2001).
- admixing of orbitals; crossings become avoided



ARPES
H. Iwasawa et al.,
PRL (2010)

sr ARPES





srARPES : splitting at Gamma point
~0.1eV
C. Veenstra et al.,
PRL 112 127002 (2014)

Haverkort et al.
PRL'08

- Spin-orbit splittings consistent with LDA and are substantial
- Does Hund’s metal picture persist in the presence of spin-orbit?

Method

- 2D Tight-Binding model which describes LDA+SOC band structure.
- DMFT computation with SOC, which involves finite ImG(τ).
- U=2.3 eV, J_H=0.4 eV.

$$H = H_0 + H_{\rm ls} + H_{\rm int}$$

$$H_{\rm int} = (U - 3J_{\rm H})\frac{\hat{N}(\hat{N}-1)}{2} - 2J_{\rm H}\vec{S}^2 - \frac{J_{\rm H}}{2}\vec{L}^2$$

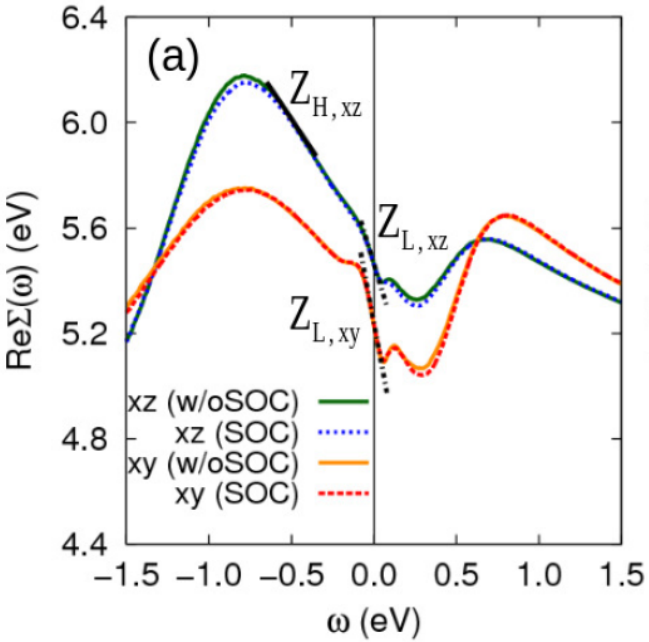
$$H_{\rm ls} = \frac{\lambda_z}{2}\sum_{m=-1}^{1} m(d^\dagger_{m\uparrow}d_{m\uparrow} - d^\dagger_{m\downarrow}d_{m\downarrow}) + \frac{\lambda_{xy}}{\sqrt{2}}\sum_{m=-1}^{0}(d^\dagger_{m+1\downarrow}d_{m\uparrow} + d^\dagger_{m\uparrow}d_{m+1\downarrow})$$

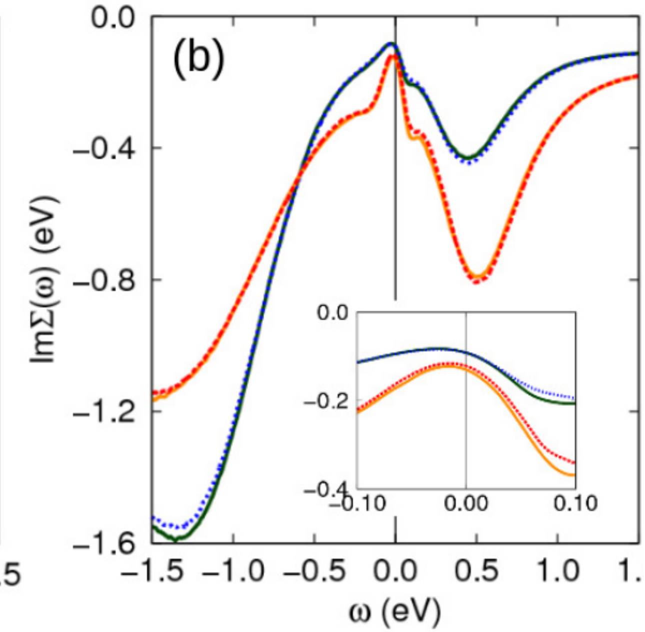
$$\lambda_{\rm xy} = \lambda_{\rm z} = \lambda_{SOC} = 100\,{\rm meV}$$

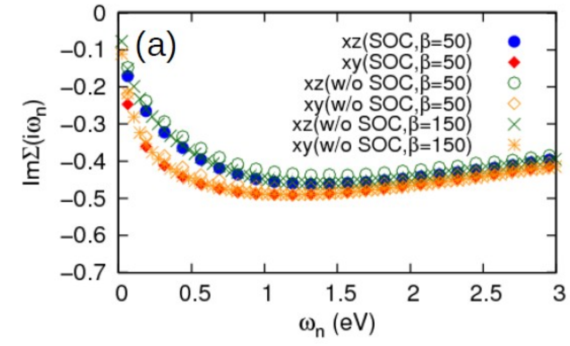
Table I. The tight-binding Hamiltonian $t^{\mathbf{R}\neq0}_{\alpha\sigma,\alpha'\sigma'}$, t=0.42, t_1=0.17, t_2=0.30, t_3=0.03, and t_4=0.04 (eV).

	xz, xz	yz, yz	xy, xy	xz, yz
$t^{\pm1,0,0}_{\alpha,\alpha'}$	$-t_2$	$-t_3$	$-t$	0
$t^{0,\pm1,0}_{\alpha,\alpha'}$	$-t_3$	$-t_2$	$-t$	0
$t^{\pm1,\pm1,0}_{\alpha,\alpha'}$	0	0	$-t_1$	$-t_4$
$t^{\pm1,\mp1,0}_{\alpha,\alpha'}$	0	0	$-t_1$	t_4

Self-energies with SOC very similar to the ones without





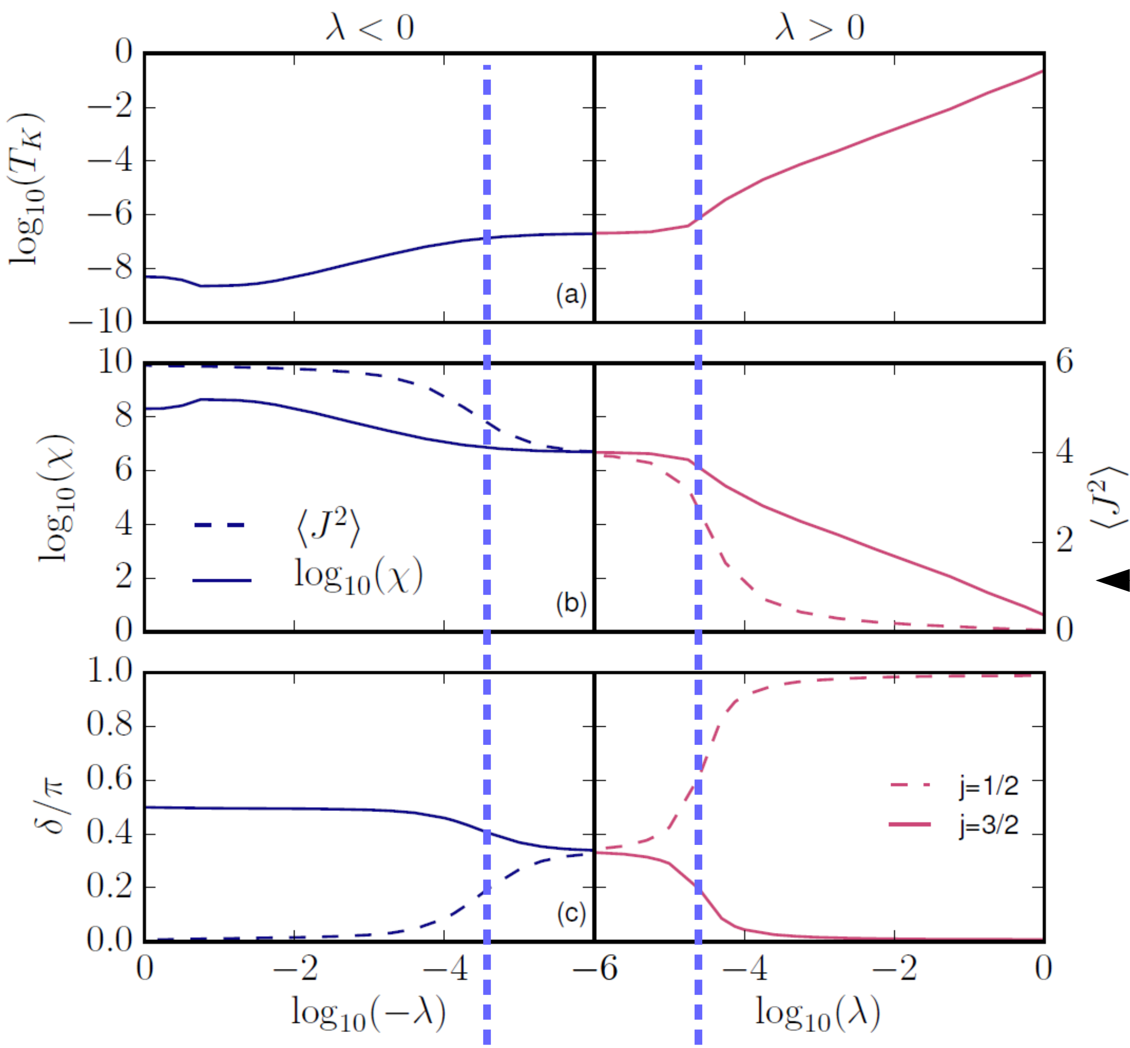


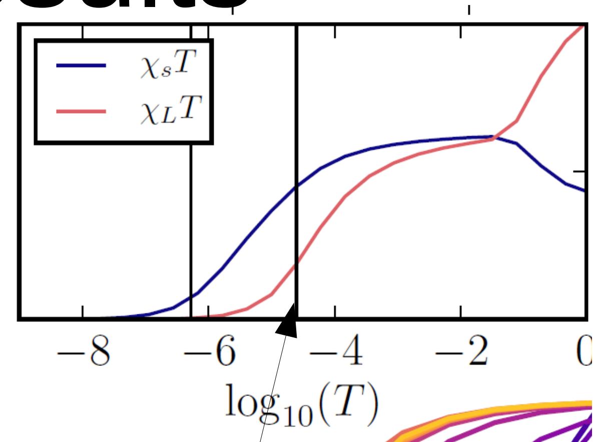
- Spin-orbit coupling does not affect electronic correlations in spite of being substantially larger than $T_{FL.}$Why?

Impurity model results

-d^2: $SrCrO_3$, $SrMoO_3$

-d^4: ruthenates





T_K^{orb}

SOC needs to exceed T_K^{orb}!

SOC J=2 metal

Hund's metal

van Vleck J=0 insulator

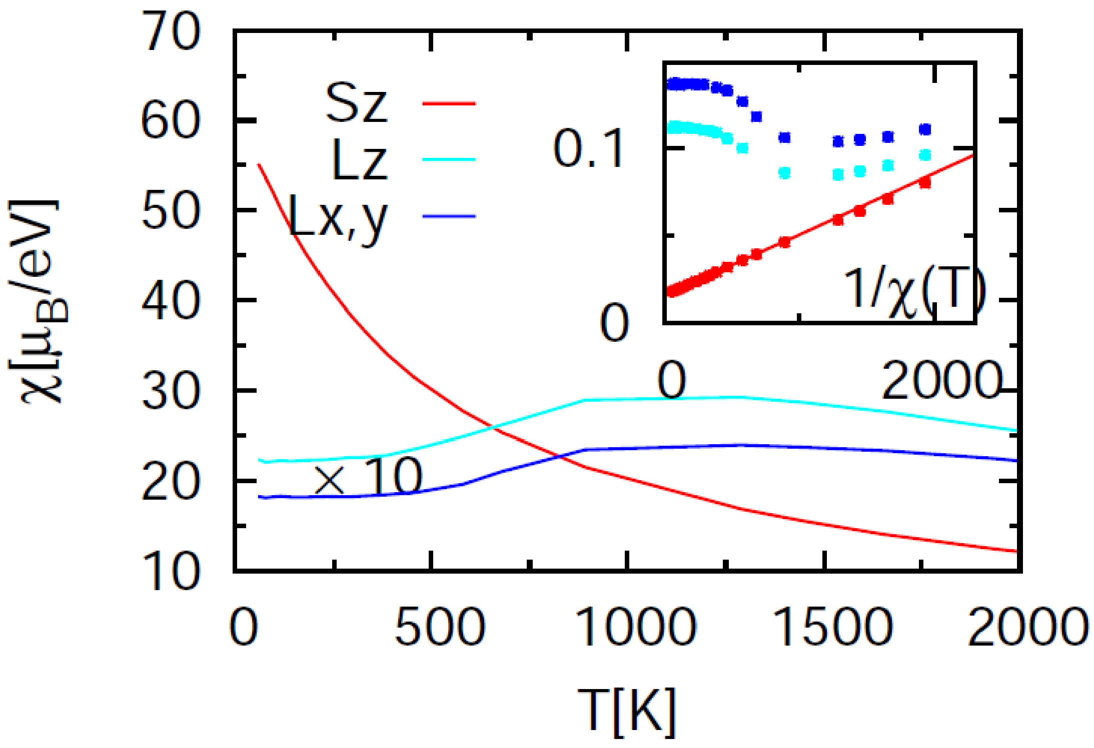
$|\lambda| < T_K^{orb}$

Horvat, Zitko, Mravlje, PRB 96 085122 (2017)

See also Kim et al.PRL 118 086401(2017).

LDA+DMFT on Sr_2RuO_4

- T_K^{orb} >0.1 eV. Orbital moments are quenched. SOC has no effect

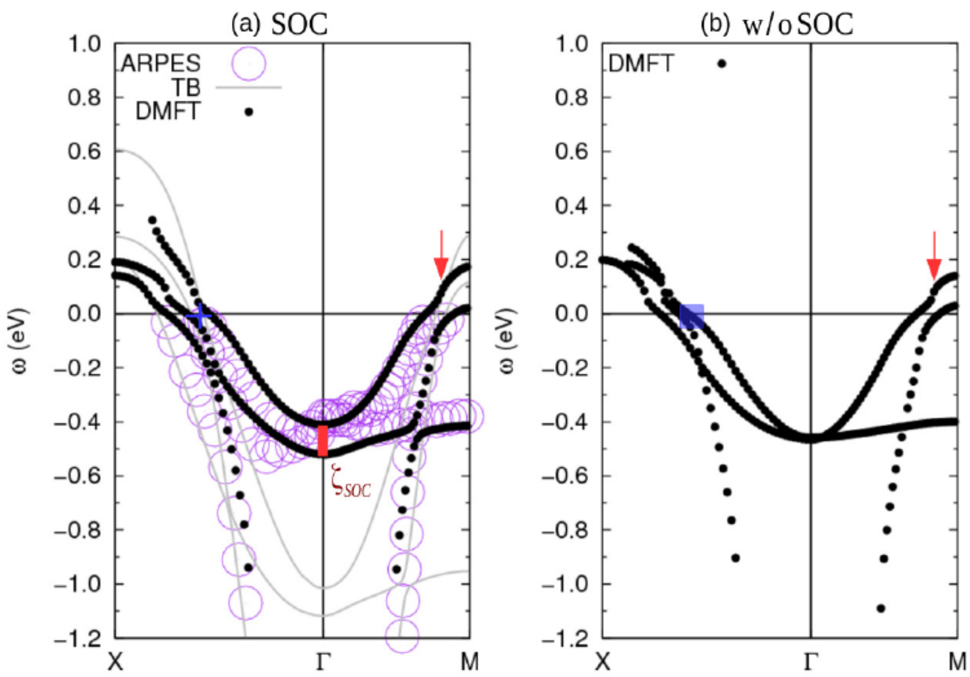


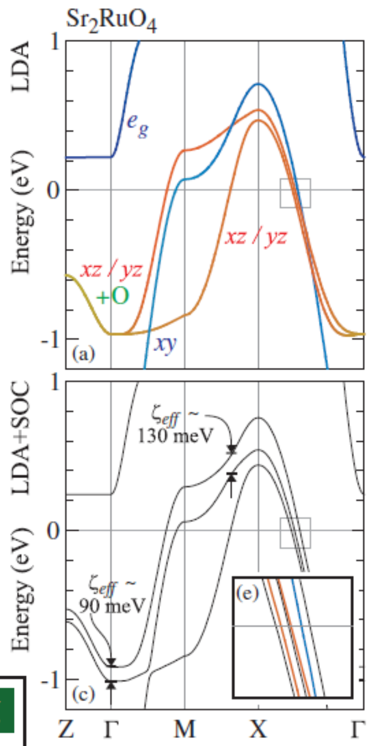
Mravlje, Georges, PRL' 117 036401 (2016).

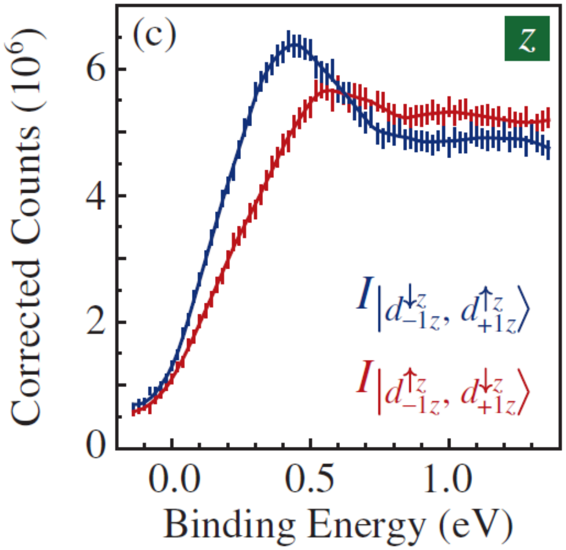
WHAT DOES THIS MEAN FOR ELEC. STRUCTURE/
AS PROBED BY ARPES?

DOES DMFT PREDICT THAT SOC IS WASHED
AWAY BY CORRELATIONS?

Not at all: SOC effects are correctly reproduced







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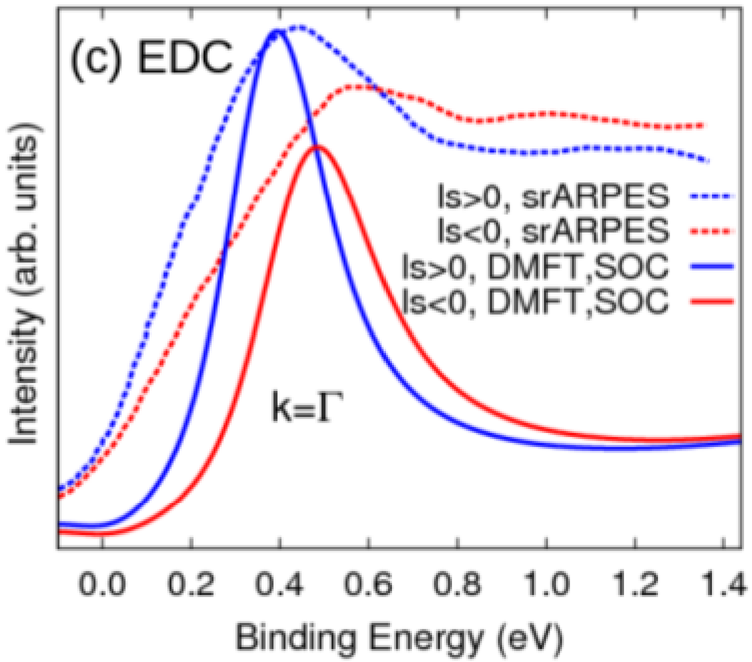
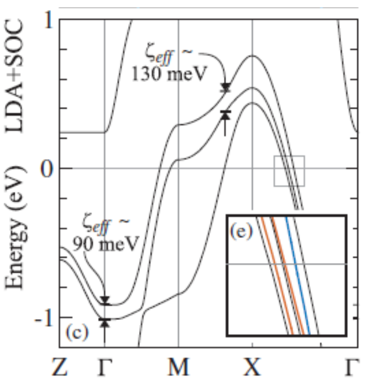
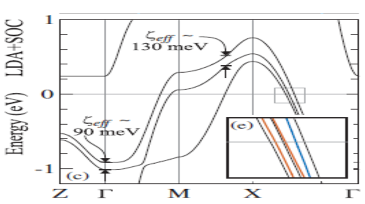


(c) EDC
ls>0, srARPES
ls<0, srARPES
ls>0, DMFT,SOC
ls<0, DMFT,SOC
k=Γ
Intensity (arb. units)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
Binding Energy (eV)

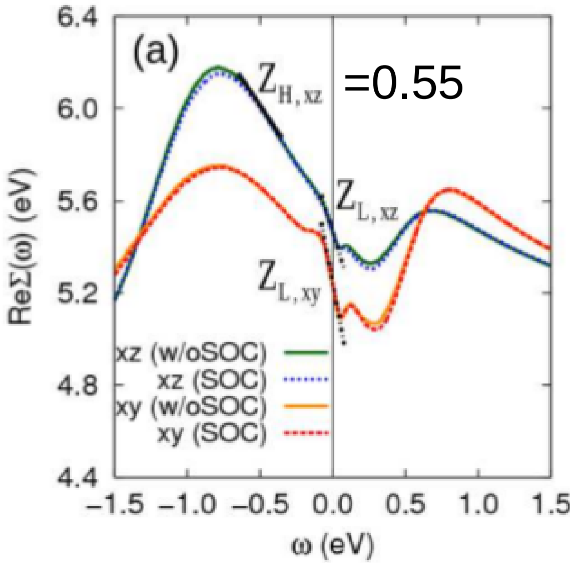
How does this work?

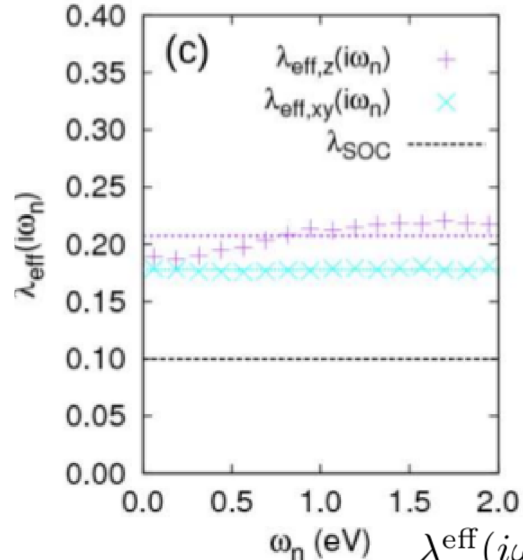
- SOC is a part of the single particle Hamiltonian, hence it is renormalized with the rest of band structure. Take a slave-boson type self-energy Re Σ= (1-1/Z) ω. Full single-particle Hamiltonian is renormalized.





- In DMFT, self-energy has more structure, slope at -0.5eV smaller.





Zhang et al. PRL 116 106402 (2016).

$$\lambda_z^{\mathrm{eff}}(i\omega_n) = \lambda_{\mathrm{SOC}} + 2\mathrm{Im}\Sigma_{xz\uparrow,yz\uparrow}(i\omega_n)$$
$$\lambda_{xy}^{\mathrm{eff}}(i\omega_n) = \lambda_{\mathrm{SOC}} - 2\mathrm{Im}\Sigma_{xz\uparrow,xy\downarrow}(i\omega_n)$$

- 2nd : there are off-diagonal parts of the self energy
- Finally, splitting at Gamma is:

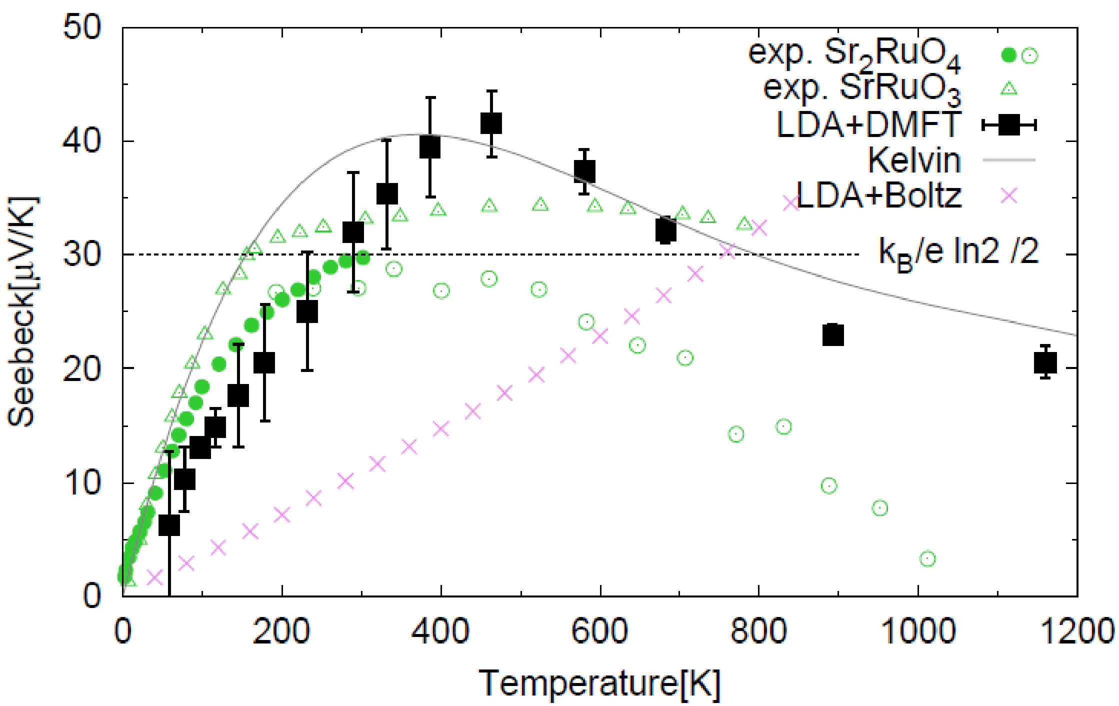
$\zeta_{\mathrm{SOC}} = Z_{H,xz}\lambda_{z,\mathrm{eff}}$ ~110 meV

- The corresponding spin-orbit at small energies is due to electronic renormalization ~5 suppressed to 40meV.

Conclusion

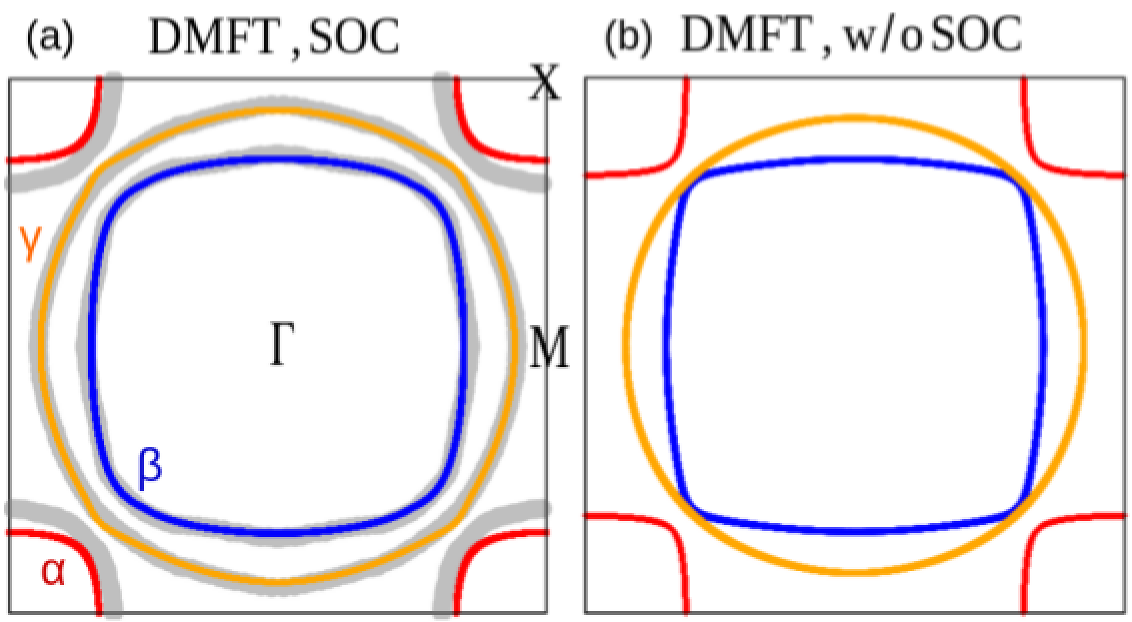
- Sr_2RuO_4 is a Fermi liquid with a low T* due to Hund's rule coupling
- Hund's metal picture is valid in spite of SOC, because $\lambda < T_K^{orb}$
- Spin-orbit effects enhanced due to off-diagonal self-energies but suppressed due to dynamical renormalization (as any other term of the single-particle Hamiltonian)
- Taking this together, Slight suppression (factor ~2) of spin-orbit at low energies, relevant to superconductivity

THANK YOU!



Silk, Terasaki, Schofield, PRB’09
Paterson, Shastry PRB’10

Fermi surface

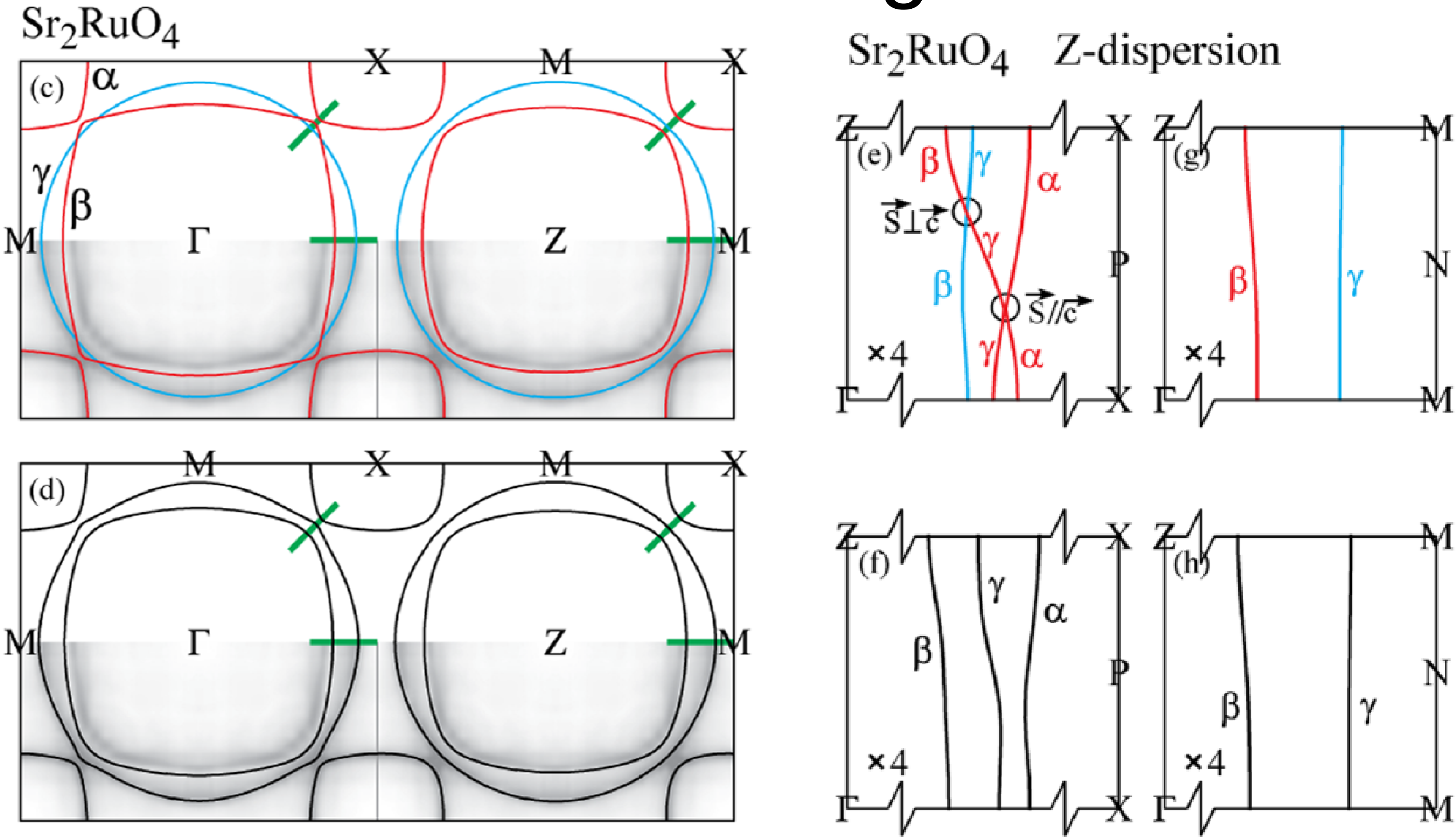


Experiment : A. Damascelli et al., PRL (2000)

SOC
n_{xy}=1.24,$n_{xz/yz}$=1.38
w/o SOC
n_{xy}=1.24,$n_{xz/yz}$=1.38

- Spin-orbit coupling affects Fermiology by inducing orbital mixing in each Fermi surface sheets
- Hund's coupling affects Fermiology by equalize orbital occupancy.

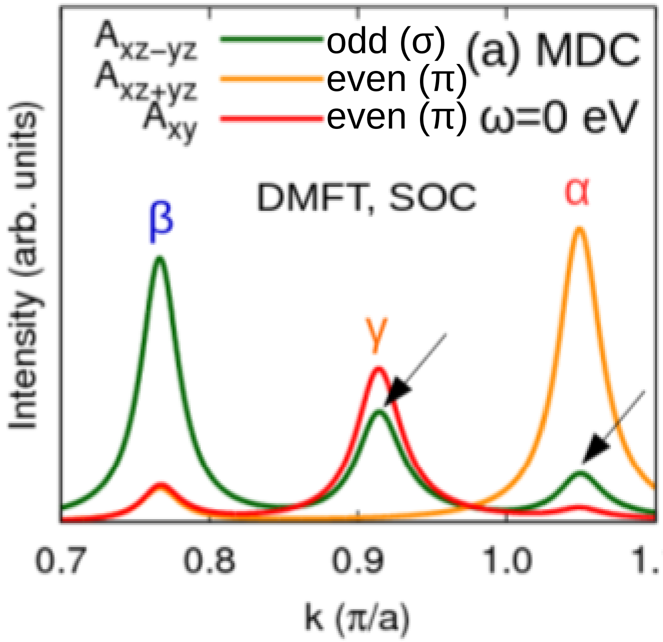
Crossing becomes an avoided crossing

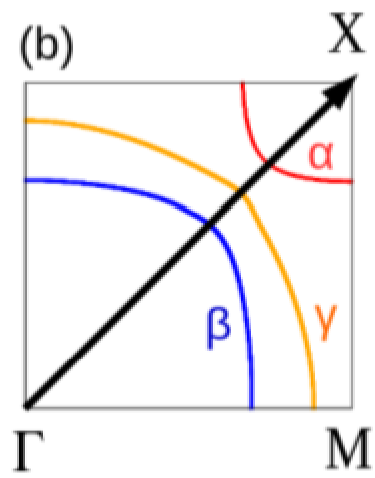


Haverkort et al.
PRL'08

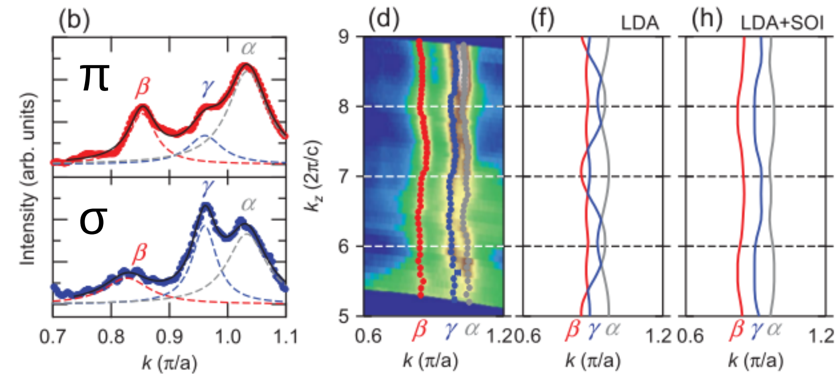
Avoided crossing more consistent with measurements of quantum oscillations, Bergemann et al., Adv. Phys.'03

SOC induced orbital mixing





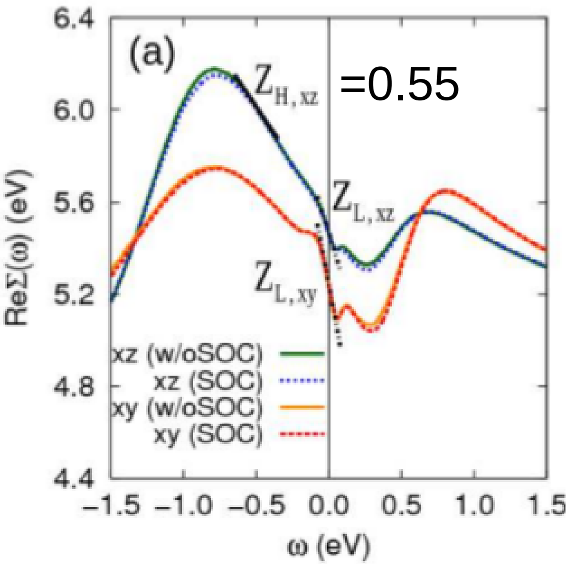
MDC

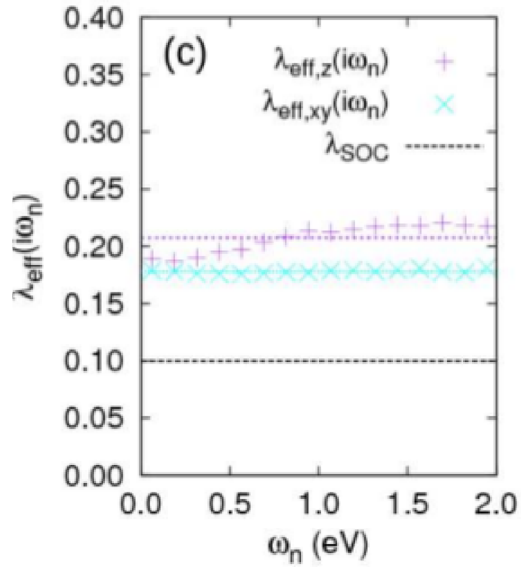


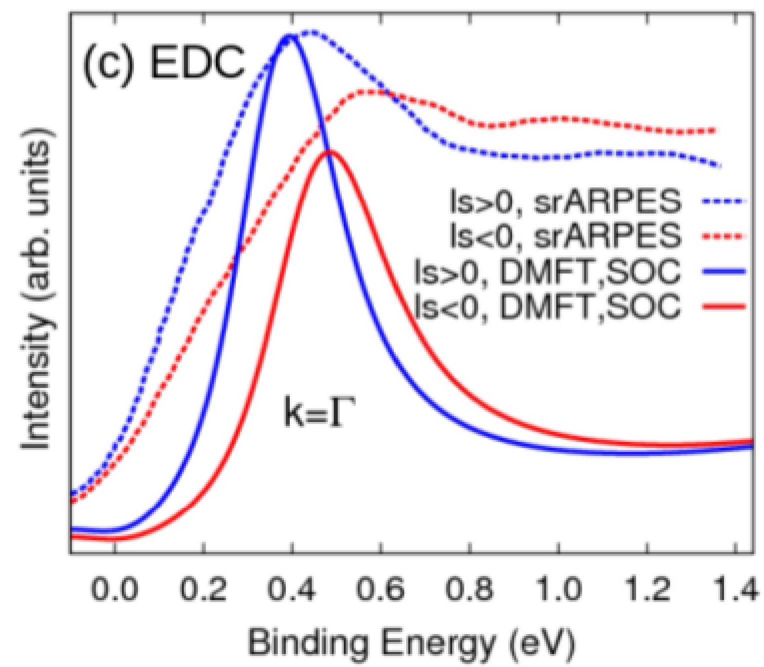
ARPES
H. Iwasawa et al.,PRL (2010)

- Spin-orbit coupling induces mixing of orbital, which is consistent with experiment.

SOC induced degeneracy lifting at Γ







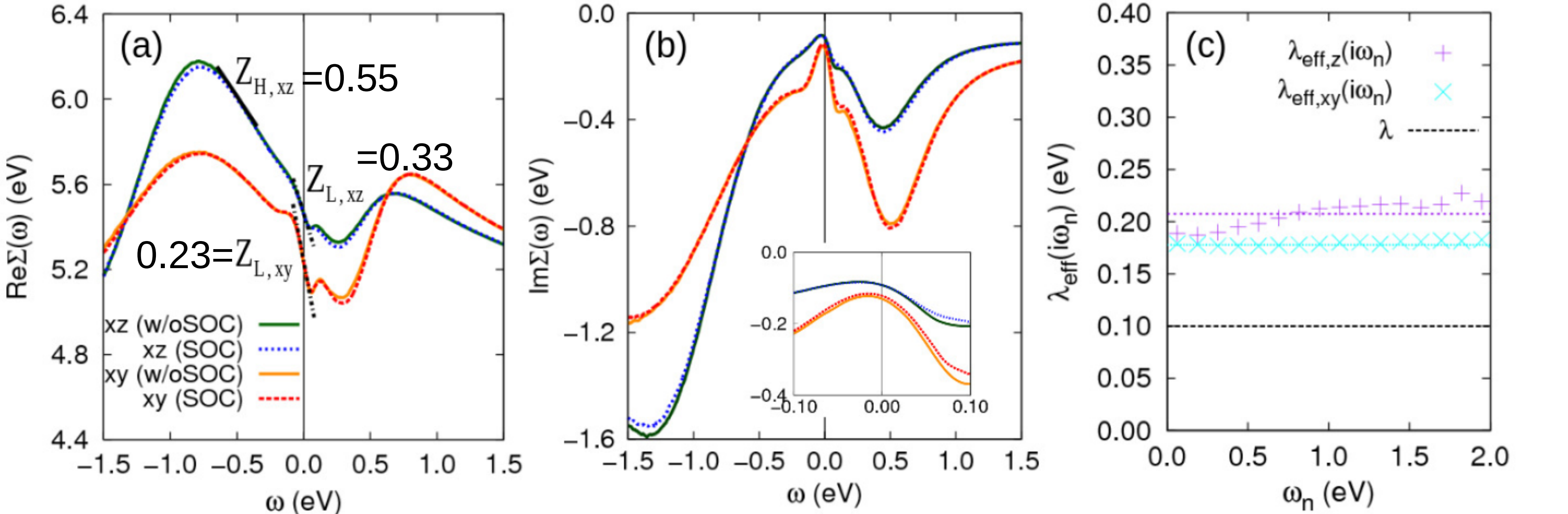
$$\zeta_{\rm SOC} = Z_{H,xz}\lambda_{z,\rm eff}$$

~110 meV

srARPES : C. Veenstra et al., PRL (2014)

- Spin-orbit coupling induced degeneracy lifting at k=Γ point is consistent with experiment.
- This consistency reflects correct renormalization of bands, and correct enhancement of effective SOC constants.

Self-energies and quasiparticle



$$\lambda_z^{\mathrm{eff}}(i\omega_n) = \lambda_{\mathrm{SOC}} + 2\mathrm{Im}\Sigma_{xz\uparrow,yz\uparrow}(i\omega_n)$$

$$\lambda_{xy}^{\mathrm{eff}}(i\omega_n) = \lambda_{\mathrm{SOC}} - 2\mathrm{Im}\Sigma_{xz\uparrow,xy\downarrow}(i\omega_n)$$

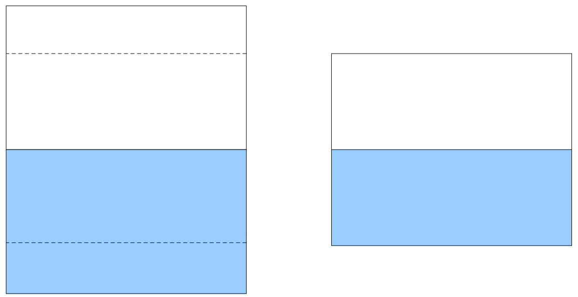
$$\det[(\omega+\mu)\delta_{\underline{a},\underline{b}} - H^0(k)_{\underline{a},\underline{b}} - \mathrm{Re}\Sigma(\omega)_a\delta_{\underline{a},\underline{b}} - \hat{\lambda}^{\mathrm{eff}}_{\underline{a},\underline{b}}] = 0$$

$\underline{a}$,$\underline{b}$: spin/orbital

- Spin-orbit coupling does not affect the nature of electronic correlation of Hund's metal.
- Electronic correlation enhances effective SOC constants without subtle energy dependence.

Who cares if ferromagnetic? → asymptotically decoupled spin; NFL!

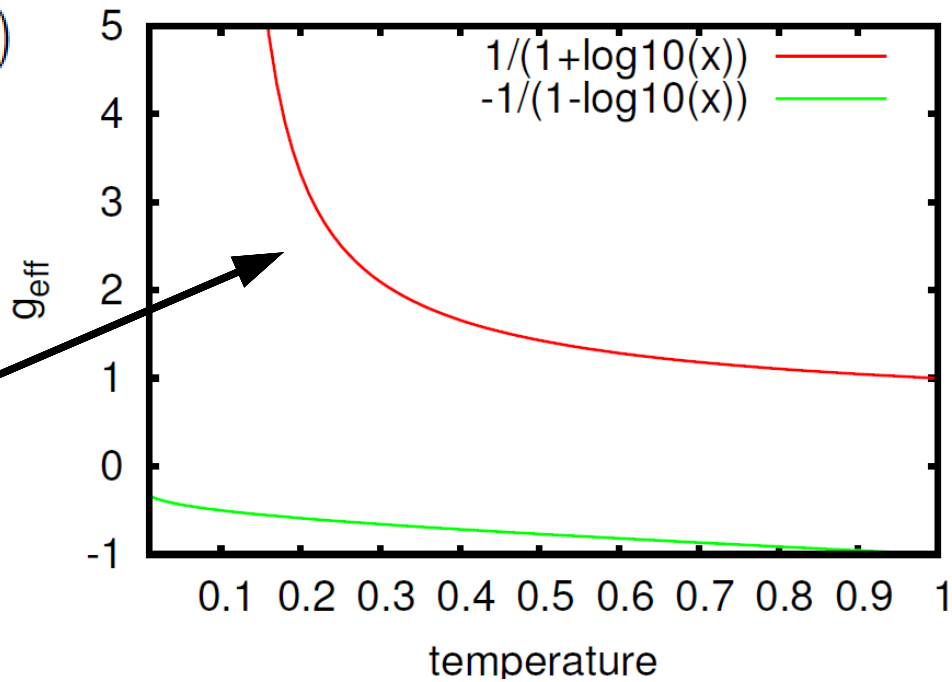
$$H = \sum_{k\sigma} \epsilon_k c^{\dagger}{}_{k\sigma} c_{k\sigma} + \overbrace{J\psi^{\dagger}(0)\vec{\sigma}\psi(0)\cdot\vec{S}_f}^{\Delta H}.$$



$$J(D') = J(D) + 2J^2\rho\frac{\delta D}{D} \qquad g = \rho J$$

$$\frac{\partial g}{\partial \ln D} = \beta(g) = -2g^2 + O(g^3)$$

$$\boxed{g(D') = \frac{g_o}{1 - 2g_o \ln(D/D')}}$$

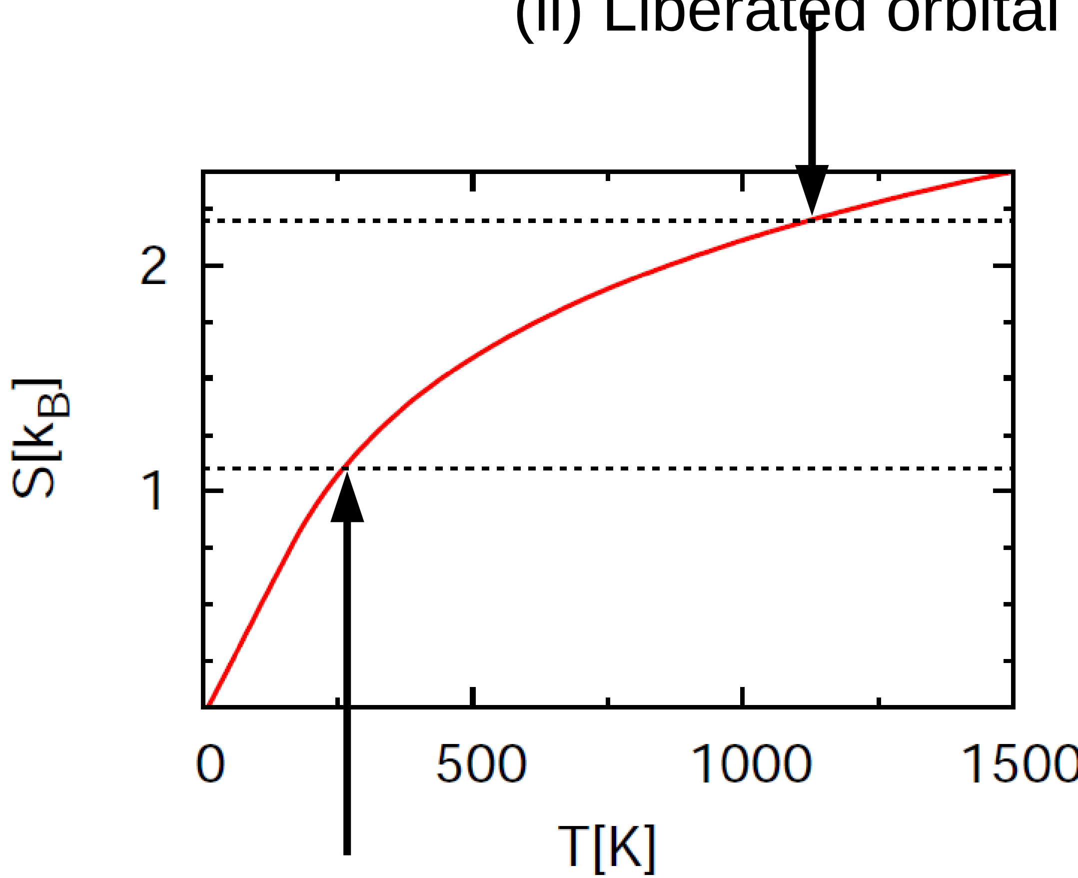


Growth of interaction at low energies for anti-ferro but not for ferro

Two-stage decoherence

- Entropy in Sr_2RuO_4 from LDA+DMFT

(ii) Liberated orbital moments



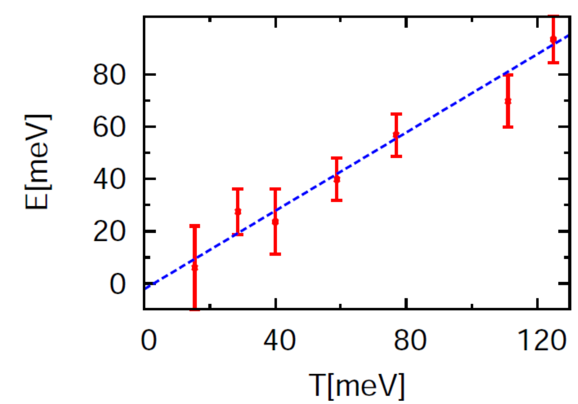
(i) Liberated spins

$$E = \gamma T^2/2$$

$$\gamma = 38\mathrm{mJ/molK^2}$$

$$S = \gamma T; T < T_0$$

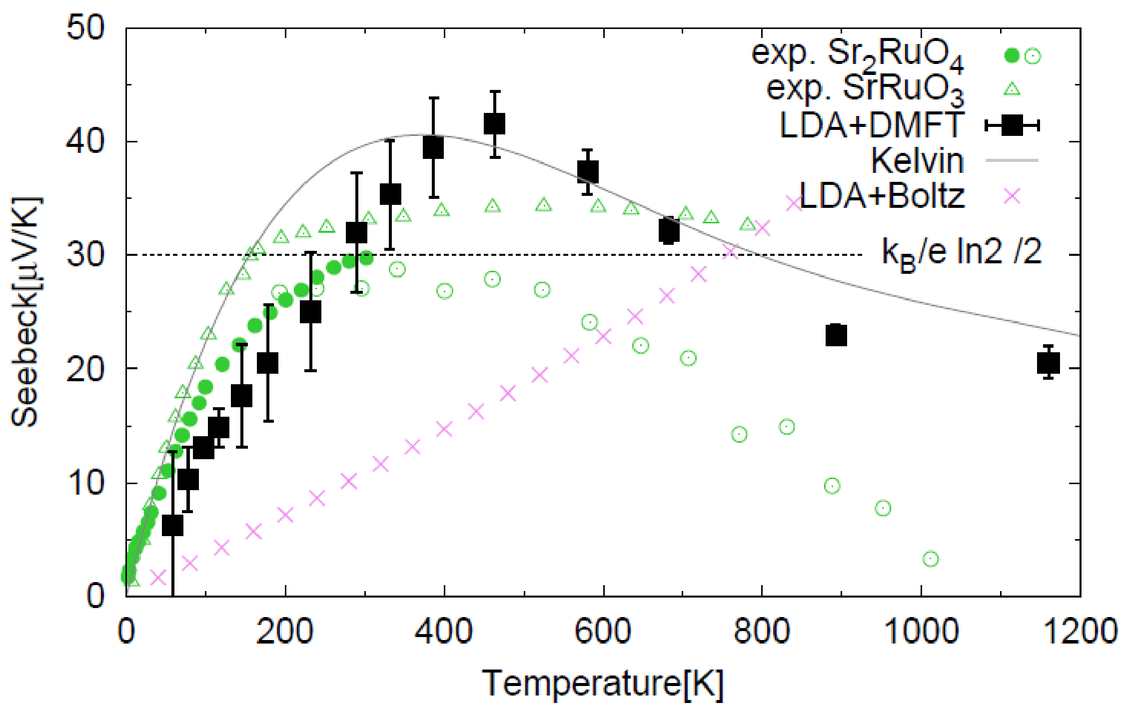
$$S = \gamma T_0 + c\log(T/T_0); T > T_0$$



$$T_0 = c/\gamma \quad c = 0.75k_B$$

Consequences of this for Seebeck

- Knowing DOF one can attempt Heikes analysis



$$S_H = k_B/2e \log(d_{N-1}/d_{N+1})$$
$$= k_B/2e \log(4/2) \approx 30\mu V/K$$

JM & Georges, PRL'16
Klein et al. PRB'06

d_{N-1}=(2S+1)=4 ; N-1=3, S=3/2
d_{N+1}=(2S+1)=2 ; N+1=5, S=1/2

Comments: retaining **just spins**!

If orbitals kept:
→ k_B/(2e)*log(4/6) = -17.5microV/K

- ab- Seebeck explainable in entropic terms and points to quenched orbitals and free spins

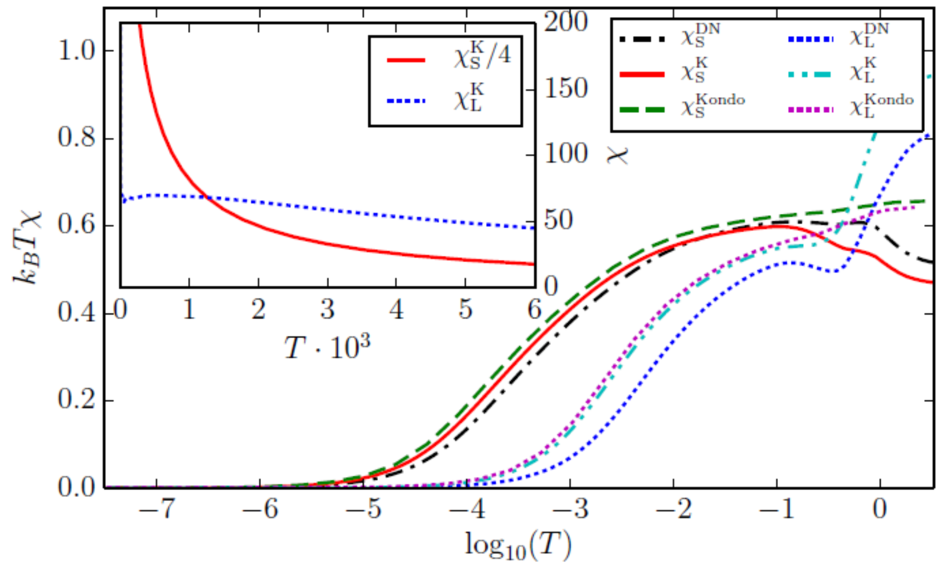
- Can Seebeck (blindly) be used as diagnostics of DOFs of warm metals?
- Is entropy a limiting factor for Seebeck coefficient?

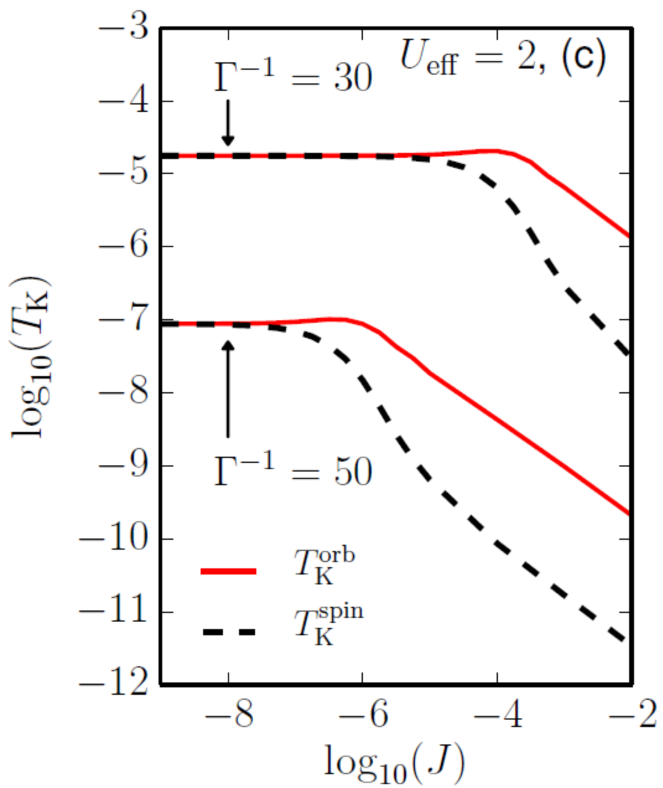
Insights from impurity model

- Kanamori impurity with NRG [S and L SU(2) symmetries]

$$H_{\text{imp}} = \frac{1}{2}(U - 3J)N_d(N_d - 1) - 2J\mathbf{S}^2 - \frac{J}{2}\mathbf{L}^2$$

- Distinct scales for screening of S and L





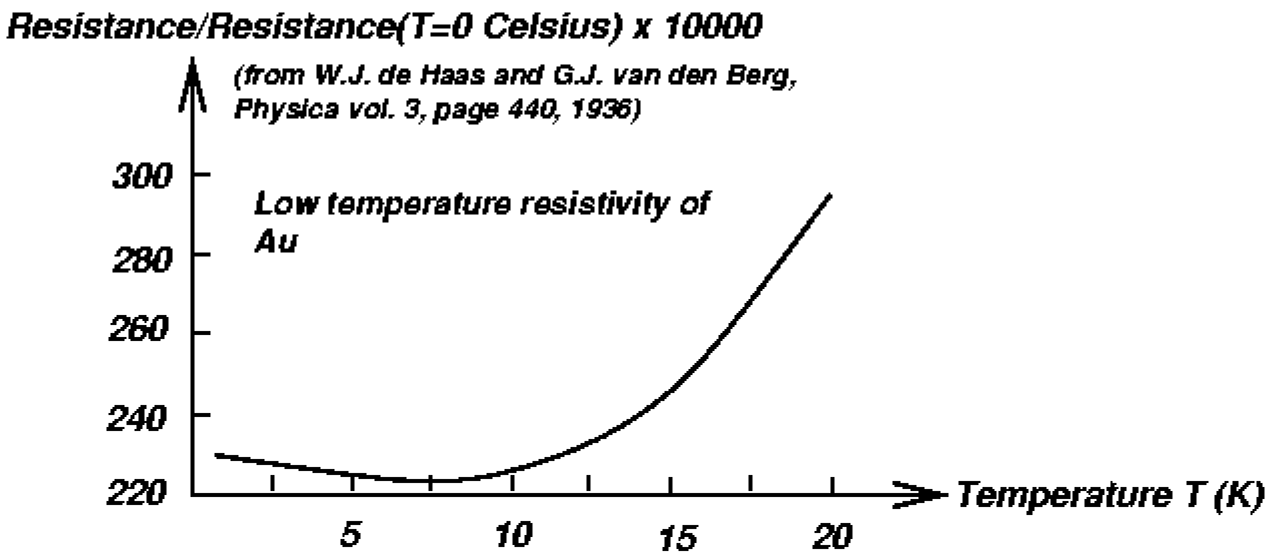
Horvat, Žitko, Mravlje PRB'16
Okada, Yosida, PTP'73
Yin, Haule, Kotliar PRB'12

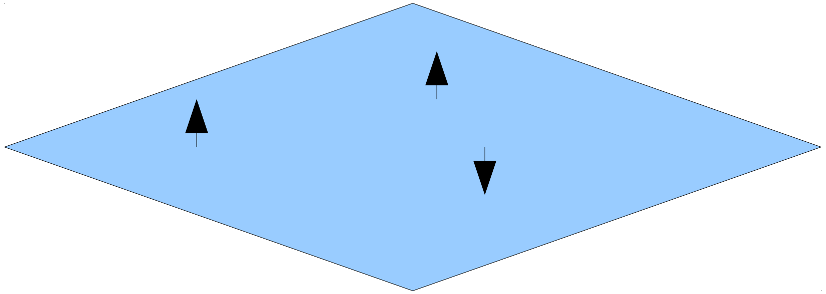
- Suppression of (both) T_K with J

- Similar results for Kanamori, Dworin-Narath,Kondo-Kanamori,

Atom in a medium : quantum impurity problem

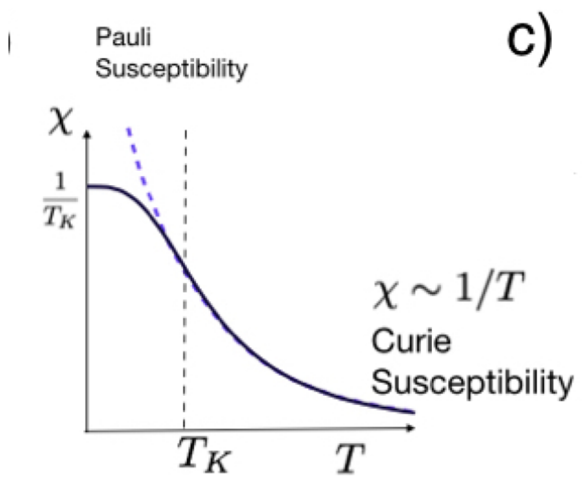
- Kondo effect

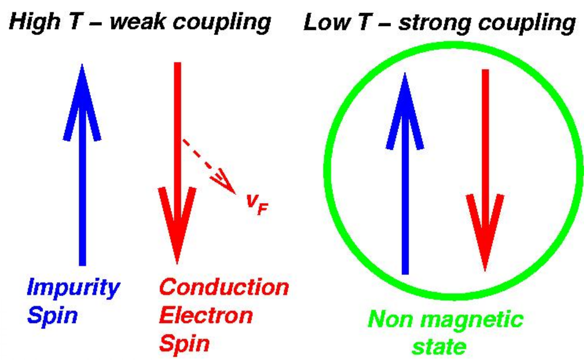


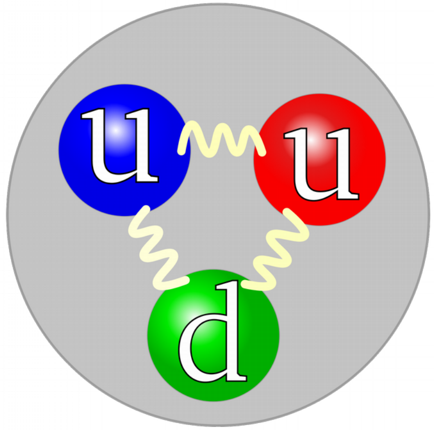


Kondo effect

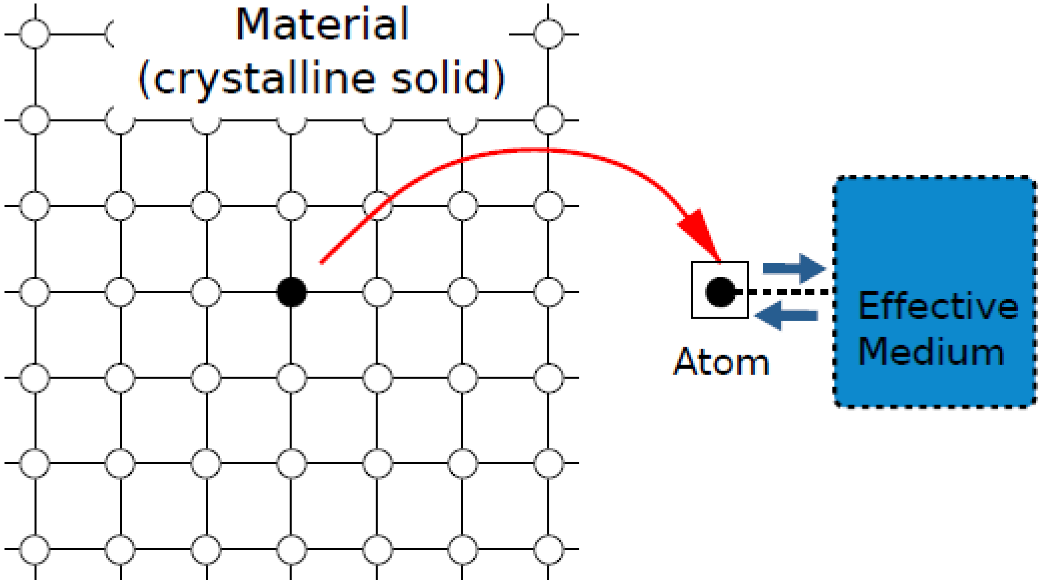
- Infrared slavery
- Screening of magnetic moments → renormalized metallic response







- Also bulk : high temperatures, local moments
- Low teperatures ; renormalized quasiparticles

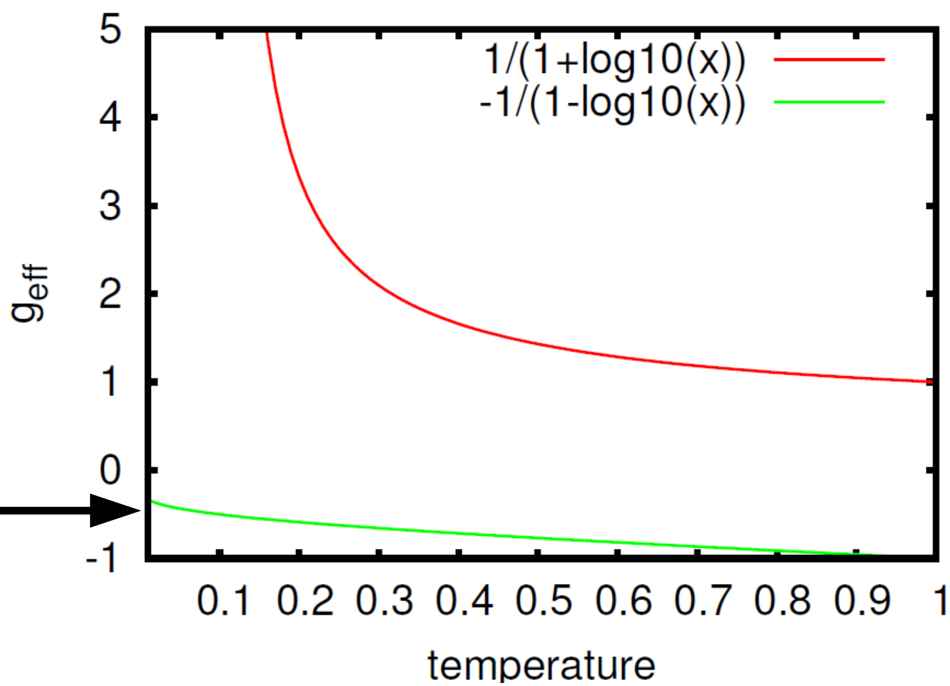


Ferromagnetic Kondo effect, infrared freedom

$$H = \sum_{k\sigma} \epsilon_k c^{\dagger}{}_{k\sigma} c_{k\sigma} + \overbrace{J\psi^{\dagger}(0)\vec{\sigma}\psi(0) \cdot \vec{S}_f}^{\Delta H} .$$

$$\boxed{g(D') = \frac{g_o}{1 - 2g_o \ln(D/D')}}$$

Free moments at
low temperatures.
Not a Fermi liquid

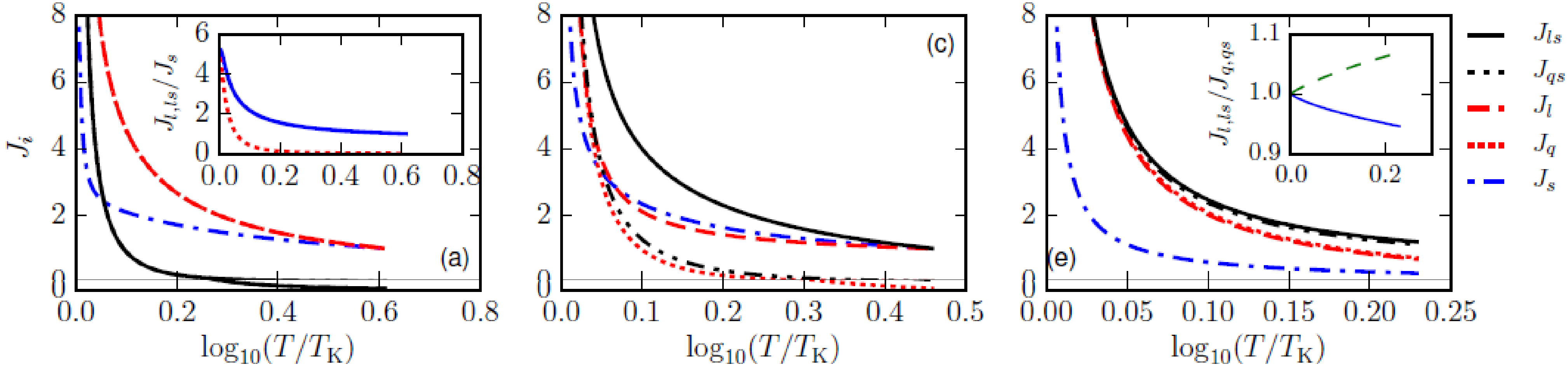


RG flow

Suppressed Jls,Jqs

Suppressed quadrupole
Jl >> Jq, Jls >> Jqs

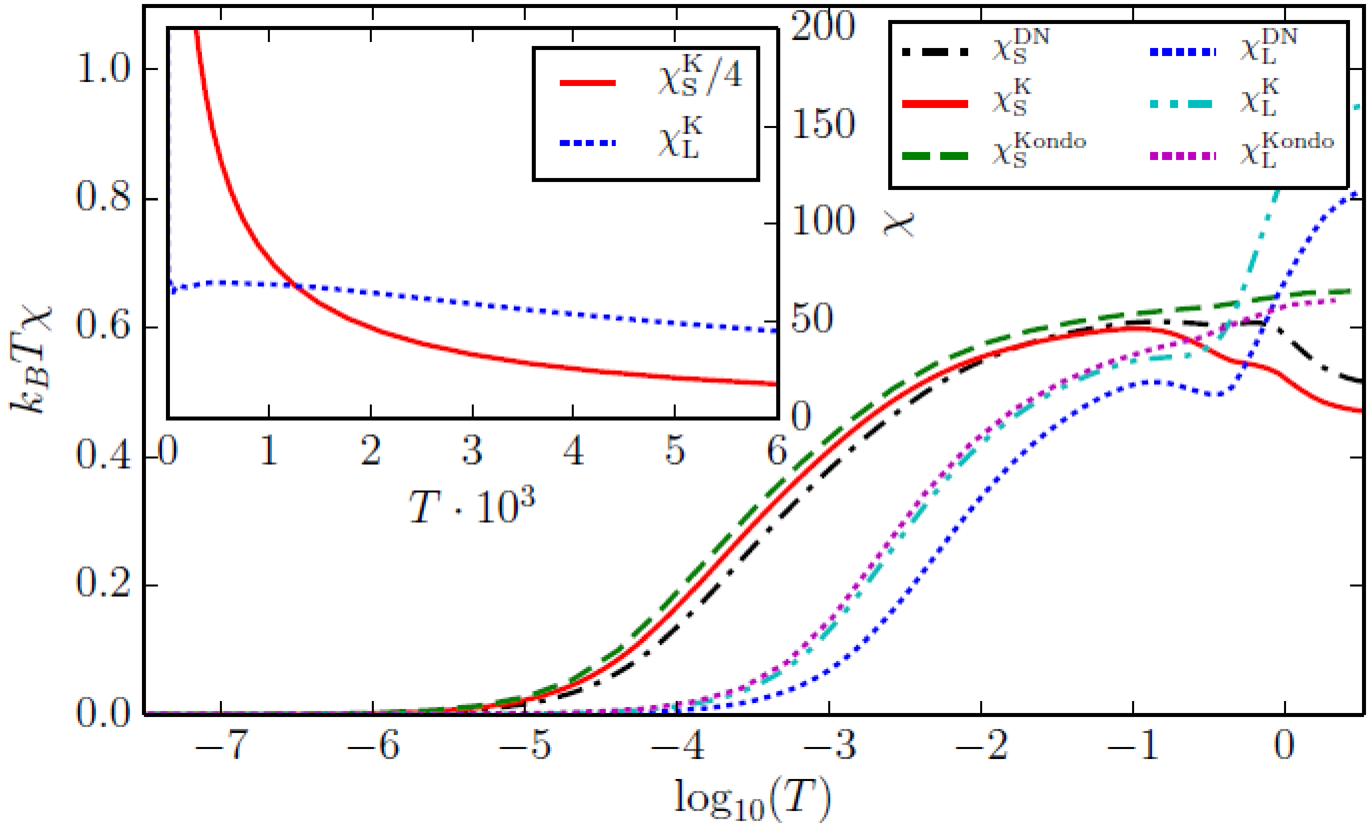
Realistic : from S-W



- Even starting with J_s=J_l,(suppressing J_{ls}=J_{qs} terms) running of J_l faster (due to larger SU(3) symmetry)
- Splitting between J_l, J_q and J_{ls}, J_{qs} becomes smaller as T is decreased → dynamic establishing of SU(3) symmetry

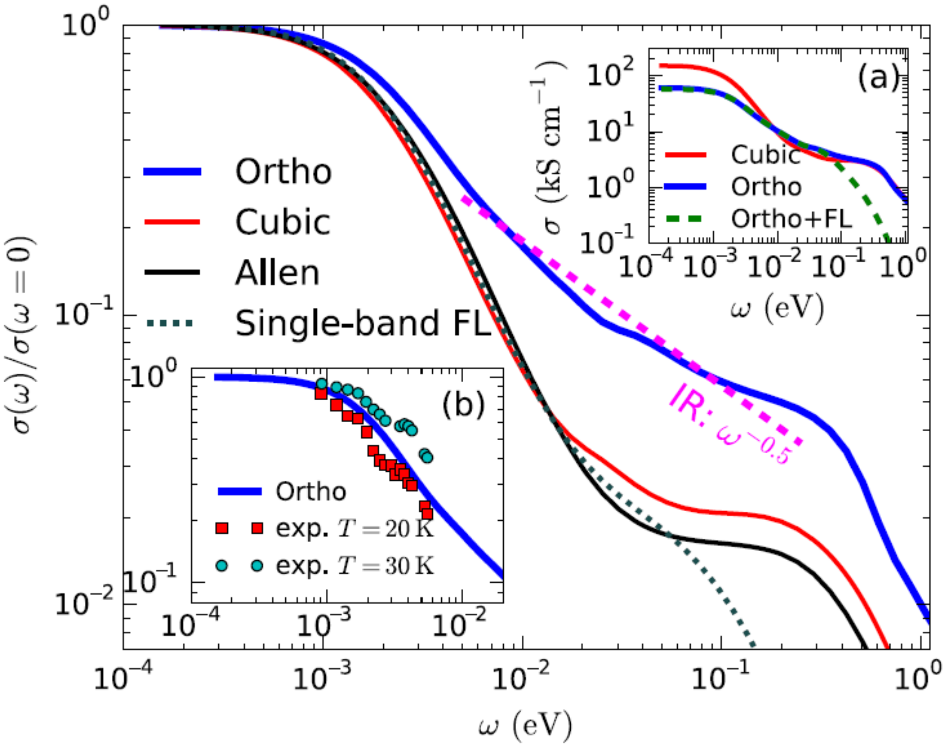
NRG results

- Hund's metal –
  - Low T - FL
  - at intermediate T : screened orbitals and fluctuating spins



Other ruthenates

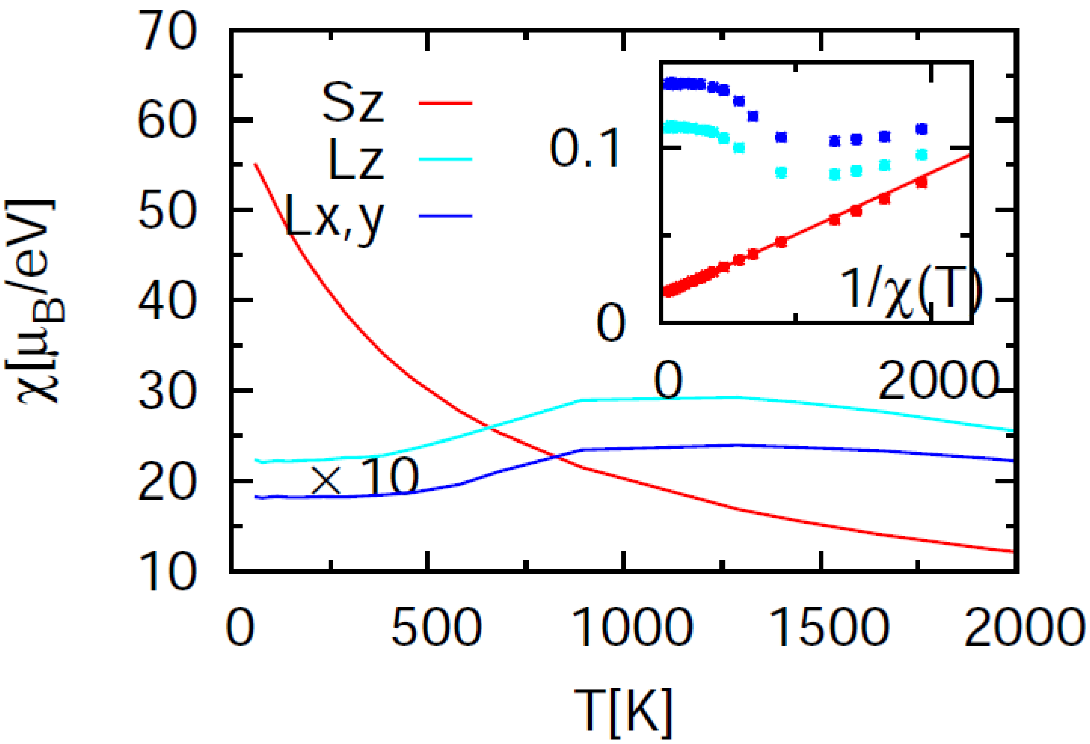
- LDA+DMFT succesfully describes also other ruthenates
- FM in $SrRuO_3$ and paramagnetism with larger renormalizations in $CaRuO_3$
- Optics in $CaRuO_3$



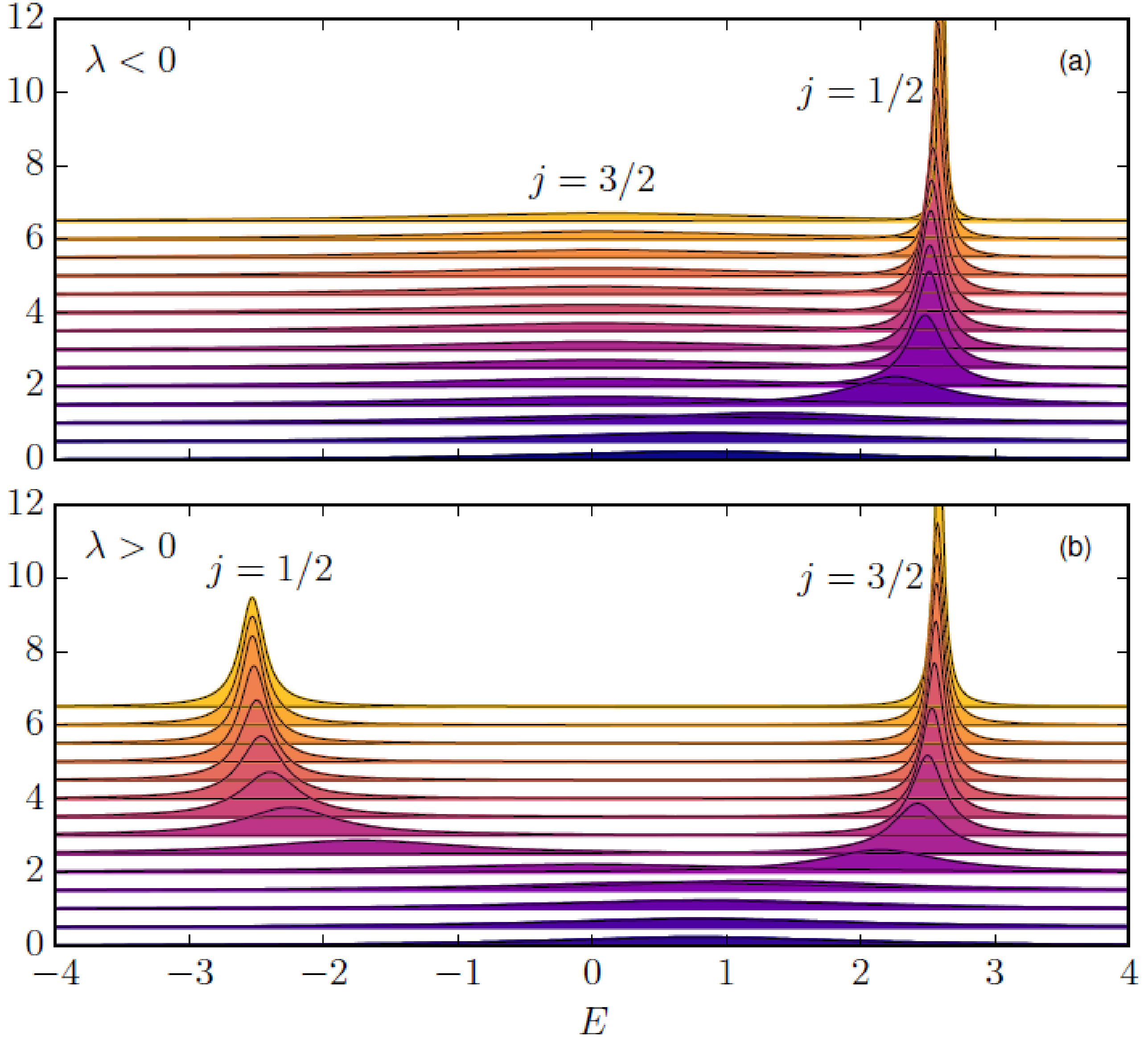
Dang, JM, Georges, Millis, PRB'15
Dang, JM, Georges, Millis, PRL'15

Returning to materials worlds … Sr_2RuO_4

- T_k^{orb} =1000K = 0.1eV; λ=0.075eV; validates qualitatively LDA+DMFT without spin-orbit (but marginally, to be investigated more)



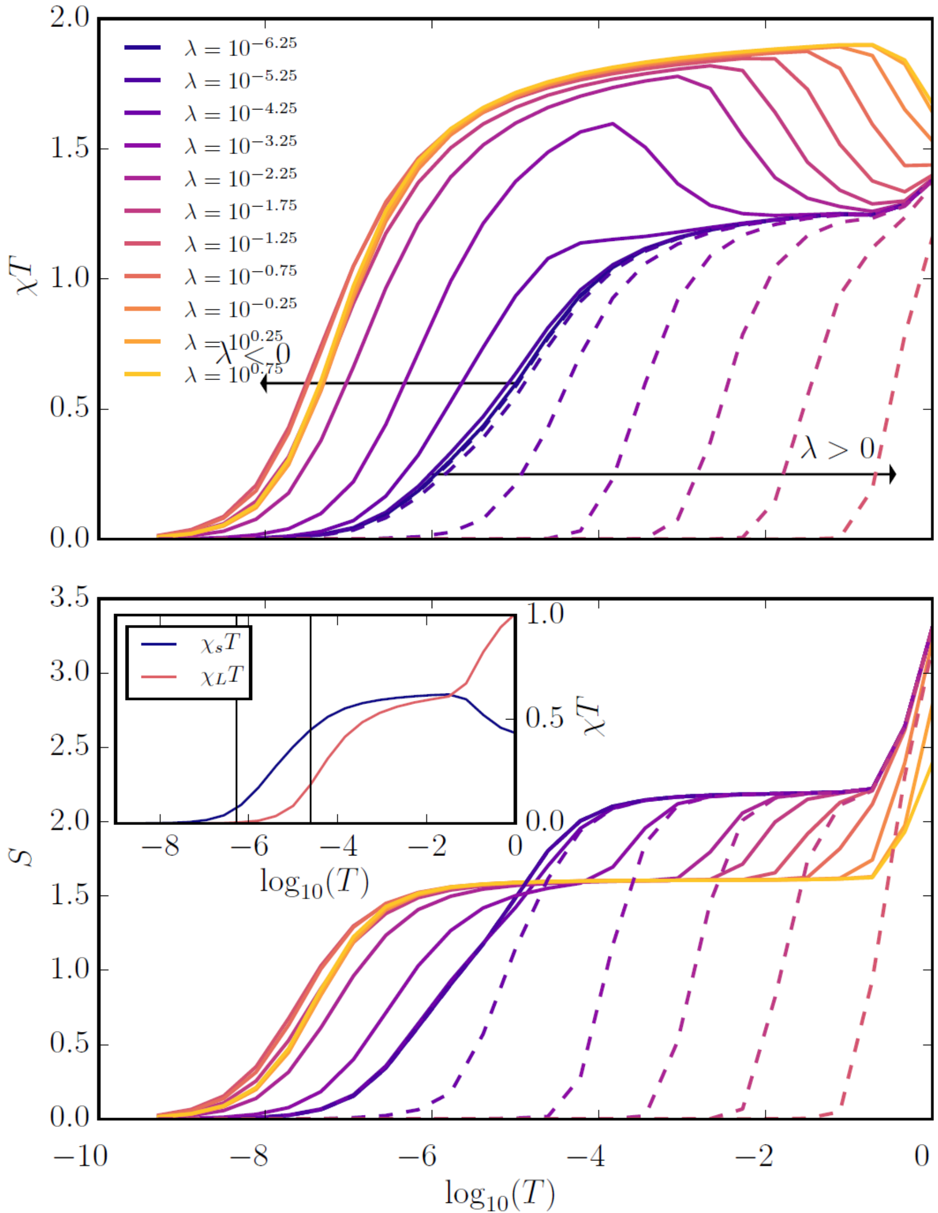
Quasiparticle resonances



What about LS coupling?

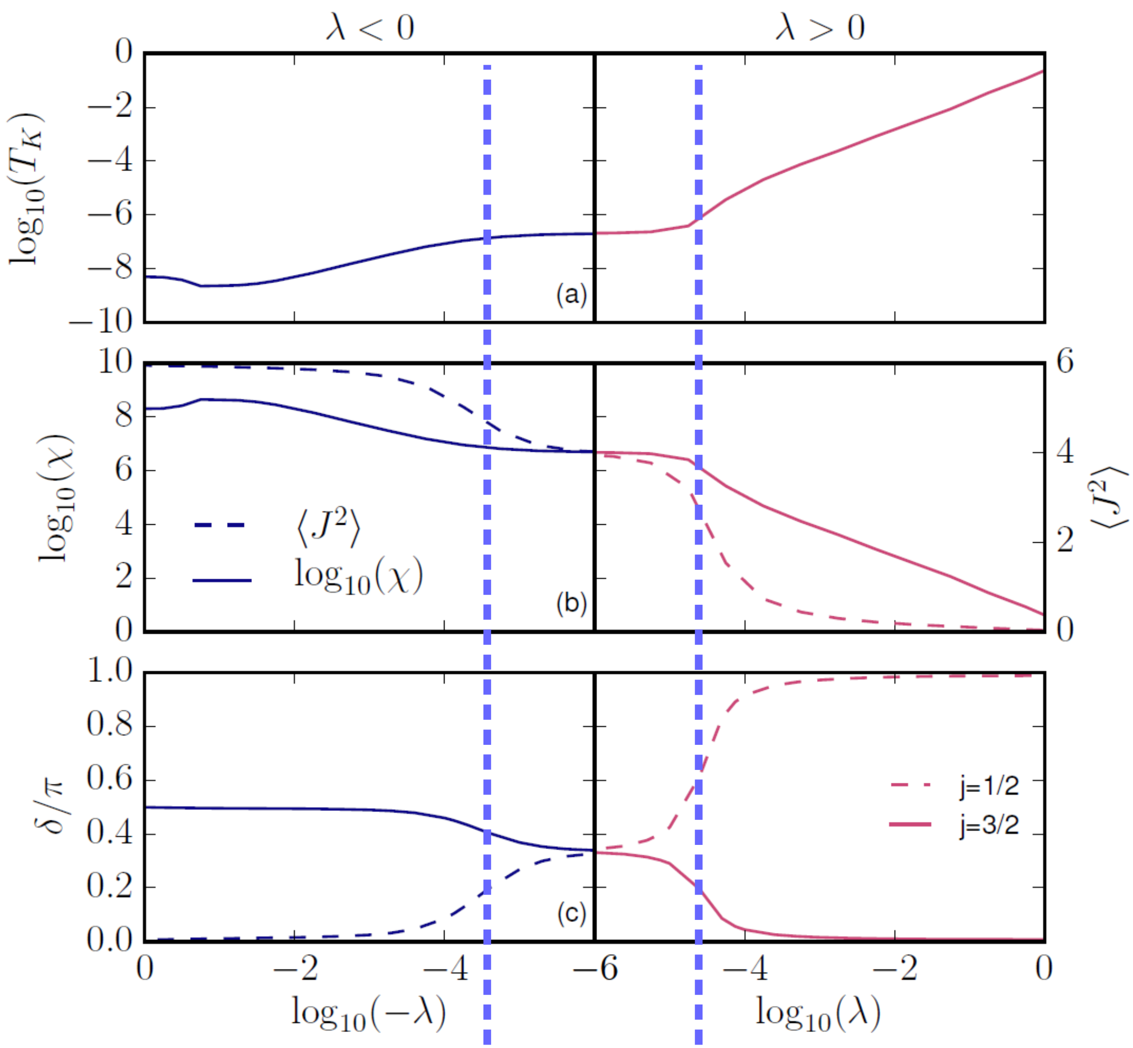
- L-S coupling not small ~0.1eV
- – not that much smaller than J_H
- What are its consequences?

NRG study :
Kanamori Hamiltonian + LS



-d^2: $SrCrO_3$, $SrMoO_3$

-d^4: ruthenates

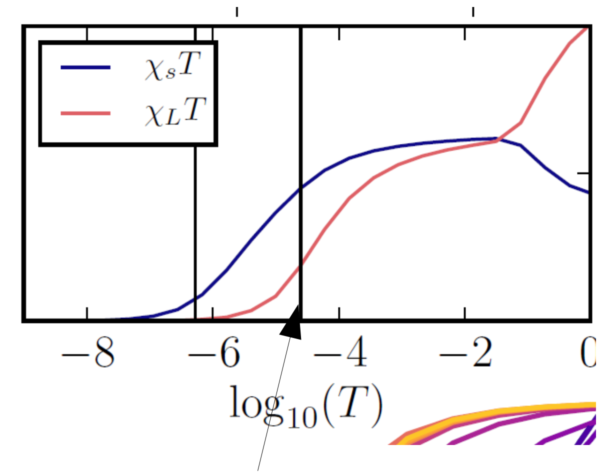


SOC J=2 metal

Hund's metal

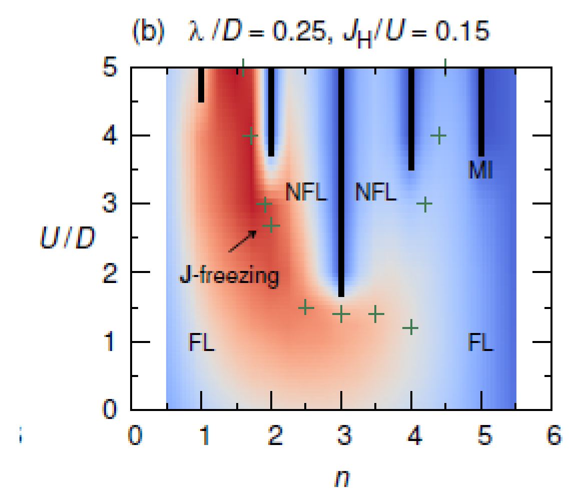
van Vleck J=0 insulator

$|\lambda| < T_K^{orb}$



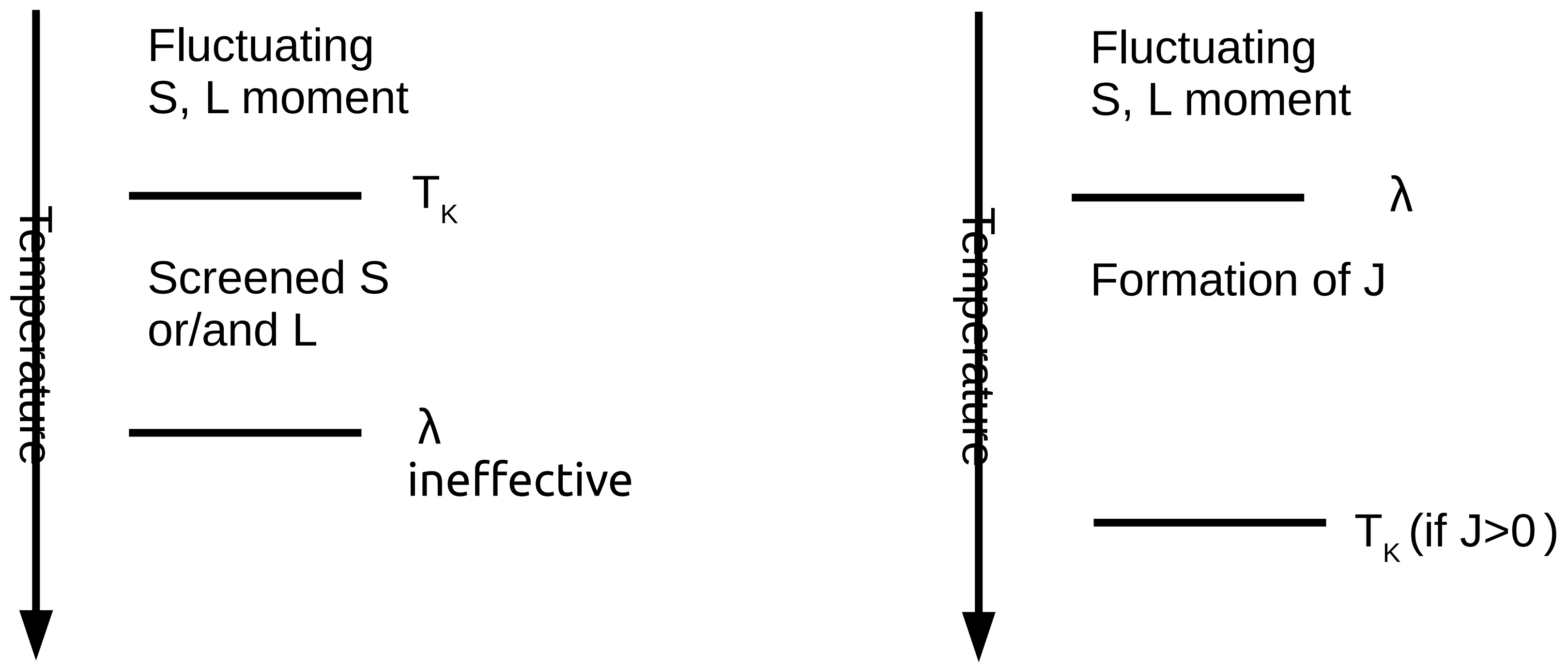
T_K^{orb}

Compare with a DMFT study of Kim et al. ArXiv:1607.05196



RG picture on relevance of λ

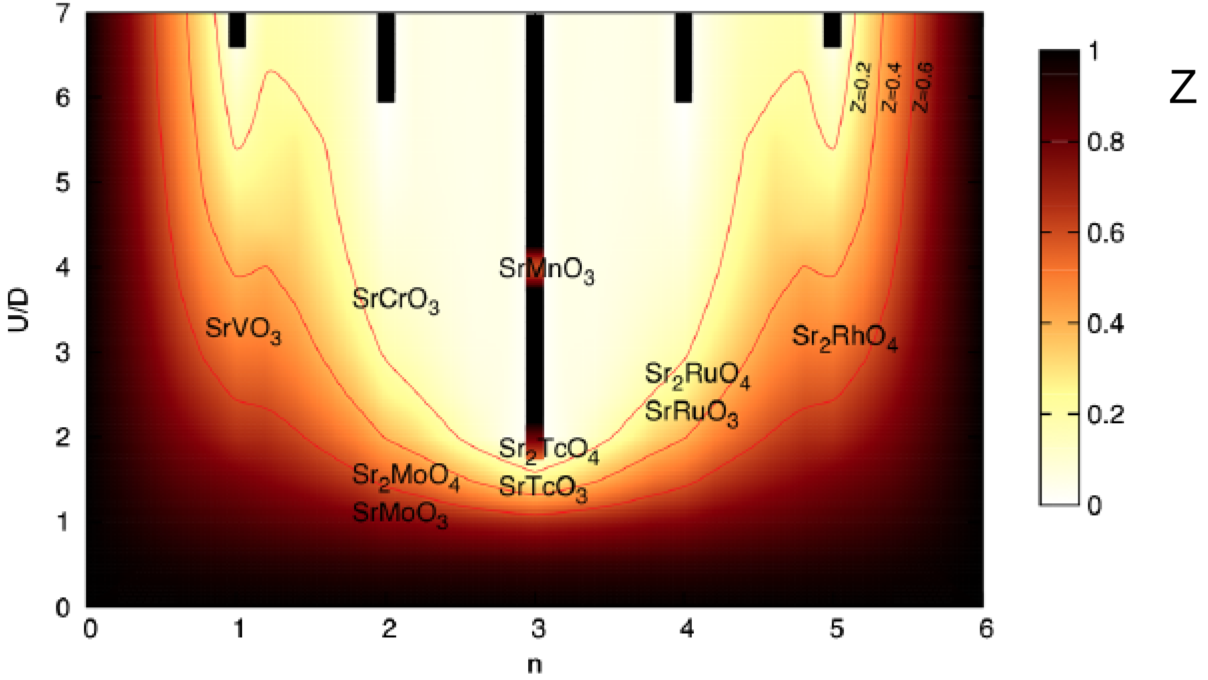
- $|\lambda| < T_K$ vs. $|\lambda| > T_K$



($T_K \rightarrow T_k^{orb}$, for Hund's metals, but more generally, first scale at which either spin/orbit moment is screened)

S

- Bright colors = small Z = strong correlations
- Bars indicate Mott insulator
- Materials placed according to specific heat enh. (if app.)

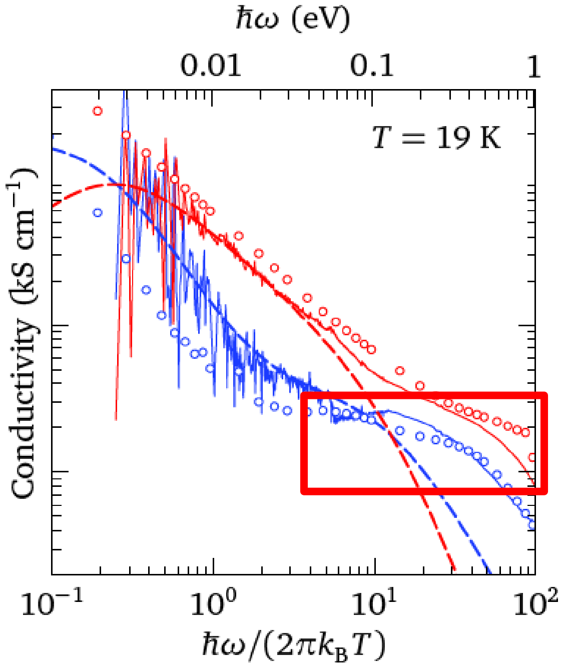


Consequences

- Existence of RQPs enables rewriting transport a la Boltzmann
- Shifts thinking from “what is going on with scattering” to “what is going on with dispersions”

Deng, JM et al, PRL'13
Wu, Kotliar, Haule, PRL'13

- Success of such thinking: explaining optics in terms of how correlations affect dispersions



Stricker, JM et al. PRL'14

Large curvature implies small cutoff (kink) scale (if mass is fixed)

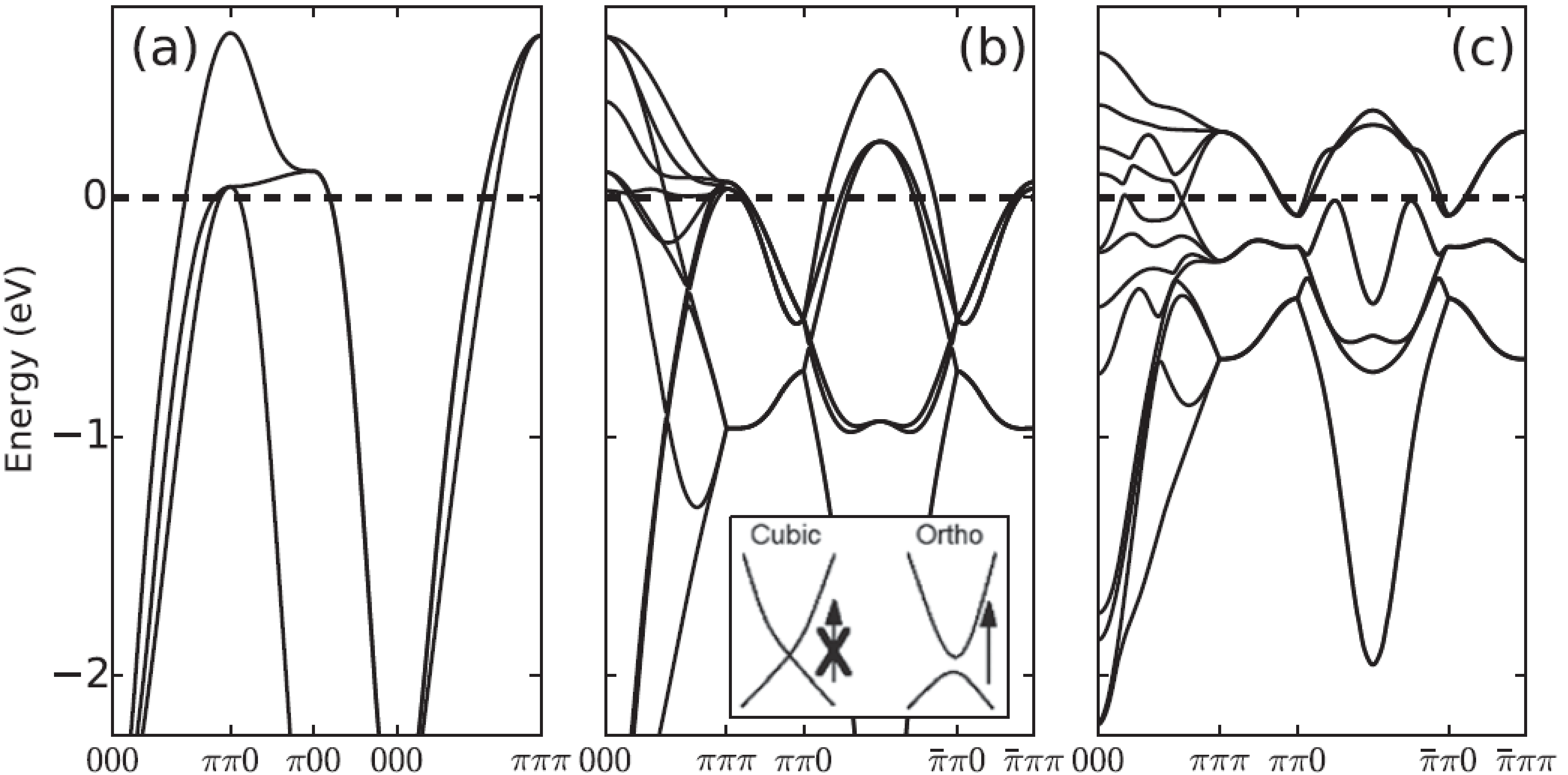
$$\mathrm{Im}\Sigma = -A\omega^2 \qquad \mathrm{Re}\Sigma = -2\omega_c A\omega + \cdots.$$

$$\mathrm{Im}\Sigma = 0 \quad |\omega| > \omega_c,$$

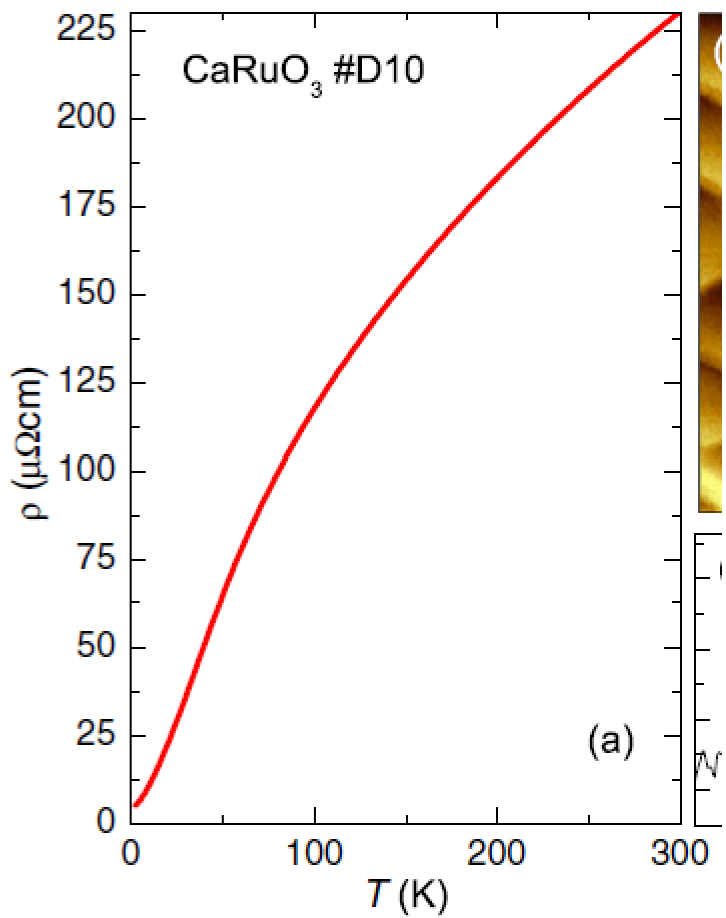
PHYSICAL REVIEW B **90**, 205131 (2014)

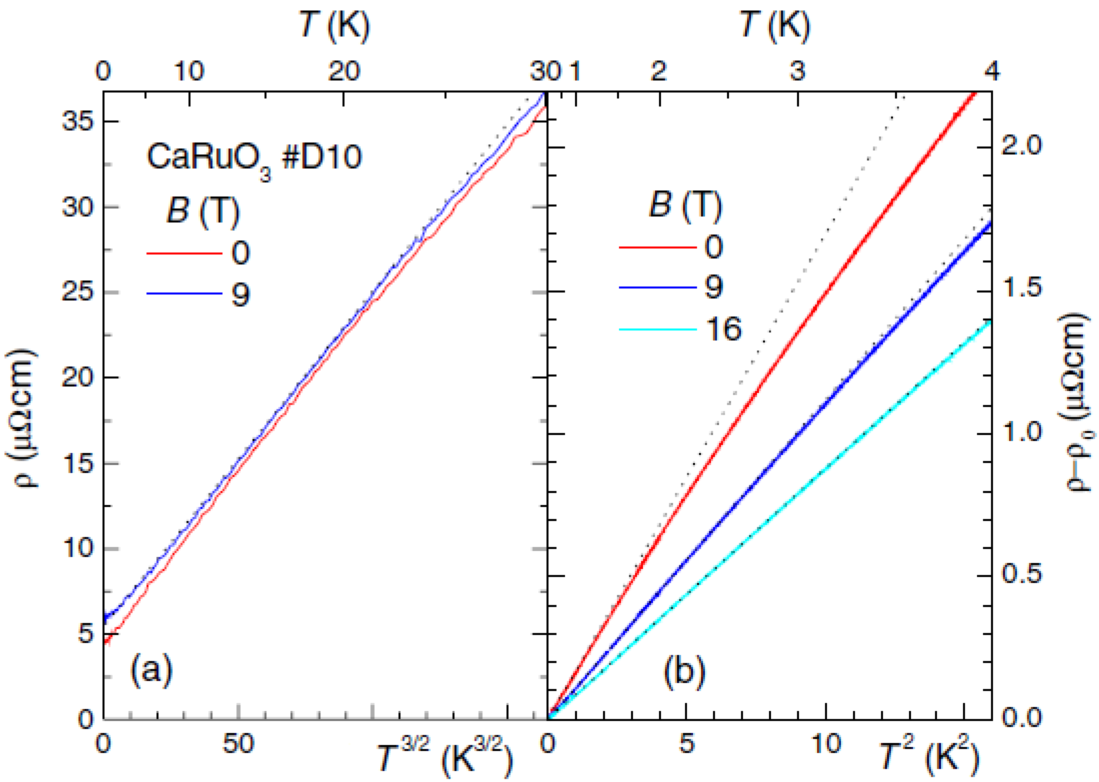
Photoemission and DMFT study of electronic correlations in $SrMoO_3$: Effects of Hund's rule coupling and possible plasmonic sideband

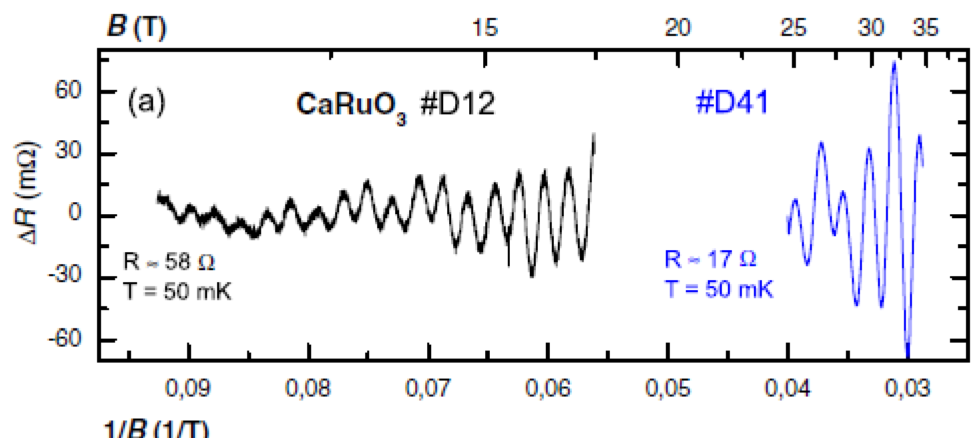
H. Wadati,[1,*] J. Mravlje,[2,3,4] K. Yoshimatsu,[5] H. Kumigashira,[5] M. Oshima,[5] T. Sugiyama,[6] E. Ikenaga,[6] A. Fujimori,[7] A. Georges,[3,4,8] A. Radetinac,[9] K. S. Takahashi,[10] M. Kawasaki,[1,10] and Y. Tokura[1,10]


(a)
(b)
(c)
Energy (eV)
0
−1
−2
000
ππ0
π00
000
πππ
000
πππ
ππ0
π̄π0
π̄ππ
000
πππ
ππ0
π̄π0
π̄ππ
Cubic
Ortho

Quantum oscillations

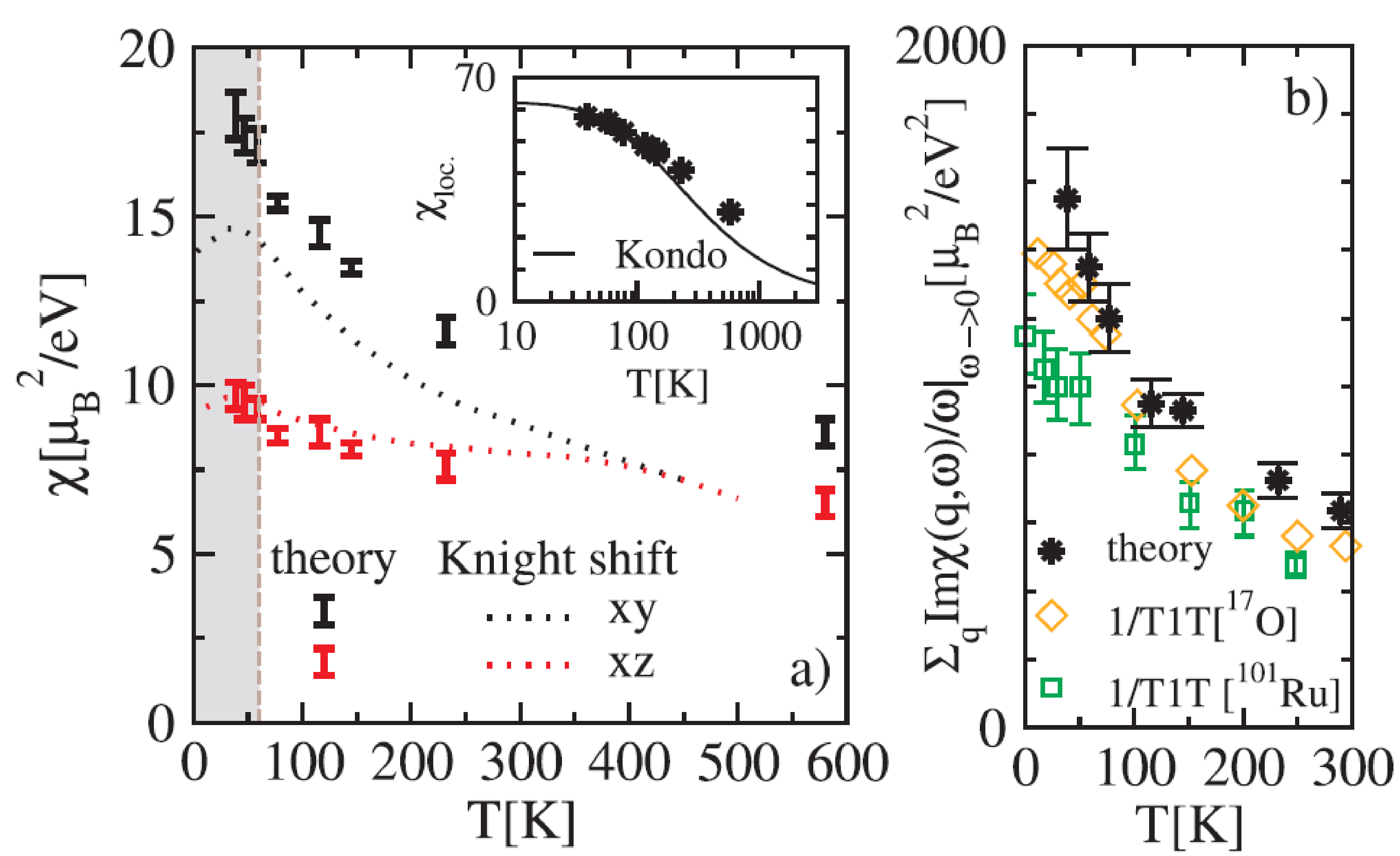




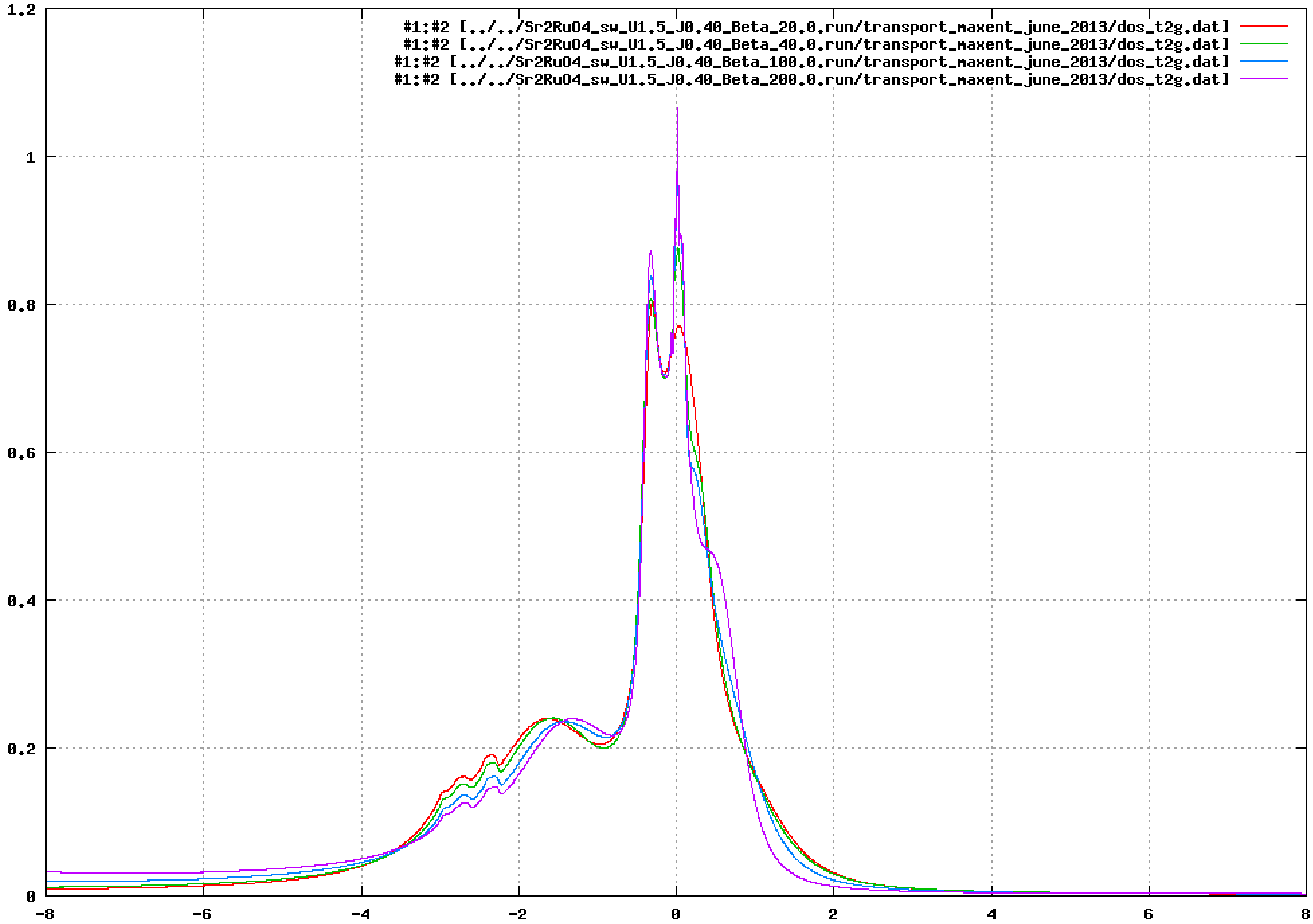


Schneider, …, Gegenwart, PRL'14

NMR



20
15
10
5
0
$\chi[\mu_B^2/eV]$
0
100
200
300
400
500
600
T[K]
70
0
$\chi_{loc.}$
Kondo
10
100
1000
T[K]
theory
Knight shift
xy
xz
a)
2000
0
$\Sigma_q \mathrm{Im}\chi(q,\omega)/\omega|_{\omega\to0}[\mu_B^2/eV^2]$
b)
theory
1/T1T[^{17}O]
1/T1T [^{101}Ru]
0
100
200
300
T[K]



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#1:#2 [../../Sr2RuO4_sw_U1.5_J0.40_Beta_200.0.run/transport_maxent_june_2013/dos_t2g.dat]
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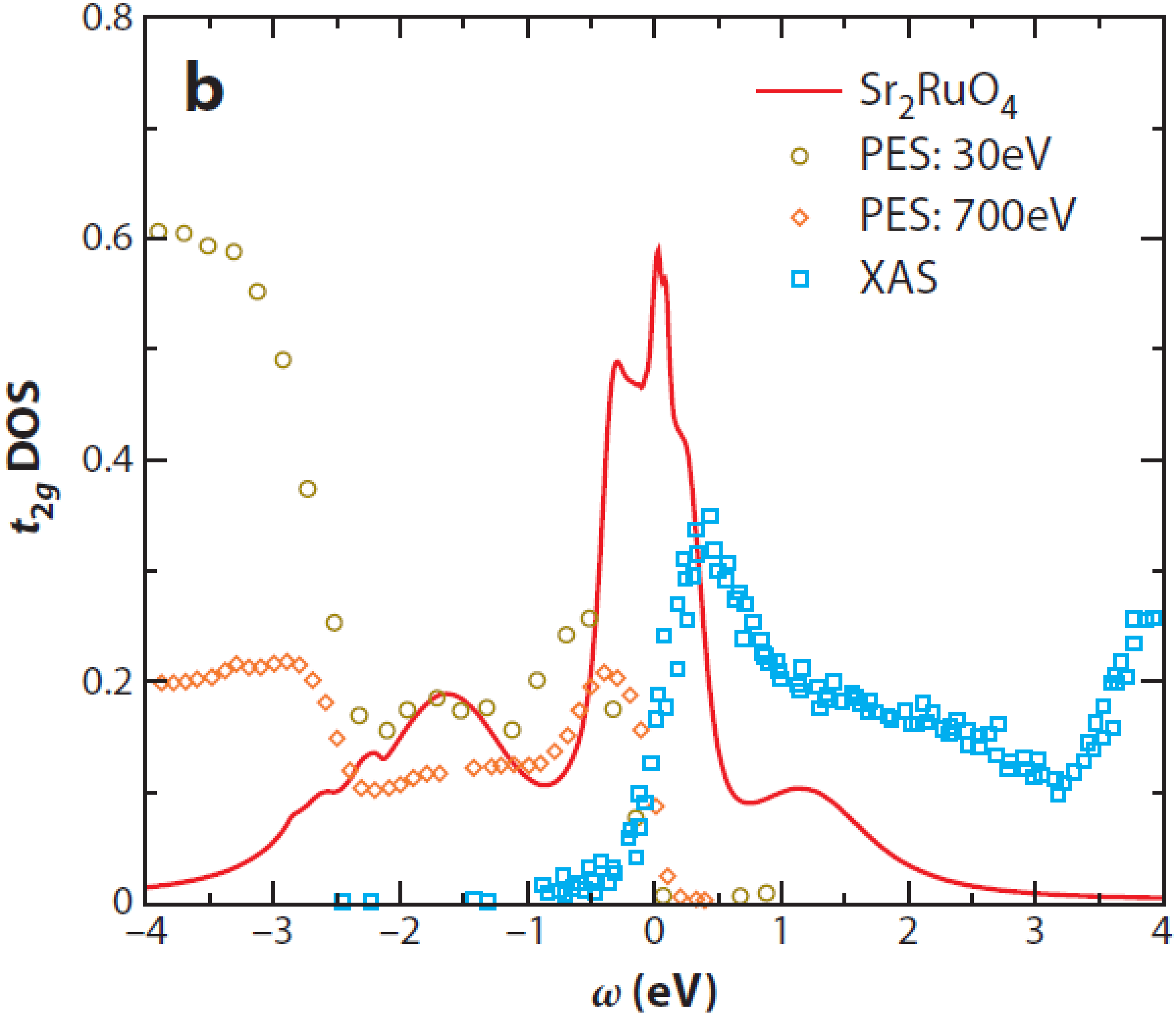
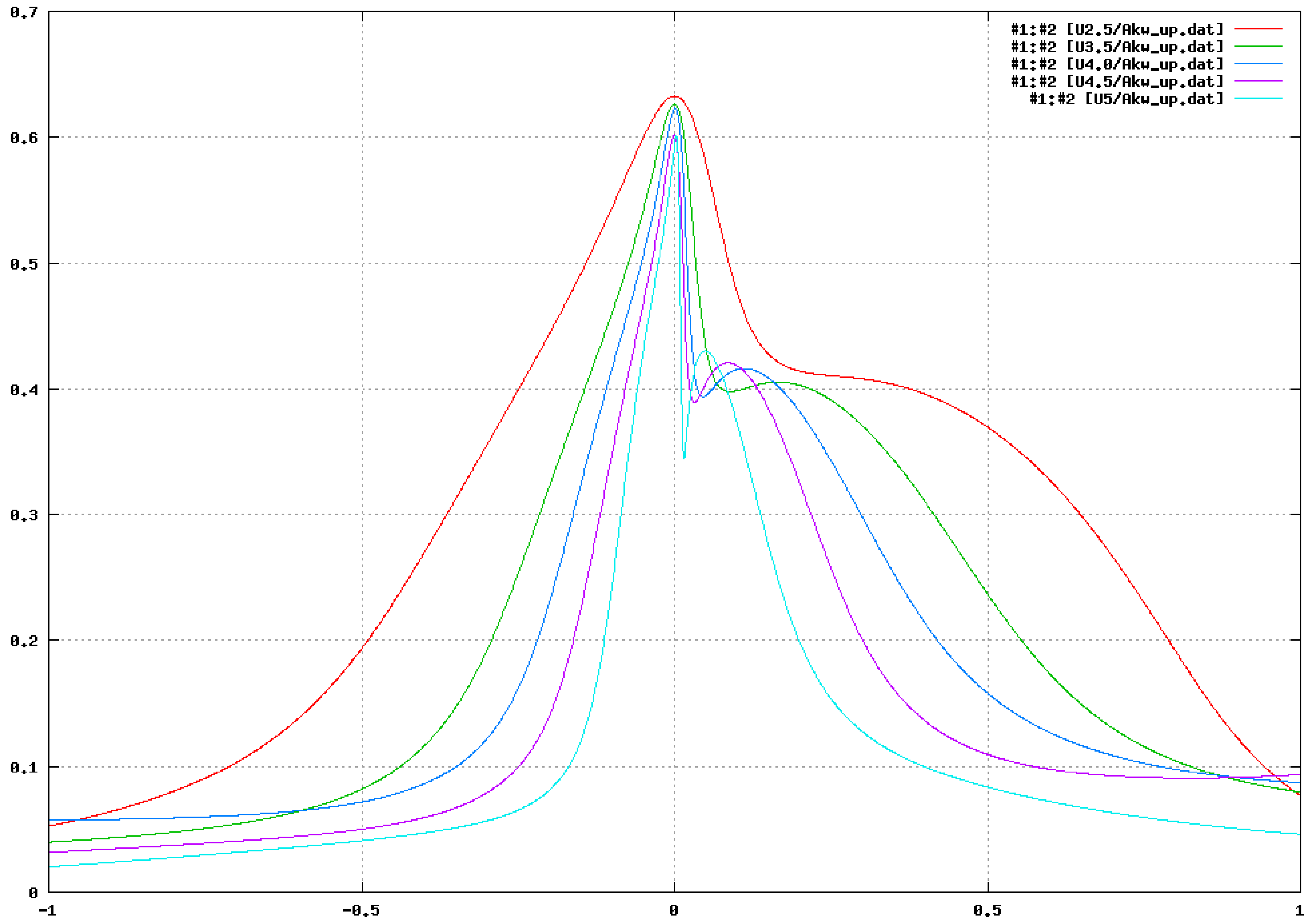
0.4
0.2
0
-8
-6
-4
-2
0
2
4
6
8

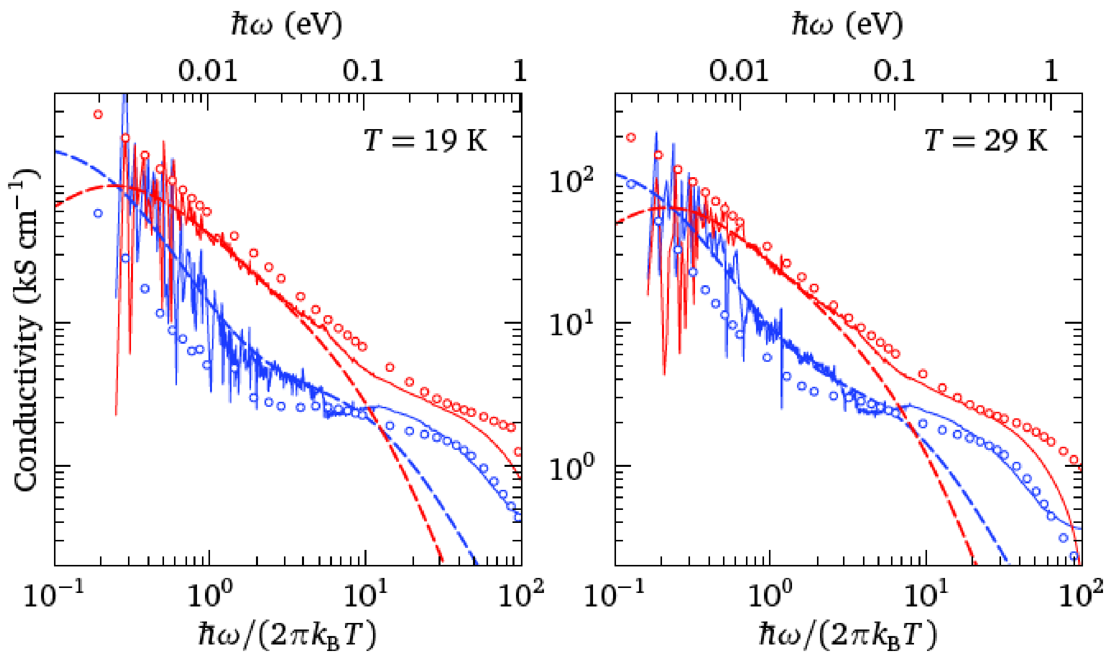

b
Sr2RuO4
PES: 30eV
PES: 700eV
XAS
t2g DOS
0
0.2
0.4
0.6
0.8
−4
−3
−2
−1
0
1
2
3
4
ω (eV)

Quasiparticle part of the spectra; J/U=1/6



LDA+DMFT on Sr_2RuO_4

- Data in close agreement with experimental ones!



$$\sigma(\omega) = \frac{2\pi e^2}{V} \sum_k \int_{-\infty}^{\infty} d\varepsilon \, \frac{f(\varepsilon) - f(\varepsilon + \hbar\omega)}{\omega} \times \mathrm{Tr}\, v_k^x A_k(\varepsilon) v_k^x A_k(\varepsilon + \hbar\omega).$$

PRL **113,** 087404 (2014) PHYSICAL REVIEW LETTERS week ending 22 AUGUST 2014

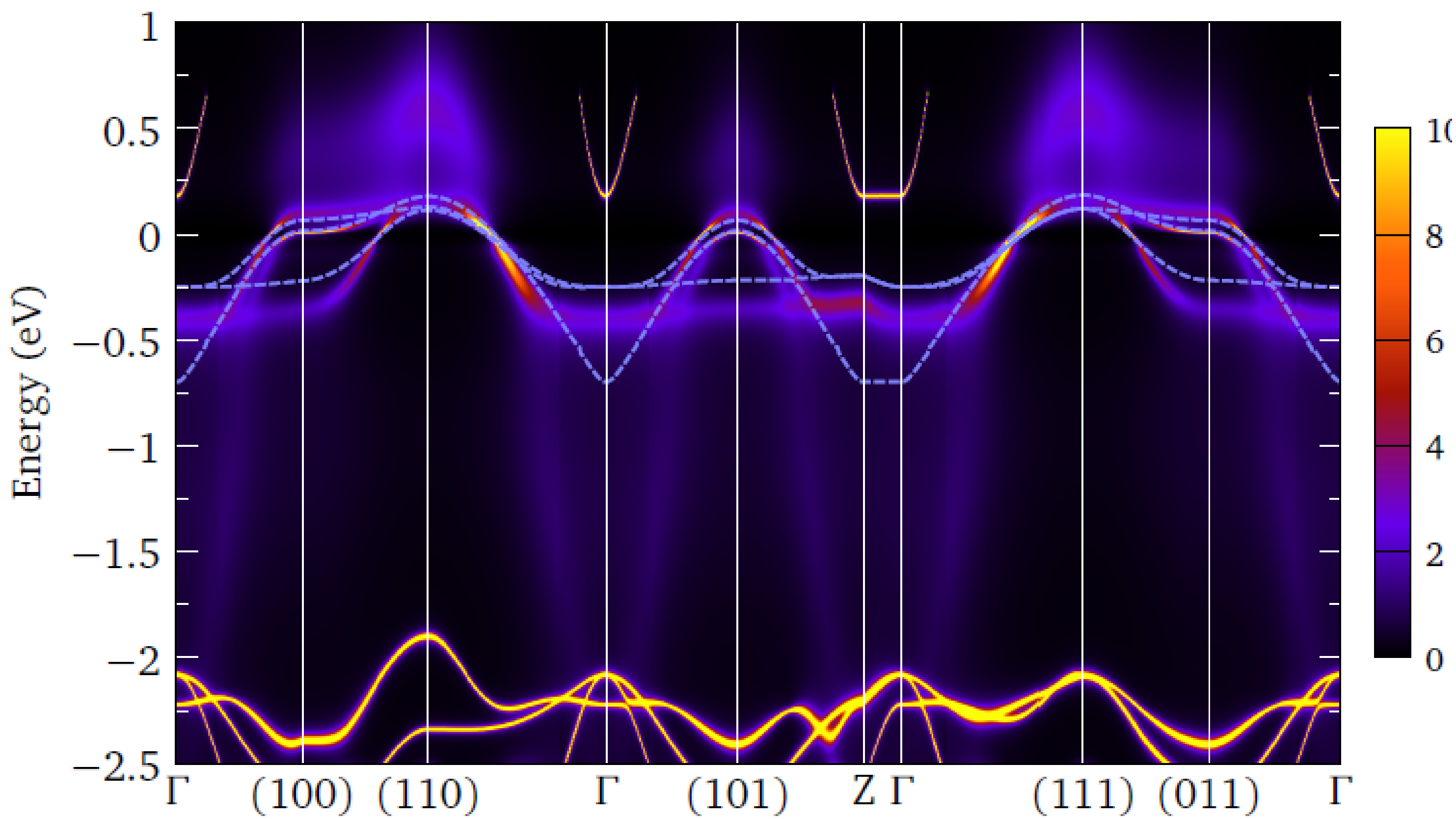
Optical Response of Sr_2RuO_4 Reveals Universal Fermi-Liquid Scaling and Quasiparticles Beyond Landau Theory

D. Stricker,[1] J. Mravlje,[2] C. Berthod,[1] R. Fittipaldi,[3] A. Vecchione,[3] A. Georges,[4,5,1] and D. van der Marel[1]

Spectral function

- Renormalized Landau QP below ~0.1eV
- Broad strongly dispersing « resilient » QPs
- Abrupt increase of dispersion at +0.1eV

Deng et al. PRL'13



D. Stricker et al., submitted

NRG study of LS coupling in impurity problem

$$
\begin{aligned}
H_{\text{imp}} = \; & \frac{1}{2}(U - 3J_{\text{H}})N_d(N_d - 1) - \\
& - 2J_{\text{H}}\mathbf{S}^2 - \frac{J_{\text{H}}}{2}\mathbf{L}^2 + \lambda \sum_m \mathbf{l}_m \cdot \mathbf{s}_m
\end{aligned}
$$

- ang. momentum **J=L+S ;** L=1, S=1 : 3rd Hund's rule→ J=2,0
- λ>0 → small J^2 (d^4 -ruthenates), λ< 0 → large J^2 (d^2 -molybdates)