Hund’s metals: overview, NRG insights, and the role of spin-orbit coupling

Jernej Mravlje

CdF, June 11, 2019

IJS

Outline

- Hund’s metals
  - Ruthenates before 2009
  - J steps in ; Basic picture: Janus
  - Hund’s impurity model : RG,NRG results
  - Characterizing the incoherent state
- Role of SOC

People

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L. Pourovskiy, EP Paris
V. Vildosola, Argentina
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T. Miyake, Japan
K. Haule, Rutgers
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A.J. Millis, Columbia

M. Kim, Rutgers
R. Triebl, G. Kraberger, Graz

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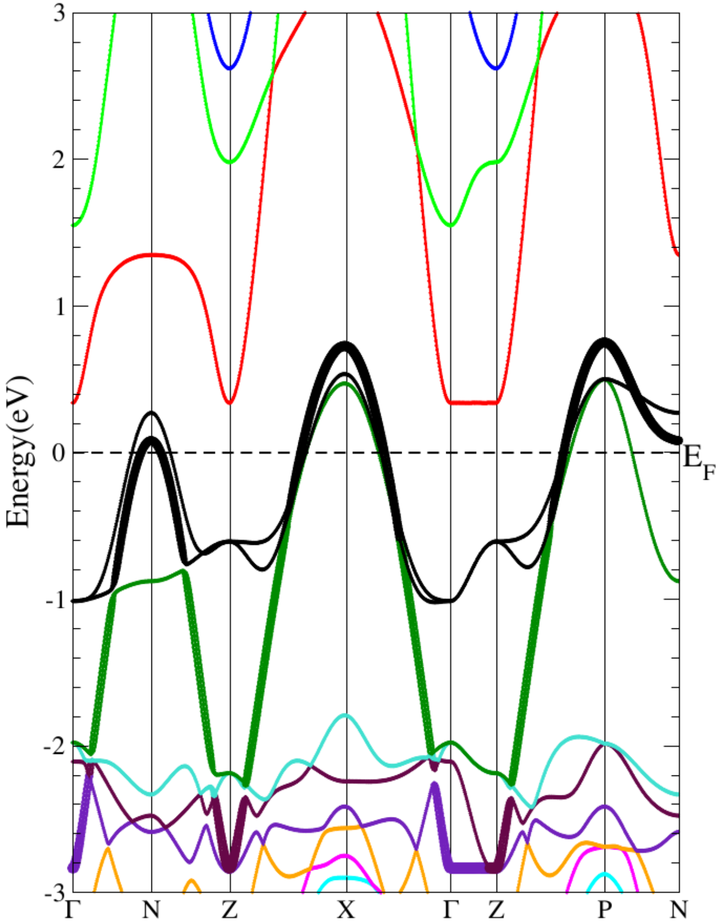
Ruthenates before 2009

Sr_2RuO_4: el. structure

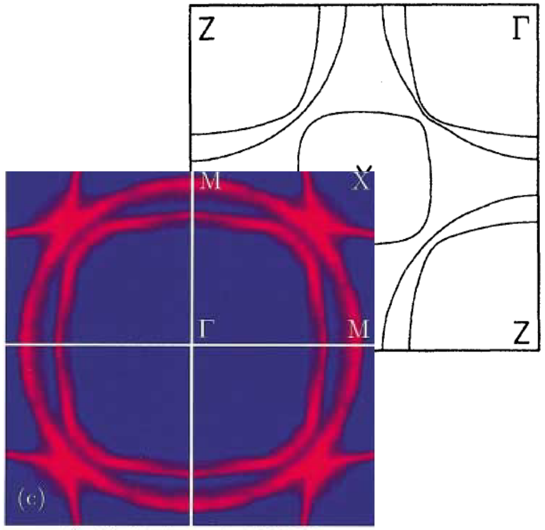


In ionic picture, 4 electrons on Ru; crystal field splitting → t_{2g} orbitals: xy and degenerate xz, yz

Wide xy band (ϒ sheet)

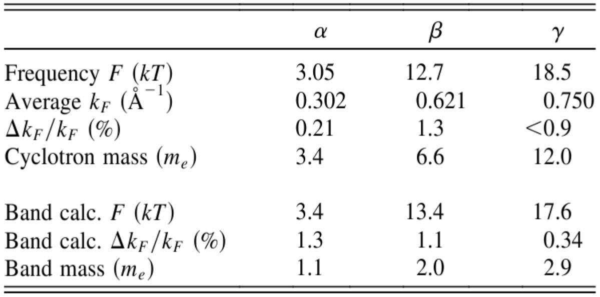
Fermi surfaces of DFT, quantum oscillations, ARPES **agree well**

Oguchi, PRB'95
Singh, PRB'95



Damascelli, Shen et al., PRL'00

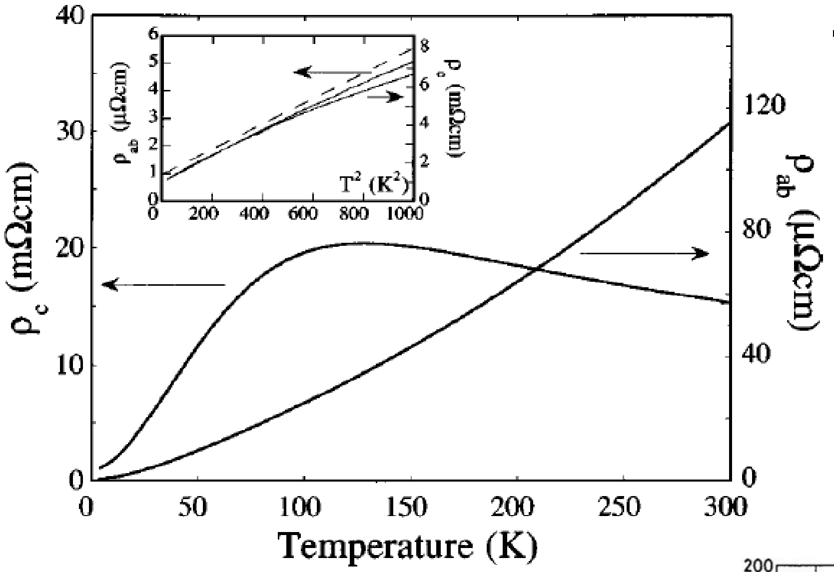
Mackenzie et al, PRL'96

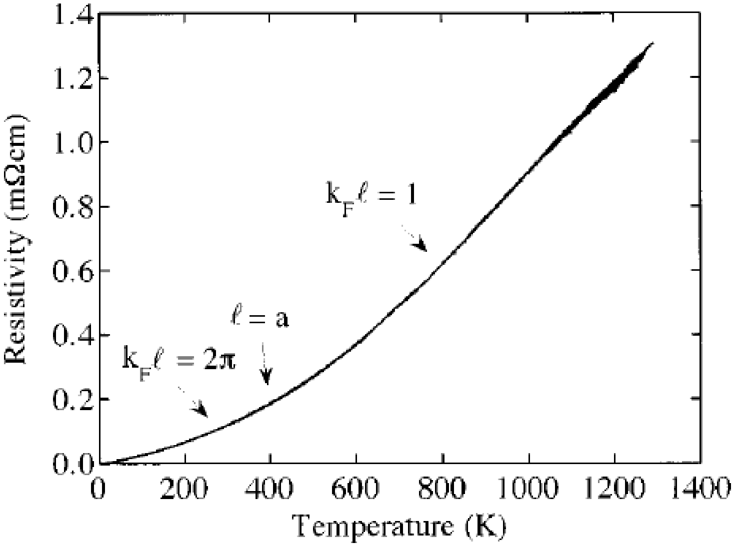


	α	β	γ
Frequency F (kT)	3.05	12.7	18.5
Average k_F (Å^{-1})	0.302	0.621	0.750
$\Delta k_F/k_F$ (%)	0.21	1.3	<0.9
Cyclotron mass (m_e)	3.4	6.6	12.0
Band calc. F (kT)	3.4	13.4	17.6
Band calc. $\Delta k_F/k_F$ (%)	1.3	1.1	0.34
Band mass (m_e)	1.1	2.0	2.9

Low coherence scale in ruthenates

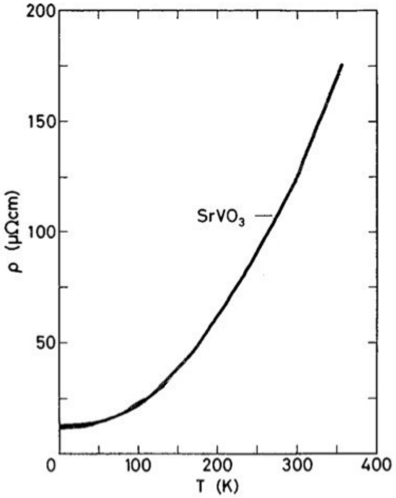
- U<W, yet strong correlations : large mass, coherence-incoherence crossover at low T* & .





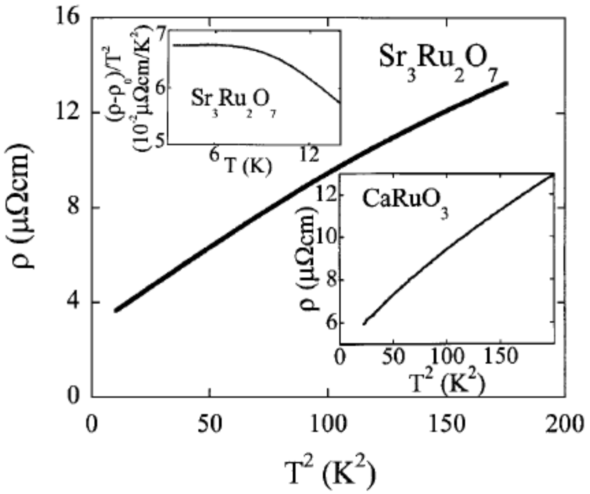
Hussey et al. PRB'98

Tyler et al. PRB'98



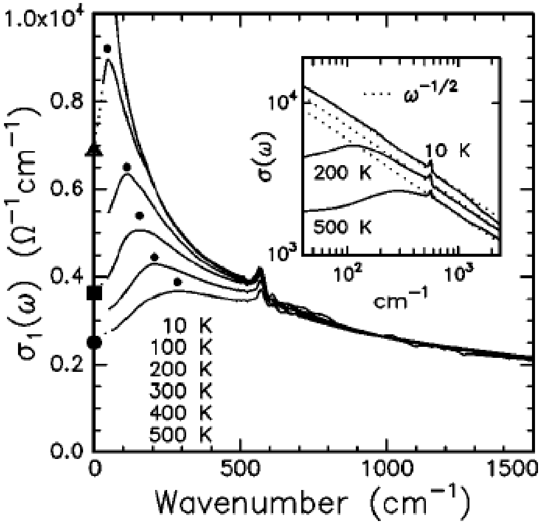
Vanadates : T^2 to a much larger T but smaller mass

Other ruthenates:also FL at a low T, and bad-metal/NFL behavior above



Capogna et al. PRL'02

SrRuO$_3$



Lee et al. PRB'02

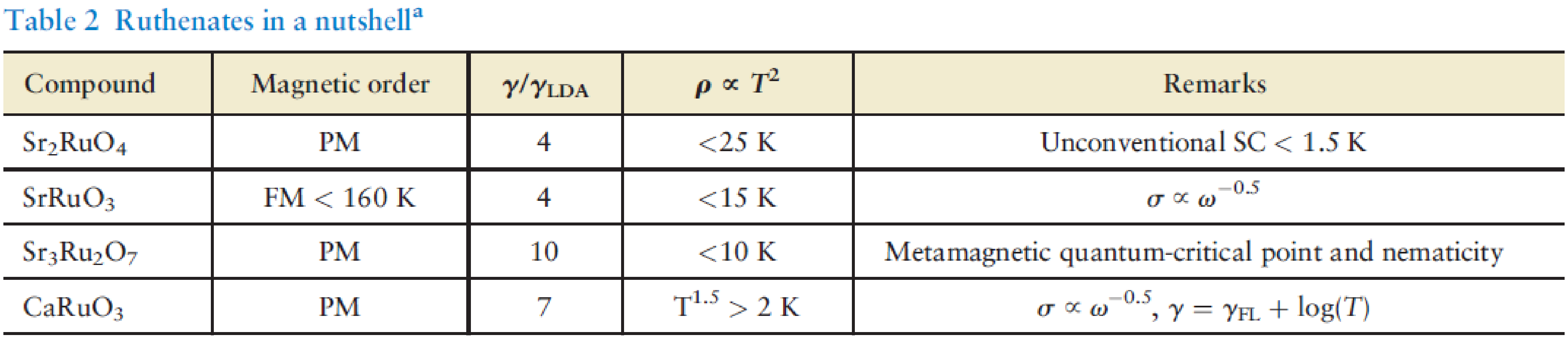


Table 2 Ruthenates in a nutshell[a]

Compound	Magnetic order	γ/γ_{LDA}	$\rho \propto T^2$	Remarks
Sr_2RuO_4	PM	4	<25 K	Unconventional SC < 1.5 K
$SrRuO_3$	FM < 160 K	4	<15 K	$\sigma \propto \omega^{-0.5}$
$Sr_3Ru_2O_7$	PM	10	<10 K	Metamagnetic quantum-critical point and nematicity
$CaRuO_3$	PM	7	$T^{1.5} > 2$ K	$\sigma \propto \omega^{-0.5}$, $\gamma = \gamma_{FL} + \log(T)$

Georges • de' Medici • Mravlje

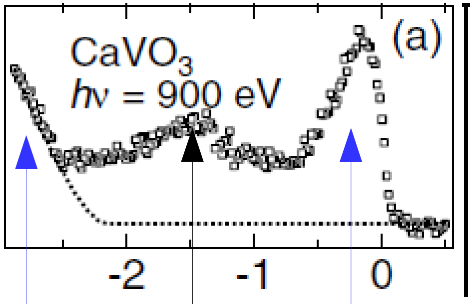
Annu. Rev. Condens. Matter Phys. 2013. 4:137–78

3d -> 4d

- Orbitals become extended
- Interactions diminish
- Bands become broad

Ruthenates : U~2eV
W~2-3eV

Vanadates : U ~ 4-5 eV
W ~ 2eV

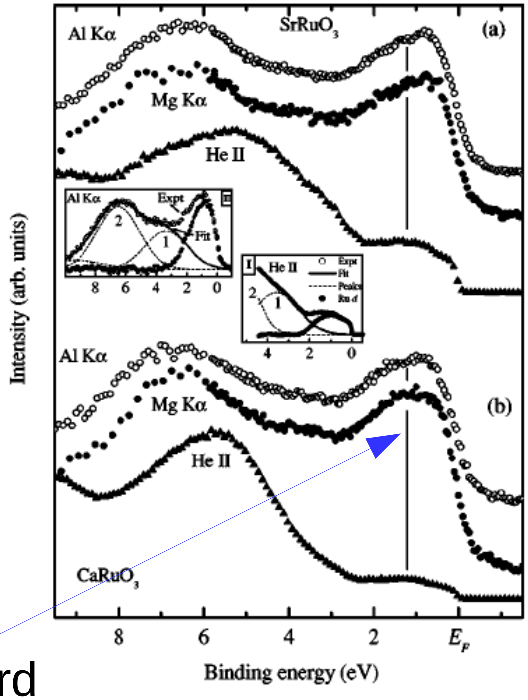


Sekiyama et al.
PRL'04

O

Hubbard
band

QP



“No” Hubbard
band (in
some cases)

PHYSICAL REVIEW B **71**, 161102(R) (2005)

Evidence against strong correlation in 4*d* transition-metal oxides CaRuO_3 and SrRuO_3

Kalobaran Maiti* and Ravi Shankar Singh

Although Sr_2RuO_4 is a fully confirmed Fermi liquid at low temperatures, its properties at temperatures of approximately 30 K and above are more anomalous, raising the question of what should set such a low “crossover” scale in a material with a relatively high Fermi temperature of greater than 1000 K [12]. The behavior of $Sr_3Ru_2O_7$ was

in thin films of $CaRuO_3$ [15]. The situation in $SrRuO_3$ is more interesting still. High frequency measurements at relatively elevated temperatures suggested an anomalous $\sqrt{\omega}$ frequency dependence, leading to the proposal of a non-Fermi liquid metallic state [16]. Observation of a T^2

L. Capogna,[1] A. P. Mackenzie,[1,2] R. S. Perry,[1] S. A. Grigera,[1,2] L. M. Galvin,[1] P. Raychaudhuri,[1] and A. J. Schofield[1]
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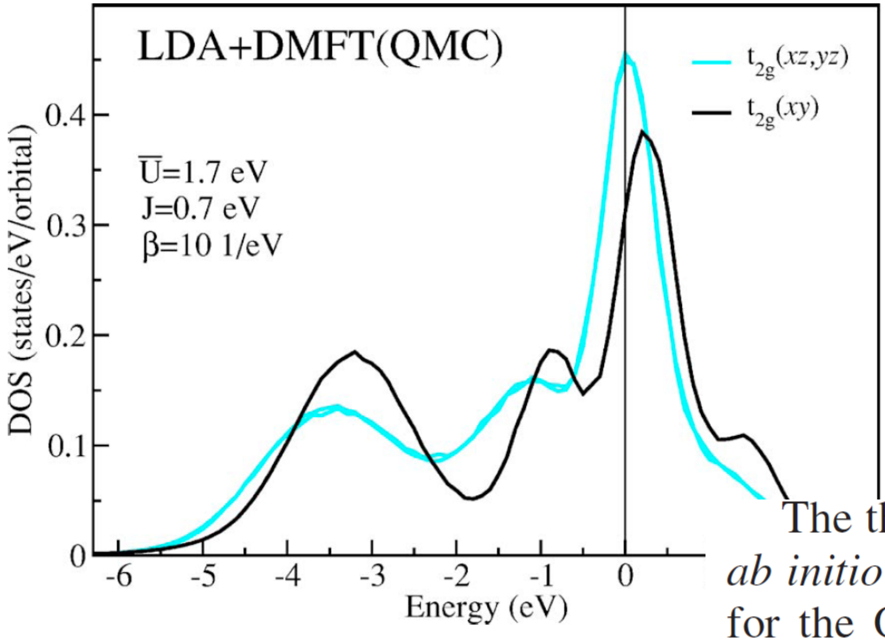
PHYSICAL REVIEW B **75**, 035122 (2007)



The three-orbital, projected Hamiltonian together with the *ab initio* Coulomb interaction parameters were used as input for the QMC simulation of the effective quantum impurity problem arising in the DMFT. The simulations were performed for an inverse temperature $\beta = 10\ \mathrm{eV}^{-1}$ using 40 imaginary time slices ($\Delta\tau = 0.25$). Although the temperature chosen for the QMC calculations appears to be rather high, it is really sufficiently low, because it is much smaller than (i) the lowest atomic excitations (see the Appendix) and (ii) the characteristic low-energy scale ~0.5 eV obtained from the

[15] Z. V. Pchelkina, I. A. Nekrasov, Th. Pruschke, A. Sekiyama, S. Suga, V. I. Anisimov, and D. Vollhardt, Phys. Rev. B **75**, 035122 (2007).

PHYSICAL REVIEW B **77**, 046101 (2008)

Comment on “Evidence for strong electronic correlations in the spectra of Sr_2RuO_4”

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(Received 26 March 2007; published 30 January 2008)

It is pointed out that O 2*p* states dominate the electronic structure of Sr_2RuO_4 in the ~ -3 eV region and can explain the observation of a peak in the density of states in photoemission experiments. This contradicts claims that a lower Hubbard band is needed at 3 eV binding energy.

To summarize, accurate LDA calculations show a prominent DOS peak in the around 3 eV binding energy. This corresponds well with a peak observed in photoemission experiments. Therefore, it may be concluded that the lower Hubbard band arising from Coulomb correlations, which was claimed to be essential to explain the observed spectra, may not be needed after all. While the possibility of important Coulomb correlations is not excluded, it seems that the evidence for strong electronic correlations in the spectra of Sr_2RuO_4, due to Hubbard interactions claimed in Ref. 15, is not yet established.

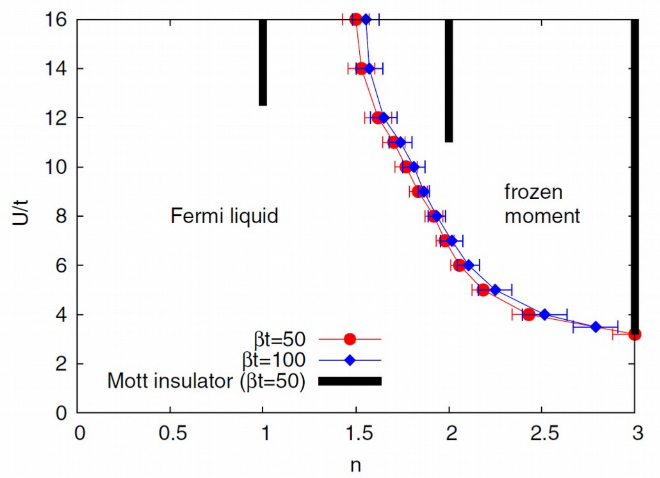
However, there are other correlation effects that can lead to mass renormalization, including interaction with itinerant electron spin fluctuations,[23,24] which as mentioned, may be important in Sr_2RuO_4, and which have been shown to be able to yield renormalizations of the observed magnitude using realistic parameters.[11,12] Besides, the physics of 4*d* ox-

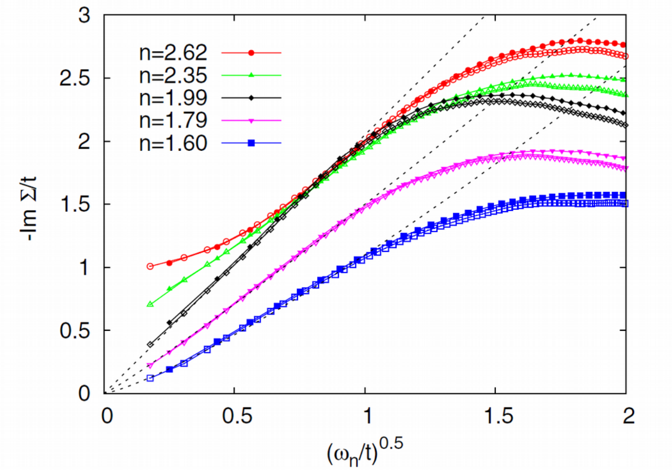
[15] Z. V. Pchelkina, I. A. Nekrasov, Th. Pruschke, A. Sekiyama, S. Suga, V. I. Anisimov, and D. Vollhardt, Phys. Rev. B **75**, 035122 (2007).

PRL **101,** 166405 (2008) PHYSICAL REVIEW LETTERS week ending 17 OCTOBER 2008

Spin Freezing Transition and Non-Fermi-Liquid Self-Energy in a Three-Orbital Model

Philipp Werner,[1] Emanuel Gull,[2] Matthias Troyer,[2] and Andrew J. Millis[1]





In conclusion, we have shown that in a model, relevant to transition metal oxides with partly filled *d*-shells, with several electrons in a threefold degenerate level, an apparent spin-freezing transition occurs. While it is possible that the effects could be due to a rapid decrease of the spin coherence scale to values below the range accessible to us, the square-root self-energy and T-linear spin-spin correlation function are strong evidence for an actual $T = 0$ transition. The frozen-moment phase results from a calcu-

PRL **100,** 226402 (2008) PHYSICAL REVIEW LETTERS week ending 6 JUNE 2008

Correlated Electronic Structure of $LaO_{1-x}F_xFeAs$

K. Haule, J. H. Shim, and G. Kotliar

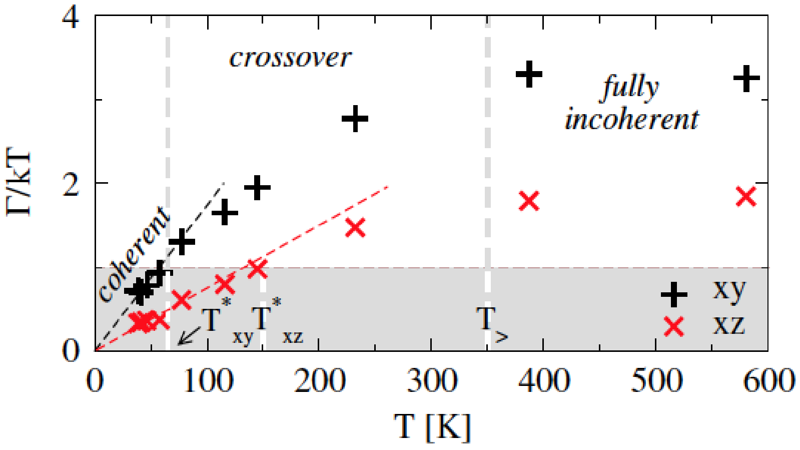
In conclusion, we studied the band structure of the newly discovered superconductor $LaO_{1-x}F_xFeAs$, and we predict the orbital and momentum resolved spectral function and optical conductivity of the compound. Density functional theory predicts that a set of Fe 3*d* bands are crossing the Fermi level with no clear splitting into the e_g and t_{2g} manifold. The Coulomb correlations among the six electrons in the set of five Fe-3*d* orbitals is strong enough to push the compound close to the metal insulator transition.

Different way of looking at ruthenates and pnictides was needed

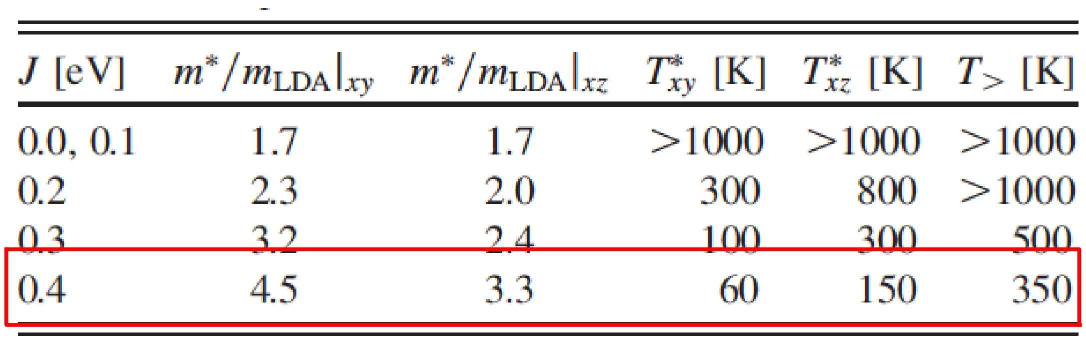
J steps in: Janus

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



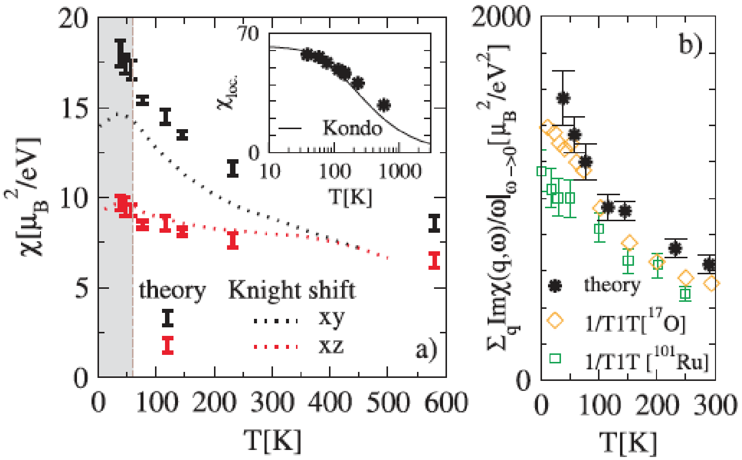
J [eV]	$m^*/m_{\mathrm{LDA}}\|_{xy}$	$m^*/m_{\mathrm{LDA}}\|_{xz}$	T^*_{xy} [K]	T^*_{xz} [K]	$T_>$ [K]
0.0, 0.1	1.7	1.7	>1000	>1000	>1000
0.2	2.3	2.0	300	800	>1000
0.3	3.2	2.4	100	300	500
0.4	4.5	3.3	60	150	350

Mravlje et al. PRL'11

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

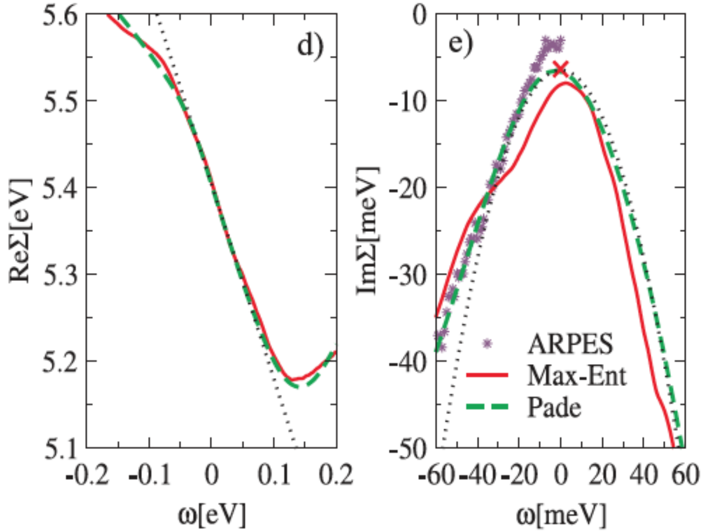
Low T*/E* in experimental observables

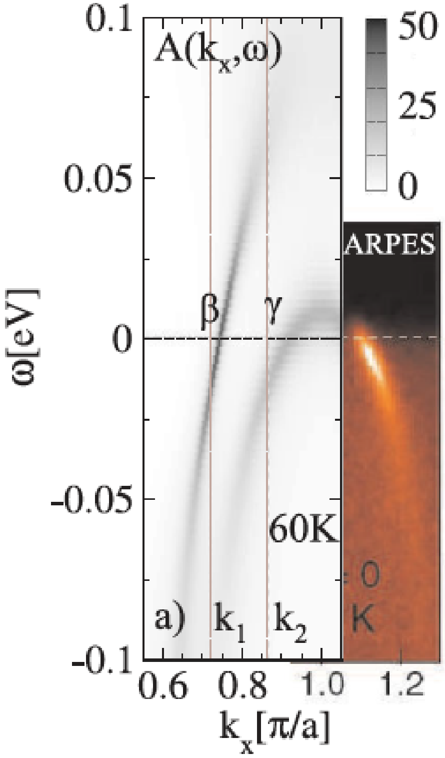
- Temperature dependences of NMR



Excellent agreement.
Only if J is properly included.

- Low frequency kink in Σ



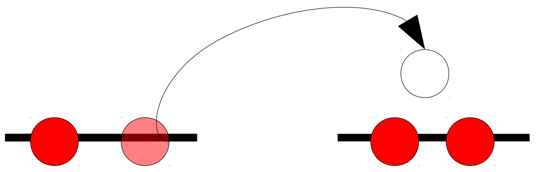


Mravlje et al. PRL'11

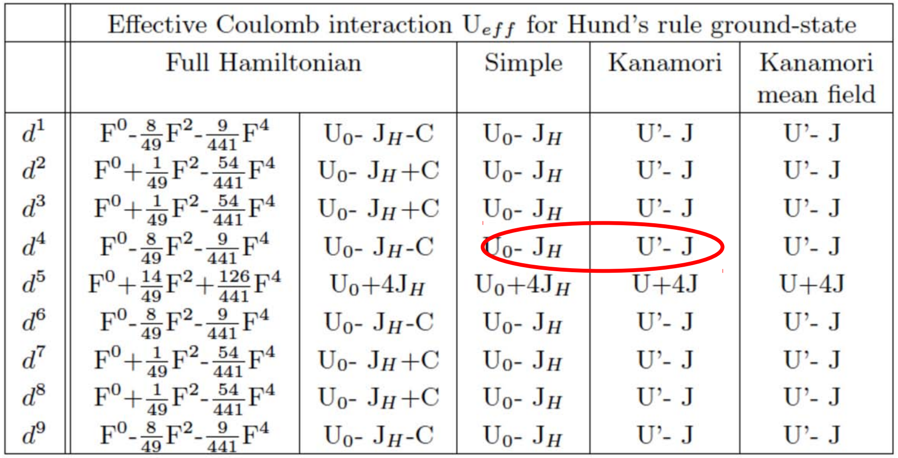
In a restaurant in Paris, Luca told me, J reduces effective repulsion

- Effective interaction

  U_{eff}=E(N+1)+E(N-1) – 2 E(N)



- U-3J away from half-filling (eff. U **diminished** by J)
- U+2J at half filling (eff. U **increased** by J)
- Slater all d-states Hamiltonian



	Effective Coulomb interaction U_{eff} for Hund's rule ground-state				
	Full Hamiltonian		Simple	Kanamori	Kanamori mean field
d^1	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	U_0-J_H-C	U_0-J_H	U'- J	U'- J
d^2	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	U_0-J_H+C	U_0-J_H	U'- J	U'- J
d^3	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	U_0-J_H+C	U_0-J_H	U'- J	U'- J
d^4	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	U_0-J_H-C	U_0-J_H	U'- J	U'- J
d^5	$F^0+\frac{14}{49}F^2+\frac{126}{441}F^4$	U_0+4J_H	U_0+4J_H	U+4J	U+4J
d^6	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	U_0-J_H-C	U_0-J_H	U'- J	U'- J
d^7	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	U_0-J_H+C	U_0-J_H	U'- J	U'- J
d^8	$F^0+\frac{1}{49}F^2-\frac{54}{441}F^4$	U_0-J_H+C	U_0-J_H	U'- J	U'- J
d^9	$F^0-\frac{8}{49}F^2-\frac{9}{441}F^4$	U_0-J_H-C	U_0-J_H	U'- J	U'- J

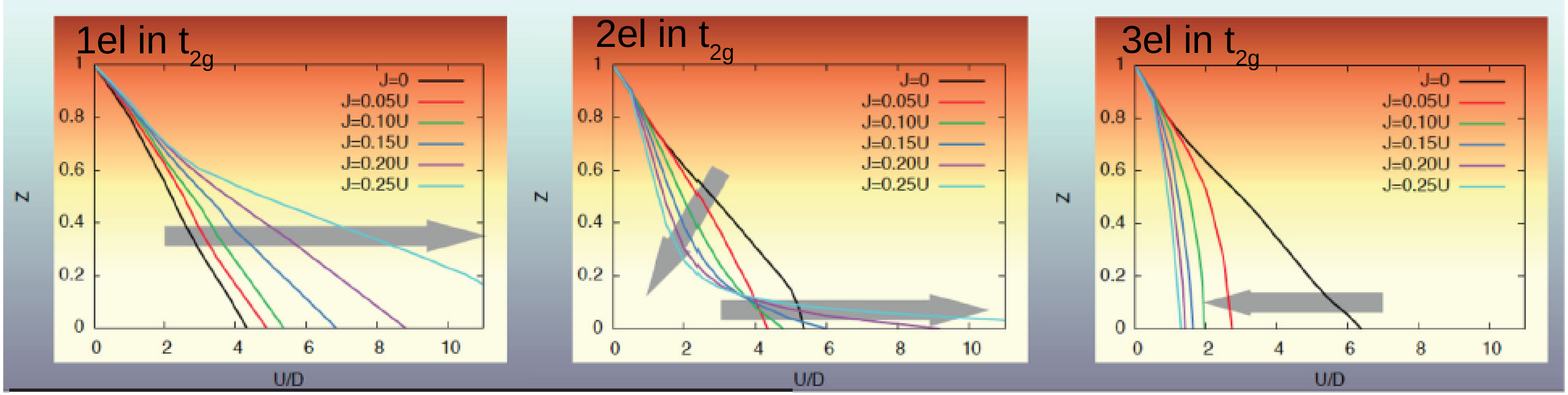
van der Marel,
Sawatzky
PRB'88
de'Medici
PRB'11

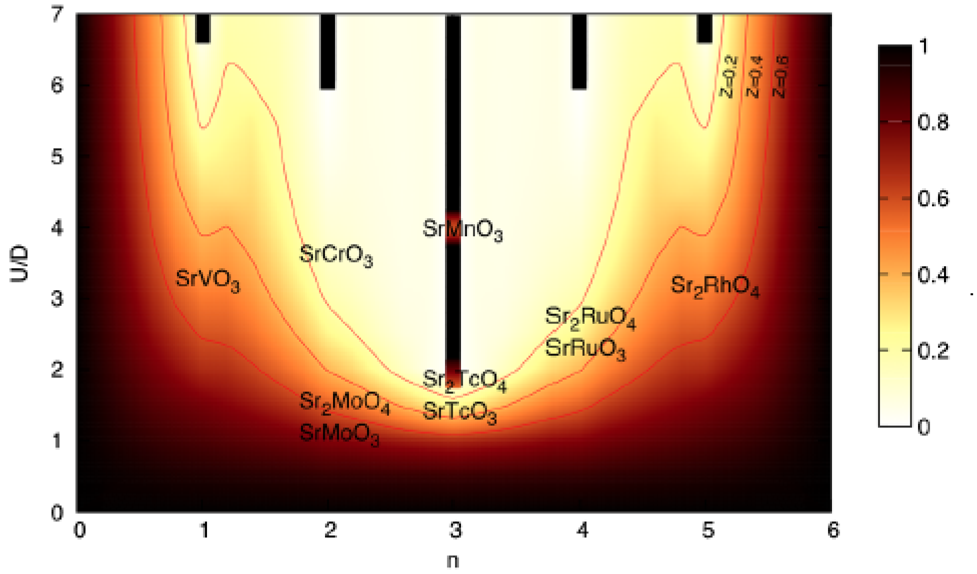
Two weeks later in Antoine’s office at Ecole Polytechnique

- Luca says: Ueff reduced → insulator further away
- Jernej says: coherence scale is reduced, thing becomes more correlated
- Antoine says: you guys might be both right!

DMFT : Hund's metals

- Quasiparticle weight Z



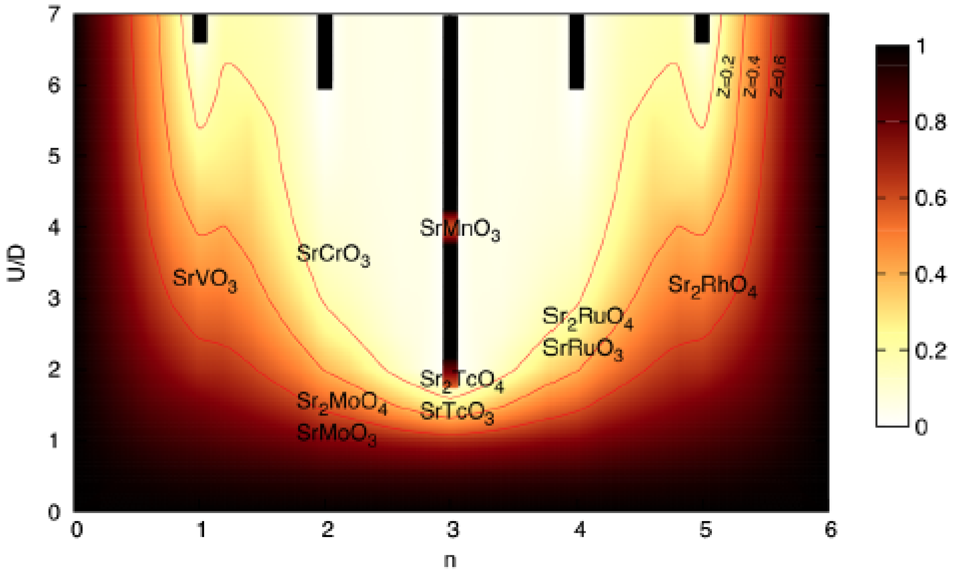


L. de'Medici, JM, A.Georges, PRL'11

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
Fanfarillo, Bascones PRB’15 ...

- Why such behavior?
- A fruitful line of thinking is to consider it as a doped half filled Mott ins.

de'Medici, Giovannetti, Capone, PRL'14
de'Medici, Hasan, Capone, Dai, PRL'09
Ishida, Liebsch, PRB'10
Misawa,Nakamura, Imada, PRL'12



- Here, I will be discussing insights from impurity models, instead

Insights from Hund’s impurity model investigation: RG,NRG results

Kanamori-Kondo model

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

- Schrieffer-Wolff

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

- Kondo model

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

For Nd=2 → S=1, L=1

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

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

Horvat, Zitko, Mravlje PRB’16

Yin, Haule, Kotliar PRB’12
Aron, Kotliar PRB’15
Stadler et al. PRL’15
Stadler et al.Annals of Phys.’19

Insights from impurity problem: Js small or even ferromagnetic

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

SU(2) angular momentum sym.

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

For Nd=2 → S=1, L=1

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

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

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

Horvat, Žitko, Mravlje PRB'16

SU(3) angular momentum sym.

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

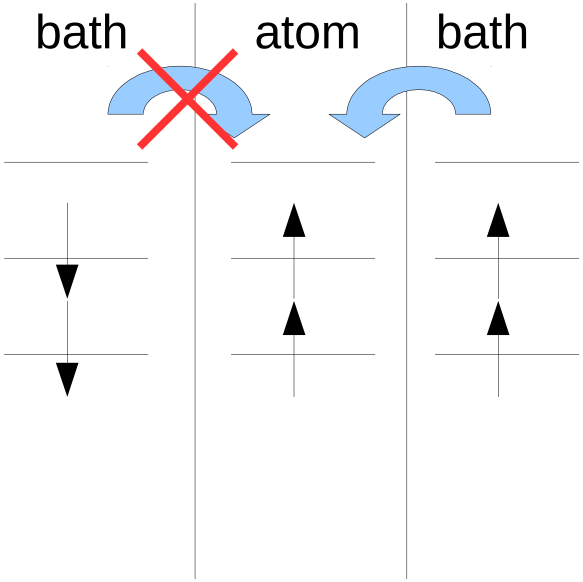
For Nd=2 → S=1, T fund.rep of SU(3)

$$\begin{aligned} H_K^{DN} = {} & J_p N_f + J_s \mathbf{S}\cdot\mathbf{s} + J_t \mathbf{T}\cdot\mathbf{t} + \\ & J_{ts}(\mathbf{T}\otimes\mathbf{S})\cdot(\mathbf{t}\otimes\mathbf{s}) \end{aligned}$$

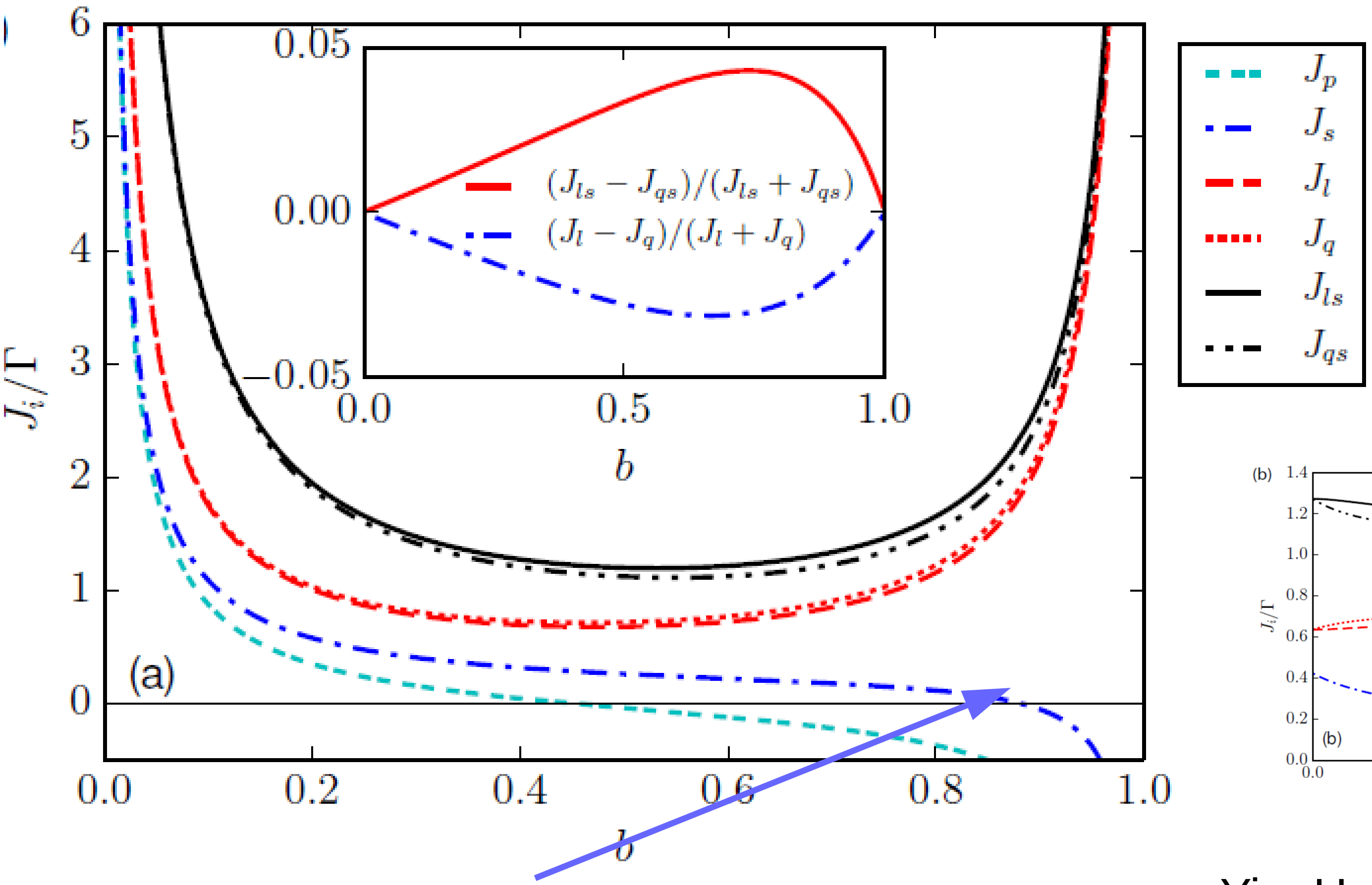
Yin, Haule, Kotliar PRB'12
Aron, Kotliar PRB'15
Stadler et al. PRL'15

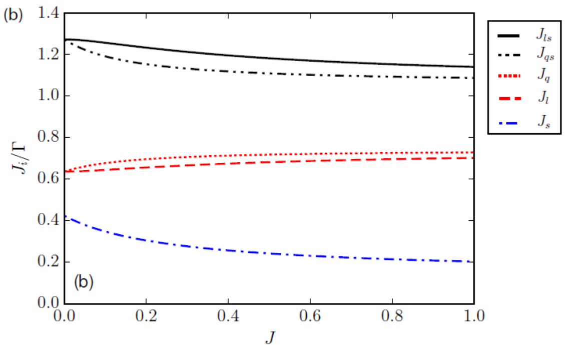
Js small or even ferromagnetic!
(ferromagnetic Kondo leads to unscreened moments)

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



Kondo coupling constants

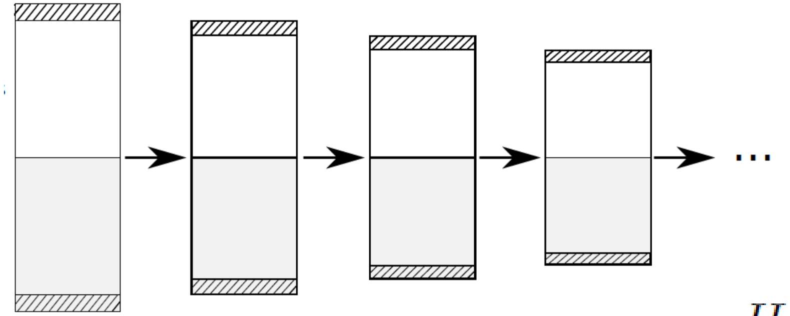




- Small or even ferromagnetic J_s
- Small splittings between quadrupole and orbital terms.
- Mixed terms are strongest.

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

RG

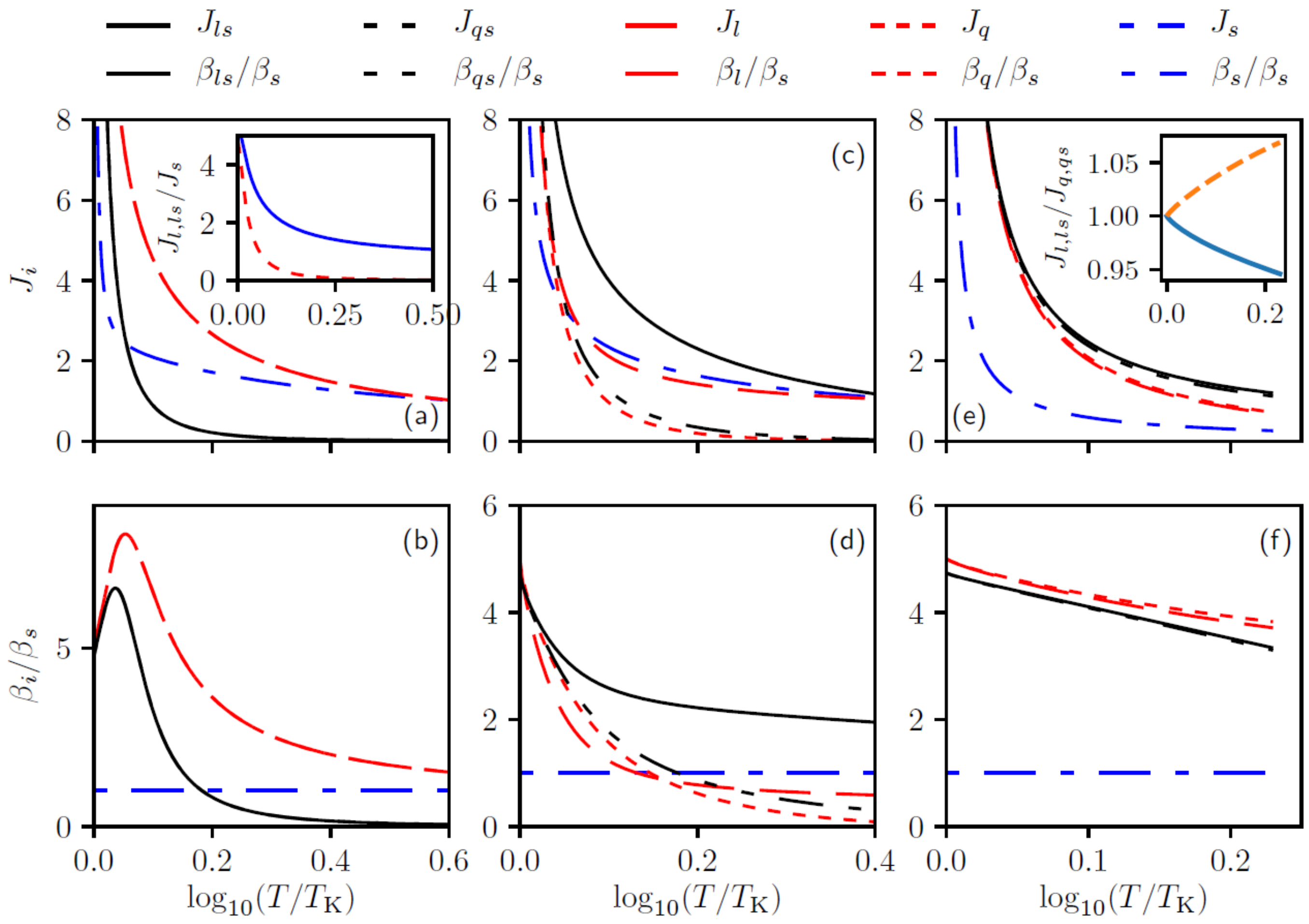


$$\beta_i = \mathrm{d}J_i/\mathrm{d}\ln(D)$$

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

$$\begin{aligned}
\beta_p &= 0, \\
\beta_s &= -\frac{1}{9}\left(3{J_{ls}}^2 + 5{J_{qs}}^2 + 9{J_s}^2\right), \\
\beta_l &= -\frac{1}{16}\left(4J_l^2 + 3{J_{ls}}^2 + 5\left(4{J_q}^2 + 3{J_{qs}}^2\right)\right), \\
\beta_q &= -\frac{3}{8}(4J_l J_q + 3J_{ls}J_{qs}), \\
\beta_{ls} &= -\frac{1}{6}(3J_l J_{ls} + 5J_{ls}J_{qs} + 12J_{ls}J_s + 15J_q J_{qs}), \\
\beta_{qs} &= -\frac{1}{12}(J_{qs}(18J_l + 7J_{qs} + 24J_s) + 3{J_{ls}}^2 + 18J_{ls}J_q).
\end{aligned}$$

- J_s,J_l influenced by mixed terms
- If $J_{ls}=J_{qs}=0$, faster running of J_l in SU(3) limit ($J_l=J_q$)
- Dynamic restoration of symmetry $J_l \rightarrow J_q$ when they differ initially.



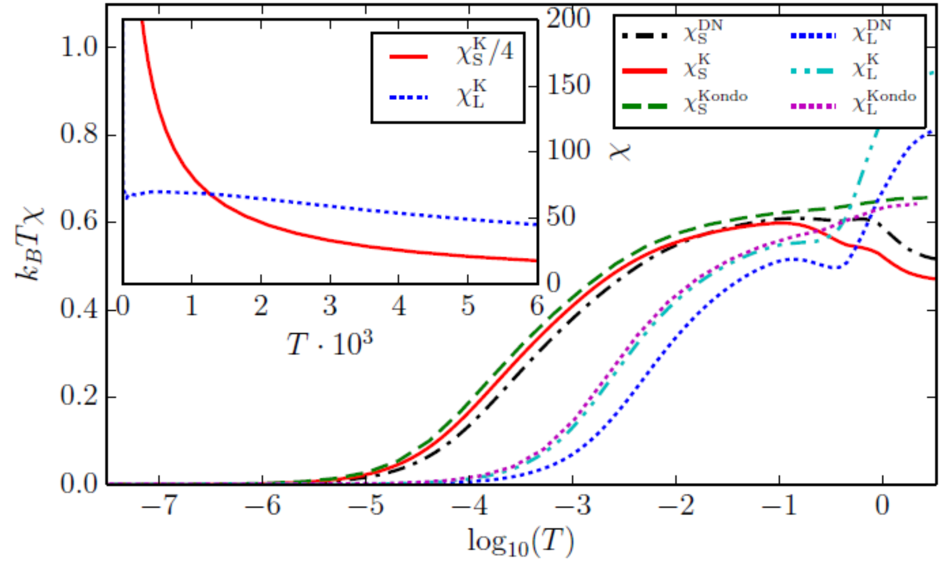
J_{ls}
J_{qs}
J_l
J_q
J_s
β_{ls}/β_s
β_{qs}/β_s
β_l/β_s
β_q/β_s
β_s/β_s
J_i
$J_{l,ls}/J_s$
0.00
0.25
0.50
(a)
(b)
(c)
(d)
(e)
(f)
$J_{l,ls}/J_{q,qs}$
1.05
1.00
0.95
0.0
0.2
β_i/β_s
$\log_{10}(T/T_{\mathrm{K}})$
$\log_{10}(T/T_{\mathrm{K}})$
$\log_{10}(T/T_{\mathrm{K}})$

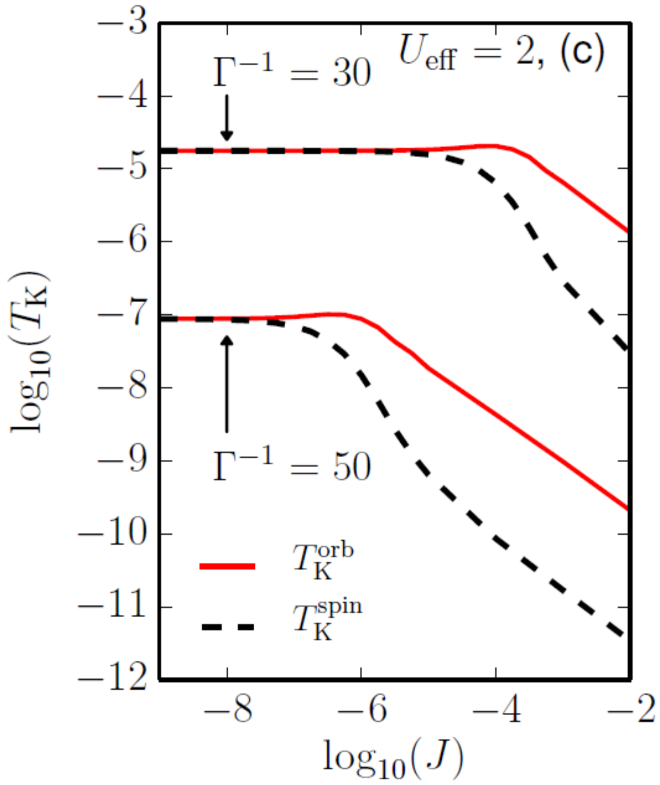
NRG results

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

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

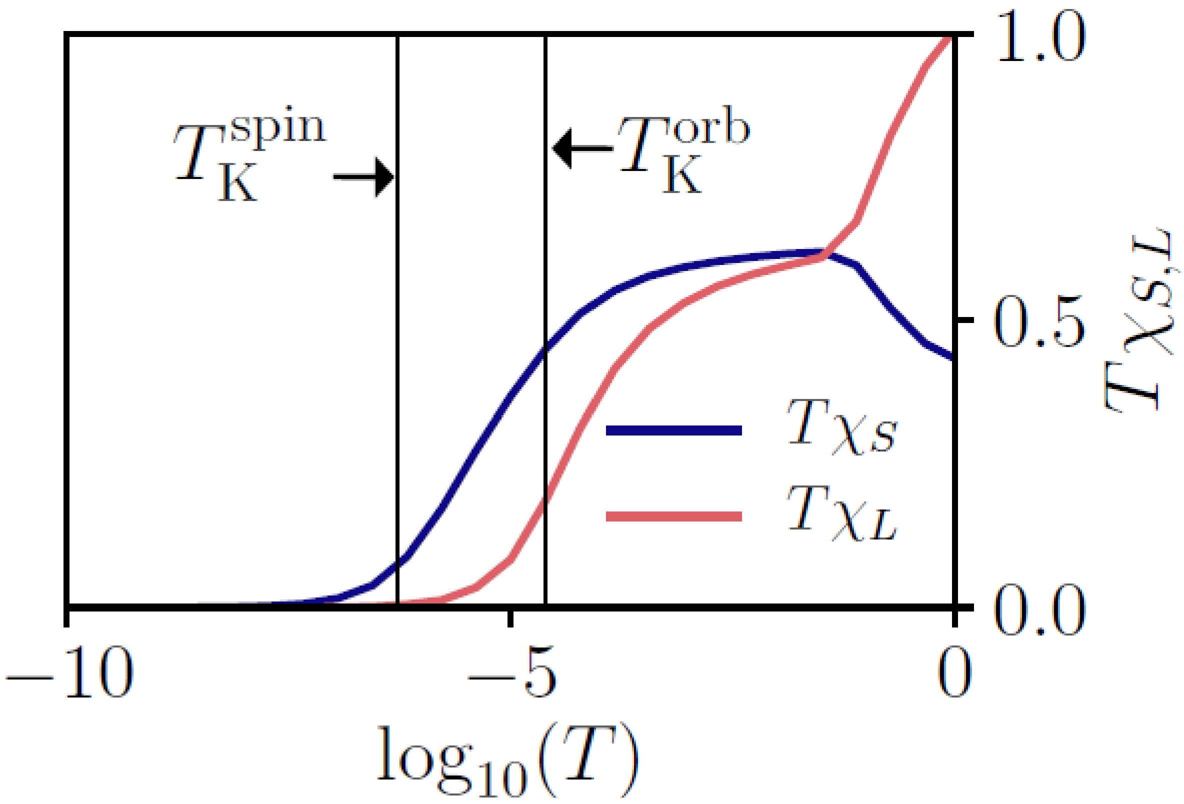
- Distinct scales for screening of S and L





- Suppression of (both) T_K with J
- Similar results for Kanamori, Dworin-Narath,Kondo-Kanamori,

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

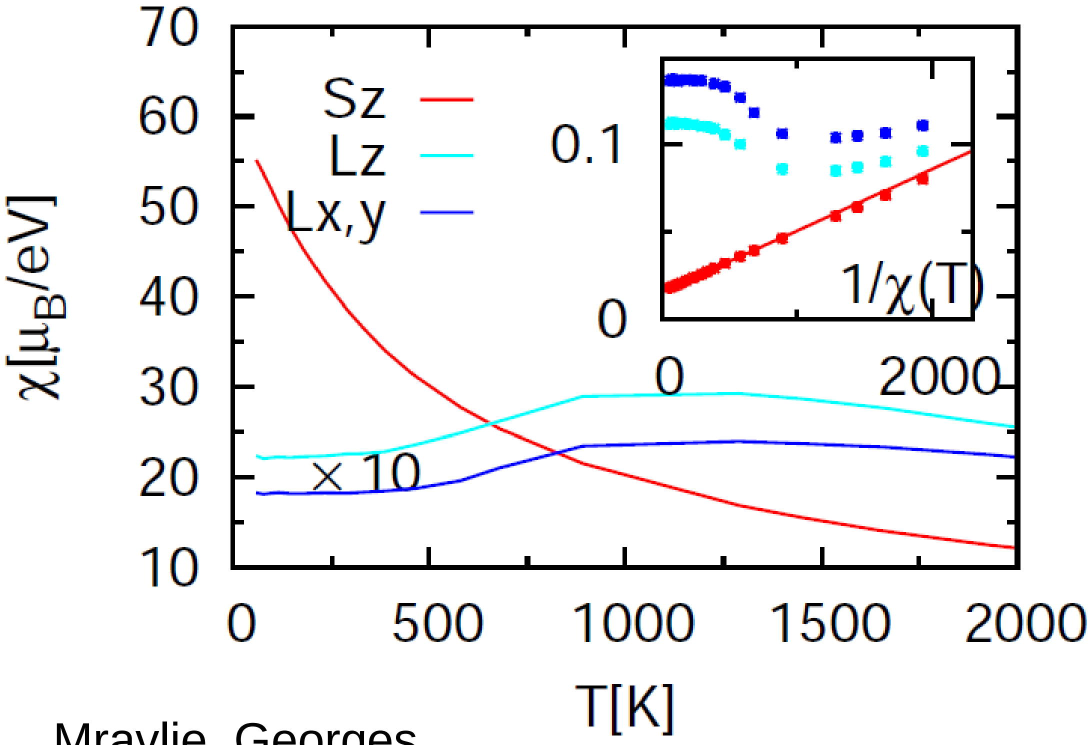


Horvat, Zitko, Mravlje PRB'16

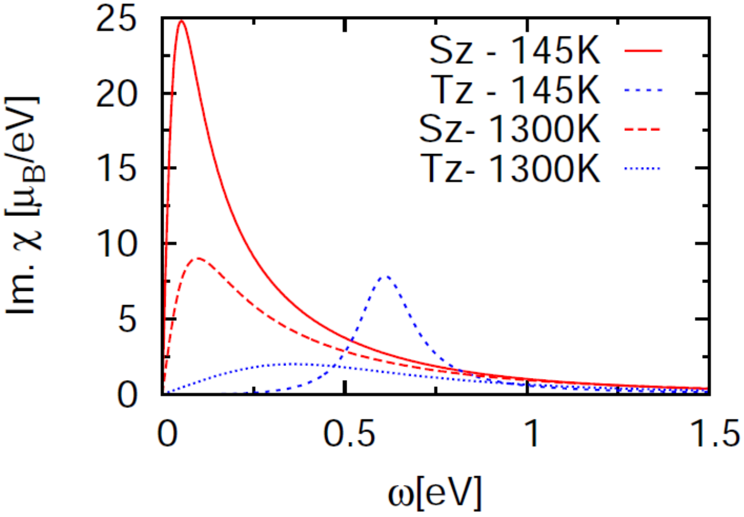
NRG for 3orbital Kanamori Hamiltonian

LDA+DMFT on Sr_2RuO_4

- This behavior found also in DMFT: Hund’s metal = quenched orbitals / slowly fluctuating spins

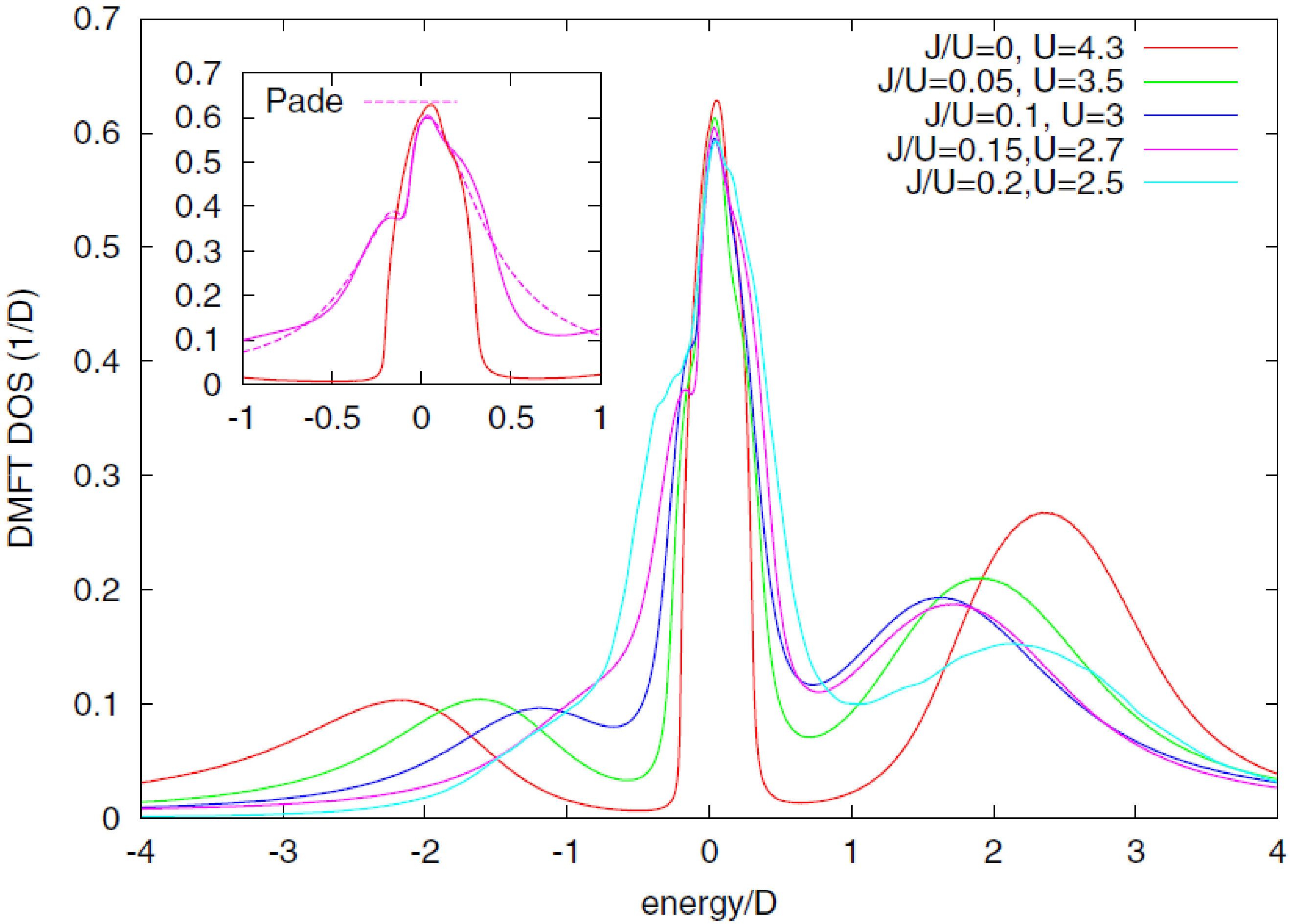


Mravlje, Georges, PRL’16



Consequence for photoemission

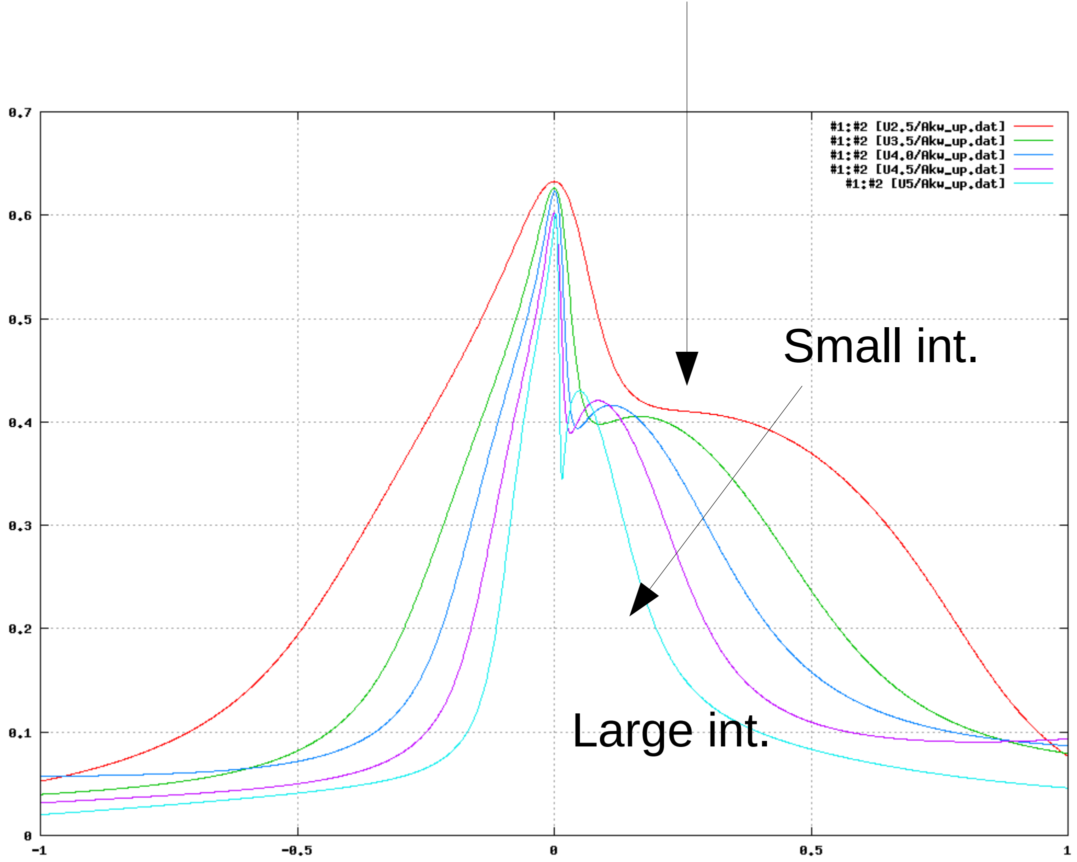
- Quasiparticle peak has structure:



Wadati, JM et al. PRB’14. Stadler et al.PRL’15, Ann. Phys.’19

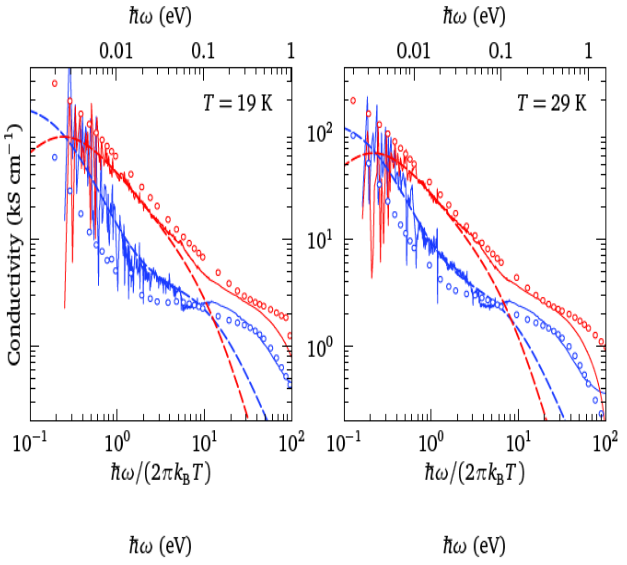
Quasiparticle part of the spectra;DMFT semicirc. J/U=1/6

Frequency of the feature given by T_K^{orb}



Small int.

Large int.

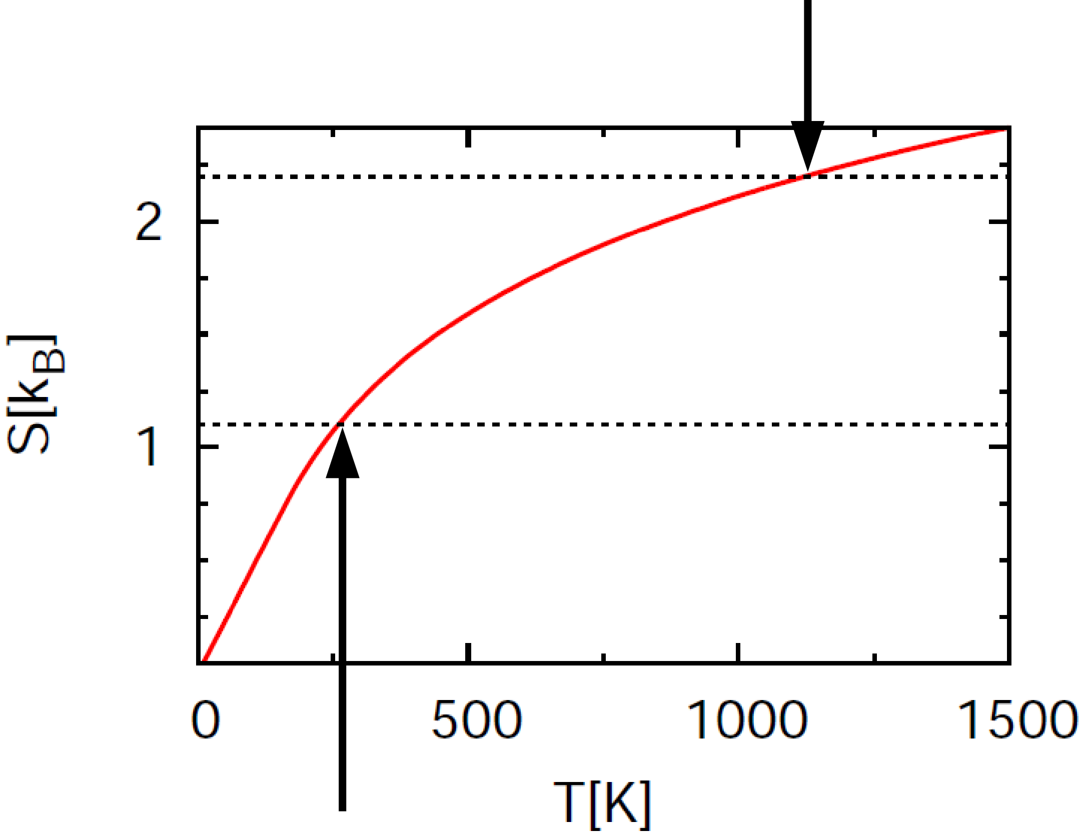


Observed in optical study of Sr_2RuO_4
Stricker,JM et al. PRL’14

Two-stage decoherence

- Entropy in Sr_2RuO_4 from LDA+DMFT

(ii) Liberated orbital moments



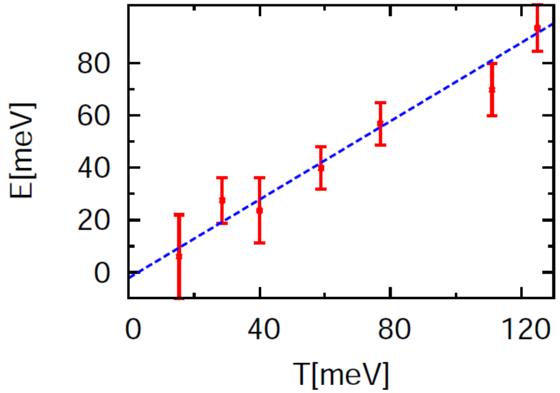
(i) Liberated spins

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

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

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

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



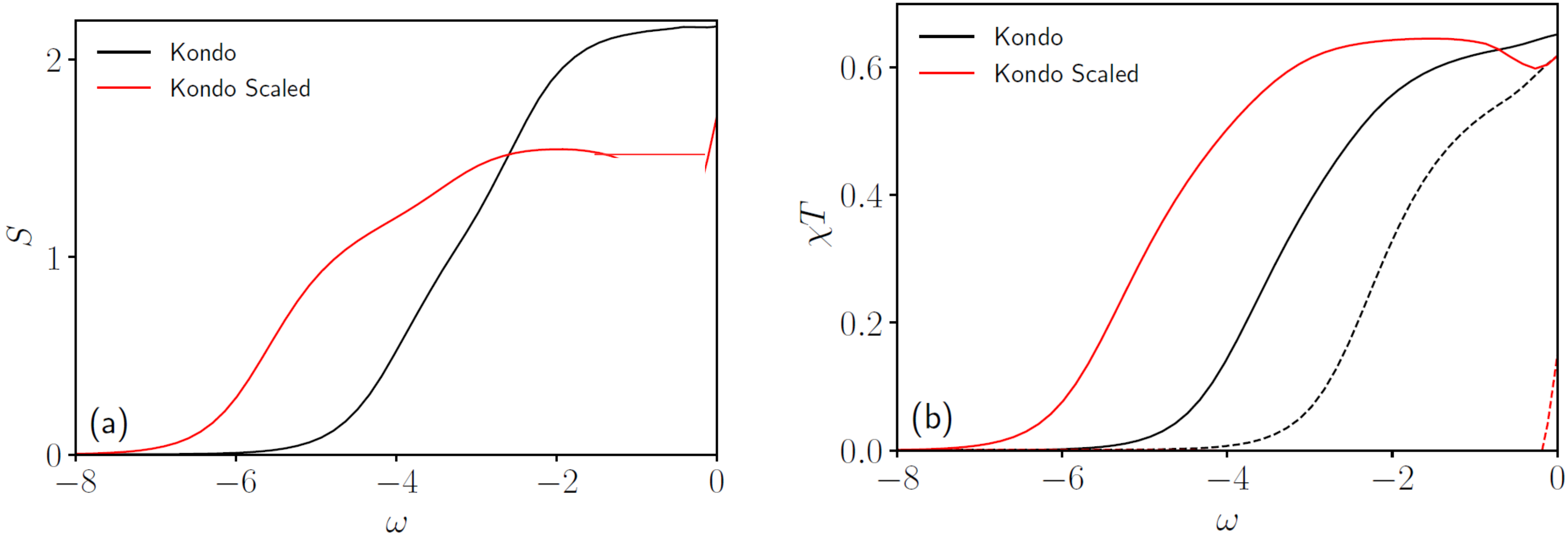
$$T_0 = c/\gamma \qquad c = 0.75k_B$$

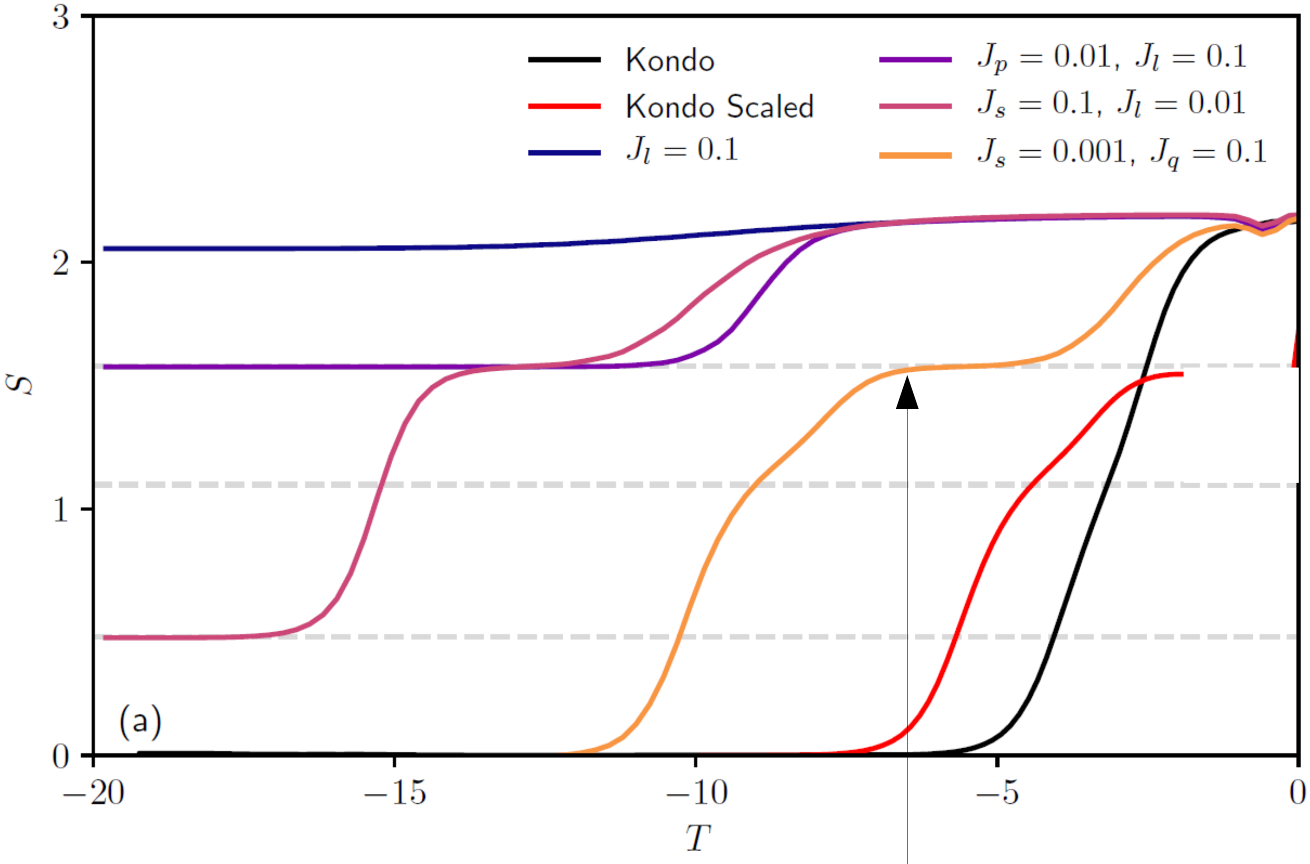
Mravlje, Georges,
PRL’16

But is this correct?

- Should one associate log 3 entropy with fluctuating spin state?That is, is the intermediate state a fluctuating spin and fully screened orbital?
- How to characterize this properly?

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

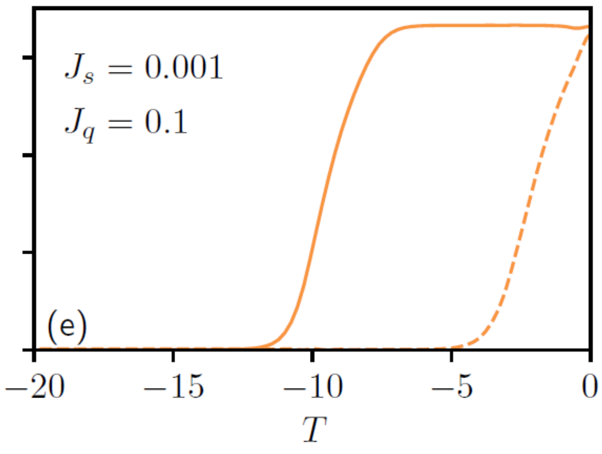




$$\log(3) + \frac{1}{2}\log\left(\frac{3+\sqrt{5}}{2}\right) \approx 1.58.$$

$$\log(3)$$

$$\frac{1}{2}\log\left(\frac{3+\sqrt{5}}{2}\right) \approx 1.58.$$



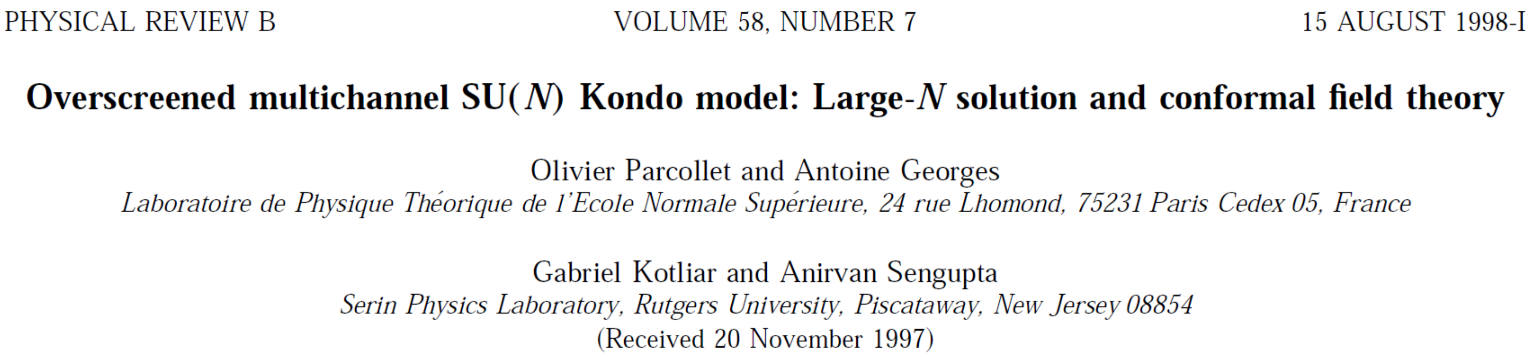
Intermediate T state exhibits a clear NFL plateau!

- J_s,J_{ts},J_p → 0 ; H= J_t T * t

$$H_K^{DN} = J_p N_f + J_s \mathbf{S}\cdot\mathbf{s} + J_t \mathbf{T}\cdot\mathbf{t} + J_{ts}(\mathbf{T}\otimes\mathbf{S})\cdot(\mathbf{t}\otimes\mathbf{s})$$

- SU(3) T (in fund. rep.) coupled to two (spin up,down) channels of cond els with SU(3)
- Intermediate NFL fixed point is two-channel overscreened SU(3): N=3,K=2

$$S_{\text{imp}} = \ln \prod_{n=1}^{Q} \frac{\sin[\pi(N+1-n)/(N+K)]}{\sin[\pi n/(N+K)]}.$$



PHYSICAL REVIEW B VOLUME 58, NUMBER 7 15 AUGUST 1998-I

Overscreened multichannel SU(N) Kondo model: Large-N solution and conformal field theory

Olivier Parcollet and Antoine Georges
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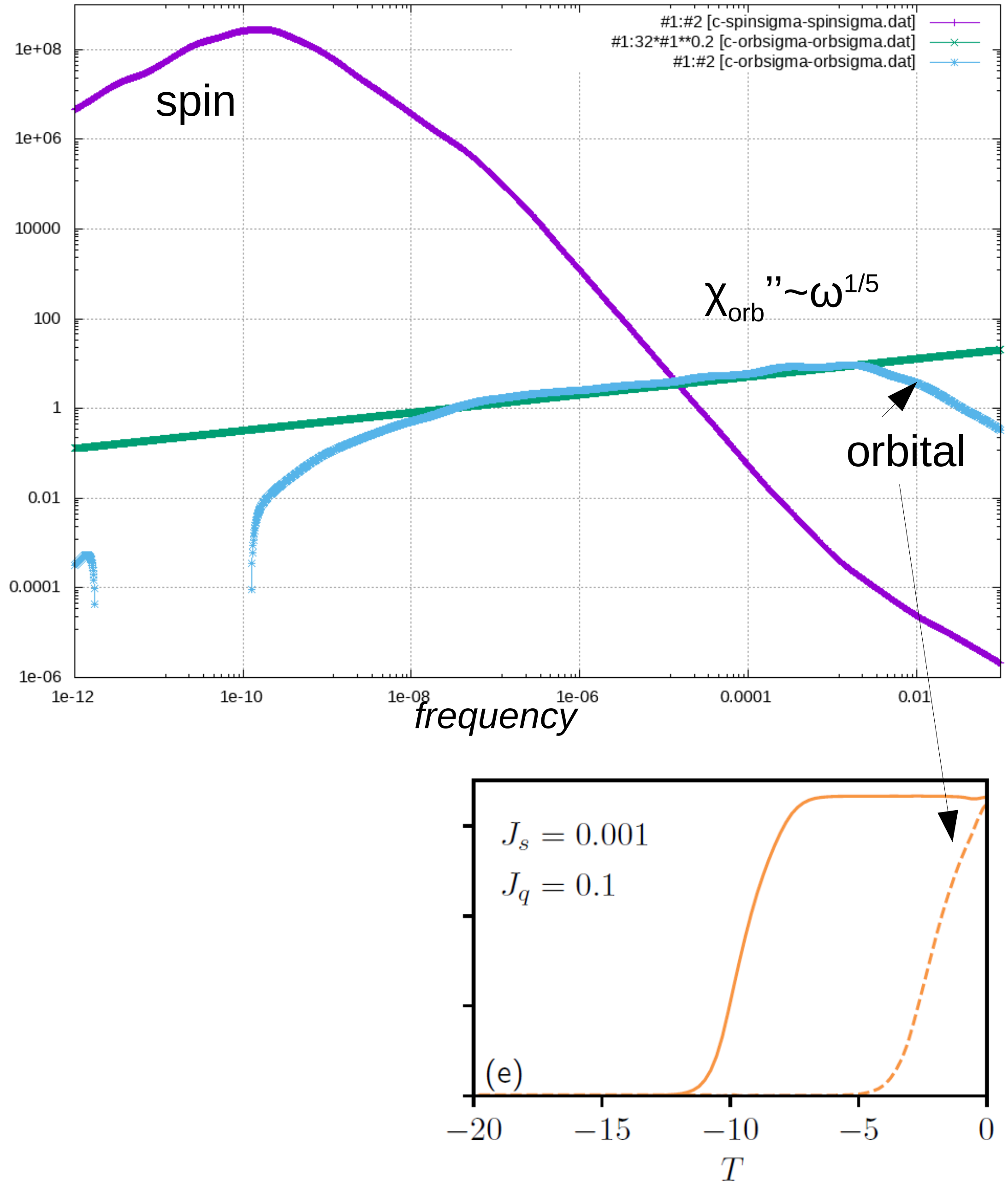
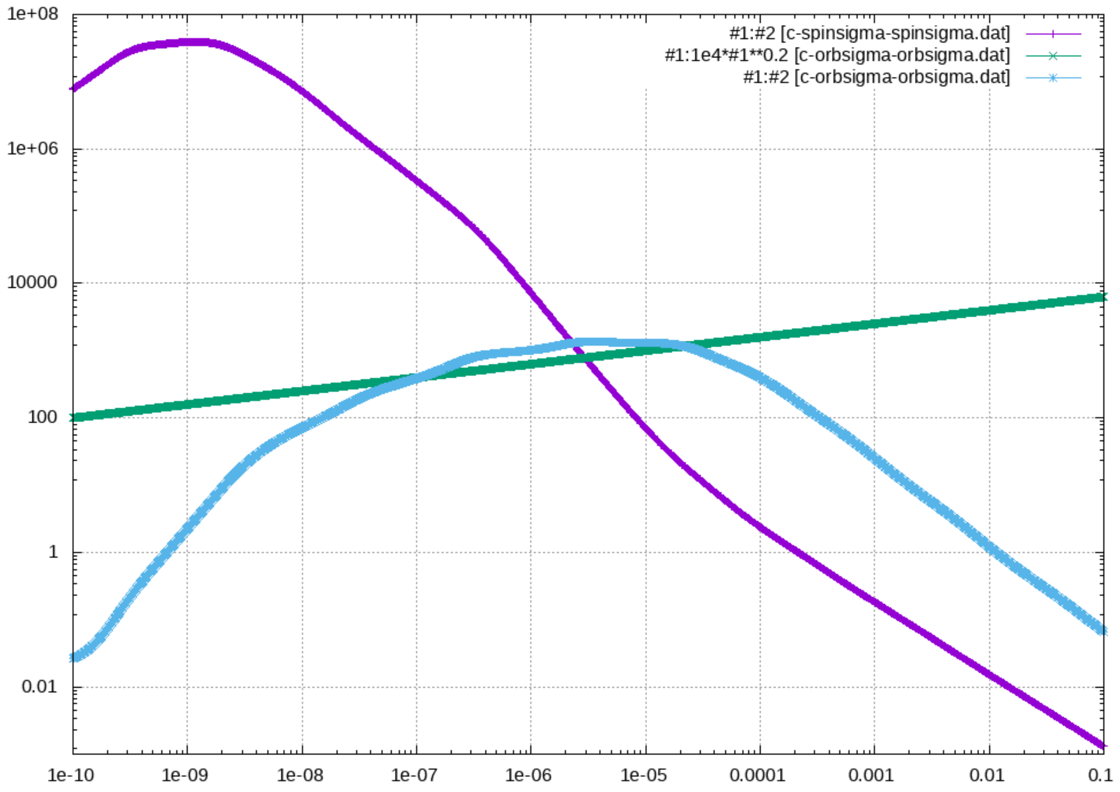
Gabriel Kotliar and Anirvan Sengupta
Serin Physics Laboratory, Rutgers University, Piscataway, New Jersey 08854
(Received 20 November 1997)

$\chi''(\omega)$


#1:#2 [c-spinsigma-spinsigma.dat]
#1:32*#1**0.2 [c-orbsigma-orbsigma.dat]
#1:#2 [c-orbsigma-orbsigma.dat]
spin
$\chi_{orb}''\sim\omega^{1/5}$
orbital
1e+08
1e+06
10000
100
1
0.01
0.0001
1e-06
1e-12
1e-10
1e-08
1e-06
0.0001
0.01
frequency
$J_s = 0.001$
$J_q = 0.1$
(e)
−20
−15
−10
−5
0
T

Is this seen for parameters for Anderson Hamiltonian, too?

- Marginaly – plateau cannot clearly be seen as the two scales are close.

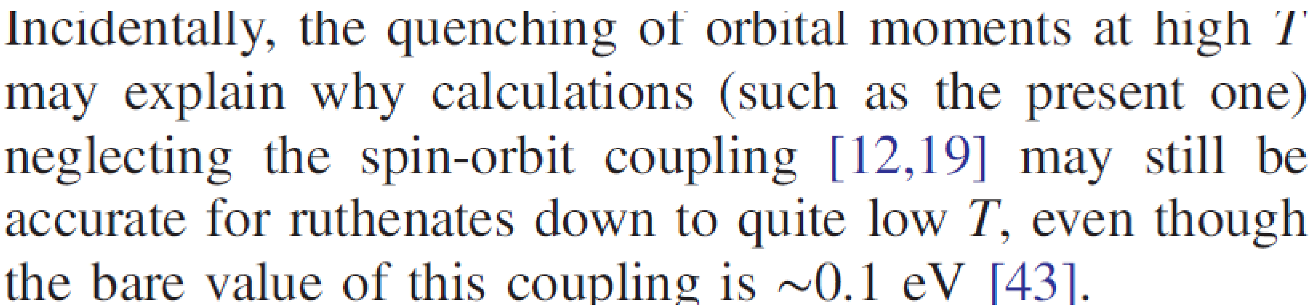


Summary this part

- Hund’s metals have a low coherence scale due to J.
- There is intermediate T state with fluctuating spins and “quenched” orbitals
- This state is influenced by NFL fixed point.
- Incoherent state of ruthenate in DMFT: two-channel overscreened SU(3)

SOC

- SOC in ruthenates nonnegligible 0.1eV, larger than T_{FL}. Its effects?

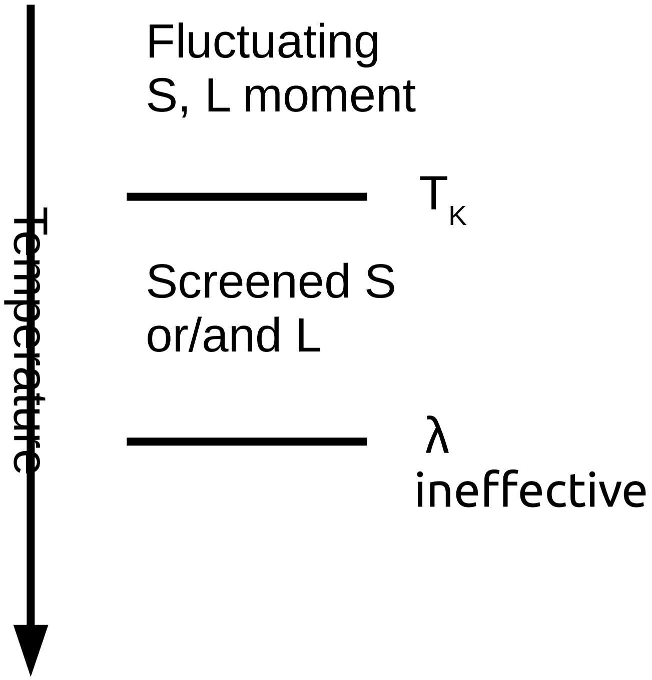


Incidentally, the quenching of orbital moments at high T may explain why calculations (such as the present one) neglecting the spin-orbit coupling [12,19] may still be accurate for ruthenates down to quite low T, even though the bare value of this coupling is $\sim$0.1 eV [43].

JM & Georges, PRL’16

RG picture on relevance of λ

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



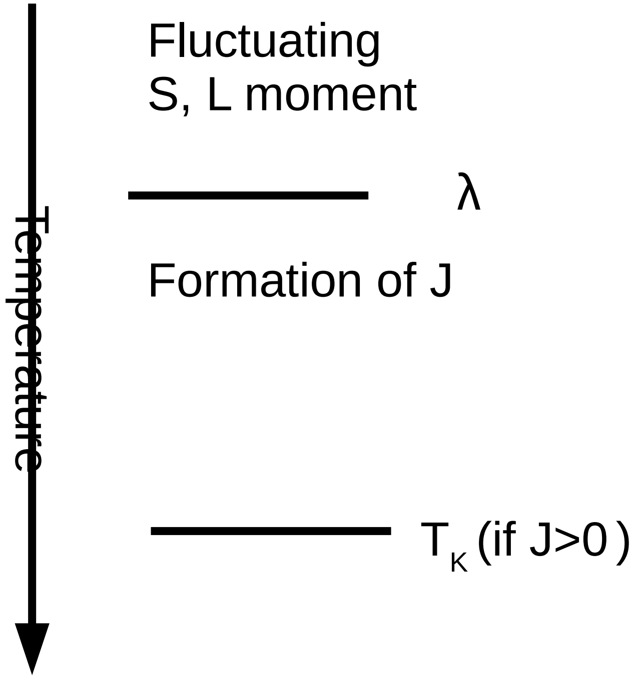
Temperature

Fluctuating
S, L moment

T_K

Screened S
or/and L

λ
ineffective



Temperature

Fluctuating
S, L moment

λ

Formation of J

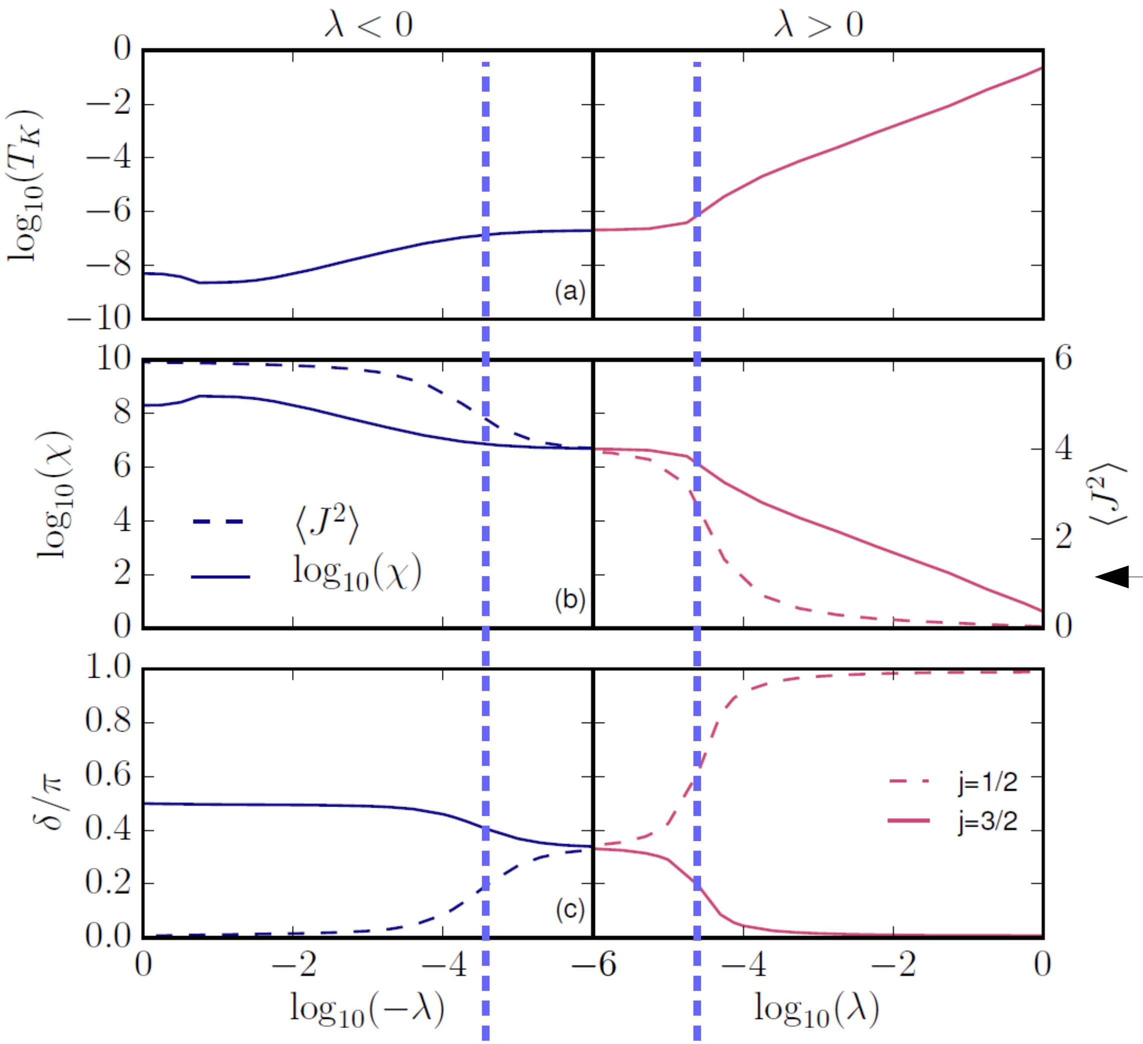
T_K (if $J>0$)

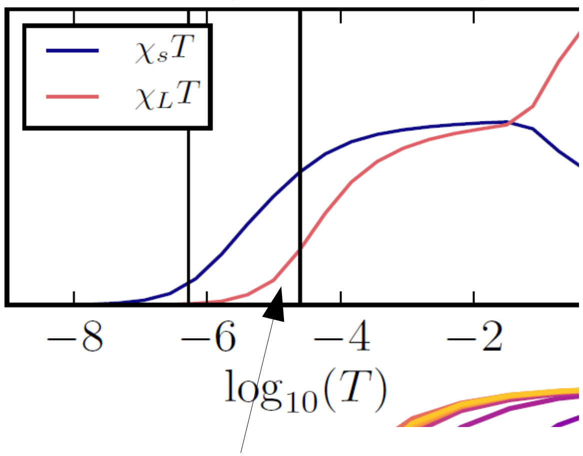
($T_K \rightarrow T_k^{orb}$, for Hund’s metals, but more generally, first scale at which either spin/orbit moment is screened)

Impurity model results

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

-d^4: ruthenates





T_K^{orb}

SOC needs to exceed T_K^{orb}!

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

SOC J=2
metal

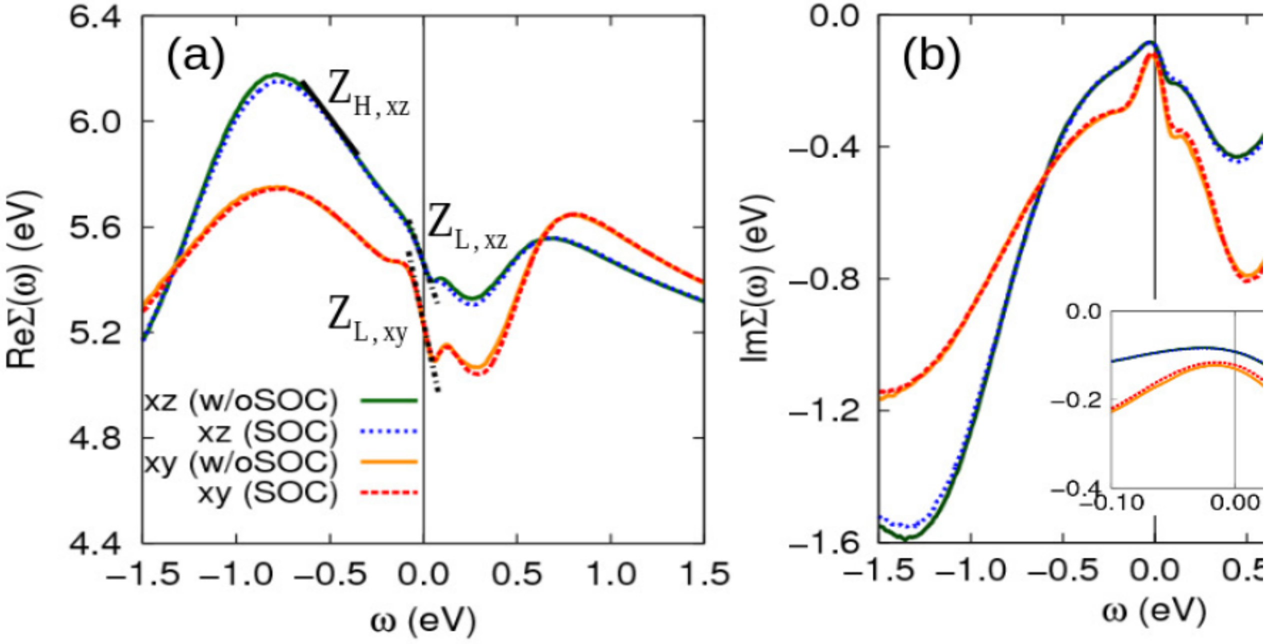
Hund's
metal

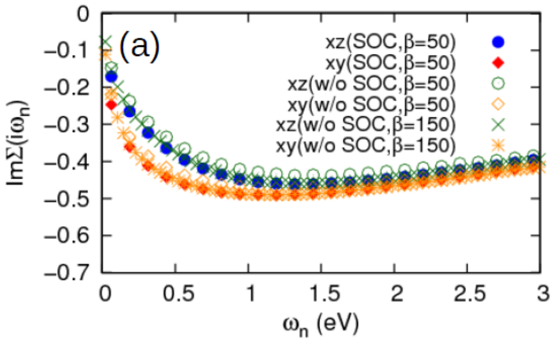
van Vleck J=0
insulator

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

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

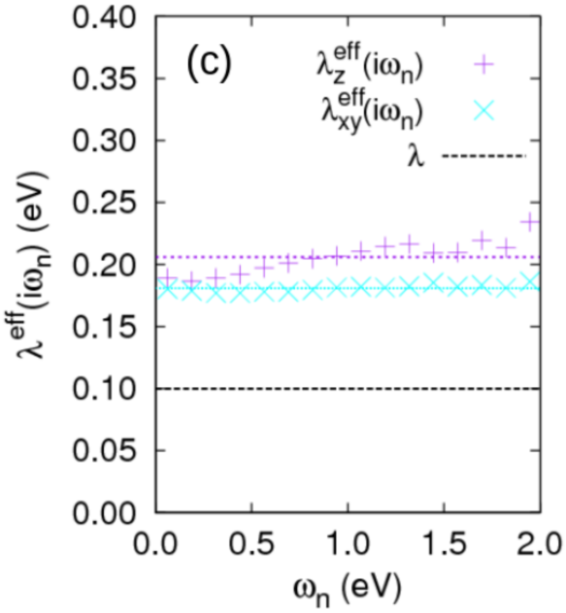
Returning to Sr_2RuO_4 within DMFT-self energies with SOC very similar to the ones without



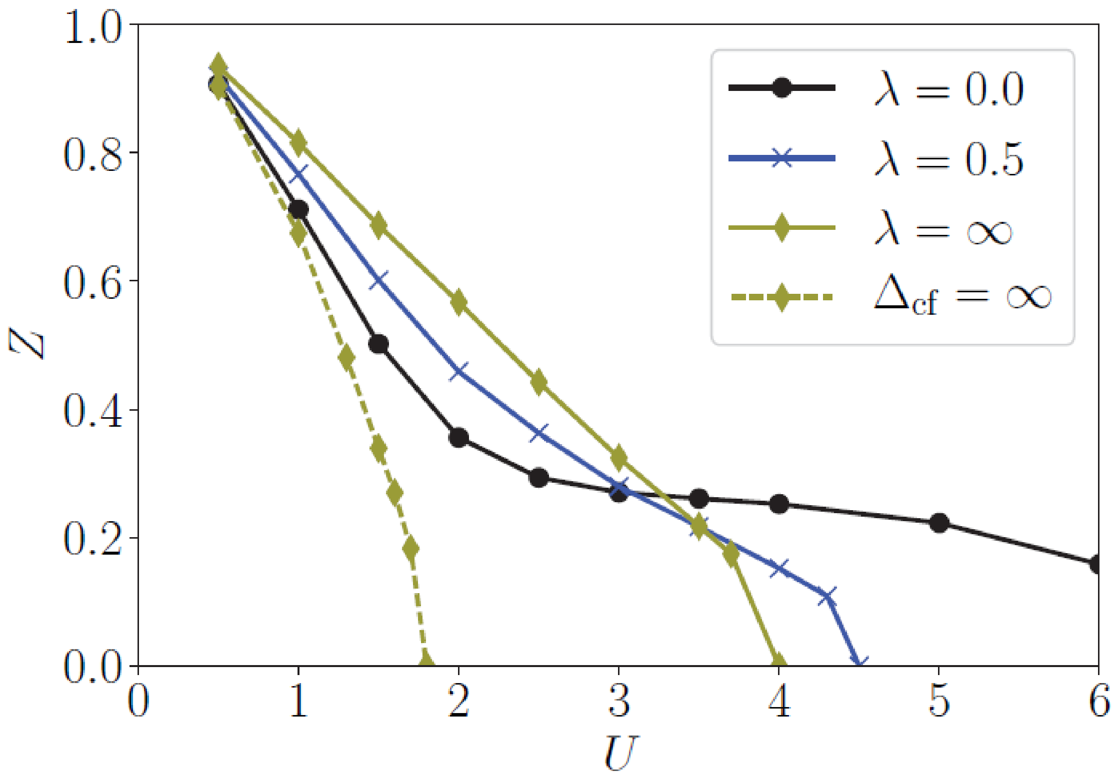


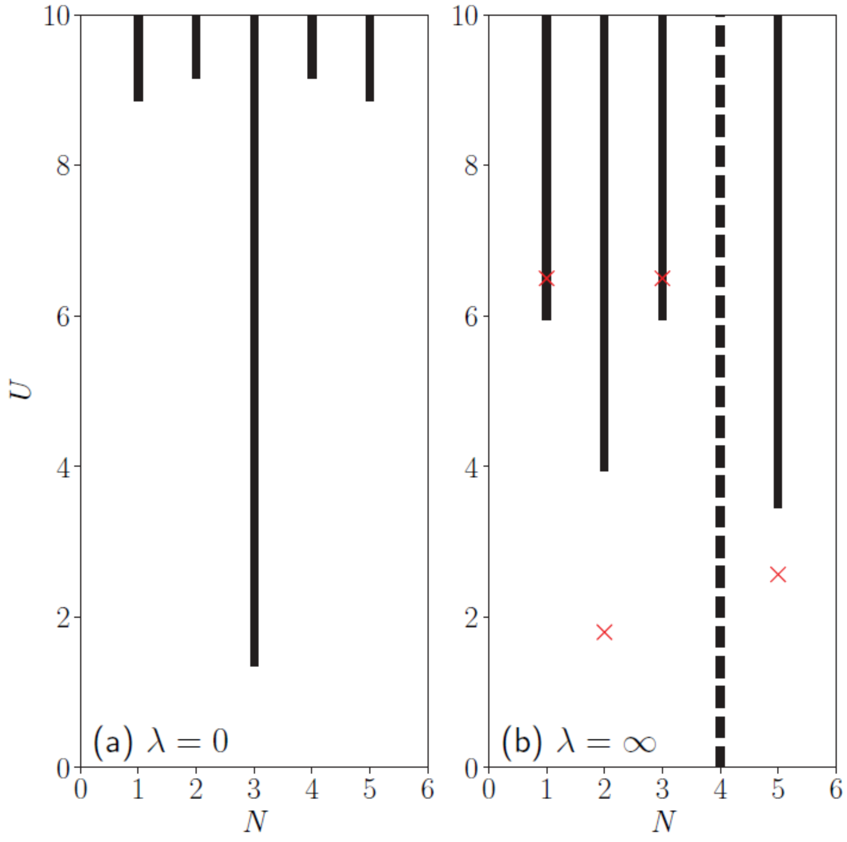
- But there is also off-diagonal term that leads to enh of SOC

Kim, JM,Ferrero,Parcollet,Georges,
PRL’18, Zhang et al. PRL’16

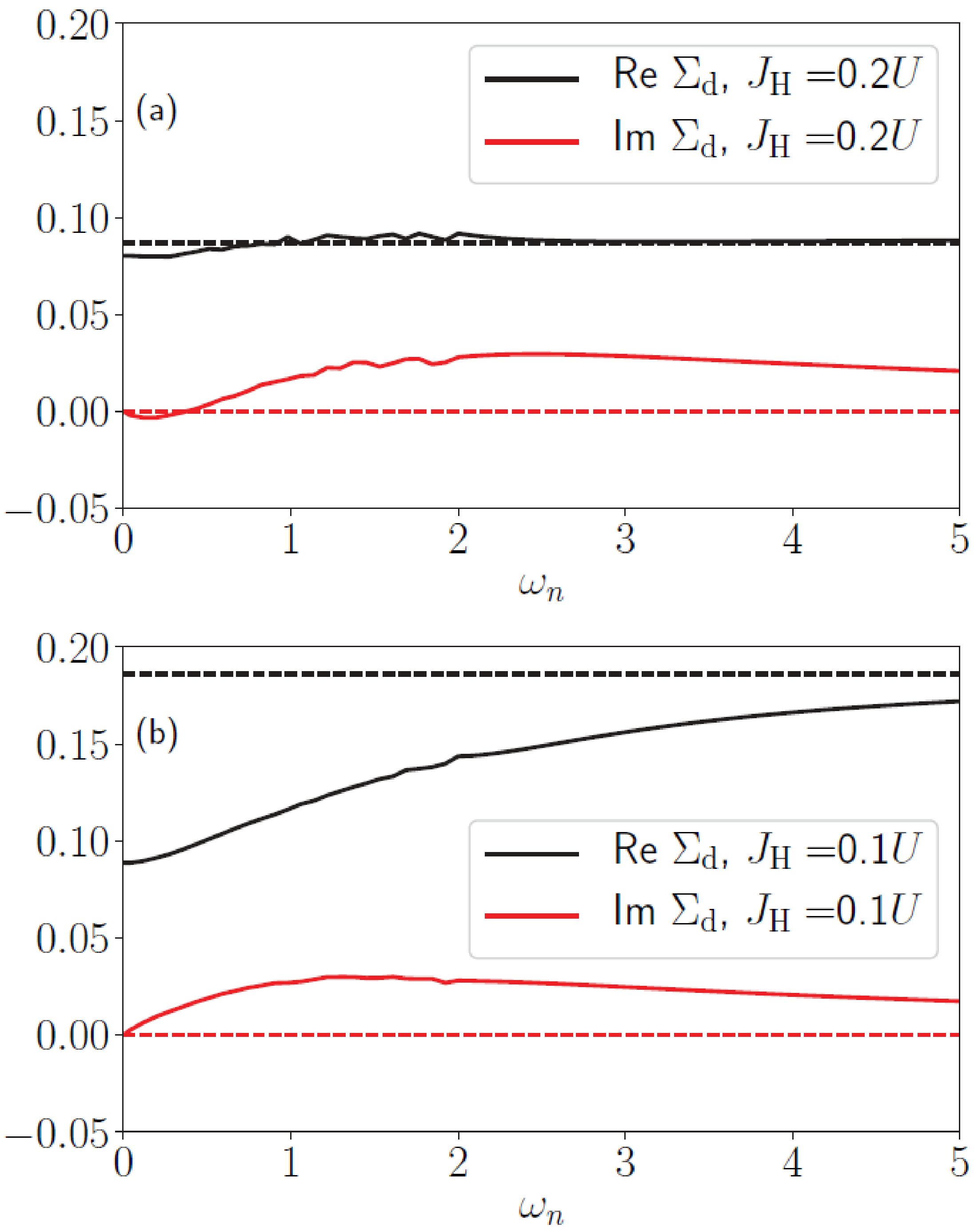


Semicircular calculation study





Triebl,
Kraberger,JM,Aichhorn,
PRB’18


(a)
Re Σ_d, J_H =0.2U
Im Σ_d, J_H =0.2U
0.20
0.15
0.10
0.05
0.00
−0.05
0
1
2
3
4
5
ω_n
(b)
Re Σ_d, J_H =0.1U
Im Σ_d, J_H =0.1U
0.20
0.15
0.10
0.05
0.00
−0.05
0
1
2
3
4
5
ω_n

Summary SOC

- For weak enough SOC its effects on correlations (but not on spectral functions) can be ignored (perhaps up to T^{K}_{orb})
- When it becomes large it destroys Hund’s metal
- Further work needed to characterize it better

Thank you!