Dynamical Mean-Field Theory:
What can we learn from it?
Where do we go from there?

Antoine Georges

TRIQS Summer School 2025

Lecture 1

OUTLINE

- DMFT: A refresher
- Putting DMFT to the test: Sr_2RuO_4
- Hund Metals: The 3rd route to strong correlations
- A few remarks about Transport
- Extensions and Generalizations of DMFT

DMFT: A Refresher
with some perspective

D-MF-T

Energy-scale dependent

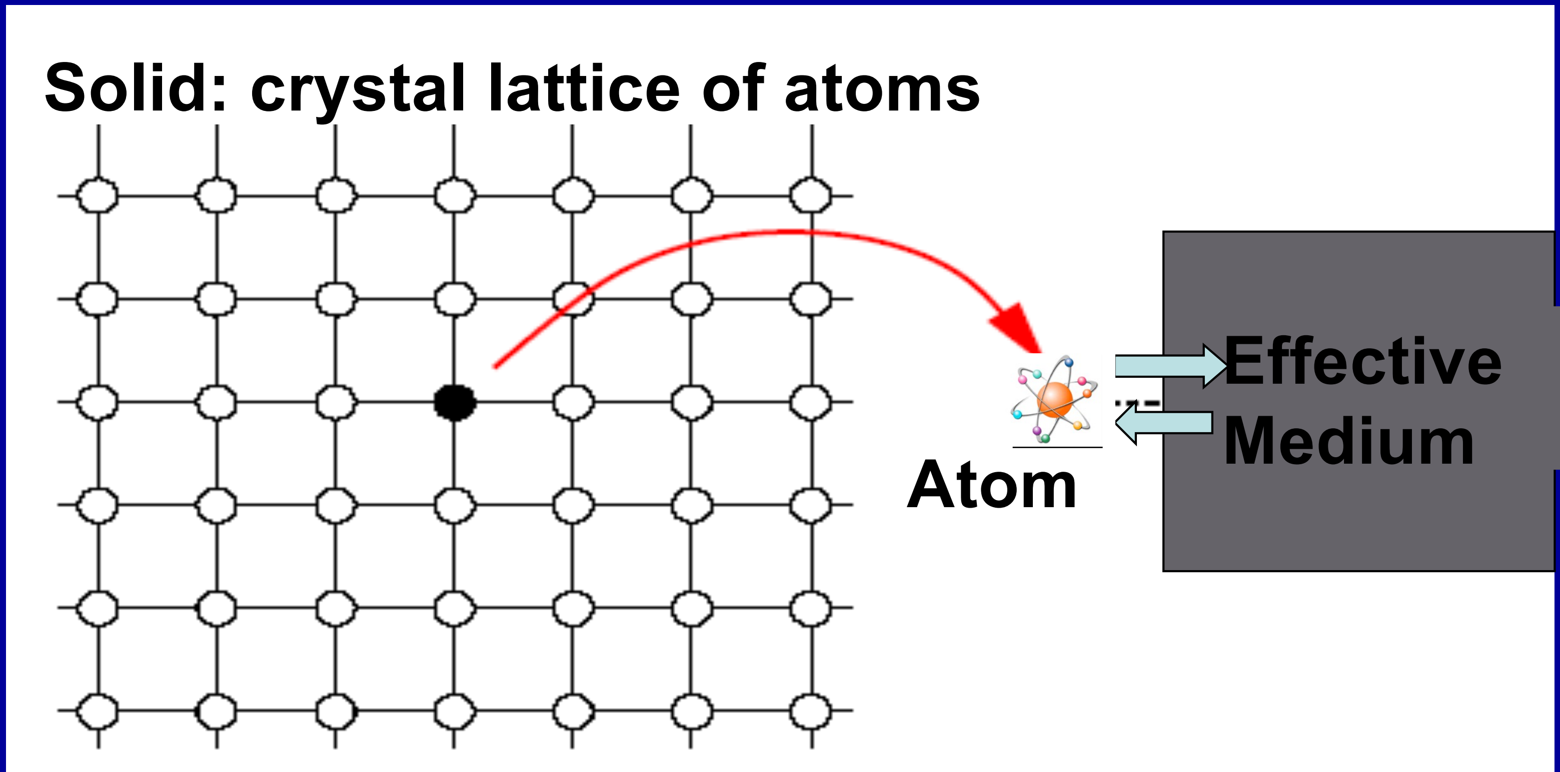
Approximation based on Locality

Dynamical Mean Field Theory

- A *theoretical and computational method* to approach the many-body quantum problem. The method becomes exact in limiting cases and can be systematically improved in a controlled way.
- A *conceptual framework* to think about materials with strong electron correlations and understand their physics

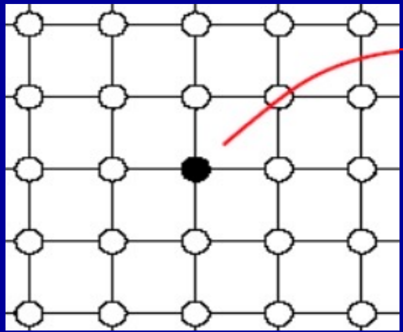
Dynamical Mean-Field Theory:

Viewing a material as an ensemble of **atoms** coupled to a self-consistent effective medium



Dynamical Mean-Field Theory equations A.G. & G.Kotliar, PRB 1992
Correlated electrons in infinite dimensions W.Metzner & D.Vollhardt, PRL 1989

The Embedding Concept



Observable: Local Green's function

$$G_{ii}(\tau - \tau') = -\langle T d_i(\tau)\, d_i^\dagger(\tau')\rangle \equiv G_{loc}$$

$\Delta(\tau - \tau')$

Effective Medium

(`Bath')

$\Delta(\tau$-$\tau')$: Dynamical Mean-Field

Quantum generalization of Weiss field

Chosen such as to reproduce the local G: $\boxed{G_{loc} = G_{imp}[\Delta]}$

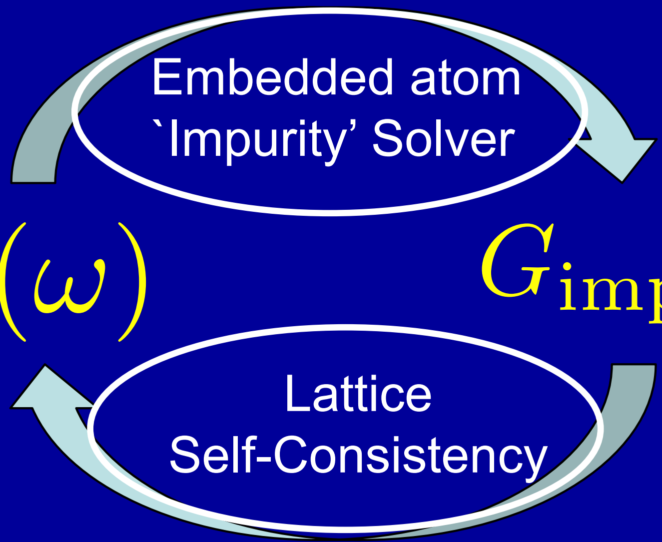
Weiss mean-field theory
Density-functional theory
Dynamical mean-field theory

Share a similar conceptual basis

TABLE 2. Comparison of theories based on functionals of a local observable

Theory	MFT	DFT	DMFT
Quantity	Local magnetization m_i	Local density $n(x)$	Local GF $G_{ii}(\omega)$
Equivalent system	Spin in effective field	Electrons in effective potential	Quantum impurity model
Generalised Weiss field	Effective local field	Kohn-Sham potential	Effective hybridisation $\Delta(\omega)$

The DMFT Self-Consistency Loop



$\Delta(\omega)$ $\quad$ $G_{\mathrm{imp}}(\omega)$

$\Rightarrow \mathrm{Self-energy} : \Sigma(\omega)$

$\Rightarrow \mathrm{Local\ Vertex} :$

$\Gamma(\omega_1, \omega_2, \omega_3)$

Gives access to the <u>lattice</u> <u>momentum-dependent</u> Green's function and response functions:

$$G(\mathrm{k}, \omega) = [\omega + \mu - H_{\mathrm{k}} - \Sigma(\omega)]^{-1}$$

$$\chi(\mathrm{q}, \omega) \sim \chi_0 + \chi_0 \star \Gamma \star \chi$$

Organizing Principle: Locality

For a single band, the DMFT approximation is:

$$\Sigma_{\mathrm{lattice}}(\mathbf{k},\omega) \simeq \Sigma(\omega) \Leftrightarrow \Sigma_{ij}(\omega) \simeq \Sigma(\omega)\,\delta_{ij}$$

With $\Sigma(\omega)$ the self-energy of the embedded atom (`impurity')

A good approximation when correlation lengths
are SMALL (e.g. high temperature,
high doping, frustration, several competing fluctuations, etc.)

Can be improved in a systematic and controlled way
by enlarging the size of the embedded fragment:
Cluster Extensions of DMFT, Generalized Embedding Methods…

Self-Energy: The DMFT *ansatz*

For a multi-band/multi-orbital material

$|\chi_m^{\mathbf{k}}\rangle$: A set of localized orbitals to which many-body interactions $U_{m1m2m3m4}$ are added: correlated Hilbert space

$|\psi_\nu^{\mathbf{k}}\rangle$: The (usually larger) set of Bloch bands (e.g. Kohn-Sham states) describing the material (larger Hilbert space)

$$\boxed{\Sigma_{\nu\nu'}(\omega,\mathbf{k}) = \sum_{mm'} \langle\psi_\nu^{\mathbf{k}}|\chi_m^{\mathbf{k}}\rangle\, \Sigma_{mm'}(\omega)\, \langle\chi_{m'}^{\mathbf{k}}|\psi_{\nu'}^{\mathbf{k}}\rangle}$$

Self-energy
\`upfolded' to
the whole system
(k-dependent)

Orbital content
of Bloch states
(k-dep)

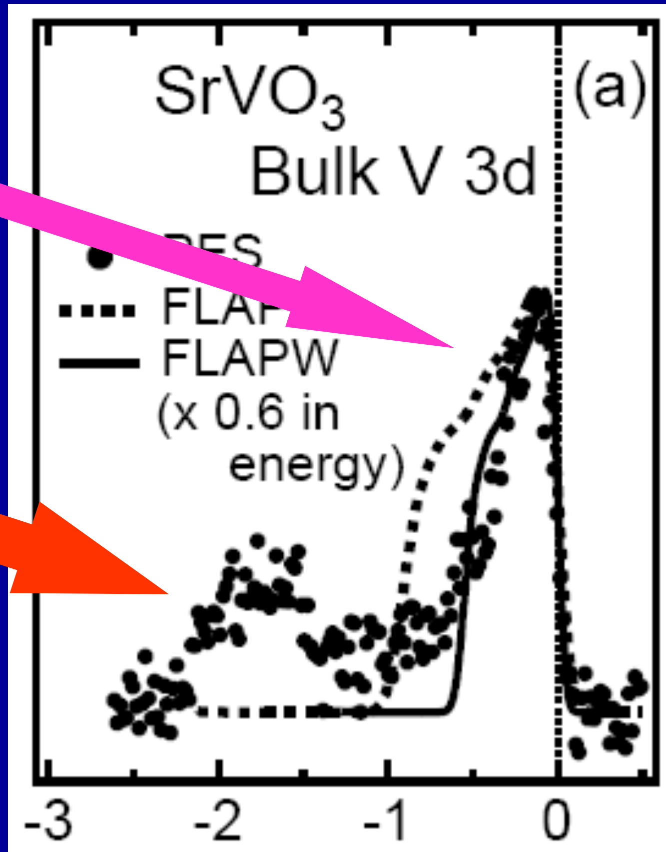
Local self-energy
In orbital space
(k-independent)

From Particles to Waves…

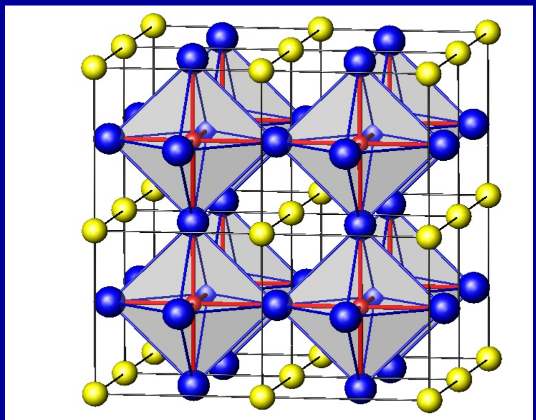
- High-energy excitations are best described as *localized particle-like atomic transitions. (cf. Mott insulators - `Hubbard bands')*
- In metals coherent *wave-like excitations emerge at low energy: quasiparticles*
- DMFT starts from atoms (each atom is a small many-body problem) and describes how quasiparticles emerge as one follows the flow from high-energy to low-energy
- *Relevance of atomic physics to the solid state!*

Correlated metals: atomic-like excitations at high energy, quasiparticles at low energy

- **Narrowing of quasiparticle bands** due to correlations (the Brinkman-Rice phenomenon)
- **Hubbard satellites** (i.e extension to the solid of atomic-like transitions)



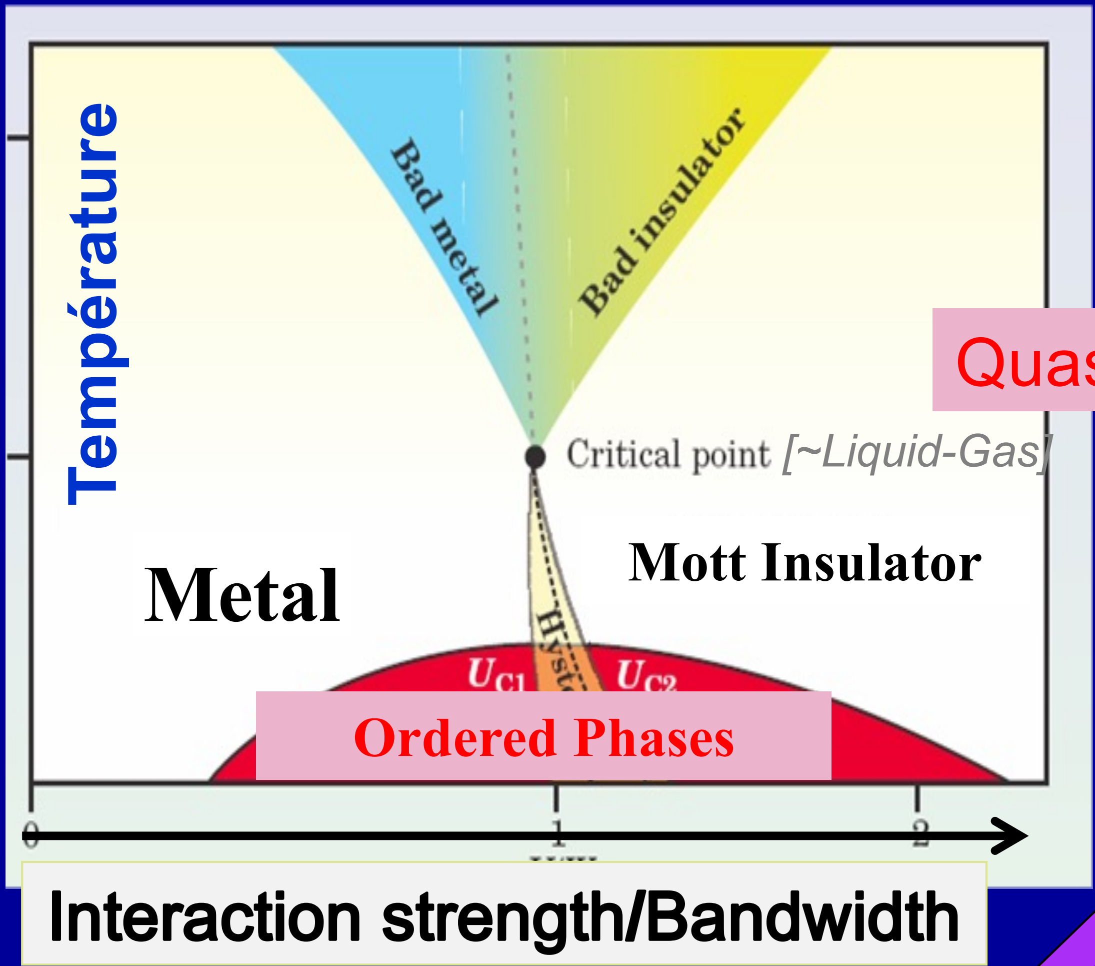
Dashed line:
Spectrum obtained from Conventional band-structure methods (DFT-LDA)

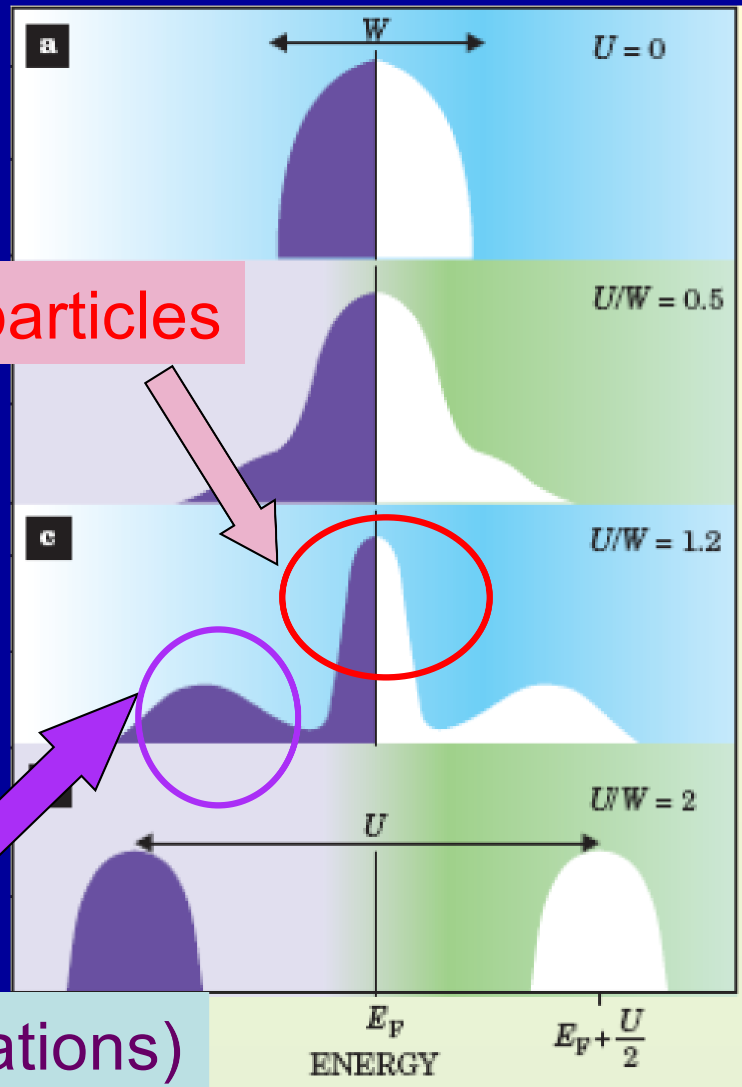


$SrVO_3$

Sekiyama et al., PRL 2004

An early success of DMFT (1992-1999)
Theory of the Mott transition



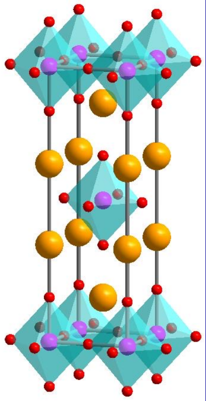


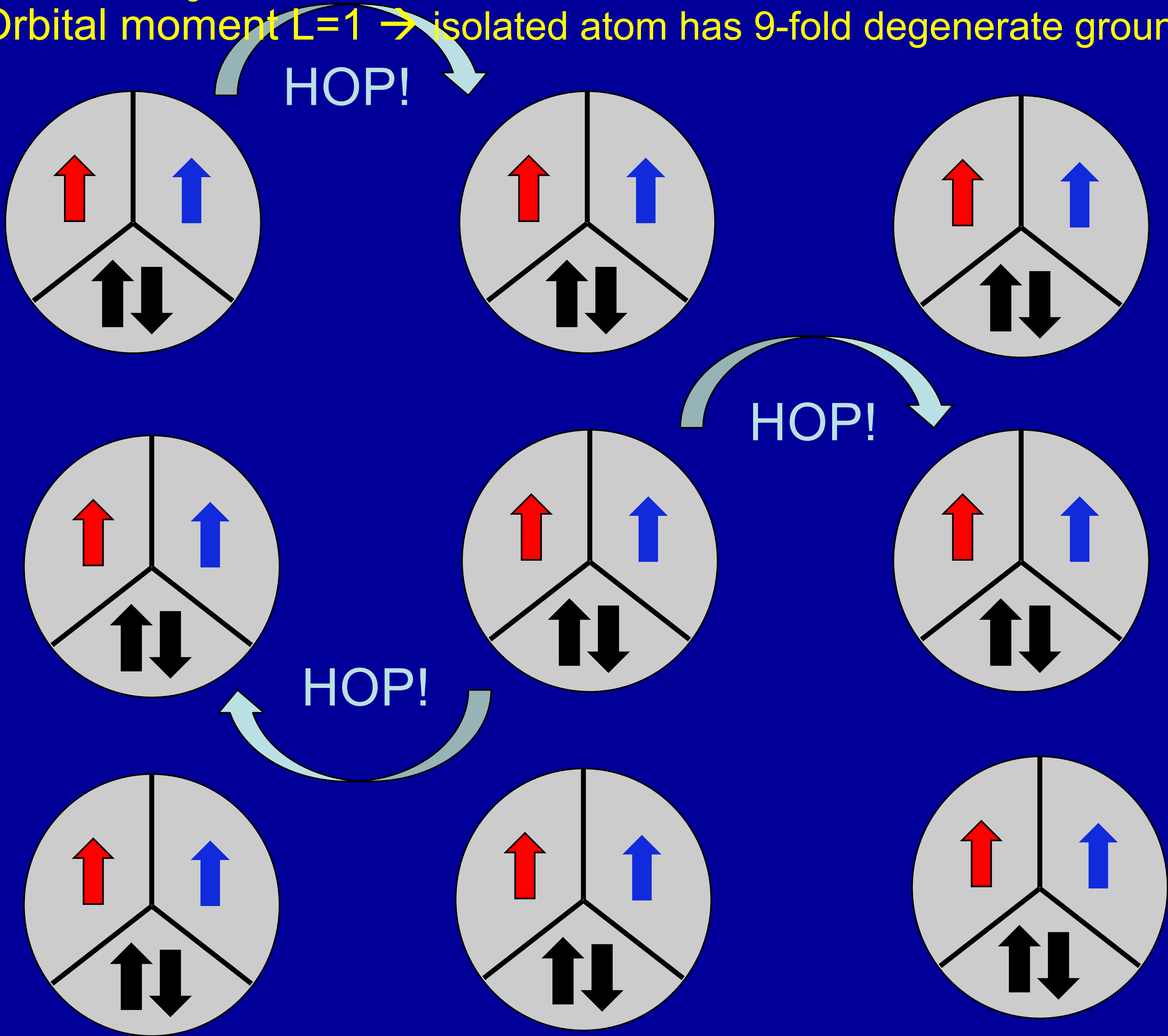
Low-frequency behavior of Δ(ω) determines nature of the phase

- Δ(ω→0) finite → local moment is screened. <u>`Self-consistent' Kondo effect</u>. Gapless metallic state.

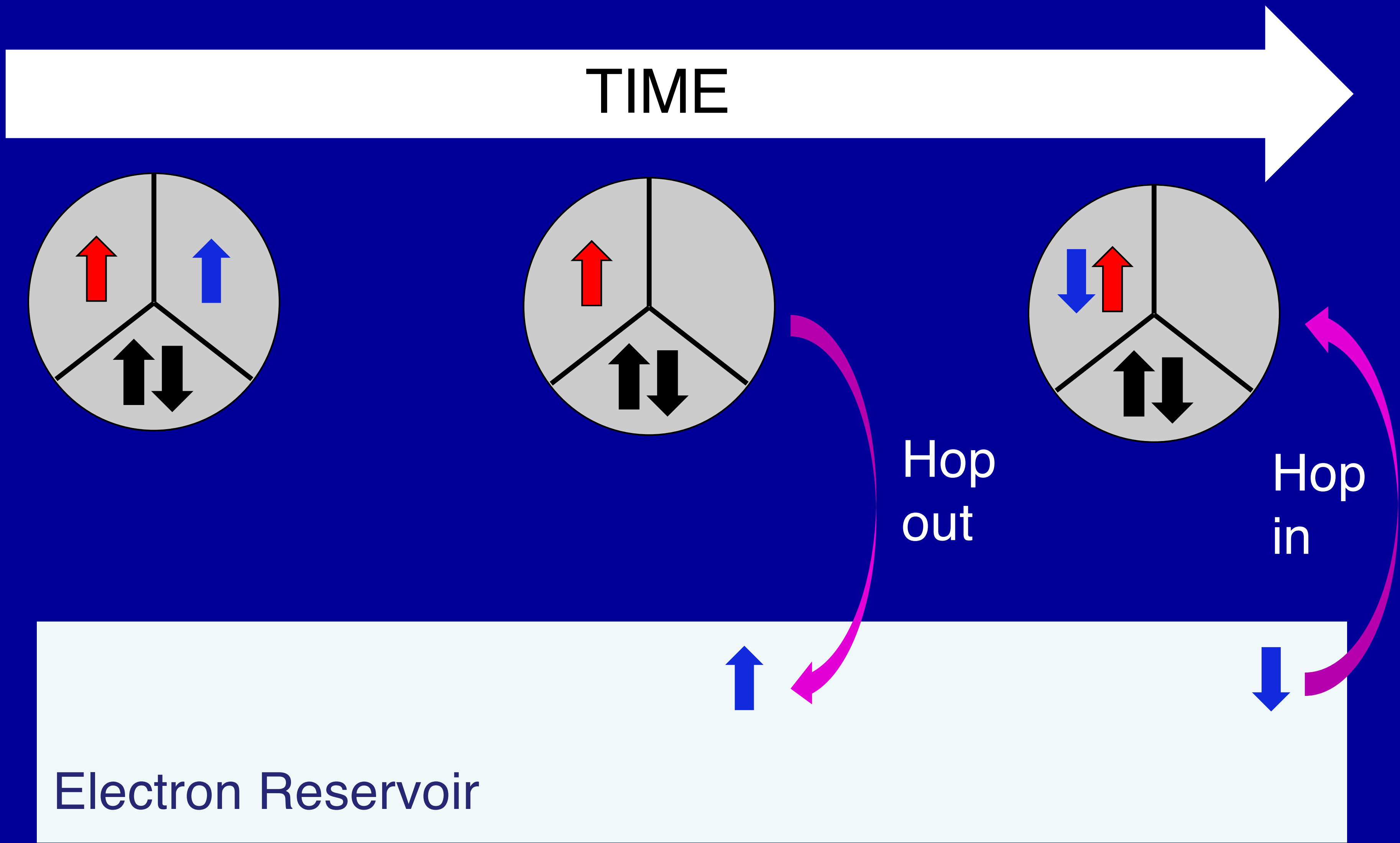
- Δ(ω) gapped → no Kondo effect, degenerate ground-state, insulator with local moments

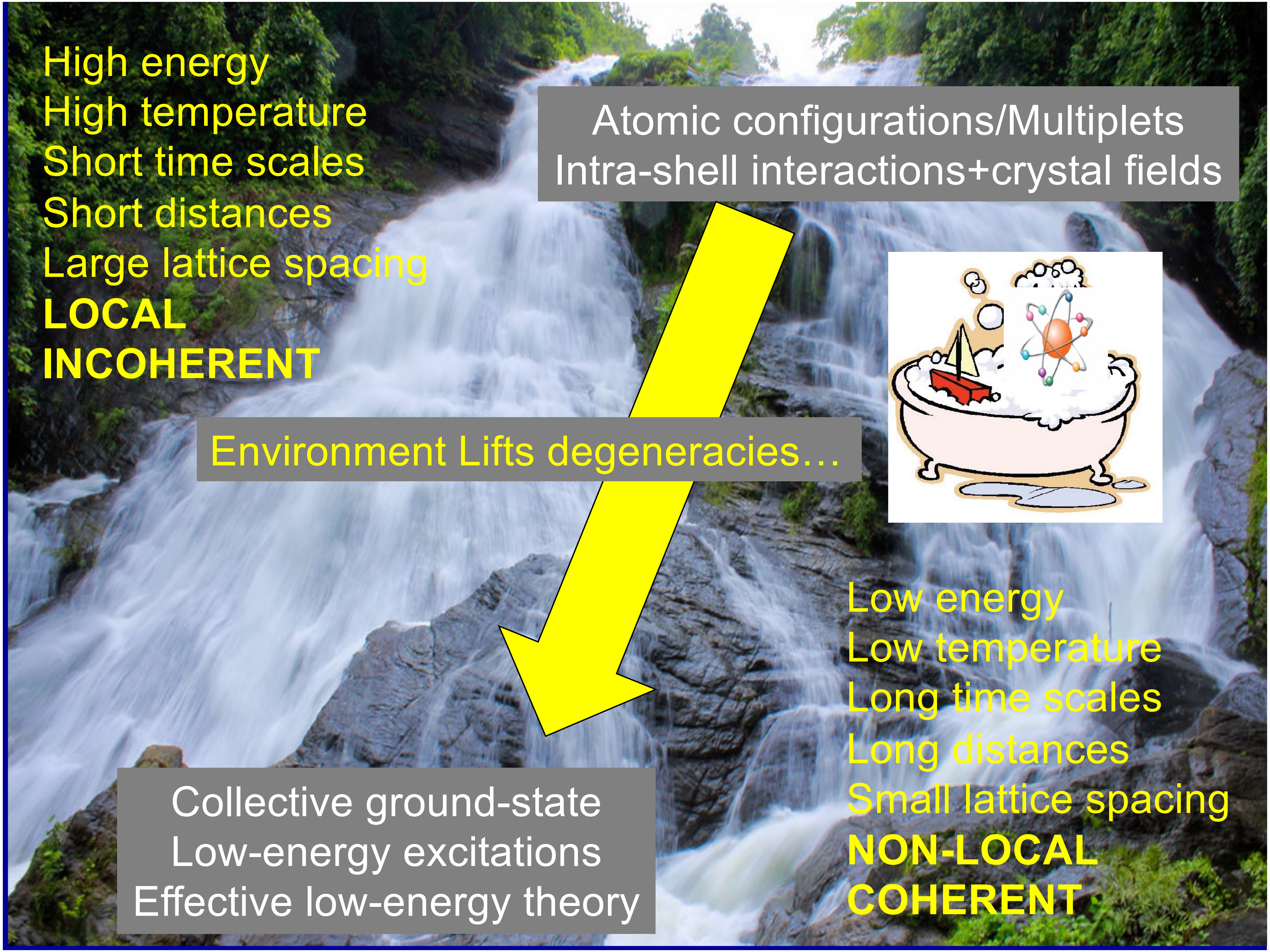
Sr_2RuO_4 t_{2g} atomic shell: 4 electrons in 3 orbitals; Spin S=1
Orbital moment L=1 → isolated atom has 9-fold degenerate ground-state





Sequence of quantum jumps between atomic configurations




High energy
High temperature
Short time scales
Short distances
Large lattice spacing
LOCAL
INCOHERENT
Atomic configurations/Multiplets
Intra-shell interactions+crystal fields
Environment Lifts degeneracies…
Low energy
Low temperature
Long time scales
Long distances
Small lattice spacing
NON-LOCAL
COHERENT
Collective ground-state
Low-energy excitations
Effective low-energy theory

A beautiful illustration of the usefulness of DMFT: Sr_2RuO_4 and Hund Metals

Sr_2RuO_4: The `Drosophila' of Strongly Correlated Oxides

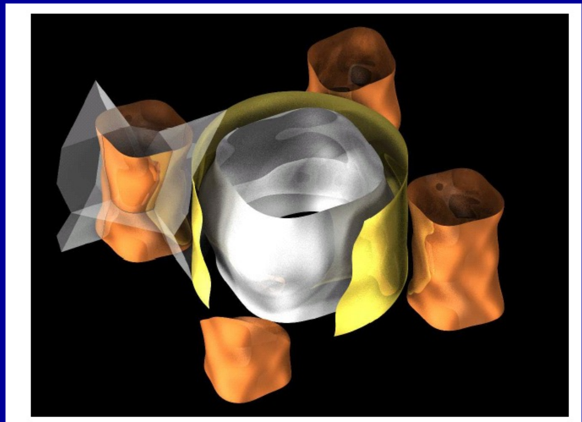
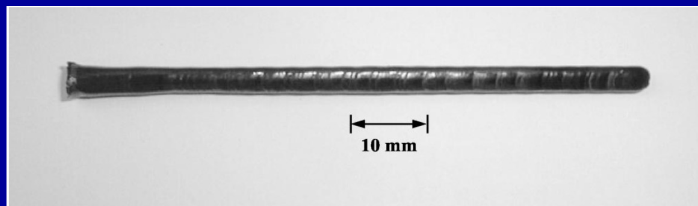
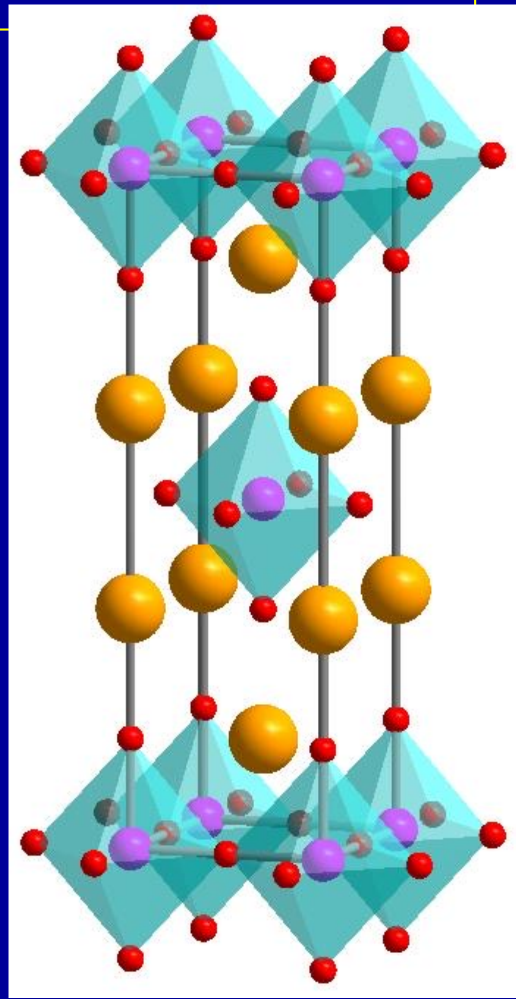


FIG. 28: Visualisation of the Fermi surface of Sr_2RuO_4. The c-axis corrugation is exaggerated by a factor of 15 for clarity.





Simple Structure

Large clean single-crystals
→ Investigated with basically <u>all techniques</u> in the experimentalist's toolbox

A.Mackenzie, Y.Maeno Rev Mod Phys 75, 657 (2003)

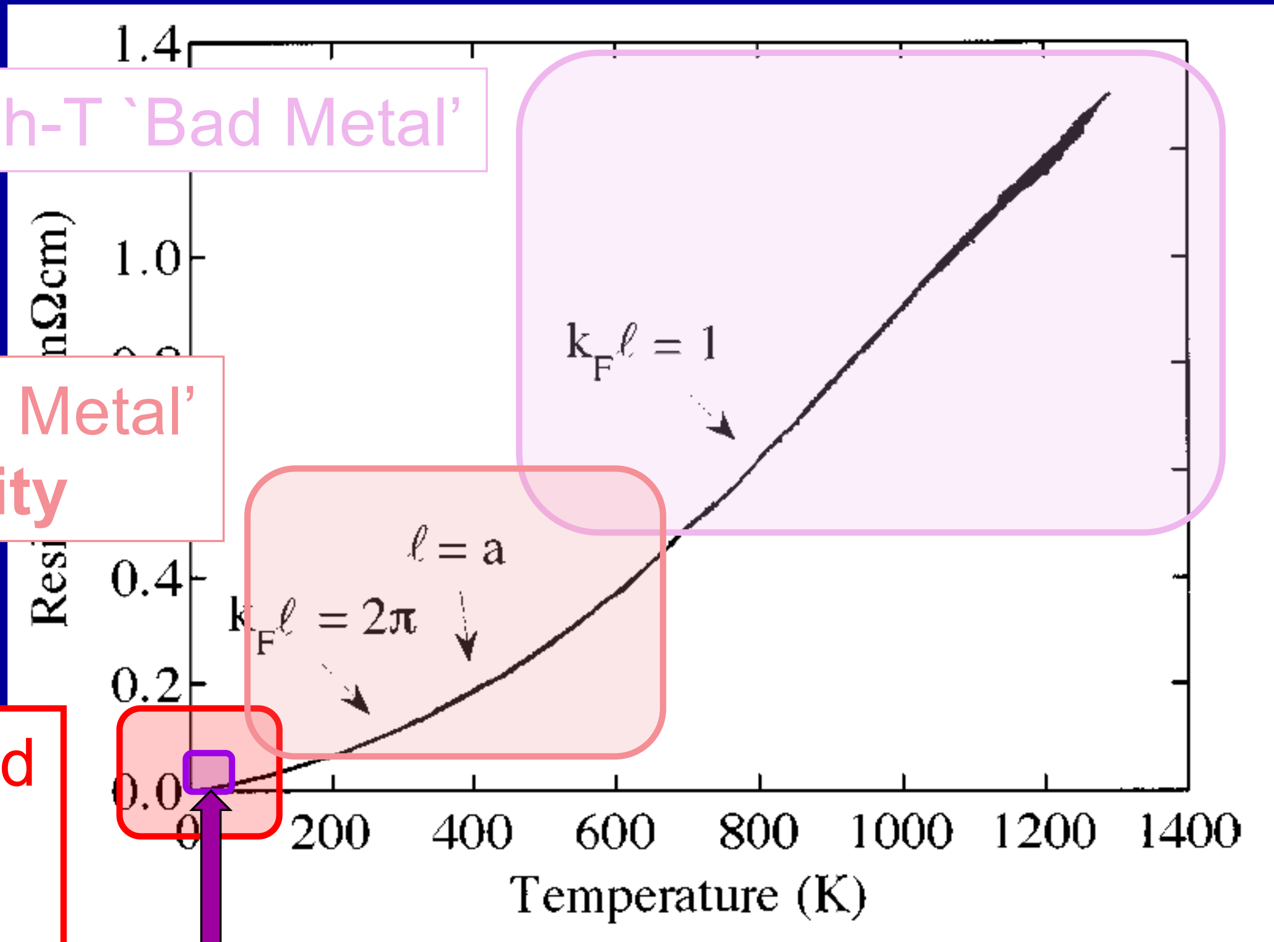
From a bad metal at high-T …
…to a superconductor at low-T (1.4K)

…The fascinating life of Sr_2RuO_4

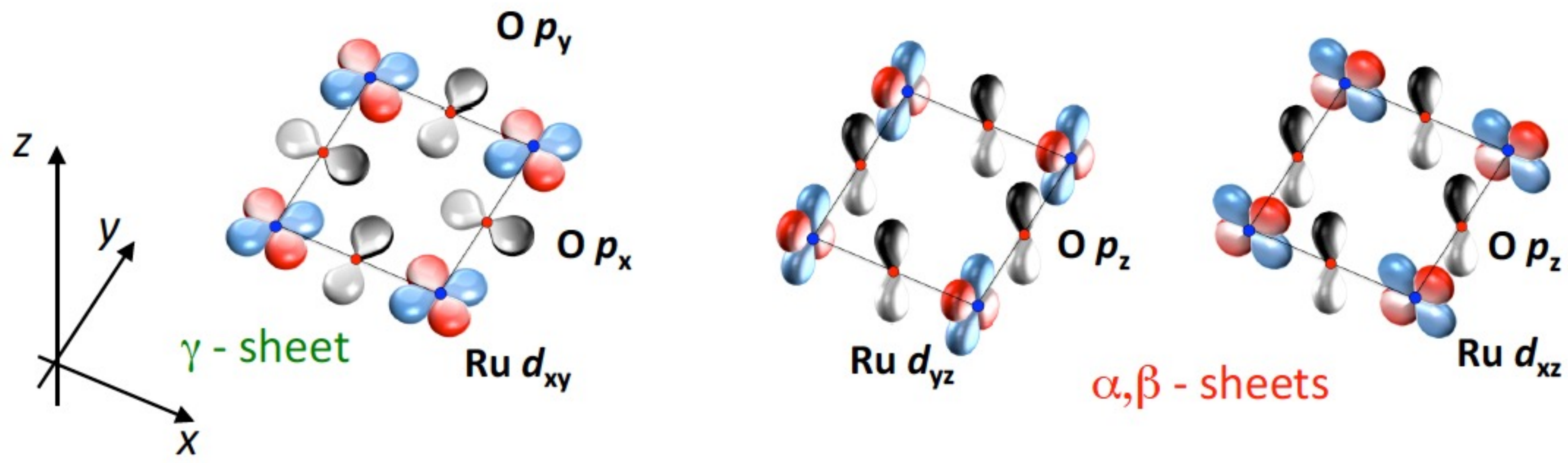
High-T \`Bad Metal'

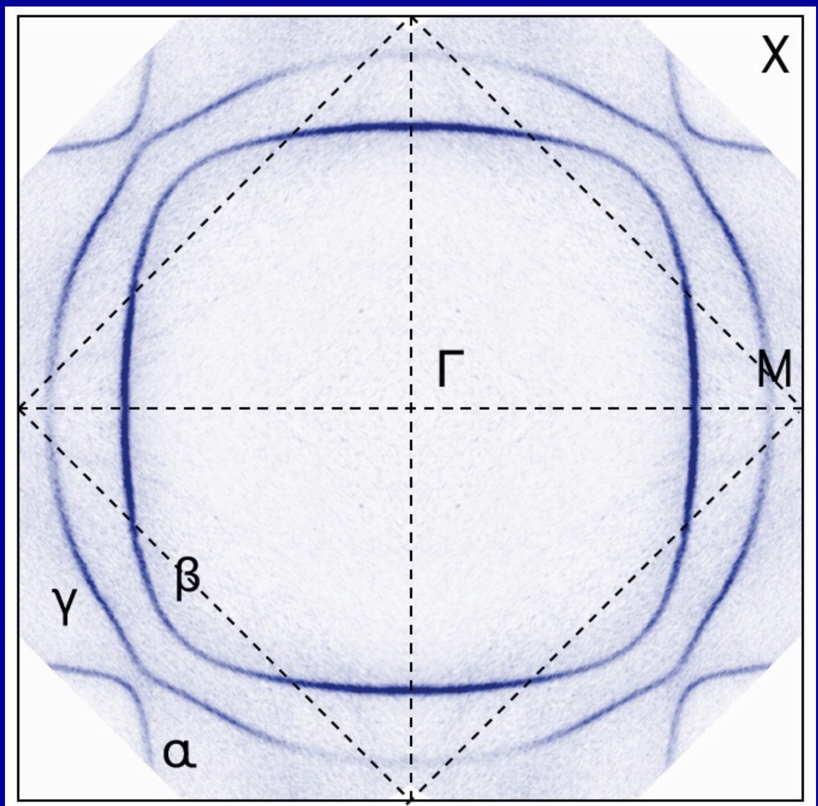
Intermediate-T \`OK Metal'
but not T^2 resistivity

Low-T Fermi Liquid
Below ~ 25 K
Good metal



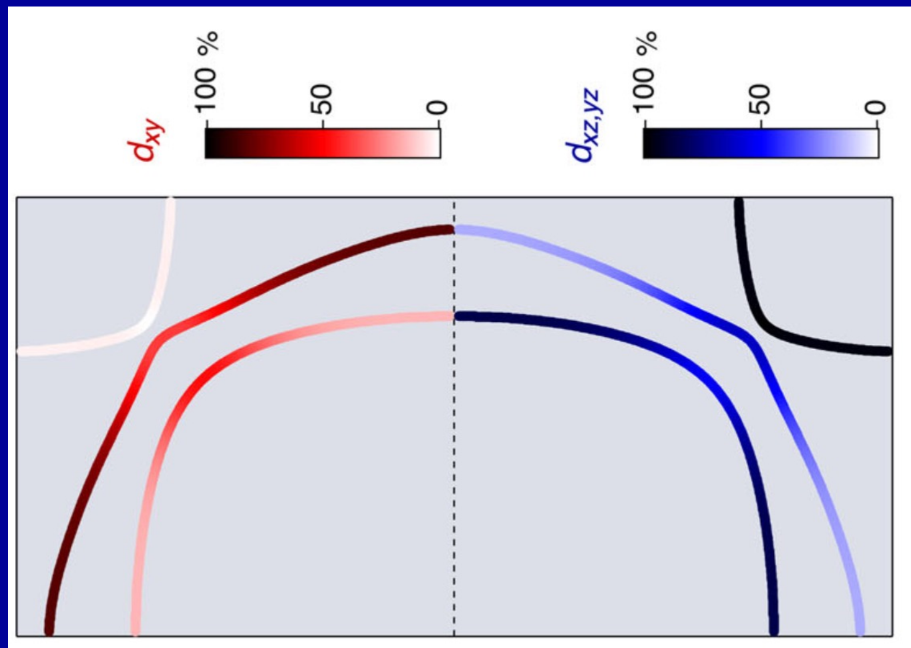
Superconductor



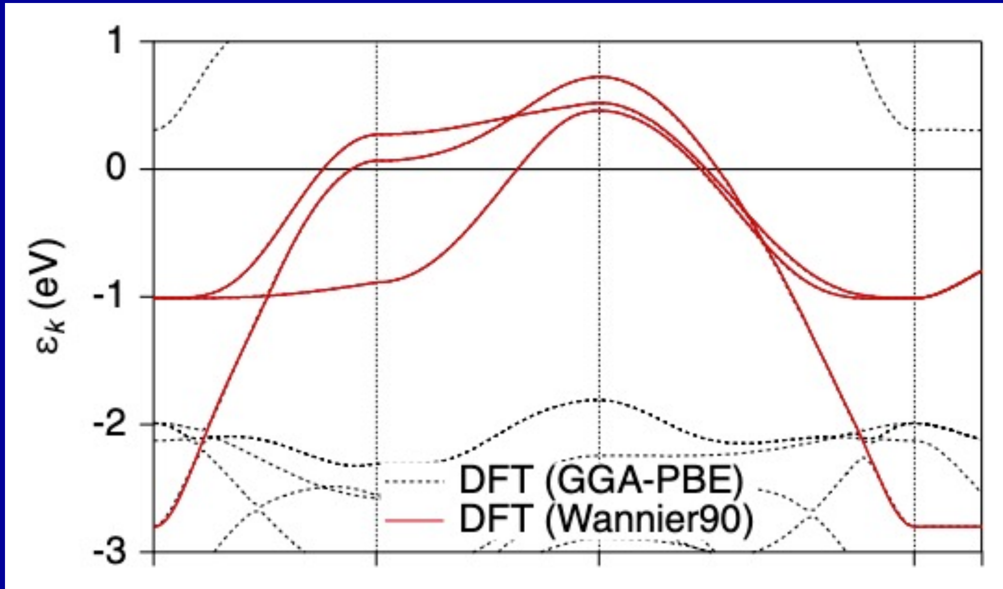


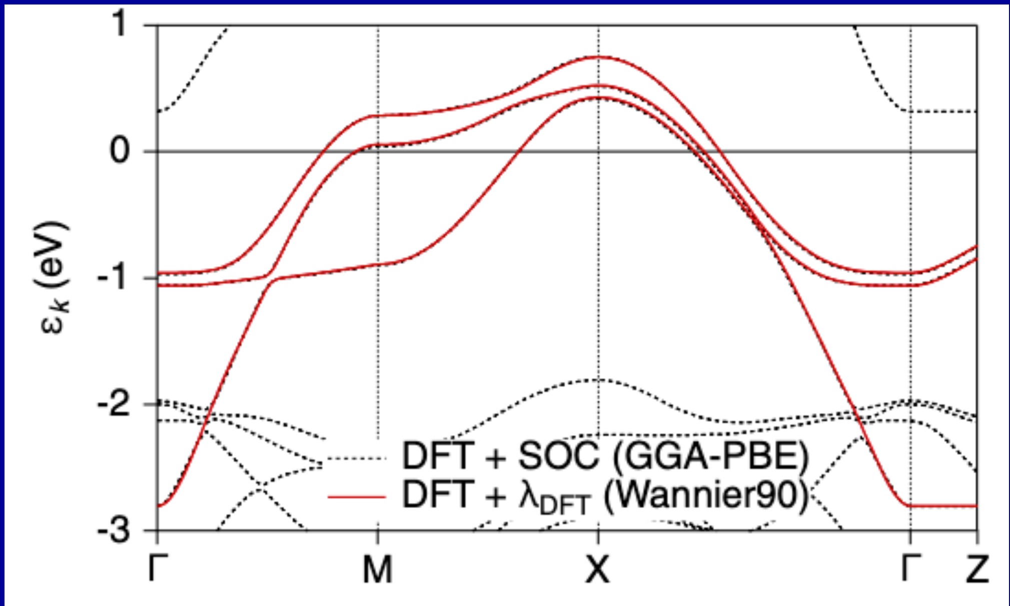
High-resolution Laser ARPES

Tamai et al. PRX 9, 021048 (2019)



Bands: Ru(4d)-xy,xz,yz+O-p → t_{2g}





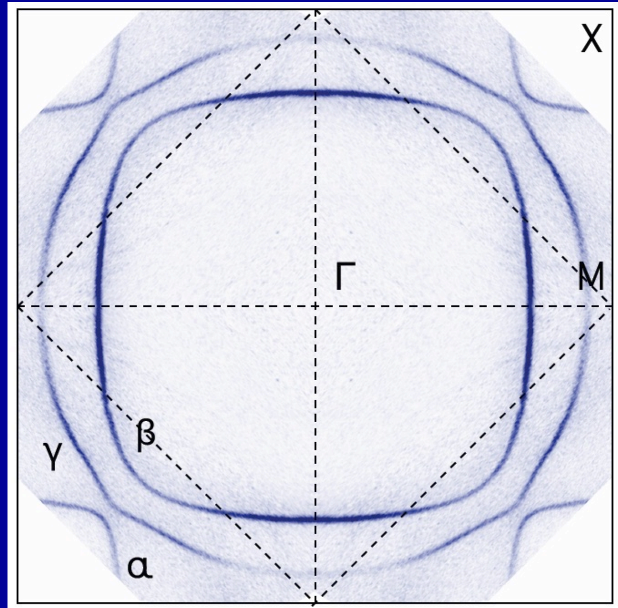


FIG. 9. DFT band structure along the high-symmetry path ΓMXΓZ compared to the eigenstates of our maximally localized Wannier Hamiltonian $\hat{H}^{\mathrm{DFT}}$ for the three t_{2g} bands. Top panel: DFT (GGA-PBE) and eigenstates of $\hat{H}^{\mathrm{DFT}}$. Bottom panel: DFT + SOC (GGA-PBE) and eigenstates of $\hat{H}^{\mathrm{DFT}} + \hat{H}^{\mathrm{SOC}}_{\lambda_{\mathrm{DFT}}}$, with a local SOC term [Eq. (8)] and a coupling strength of $\lambda_{\mathrm{DFT}} = 100$ meV.

Tamai et al. PRX 9, 021048 (2019)
Calculation by Manuel Zingl

Interactions: Kanamori hamiltonian:

[J.Kanamori, Prog. Theor. Phys. 30 (1963) 275]

$$H_{\mathrm{K}} = U \sum_{m} \hat{n}_{m\uparrow}\hat{n}_{m\downarrow} + U' \sum_{m\neq m'} \hat{n}_{m\uparrow}\hat{n}_{m'\downarrow} + (U'-J) \sum_{m<m',\sigma} \hat{n}_{m\sigma}\hat{n}_{m'\sigma} +$$
$$-J \sum_{m\neq m'} d^{+}_{m\uparrow} d_{m\downarrow} d^{+}_{m'\downarrow} d_{m'\uparrow} + J \sum_{m\neq m'} d^{+}_{m\uparrow} d^{+}_{m\downarrow} d_{m'\downarrow} d_{m'\uparrow}$$

EXACT for a t_{2g} shell

with U'=U-2J

Useful reference: Sugano, Tanabe & Kamimura,
Multiplets of transition-metal ions in crystals
Academic Press, 1970

For Sr2RuO4, c-RPA calculations (see lectures on Friday) yield U in the range 2.2eV (xz,yz)-2.5 eV (xy) and J of order 0.25 eV. Best fit to experiment is obtained for U ~ 2.4eV and J~0.4eV

Origin of Correlations in Sr_2RuO_4: Hund Coupling + van Hove

PRL **106**, 096401 (2011) PHYSICAL REVIEW LETTERS week ending 4 MARCH 2011

Coherence-Incoherence Crossover and the Mass-Renormalization Puzzles in Sr_2RuO_4

Jernej Mravlje,[1,2] Markus Aichhorn,[3,1] Takashi Miyake,[4,5] Kristjan Haule,[6] Gabriel Kotliar,[6] and Antoine Georges[1,7,5]

Jernej Mravlje
Joszef Stefan Institute
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& École Polytechnique

PHYSICAL REVIEW LETTERS **124**, 016401 (2020)

Strongly Correlated Materials from a Numerical Renormalization Group Perspective: How the Fermi-Liquid State of Sr_2RuO_4 Emerges

Fabian B. Kugler,[1] Manuel Zingl,[2] Hugo U.R. Strand,[2] Seung-Sup B. Lee,[1]
Jan von Delft,[1] and Antoine Georges[3,2,4,5]

Effective masse enhancements from DMFT: comparing with quantum oscillations

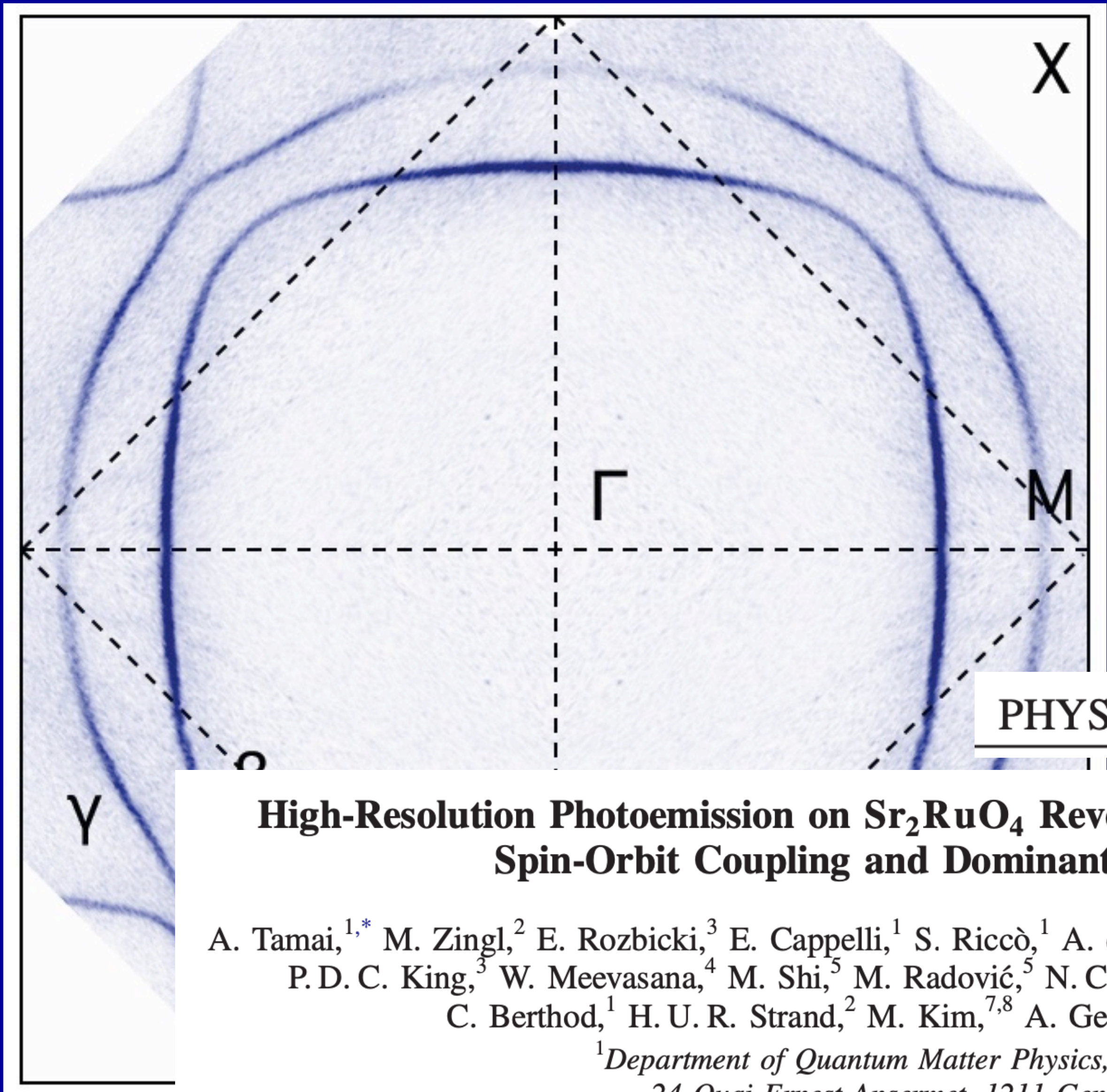
J [eV]	$m^*_{xy}/m_{\mathrm{LDA}}$	$m^*_{xz}/m_{\mathrm{LDA}}$	T^*_{xy}[K]	T^*_{xz}[K]	$T_>$[K]
0.0, 0.1	1.7	1.7	> 1000	> 1000	> 1000
0.2	2.3	2.0	300	800	> 1000
0.3	3.2	2.4	100	300	500
0.4	4.5	3.3	60	150	350

Table I. Mass enhancement of the xy and xz orbitals, as a function of Hund's coupling, for $U = 2.3$ eV. Other columns: coherence temperatures as defined in the text.

U=2.3 eV

- Increase of effective mass as J is increased
- Orbital differentiation: xy heavier (due to van Hove singularity)
- Comparable mass enhancement would require U=5eV at J=0 !

Putting DMFT to the test with high-resolution ARPES



PHYSICAL REVIEW X **9**, 021048 (2019)

High-Resolution Photoemission on Sr_2RuO_4 Reveals Correlation-Enhanced Effective Spin-Orbit Coupling and Dominantly Local Self-Energies

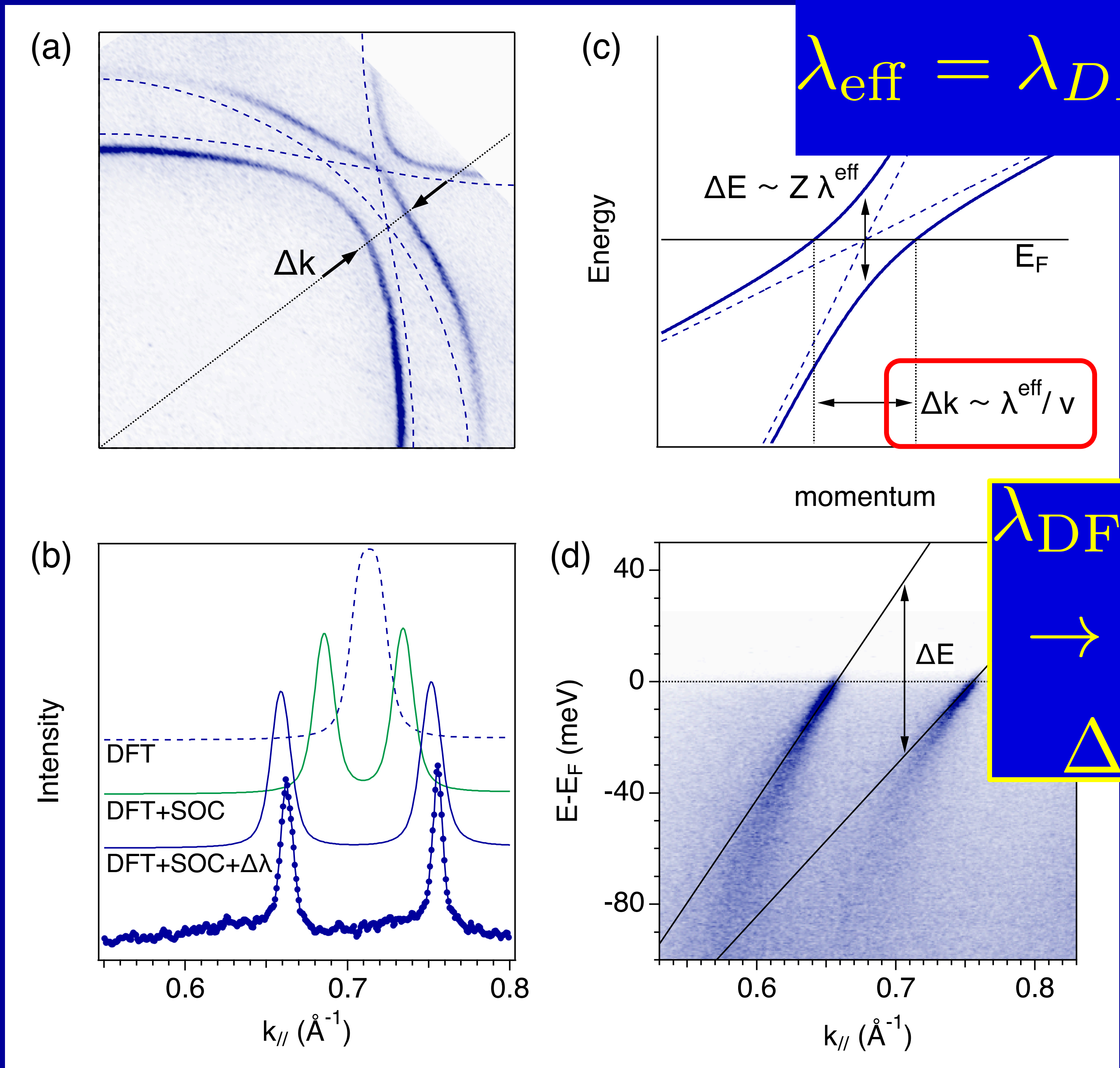
A. Tamai,[1,*] M. Zingl,[2] E. Rozbicki,[3] E. Cappelli,[1] S. Riccò,[1] A. de la Torre,[1] S. McKeown Walker,[1] F. Y. Bruno,[1] P. D. C. King,[3] W. Meevasana,[4] M. Shi,[5] M. Radović,[5] N. C. Plumb,[5] A. S. Gibbs,[3,†] A. P. Mackenzie,[6,3] C. Berthod,[1] H. U. R. Strand,[2] M. Kim,[7,8] A. Georges,[9,2,8,1] and F. Baumberger[1,5]

[1]*Department of Quantum Matter Physics, University of Geneva,*
24 Quai Ernest-Ansermet, 1211 Geneva 4, Switzerland

Fermi Surface reveals Enhancement of effective Spin-Orbit coupling in comparison to the DFT band-structure value

- This effect was predicted theoretically:
- From general perturbation-theory considerations: Liu et al PRL 101, 026408 (2008)
- From Dynamical Mean-Field Theory calculations on Sr_2RuO_4: Zhang et al. 116, 106402 (2016); Kim et al. PRL 120, 126401 (2018)

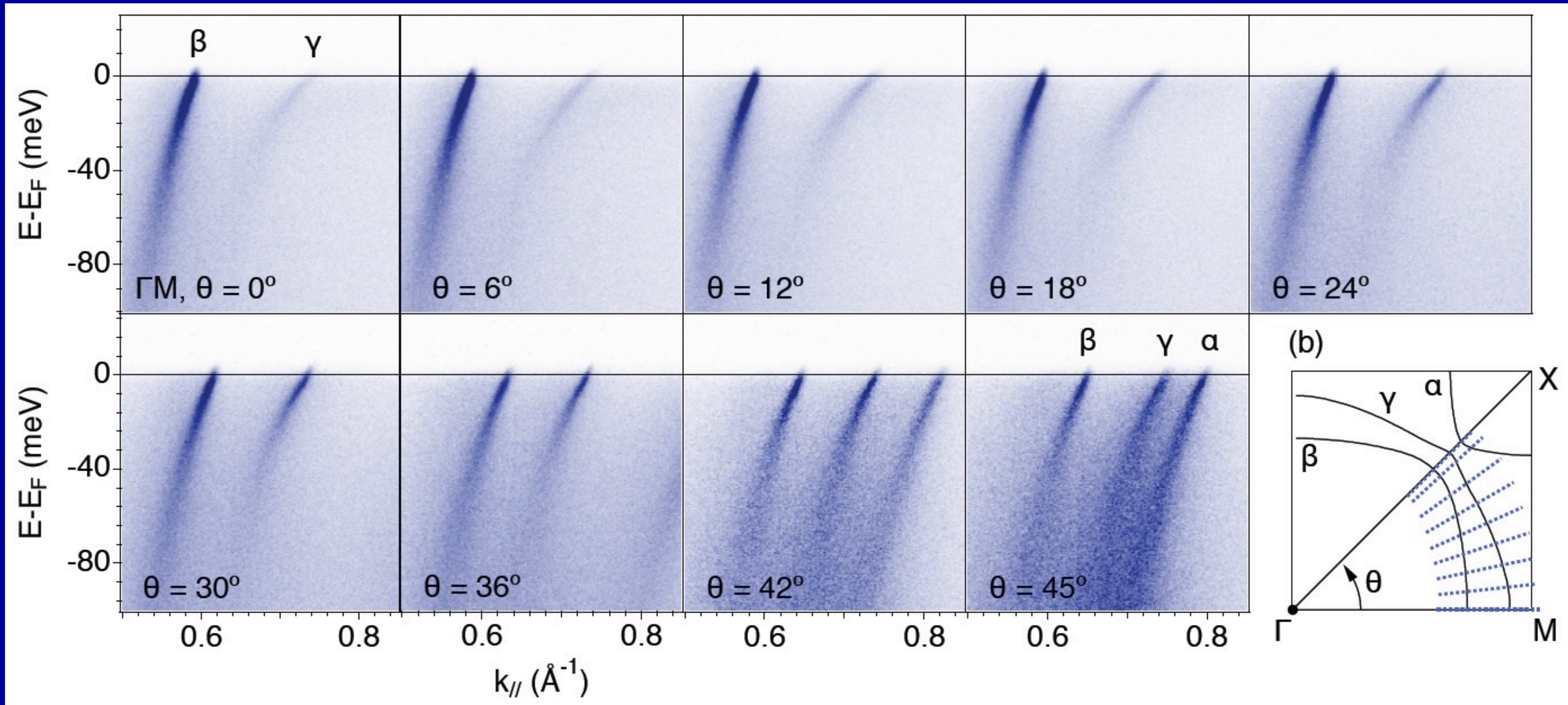
$$\lambda_{\text{eff}} = \lambda_{DFT} \frac{\Delta k_{exp}}{\Delta k_{DFT}}$$



$$\lambda_{\text{DFT}} \simeq 0.1\, eV$$
$$\rightarrow \lambda \simeq 0.2\, eV$$
$$\Delta\lambda \simeq 0.1\, eV$$

A prediction from theory. Confirmed !

Extract self-energy for each angle θ: Quasiparticle vs. Orbital basis



Extracting Self-Energy from Data:

- Reference single-particle Hamiltonian: H_0
- Natural choice: DFT+SOC+Δλ
- Green's function:

$$\hat{G}(\omega, \mathbf{k})^{-1} = \omega - \hat{H}_0 - \hat{\Sigma}(\omega, \mathbf{k})$$

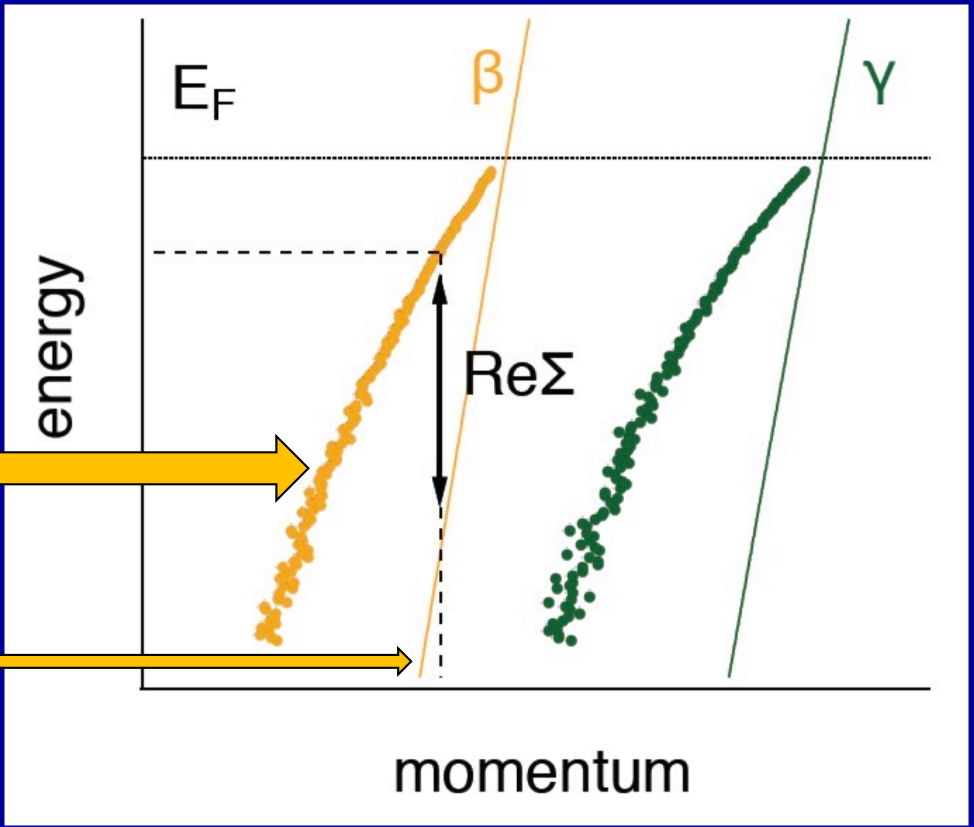
- The self-energy Σ encodes the effect of correlations
- e.g. Quasiparticle dispersions solutions of:

$$\det\left[\hat{H}_0 + \hat{\Sigma}(\omega, \mathbf{k}) - \omega\right] = 0 \to \omega_\nu(\mathrm{k})$$

Self-energy from data (1) - naïve approach

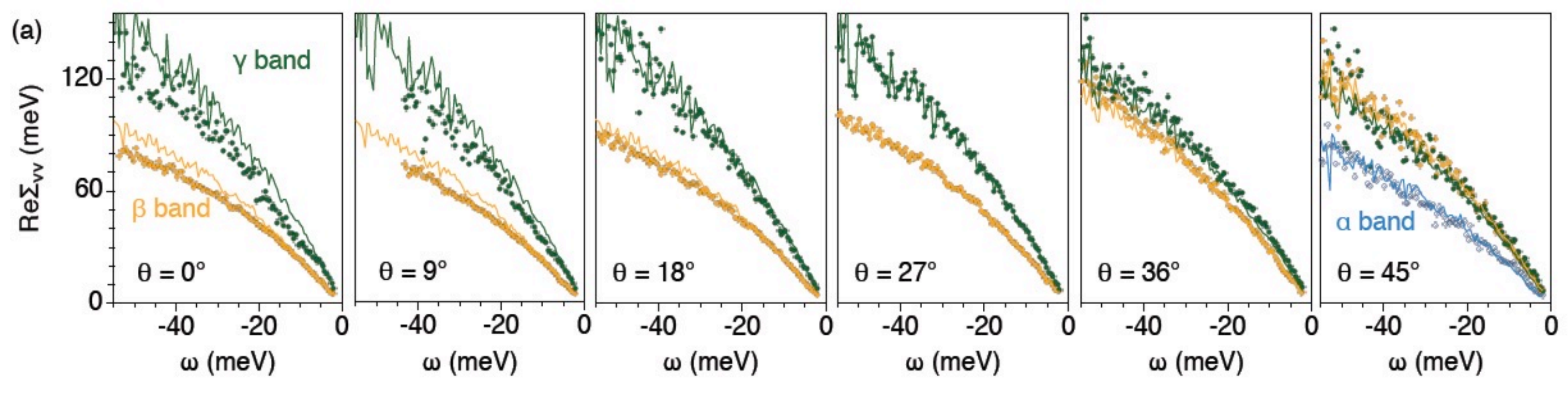
- Self-energy is a matrix $\Sigma_{\nu\nu'}$ three-band system
- $\nu,\nu'=\alpha,\beta,\gamma$ BAND index
- Assume this matrix

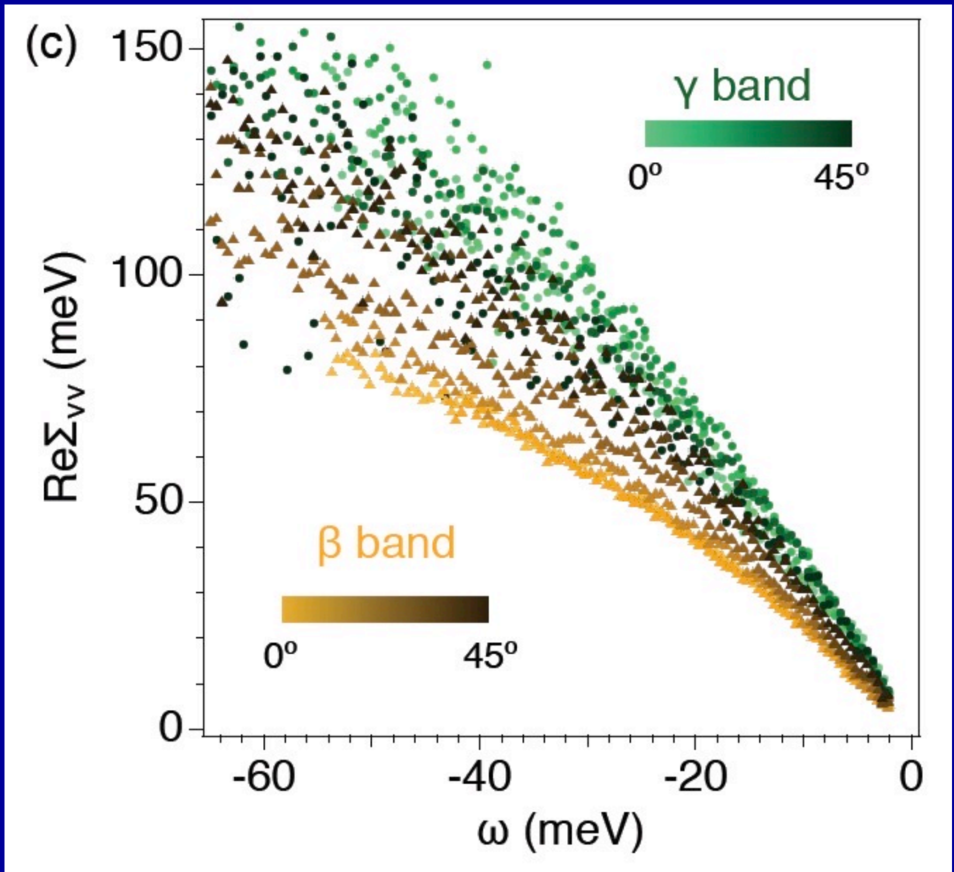
is ~ diagonal



Measured quasiparticle dispersion (from ARPES MDC)

One-particle band (from H_0)





Self-energy strongly depends on ANGLE (i.e. momentum) when extracted in band Basis (Σ_ν , ν=αβγ)

Does this indicate a failure of the DMFT approximation?

Self-Energy: The DMFT *ansatz*

For a multi-band/multi-orbital material

$|\chi_m^{\mathbf{k}}\rangle$: A set of localized orbitals with many-body interactions $U_{m1m2m3m4}$ are added: correlated Hilbert space

$|\psi_\nu^{\mathbf{k}}\rangle$: The (usually larger) set of Bloch bands (e.g. Kohn-Sham states) describing the material (larger Hilbert space)

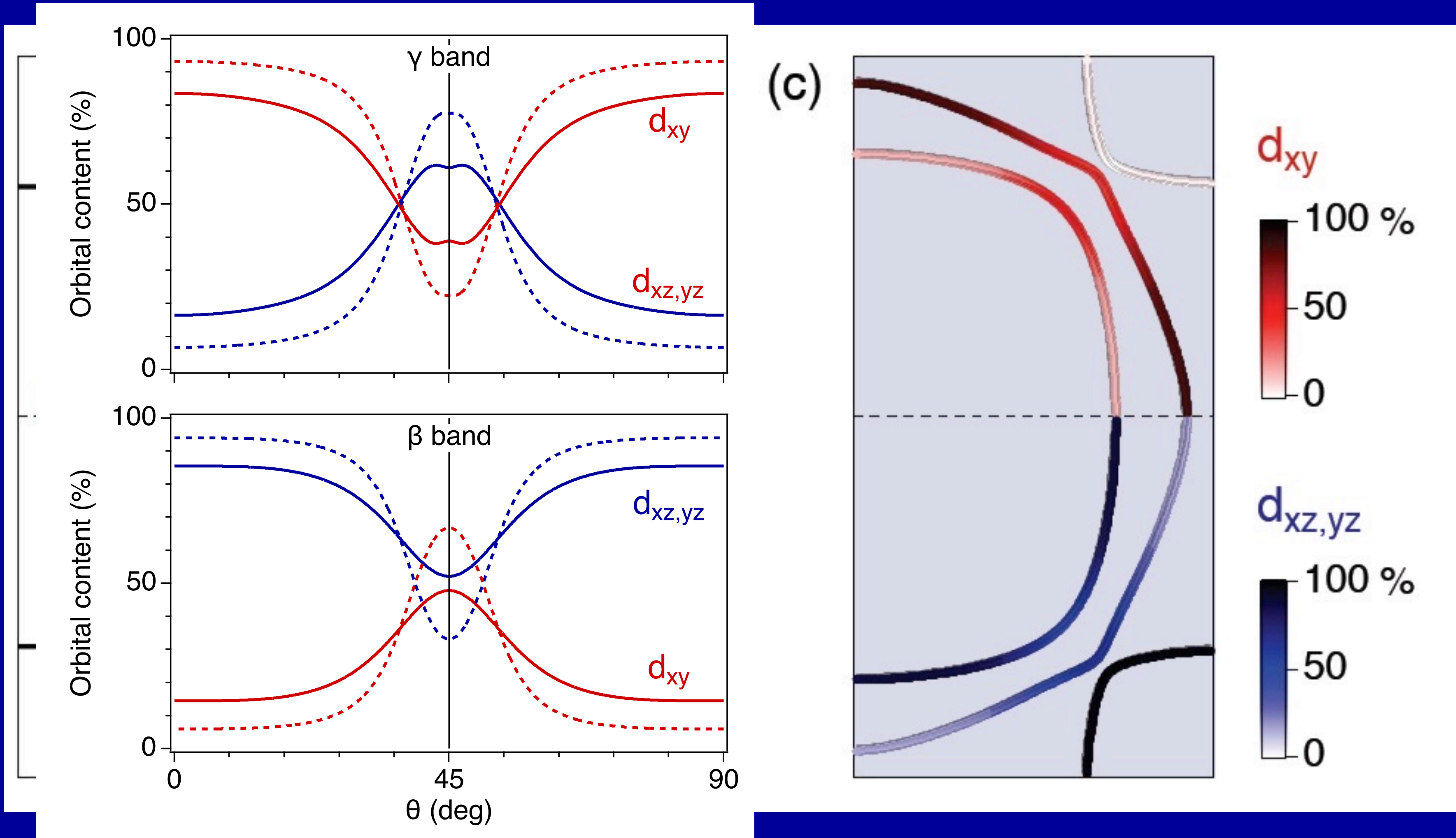
$$\boxed{\Sigma_{\nu\nu'}(\omega,\mathbf{k}) = \sum_{mm'} \langle\psi_\nu^{\mathbf{k}}|\chi_m^{\mathbf{k}}\rangle\, \Sigma_{mm'}(\omega)\, \langle\chi_{m'}^{\mathbf{k}}|\psi_{\nu'}^{\mathbf{k}}\rangle}$$

Self-energy \`upfolded' to the whole system (k-dependent)

Orbital content of Bloch states (k-dep)

Local self-energy

Orbital Content of Quasiparticle States is strongly angular dependent due to spin-orbit

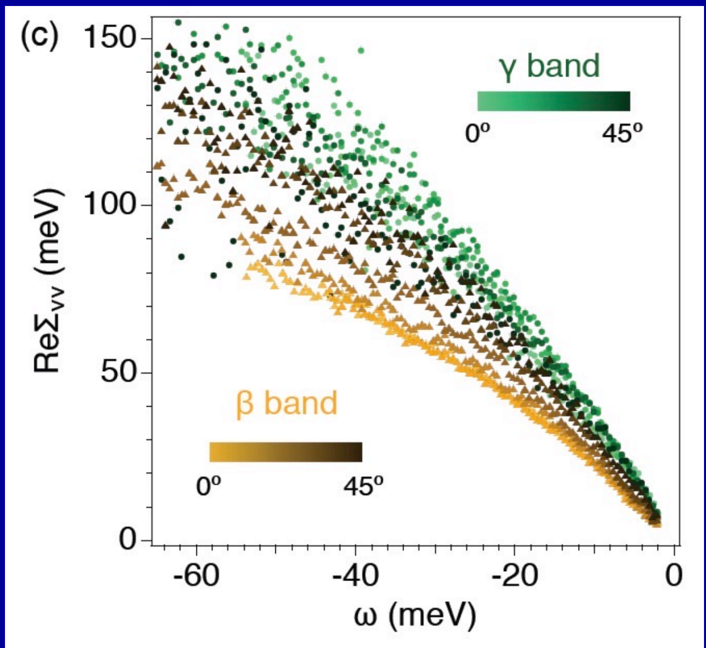


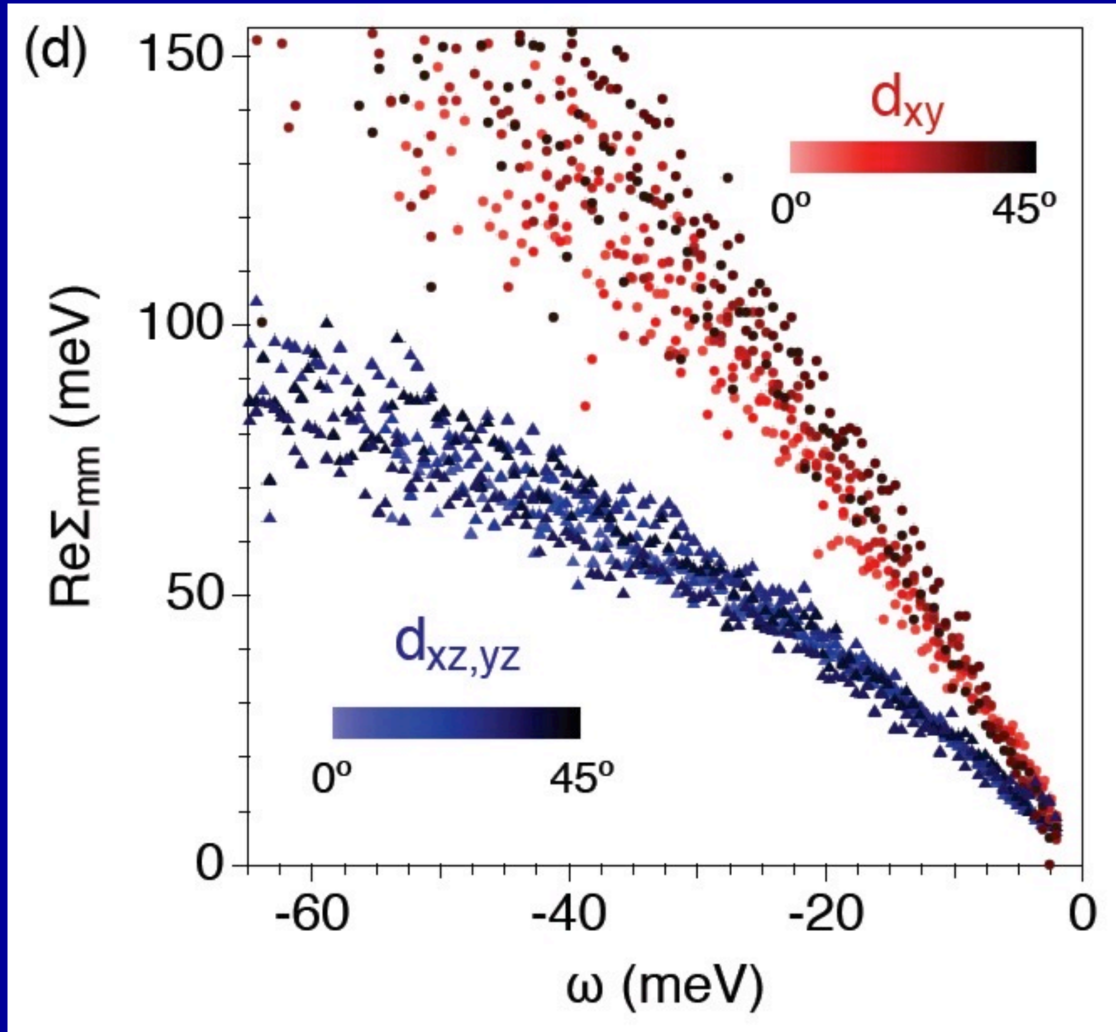
DMFT prediction (Pavarini et al PRL 2016; Kim et al. PRL 2018):
Effective enhancement $\Delta\lambda$ of SOC → Confirmed by experiments!

~ In orbital basis: Collapse of data corresponding to different angles !

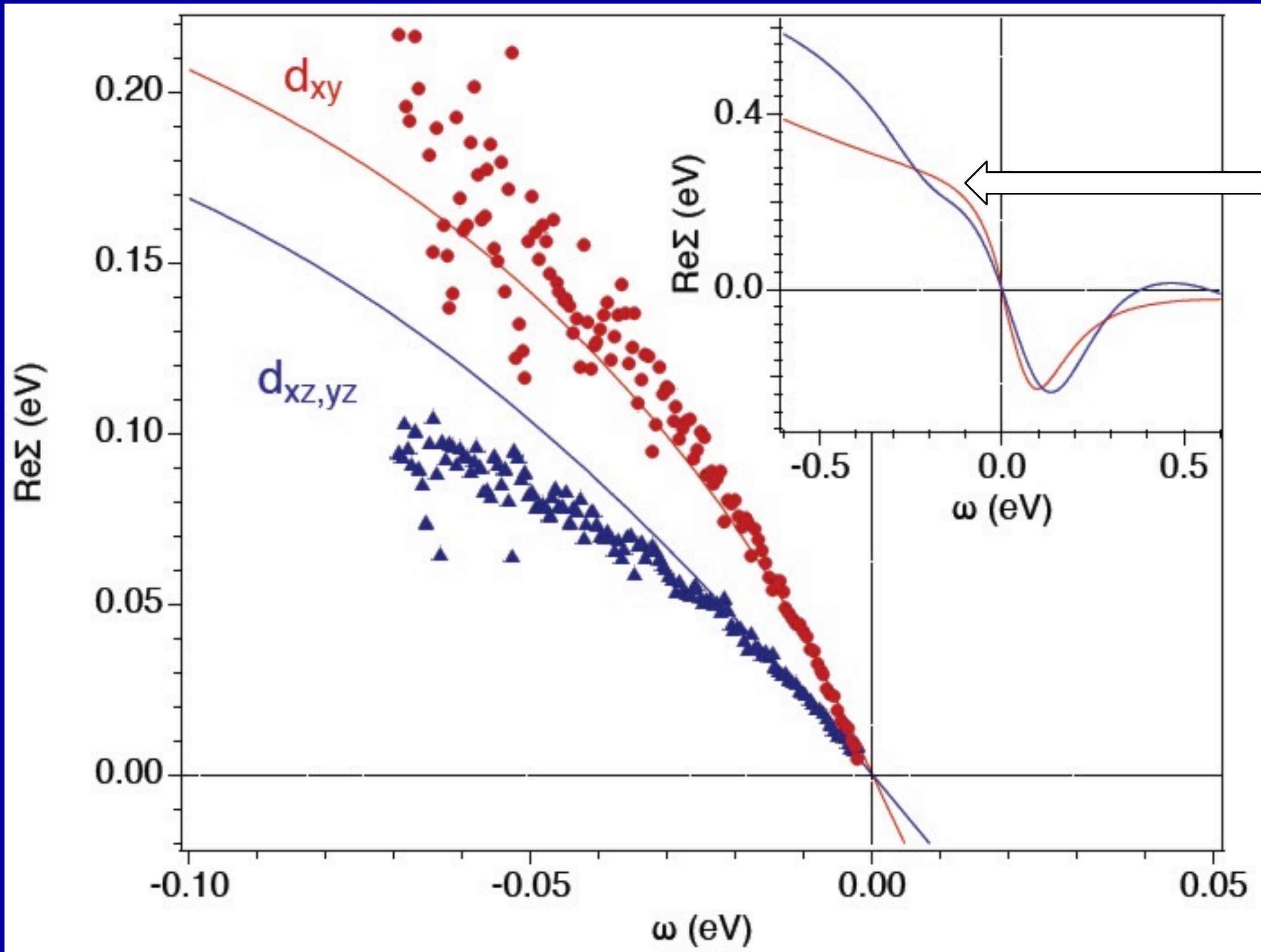
→ DMFT `Locality *ansatz*' is a good approximation

In contrast: strong angular dependence in band basis!





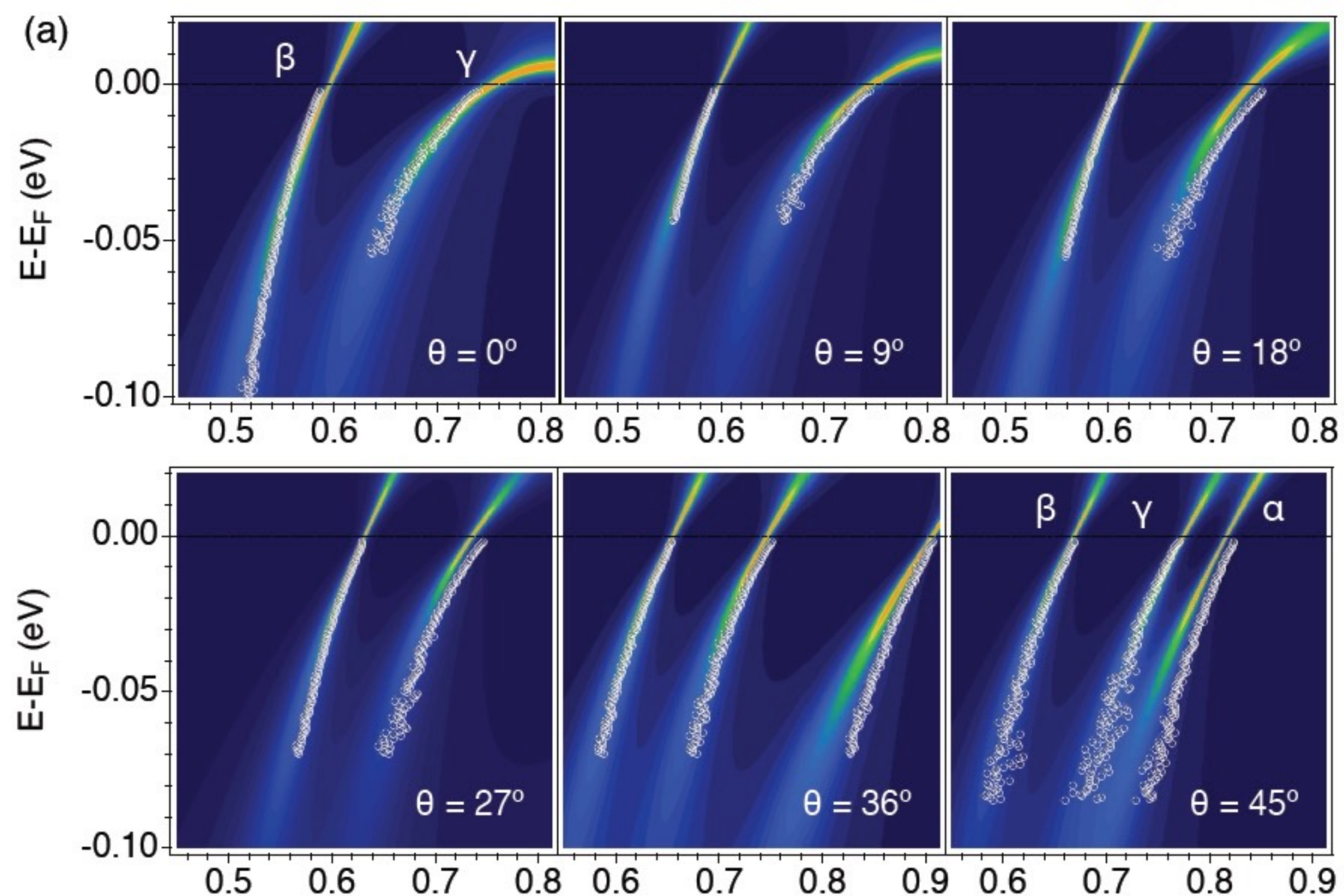
Comparison to LDA+DMFT self-energies



Kink
(electronic
origin
at ~ 100meV)

Comparing DMFT to ARPES

(Dots: ARPES MDCs. Colors: DMFT spectral intensity)



So we have learnt/discovered that:

- The locality assumption behind DMFT can be quite accurate even in a quasi-2D system
- → Why?
- The Hund coupling can be the main source of strong correlations
- → This is just the tip of the iceberg: A broad class of materials are indeed `Hund metals' !
- Other features of electronic structure have an interplay with strong correlations, such as a an Hove singularity
- [Mention SOC]

Reconciling locality with the nature of Spin Fluctuations in Sr_2RuO_4

Sidis et al. PRL 1999 (PhD thesis)

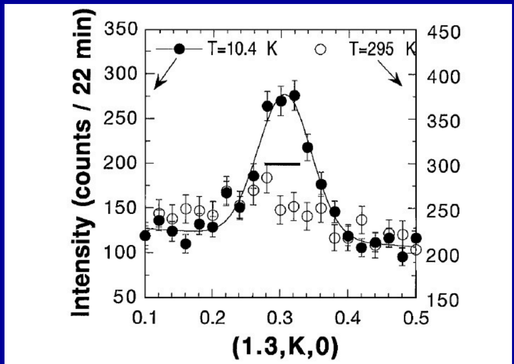
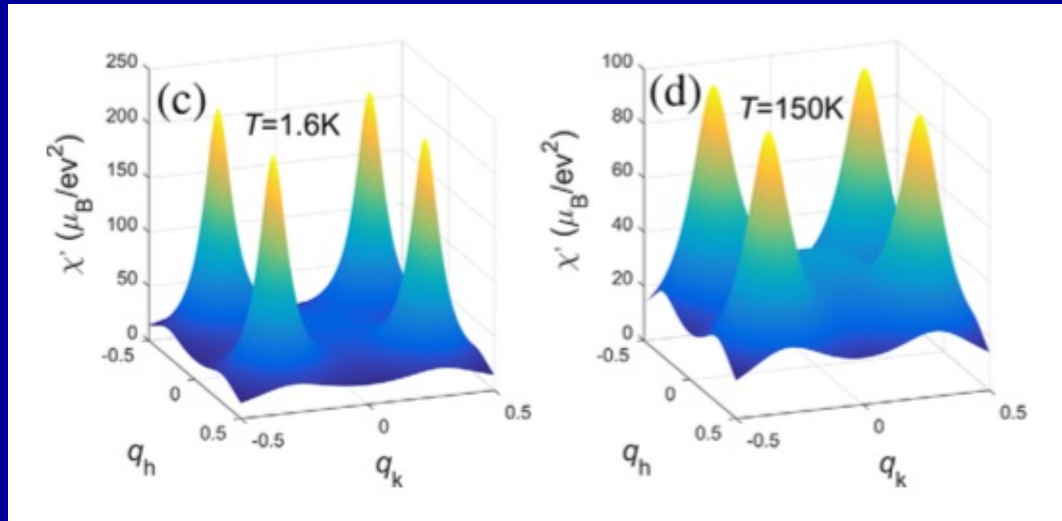


FIG. 1. Constant-ω scans performed at $\hbar\omega = 6.2$ meV around $\mathbf{Q} = (1.3, 0.3, 0)$ along the $(0, 1, 0)$ direction: $T = 10.4$ K (•), $T = 295$ K (∘).



Two-component Spin response:
(Neutrons, Steffens et al. PRL 122, 047004 (2019)):

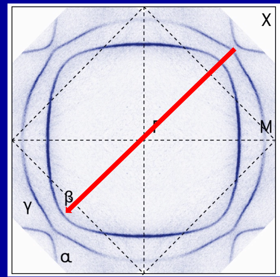
- SDW incommensurate peaks: correlation length is only ~2.5 lattice spacing at T=1.6K
- Broad signal centered at Q=0, w/ width ½ of zone and carrying substantial spectral weight

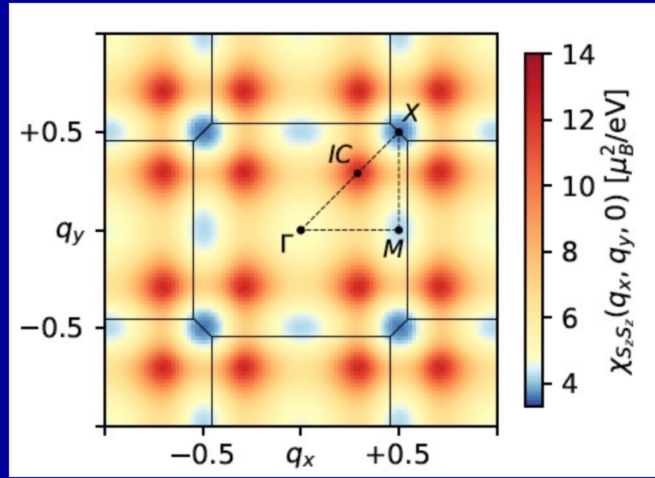
Comparison to DMFT calculations links this broad part of the spectrum to local spin fluctuations enhanced by Hund's coupling

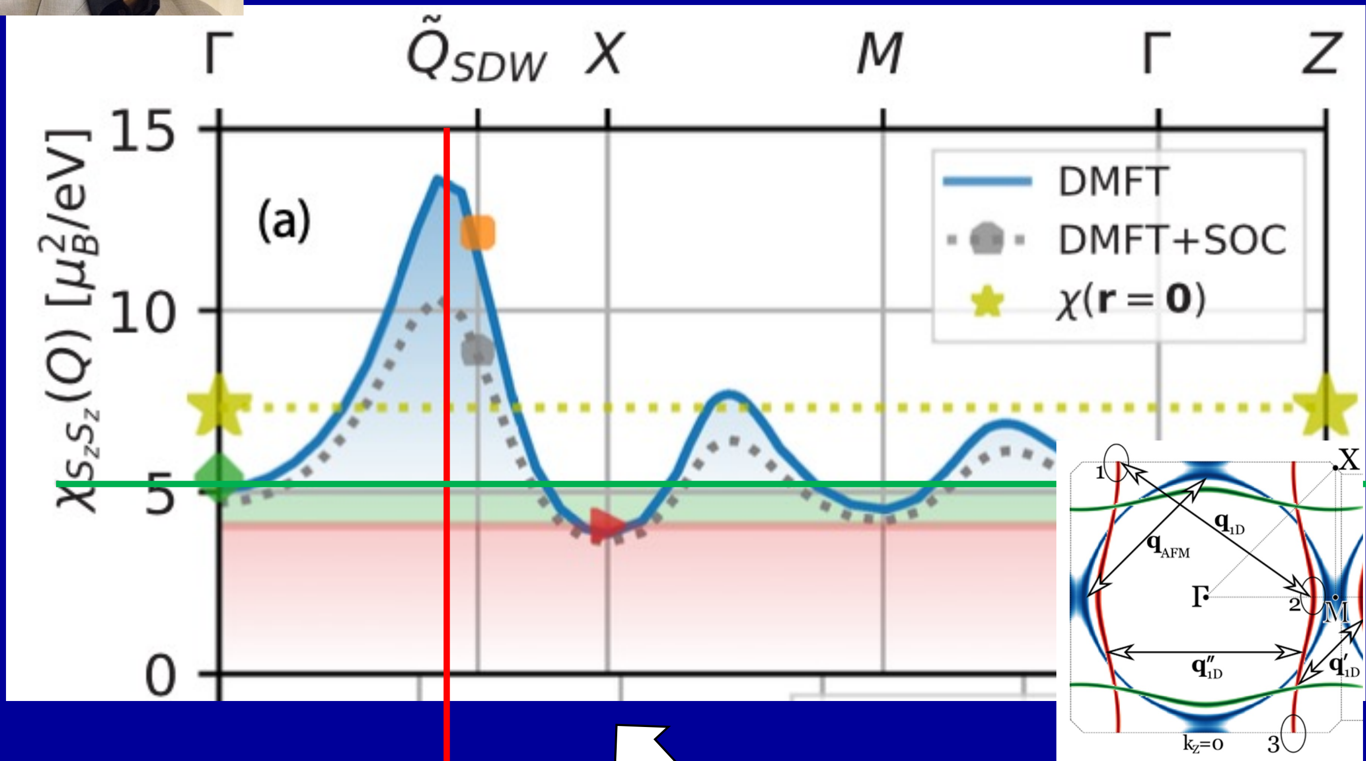
$\chi(\vec{Q})$ from DMFT w/ full vertex

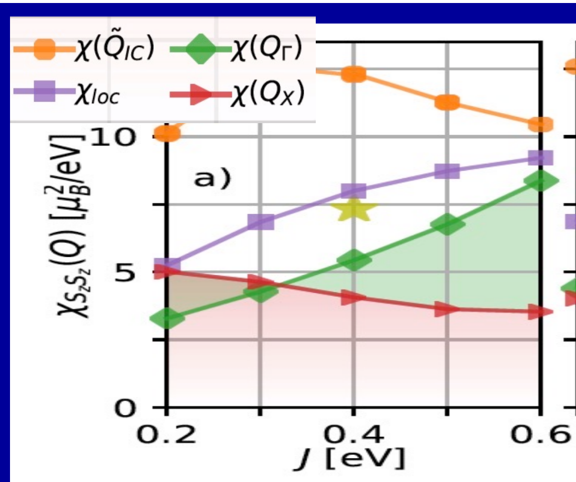
Strand et al. PRB 100, 125120 (2019)

Hugo Strand
CCQ → Orebrö









Q-independent Background: Hund's metal spin dynamics

Q_{SDW}

Response at X=(π,π) is SUPPRESSED: NOT captured by RPA

Physics
Today
April 2024

Antoine Georges is a professor of physics at the Collège de France in Paris and director of the Center for Computational Quantum Physics of the Flatiron Institute, Simons Foundation, in New York City. He is also affiliated with the University of Geneva in Switzerland and École Polytechnique in Palaiseau, France. **Gabriel Kotliar** is a Board of Governors Professor of physics at Rutgers University in Piscataway, New Jersey, and is also affiliated with Brookhaven National Laboratory.

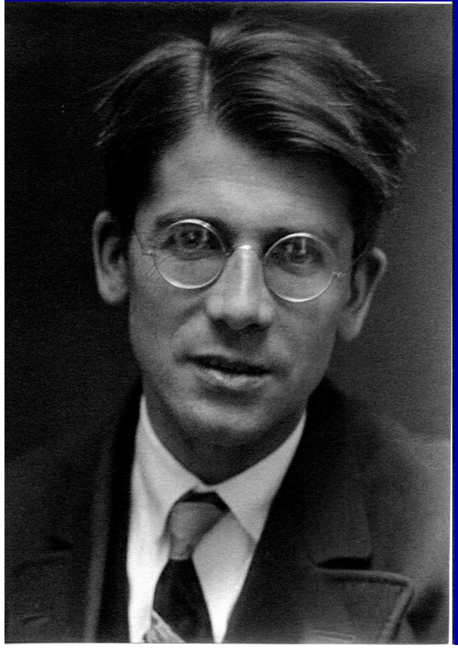
The Hund-metal path to strong electronic correlations

Antoine Georges and Gabriel Kotliar

A new type of metal has taken the scientific community by surprise. Classic concepts from atomic physics—the electrons' orbitals and spin alignment—are key to understanding it.

The Platters said:

« Only U can do make all this world seem right… »



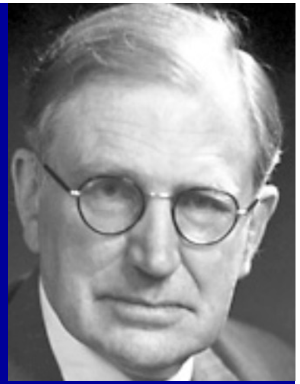
… Take-home message of this talk:
« Not only U, also J_{Hund} » !

Friedrich Hund
1896-1997

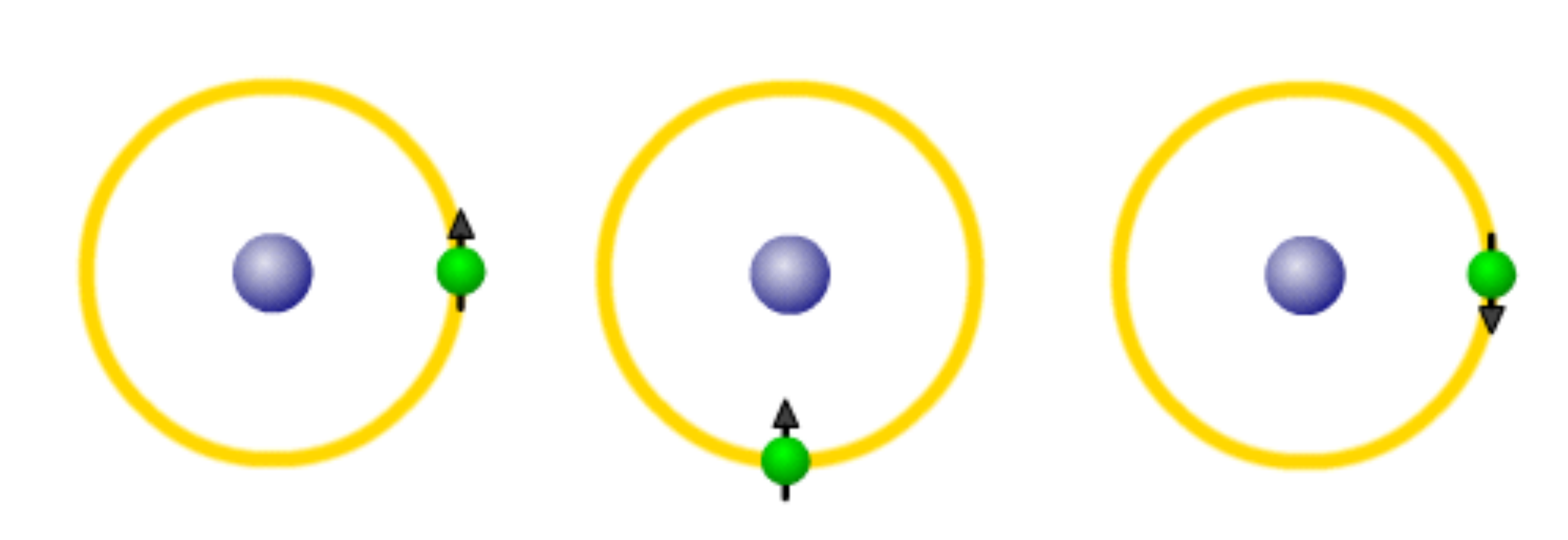
Two Classic Routes to Strong Correlations

- Mott Insulators and Metals close to the Mott transition: Hubbard U prevents electrons to move/blocks charge degrees of freedom
- Heavy Fermion Materials: Two fluids of electrons – localized and itinerant. Their hybridization impeded by U lead to very large quasiparticle masses (Kondo effect)

Strong Electronic Correlations: The Mott Route



Nevil Mott



U < t: Metal indeed (1/2-filled band)

U > t: Motion BLOCKED by repulsive interaction

→ INSULATOR

Mott insulators: charge blocking due to repulsive interaction → an incompressible state of matter!

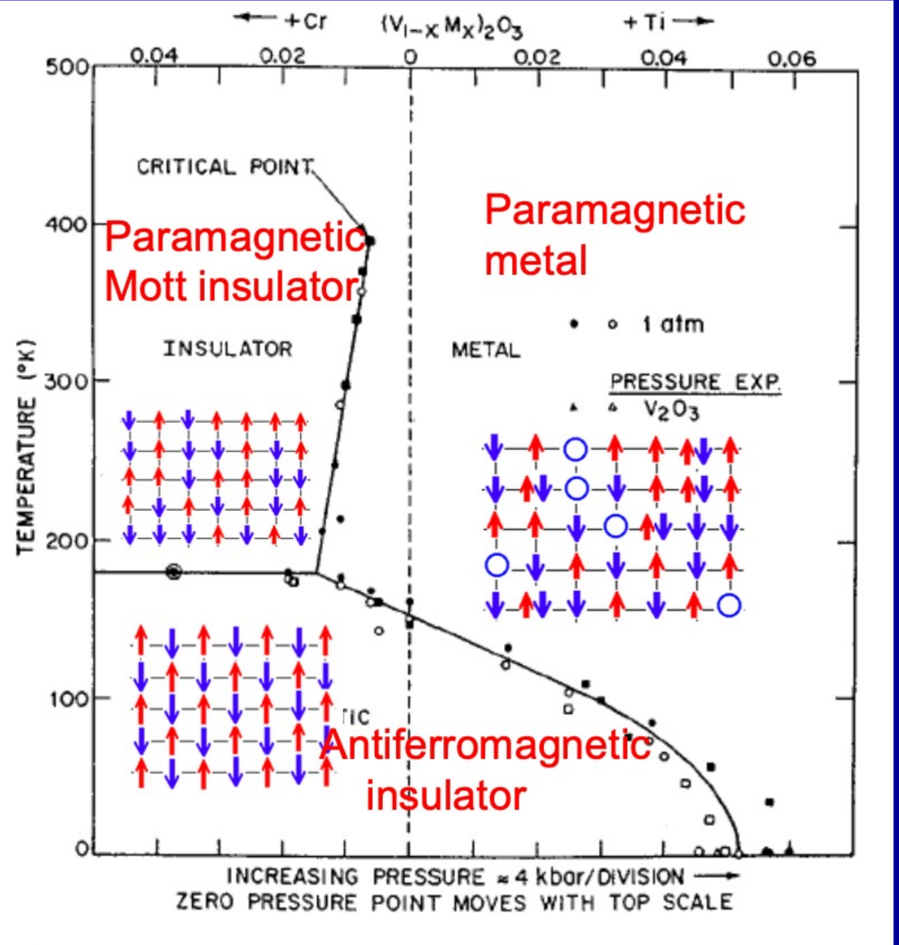
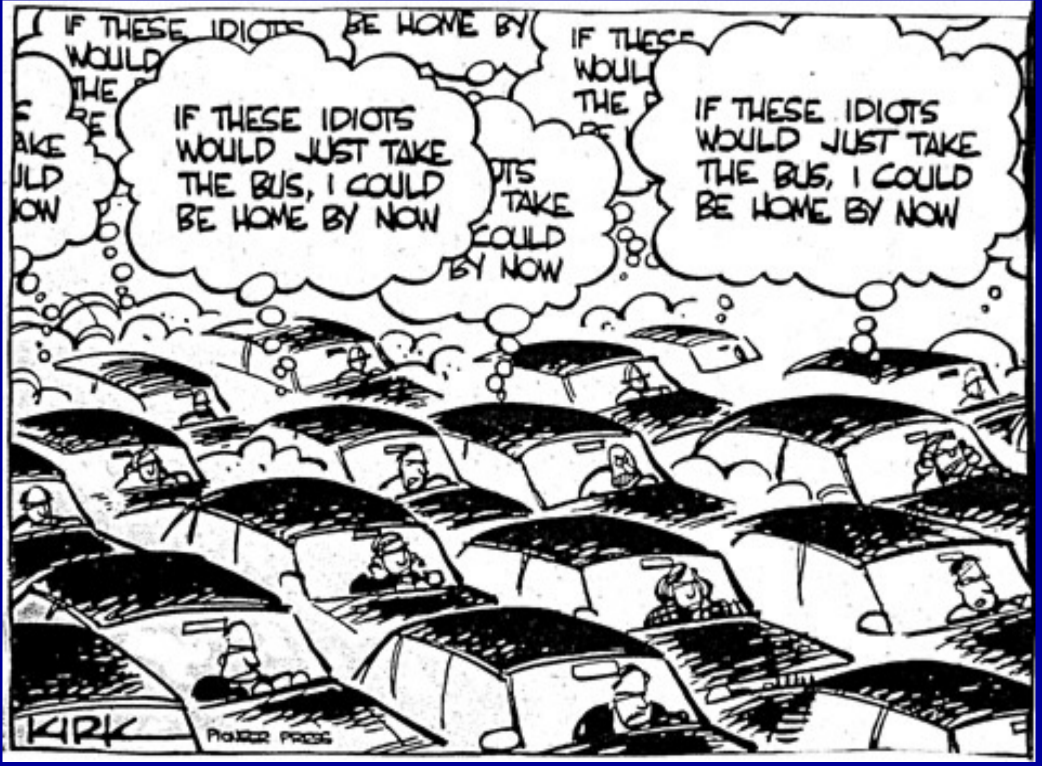


FIG. 70. Phase diagram for doped V_2O_3 systems, $(V_{1-x}Cr_x)_2O_3$ and $(V_{1-x}Ti_x)_2O_3$. From McWhan *et al.*, 1971, 1973.



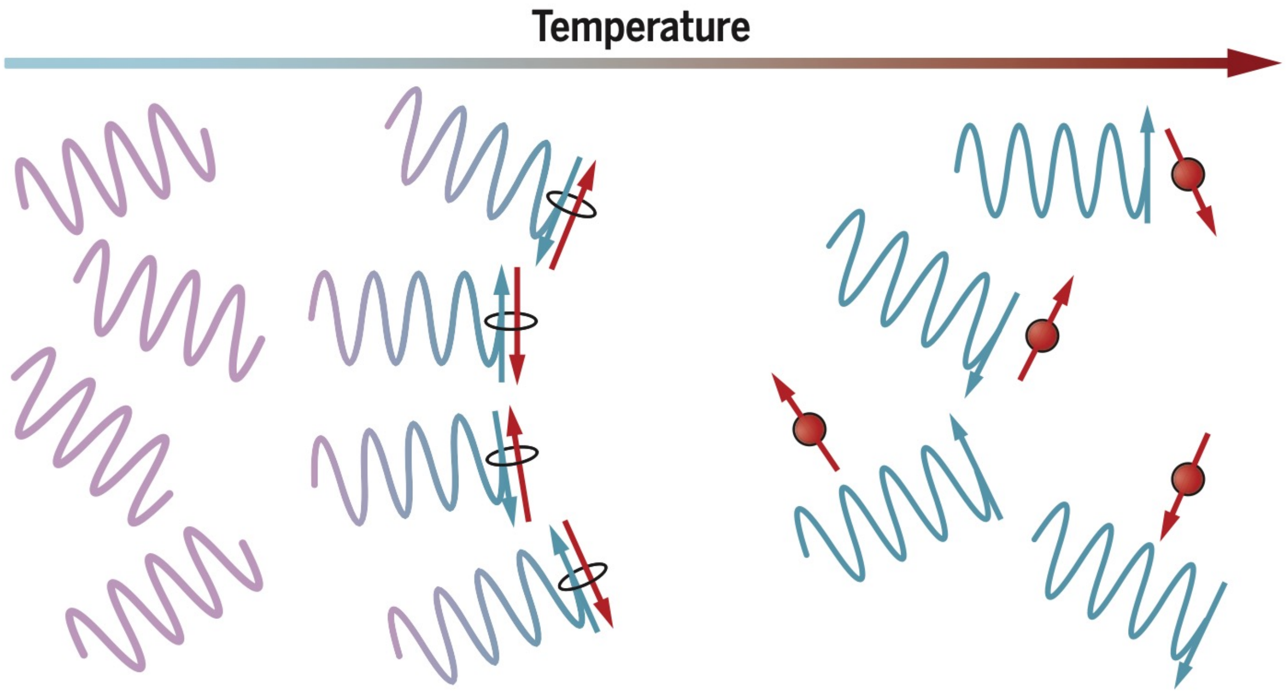
Analogy: Yoshi Maeno

Conventional (Band) Insulators:
No carriers
(~ Dry River)

Mott Insulators:
Charge carriers are BLOCKED by their mutual interactions
~ Frozen River

Heavy Fermions: From High to Low Energy

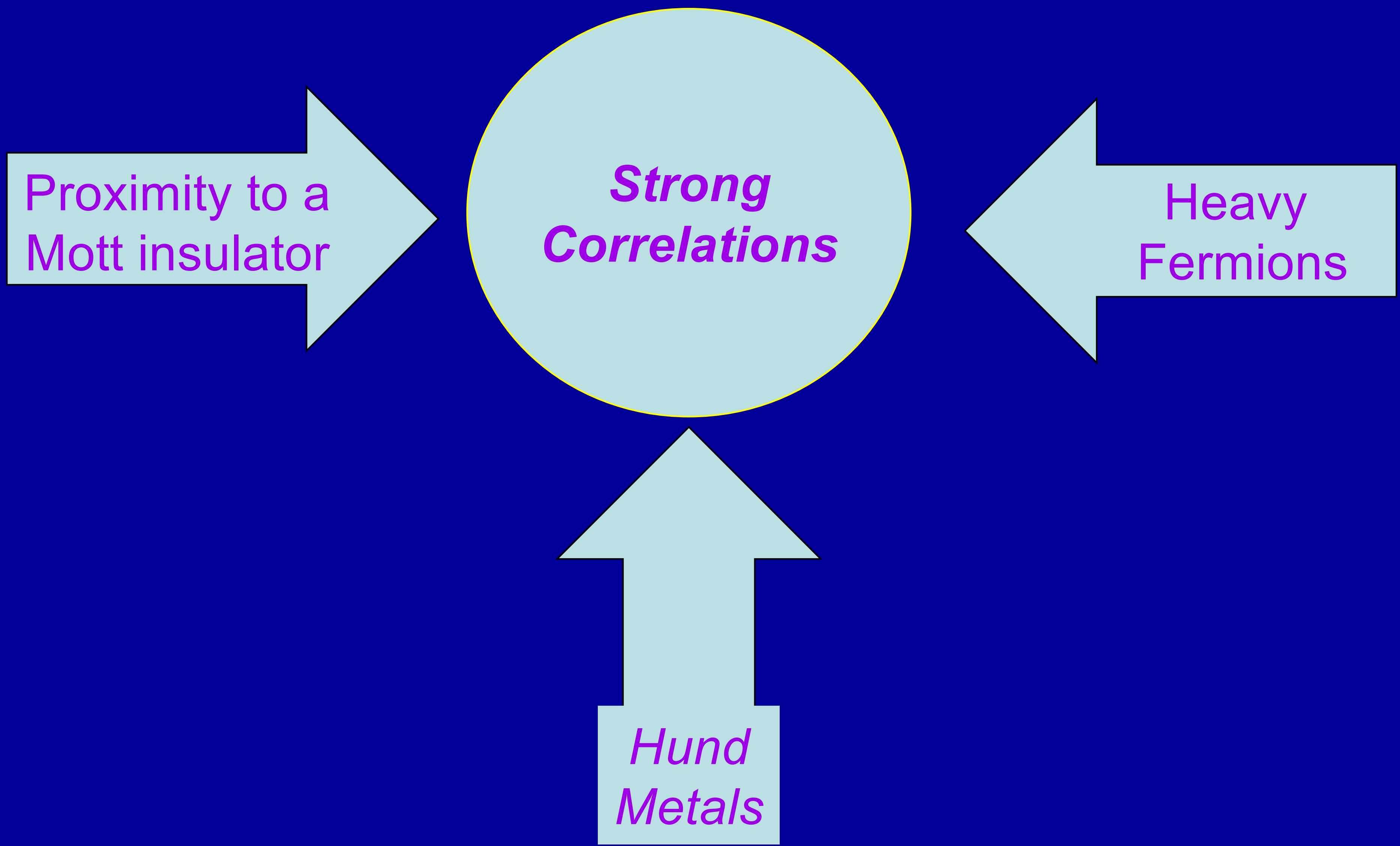
In the cerium-palladium compound ($CePd_3$) studied by Goremychkin *et al*., coherent wavelike excitations emerge at low energy, as a result of the entanglement between conduction electrons and localized spins.



Progressive binding of conduction electrons to Ce 4f electron spins lead to coherent (wavelike) excitations at low energy.

At high energy, the localized spins of the Ce 4f electrons interact weakly with the wavelike delocalized conduction electrons.

Hund Metals: A distinct route to strong electronic correlations



The big and happy family of `Hund Metals'

- Oxides of 4d Transition Metals e.g. Sr_2RuO_4
- Iron-Based Superconductors
- In the case of Sr2RuO4, proximity to van Hove singularity also plays an important role, cf. comparison to Sr_2MoO_4 Karp et al. 125, 166401 (2020)
- Hund Metals: Haule and Kotliar New J. Phys. 11, 025021 (2009); Werner, Gull, Troyer and Millis, PRL 101, 166405 (2008); Mravlje et al. PRL106, 096401 (2011); Yin, Haule and Kotliar Nat Mat 10, 932 (2011); de'Medici et al. PRL 107, 256401 (2011); AG, de'Medici and Mravlje, Ann Rev Cond. Mat. Phys Vol 4 (2013), and many more…
- Precursor articles: D.*van der Marel and G.Sawatzky PRB 37 (1988) 10674; A.Fujimori et al. PRB 44, 163 (1991)*

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Manuel Zingl

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Formerly at Collège de France,
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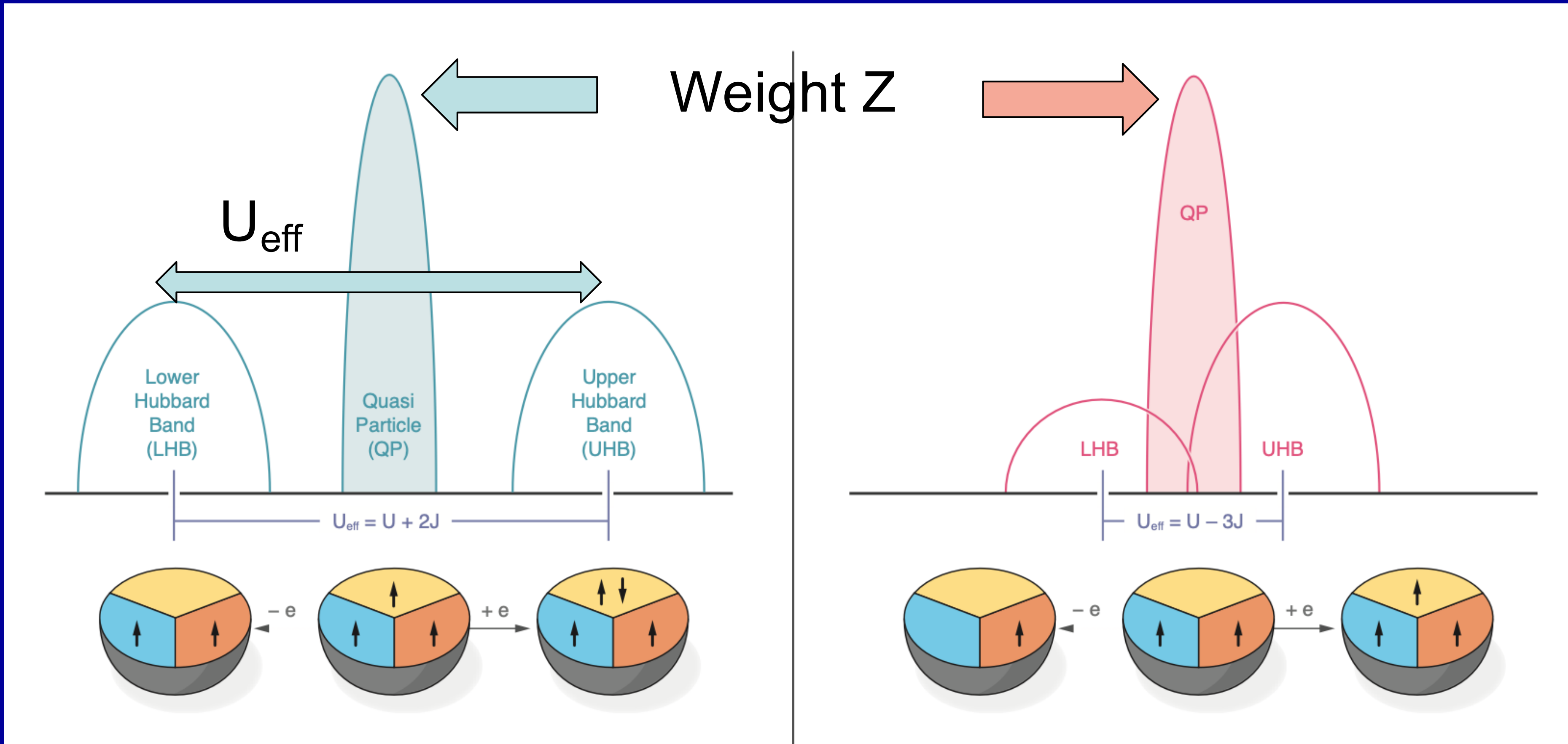
Fabian
Kugler

F.Baumberger, A.Tamai (ARPES, Geneva)

→ *Review article*
(Annual Reviews, Vol.4, 2013)
arXiv:1207.3033

Thanks also to:
S.Beck, M.Ferrero,
O.Gingras, Seung-Sup Lee,
J. Von Delft, O.Parcollet,
H.Strand, P.Hansmann,…

Spectroscopy: Mott vs. Hund



Half-Filled Shell
[Mott]

Non Half-Filled
[Hund]

U_{eff} and the MIT

cf. van der Marel&Sawatzky PRB 37 (1988) 10674 ; L. de' Medici PRB 83 (2011) 205112; A.Fujimori et al. PRB 44, 163 (1991)

N electrons in M orbitals ($0 \leq N \leq 2M$)

1) If M<N (or M>N) non half-filled shell: only the interaction between parallel spins matters U'-J=U-3J

$$U_{\text{eff}} = (U' - J)\left[\frac{(N+1)N}{2} + \frac{(N-1)(N-2)}{2} - 2\frac{N(N-1)}{2}\right] = U - 3J$$

U_{eff} = U' = U-3J

The Hund's coupling <u>reduces</u> U_{eff}

2) If N=M (half-filled shell)

$$|\uparrow\downarrow,\uparrow,\uparrow\rangle$$

$$E_0(N+1) = (U' - J)\frac{N(N-1)}{2} + U + U'(N-1)$$

$$U_{\text{eff}} = (U' - J)\left[\frac{N(N-1)}{2} + \frac{(N-1)(N-2)}{2} - 2\frac{N(N-1)}{2}\right] + U + U'(N-1)$$

$$= U + (N-1)J$$

U_{eff} = U+(N-1)J

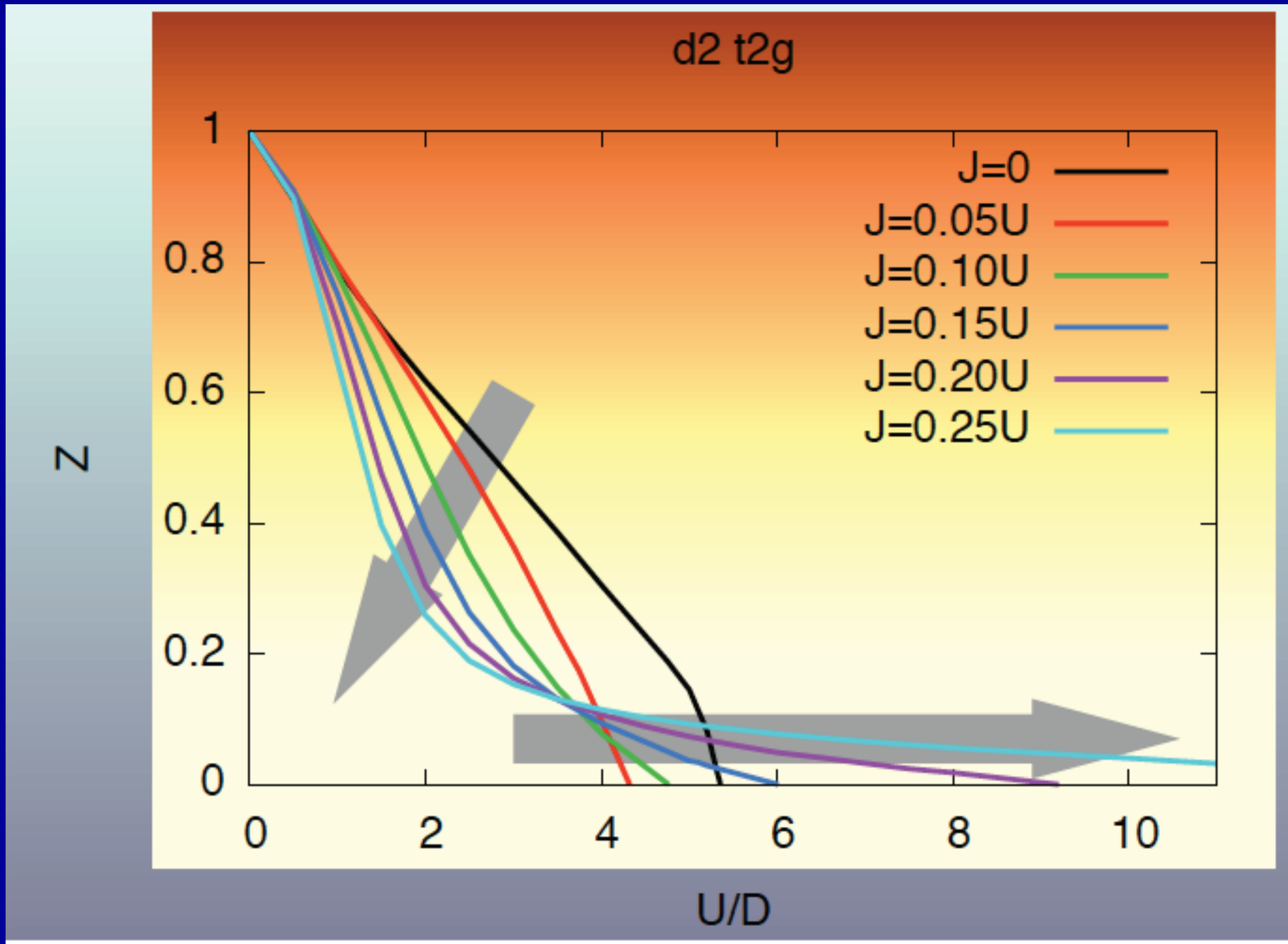
The Hund's coupling <u>increases</u> U_{eff}

→ Half-filled (sub)shells are usually robust Mott insulators

For all filling except ½-filling and a single electron and hole:

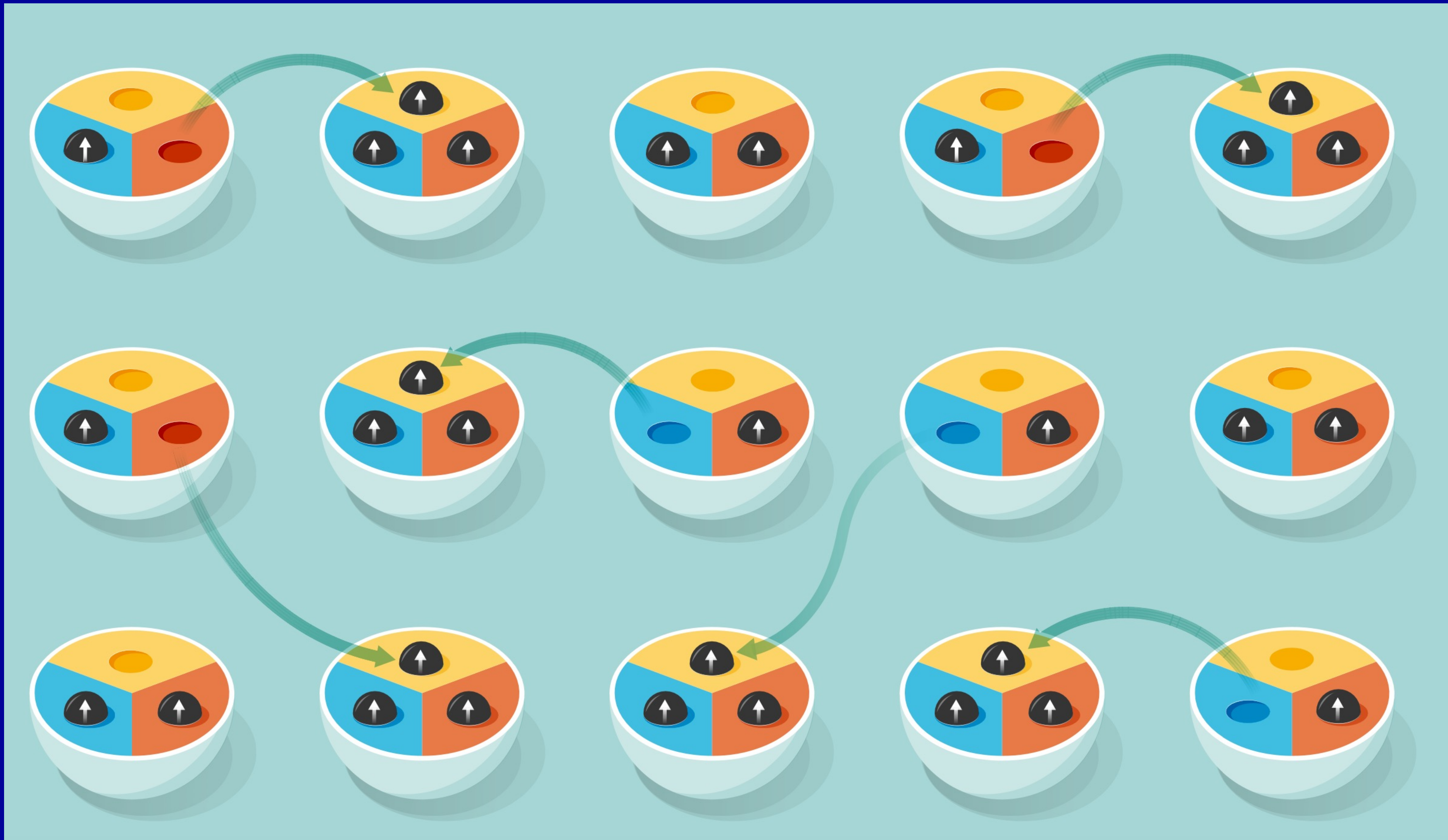
Hund's coupling suppresses coherence scale →

Reduces quasiparticle coherence scale, smaller Z, larger m*/m



But also increases U_c → Enhances range of metallic state

Spin Blocking → Reduced Phase Space → Lower Z, Enhanced Mass



Hence, the Hund coupling has two antagonistic effects (if not ½ filling)

- Drives the system

away from the Mott state

- But at the same time lowers the quasiparticle coherence scale

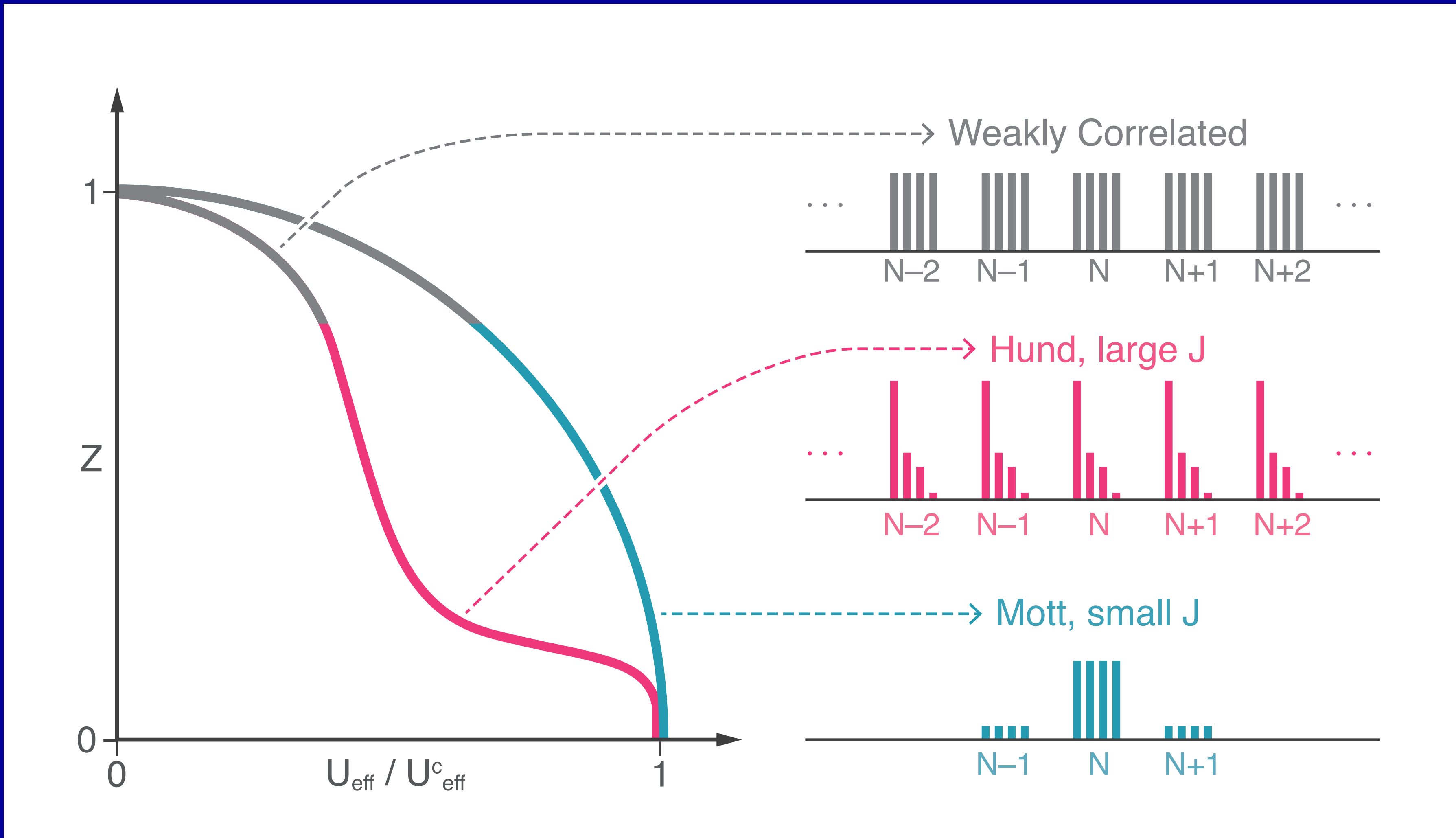
(below which the local atomic multiplet is quenched)

i.e makes the metal more correlated

PRL **107,** 256401 (2011) PHYSICAL REVIEW LETTERS week ending 16 DECEMBER 2011

Janus-Faced Influence of Hund's Rule Coupling in Strongly Correlated Materials

Luca de' Medici,[1] Jernej Mravlje,[2,3,4] and Antoine Georges[2,4,5,6]

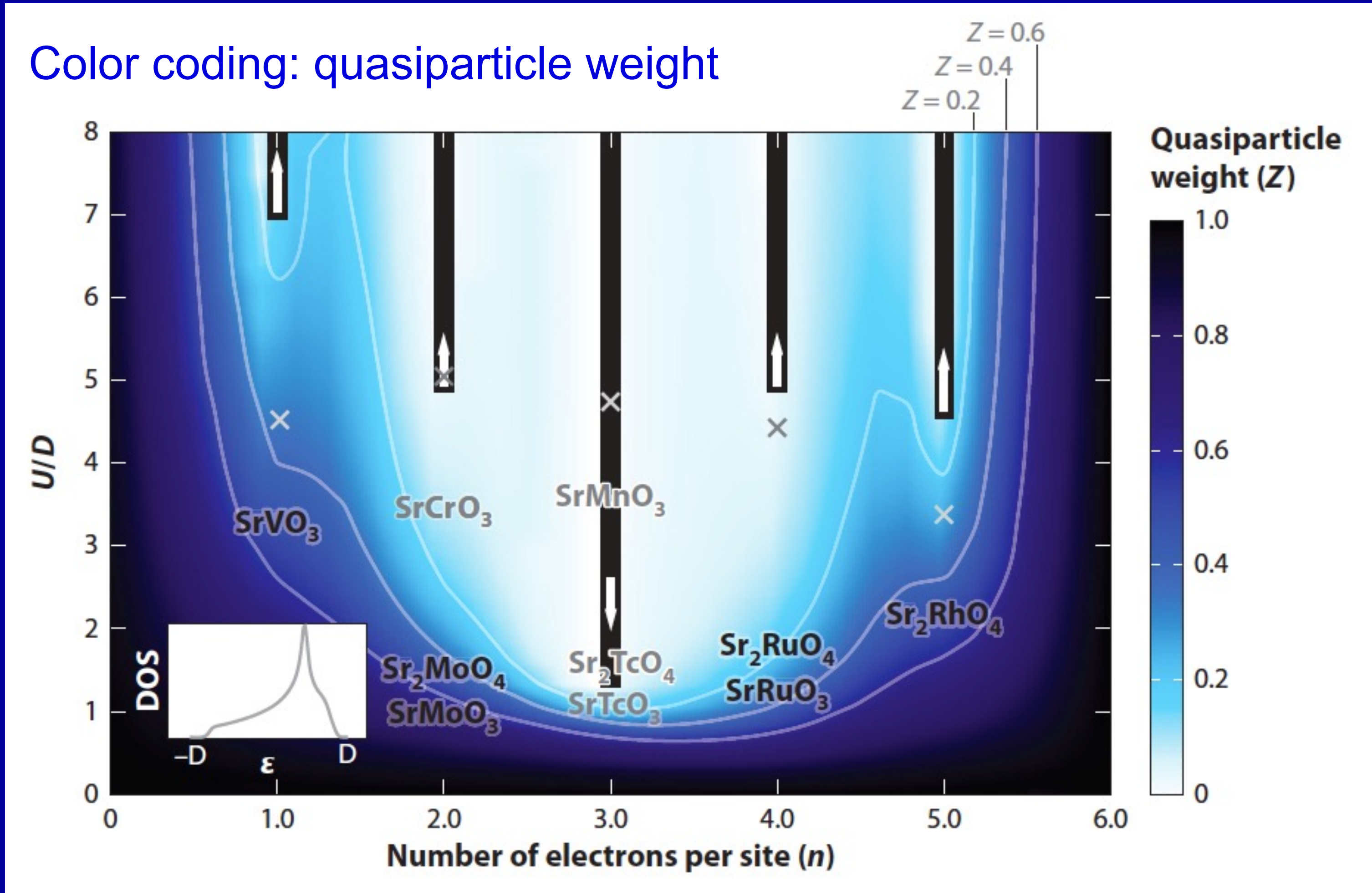


Histogram of atomic configurations
in the ground-state

Correlation effects in 4d oxides due to J, not to Mott physics

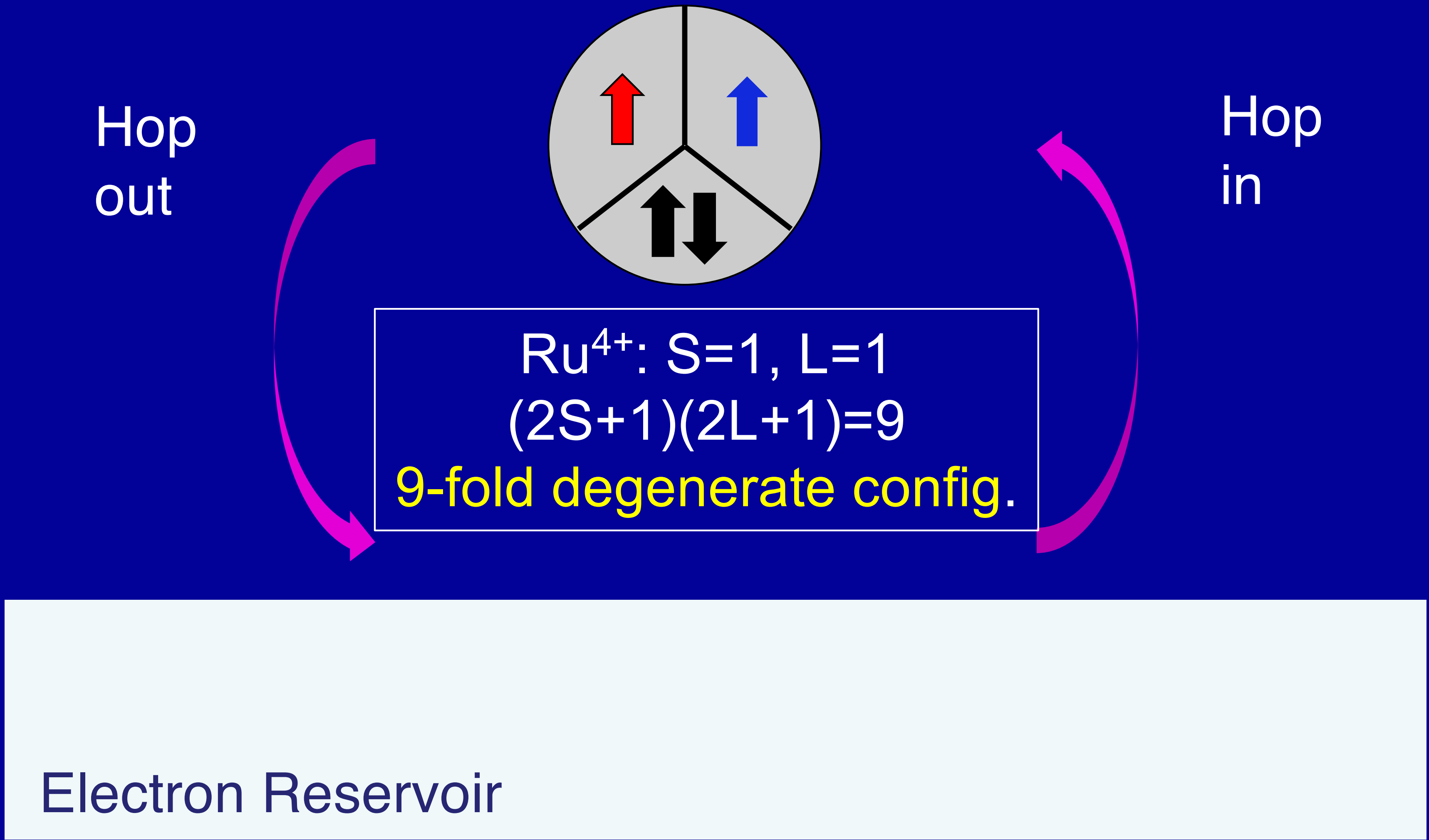
(except when ½ filled shell or strong Xtal field between orbitals)

3d oxides: U/D ~ 4
4d oxides: U/D ~ 2



Hund metals: Werner, Gull, Troyer and Millis PRL 2008; Haule and Kotliar NJP 2009; Review: A.G., de'Medici and Mravlje, Annual Reviews Cond. Mat Phys (2013)

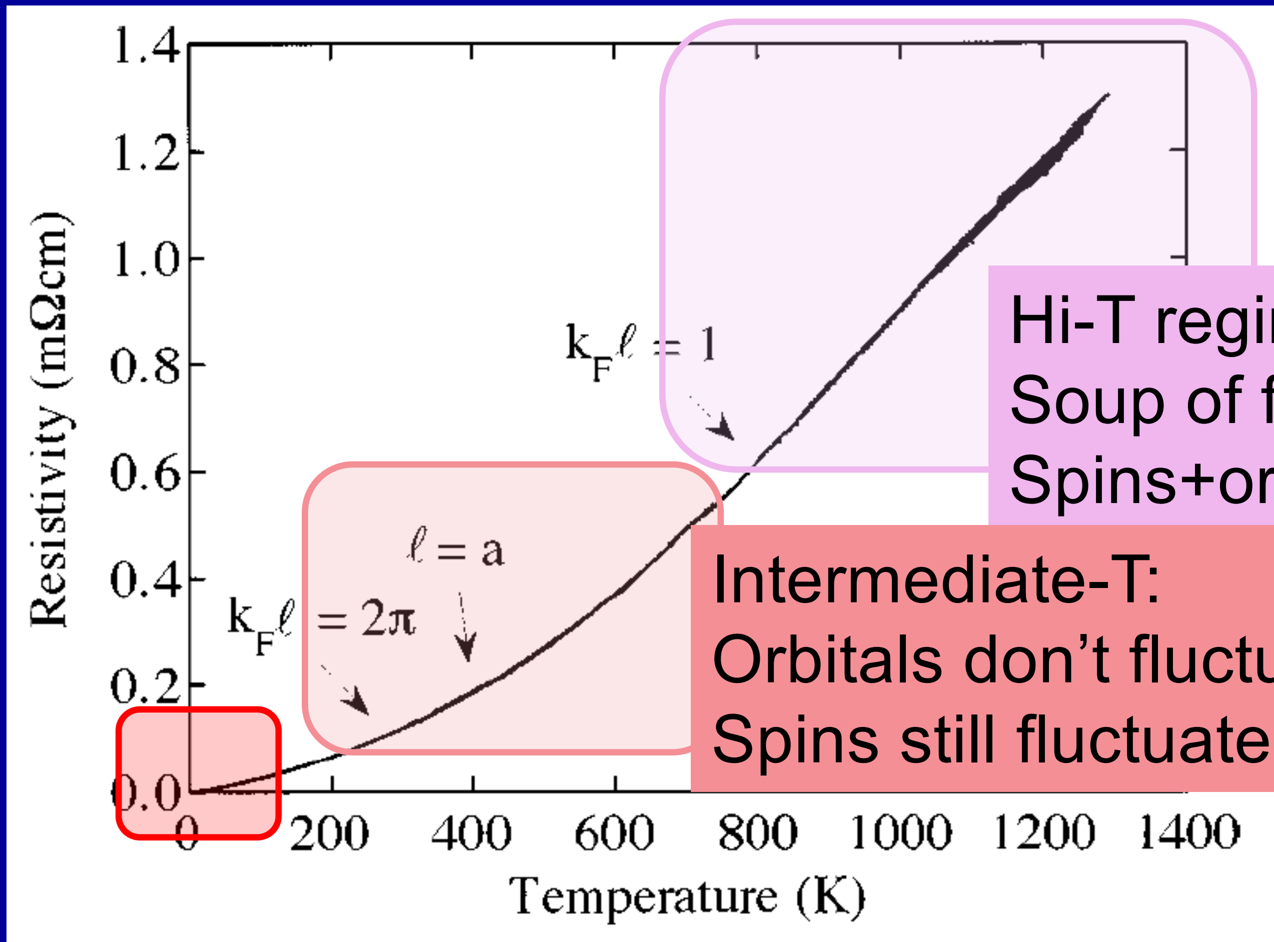
Distinct Scales for Orbital and Spin Fluctuations



Hund's metals: distinct crossover scales for orbital and spin degrees of freedom

Now beautifully understood from a renormalization-group perspective, cf. work by von Delft, Kotliar, Aron et al. and Mravlje et al.

Spin-Orbital Separation and Transport Crossovers

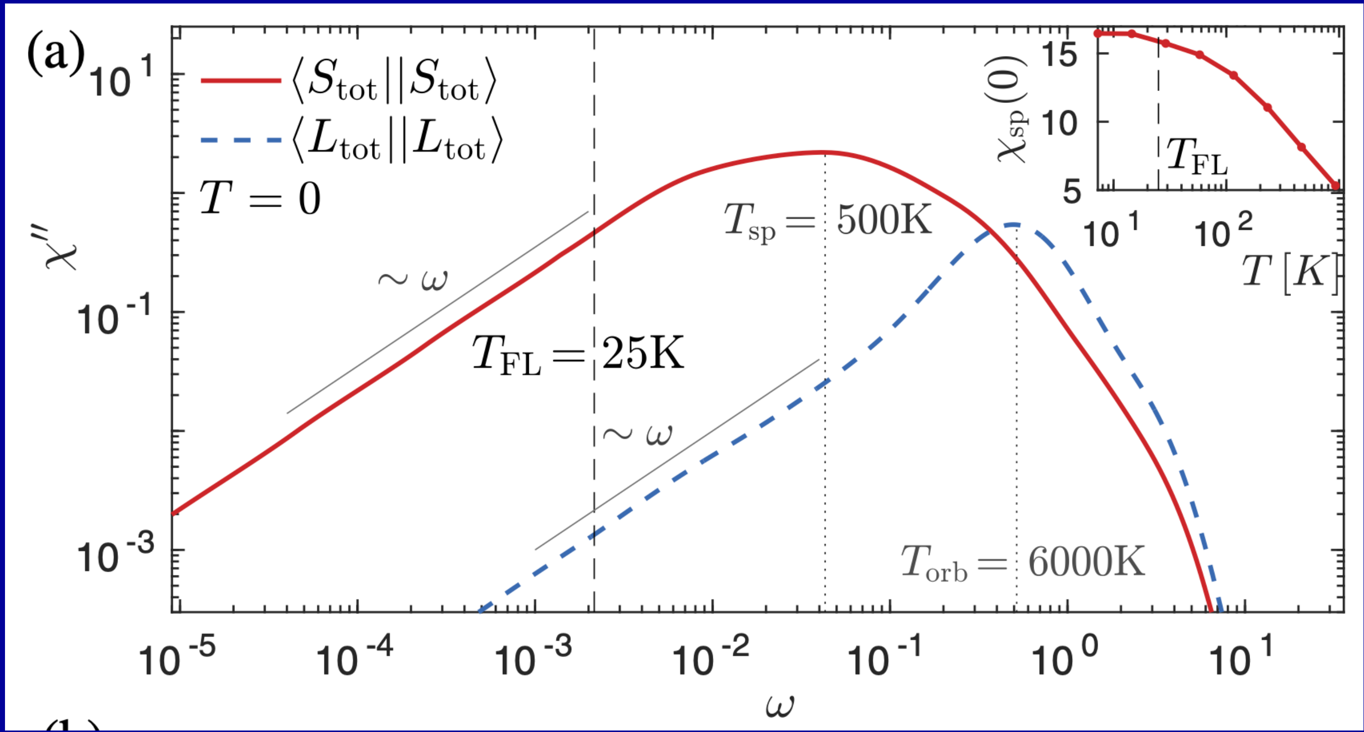


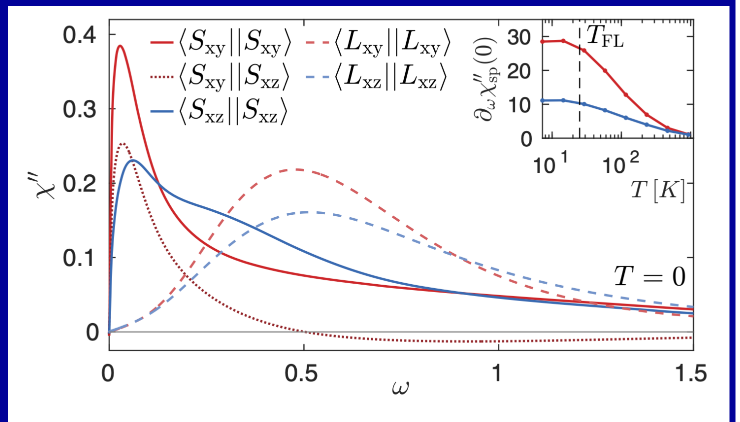
Hi-T regime:
Soup of fluctuating
Spins+orbitals

Intermediate-T:
Orbitals don't fluctuate
Spins still fluctuate

Low-T Fermi Liquid:
Spins and Orbitals
Have Pauli susceptibilities

Sr_2RuO_4: DMFT+Wilson RG

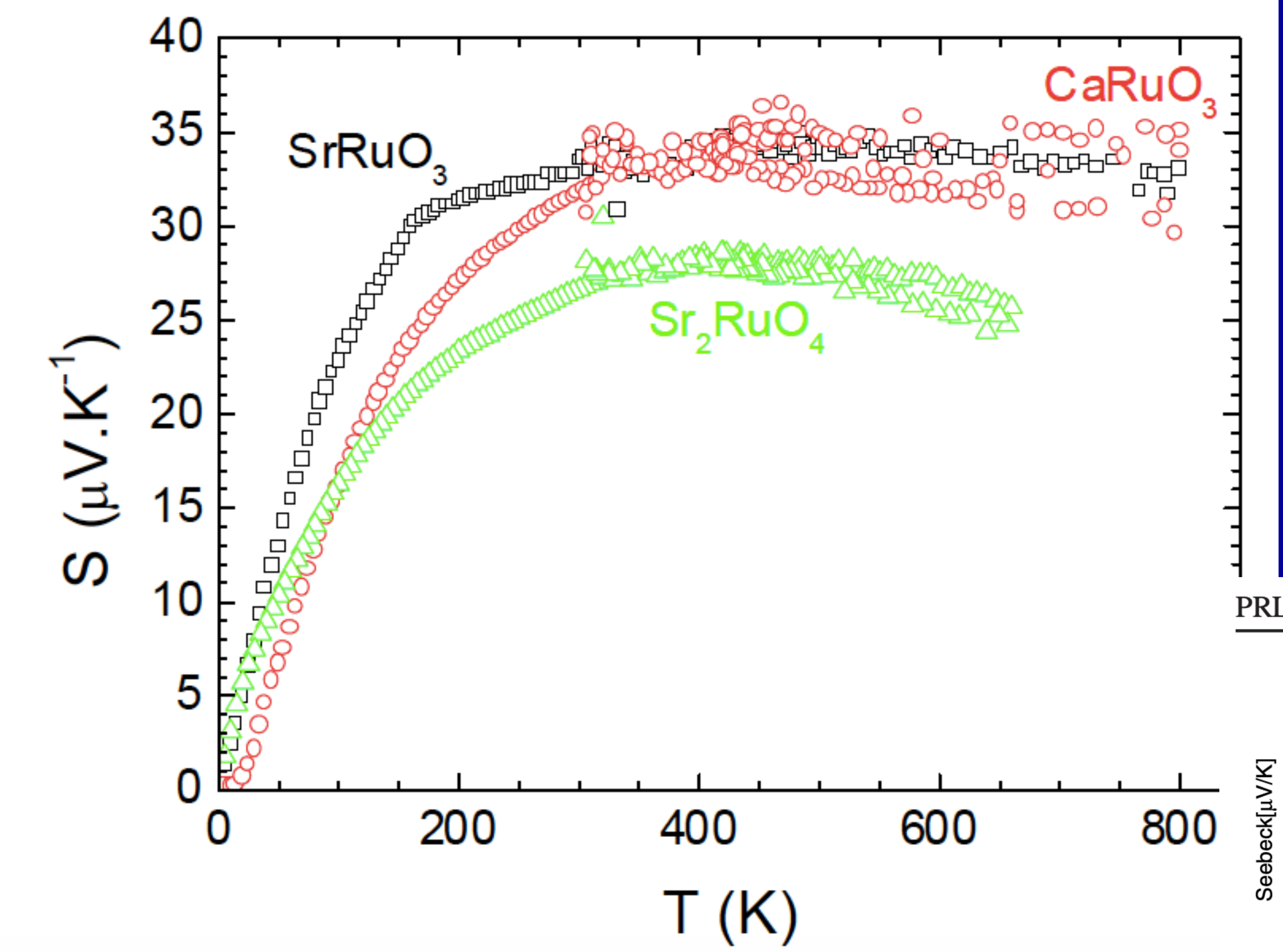




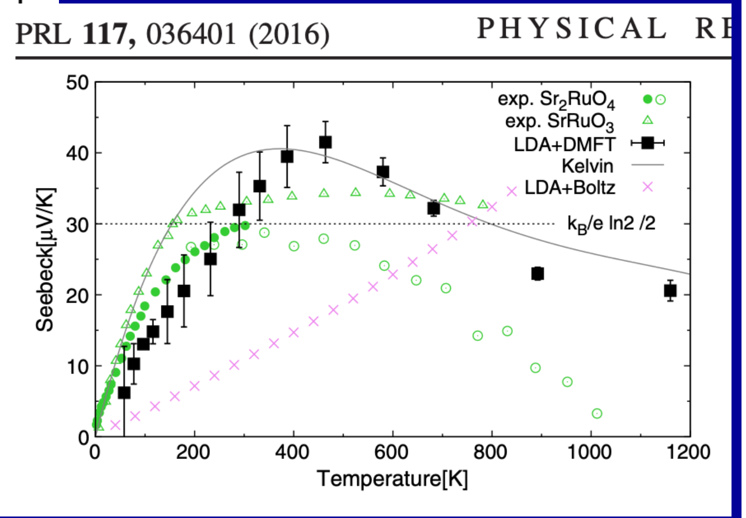
Kugler et al.
PRL (2020)

Ruthenates: Seebeck $S \equiv -\Delta V/\Delta T$

Yoshino et al. JPSJ 1996, Fu et al. PRL 2008, Keawprak Mat Trans 2008, Klein et al. PRB 2006; Present graph from Klein PhD thesis, Caen, 2006



Conspicuous plateau at ~ 25-35μV/K around room temperature



	Ru^{3+}	Ru^{4+}	Ru^{5+}
Configuration électronique	↑↓ ↑↓ ↑	↑↓ ↑ ↑	↑ ↑ ↑
Dégénérescence de spin ($\Gamma^{\sigma}=2S+1$) SPIN	2	3	4
Dégénérescence orbitalaire (Γ) ORBITAL	3	3	1
Dégénérescence totale ($\beta = \Gamma.\Gamma^{\sigma}$) TOTAL	6	9	4

Spin and Orbital degeneracies for Ru t2g shell (Klein, PhD)

Spin + orbital leads to, for a Ru^{4+} shell

$$\alpha_H = \frac{k_B}{2e} \ln \frac{4}{6} \simeq -17.66\,\mu V/K < 0\,!$$

SPIN-ONLY (as suggested by Klein, Hebert Maignan et al) leads to, according to this revisited Heikes analysis:

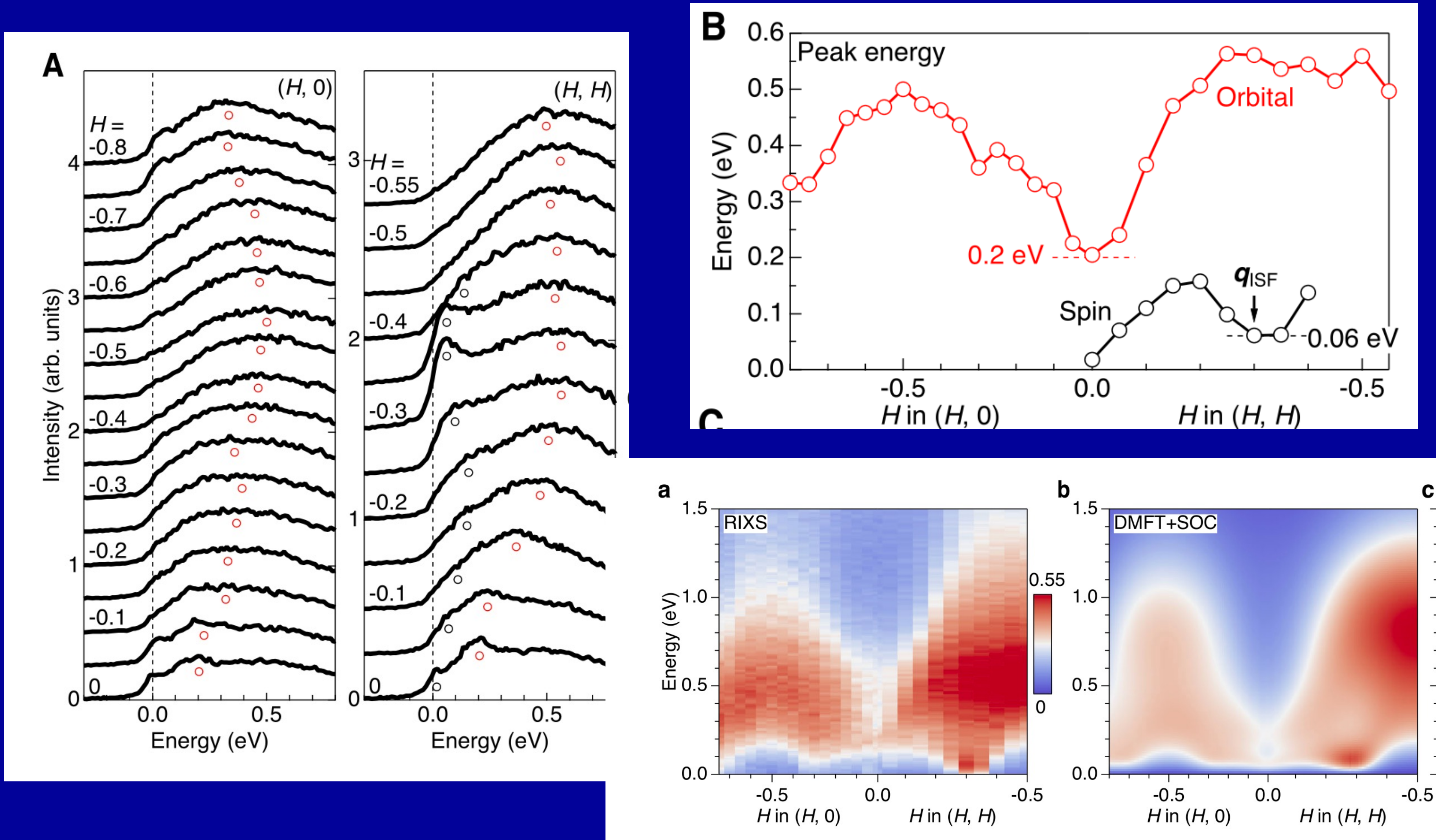
$$\boxed{\alpha_H = \frac{k_B}{2e} \ln \frac{4}{2} \simeq 30\,\mu V/K}$$

Signature of Hund metal from spectroscopies

- RIXS (H.Suzuki et al.Nature Comm 2023)
- Raman (G.Blesio, S.Beck et al. Phys Rev Research 6, 023124 (2024))
- Optics (D.Stricker et al. PRL 113, 087404 (2014))
- Wanted: Inverse-photoemission! Stricker et al. (or more studies of Sr_2MoO_4, see PRL 126, 166401 (2020))

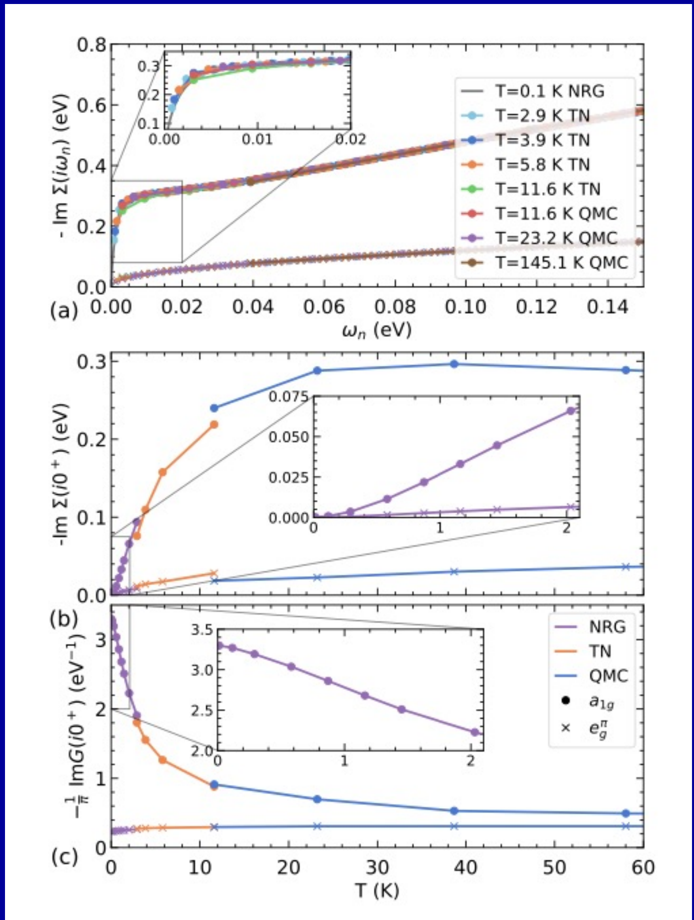
Recent Direct Evidence: RIXS

Suzuki et al. Nature Comm 14, 7042 (2023)

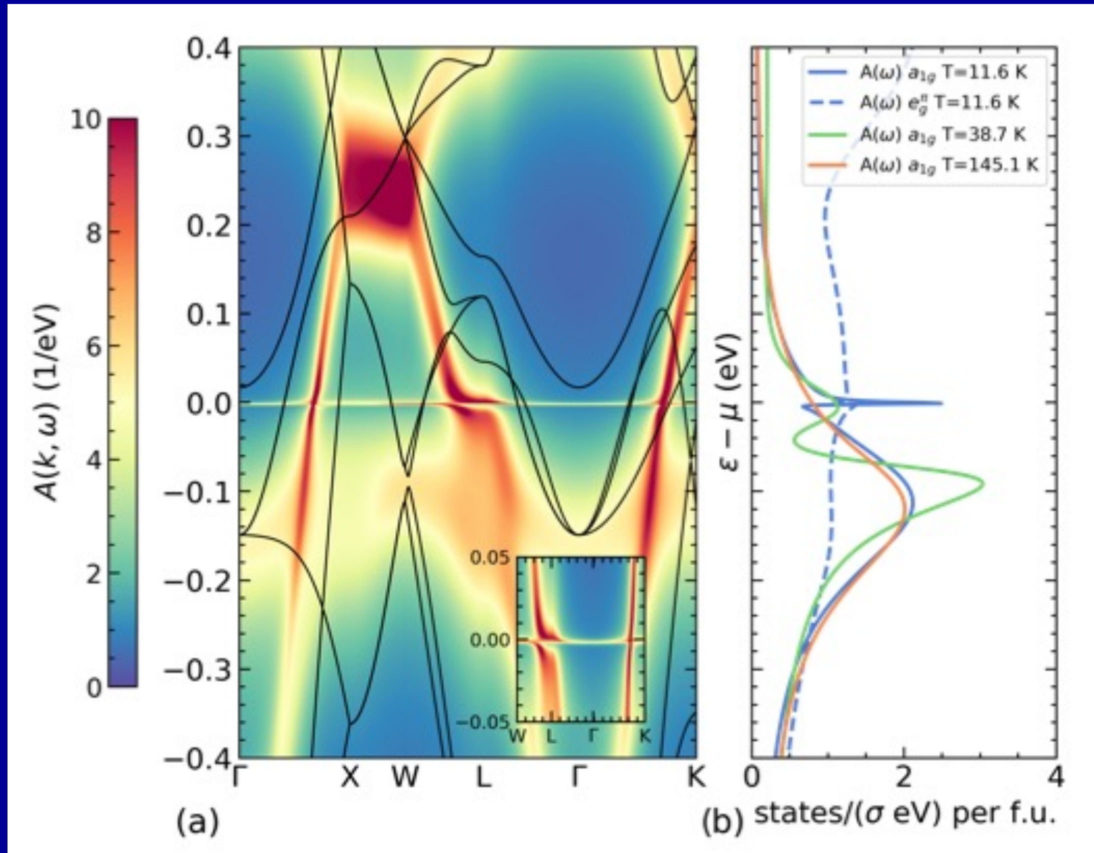


One of the latest demonstration of the importance of Hund's coupling: LiV_2O_4

Grundner et al. arXiv:2409.17268; Backes et al. arXiv:2410.08515



DMFT w/ NRG, DMRG and QMC solvers



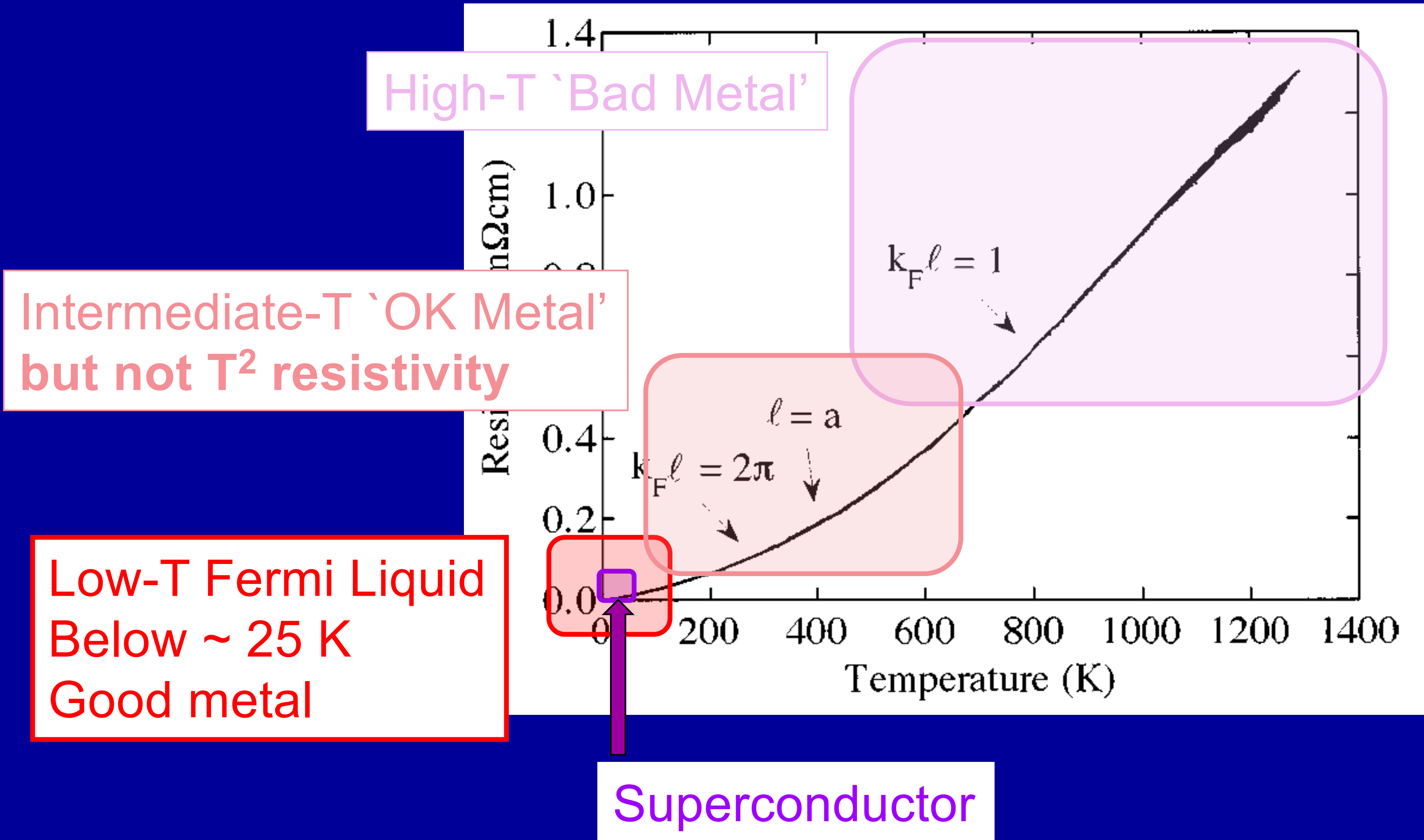
Correlation –induced flat band
Hund-assisted orbital-selective Mott

Low-frequency delicacies: Transport

(and transfers of spectral weight in spectroscopies)

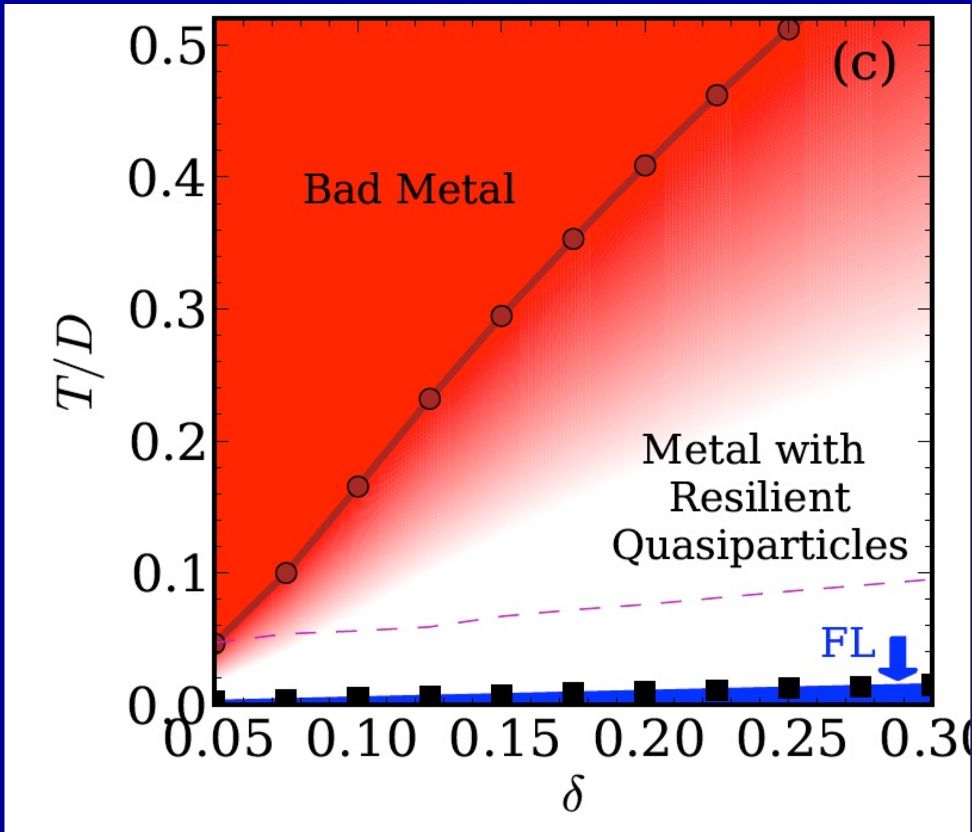
From a bad metal at high-T …
…to a superconductor at low-T (1.4K)

…The fascinating life of Sr_2RuO_4

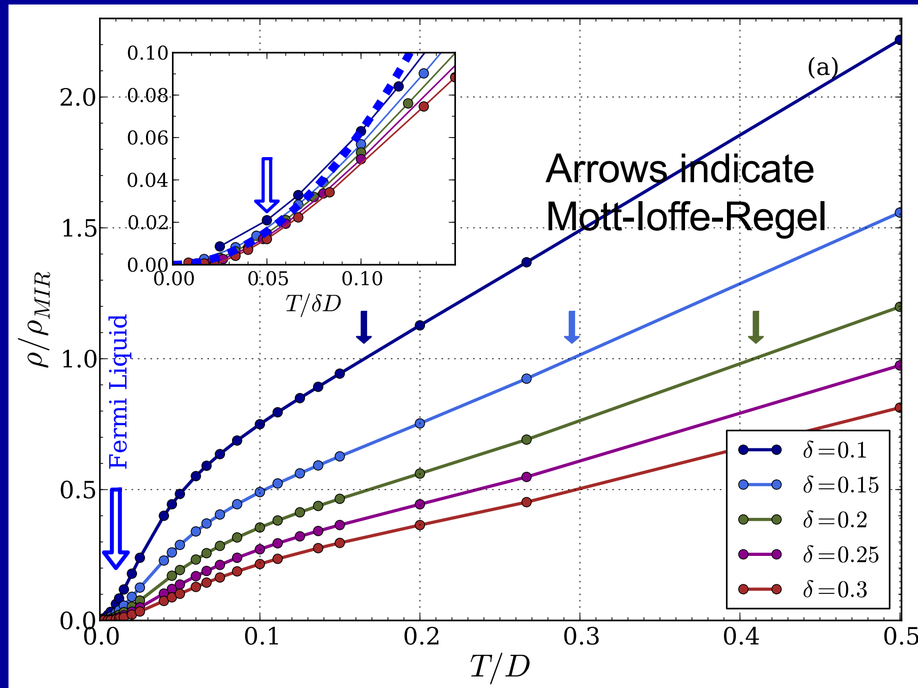


DMFT insight into a long-standing problem: "How bad metals become good"

`Resilient' *quasiparticles* beyond Landau Theory



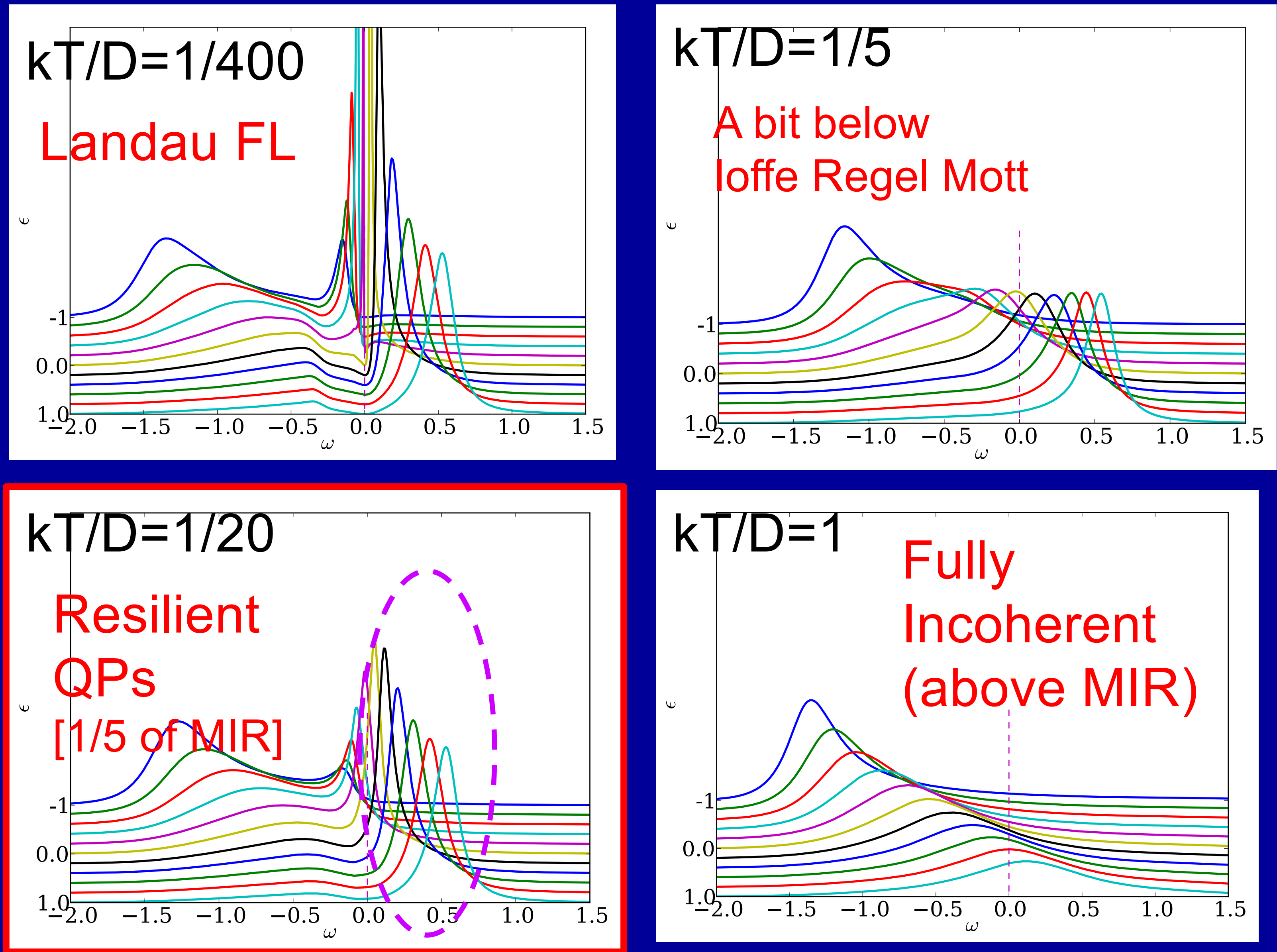
Resistivity: from a Fermi Liquid to a bad metal above Mott-Ioffe Regel



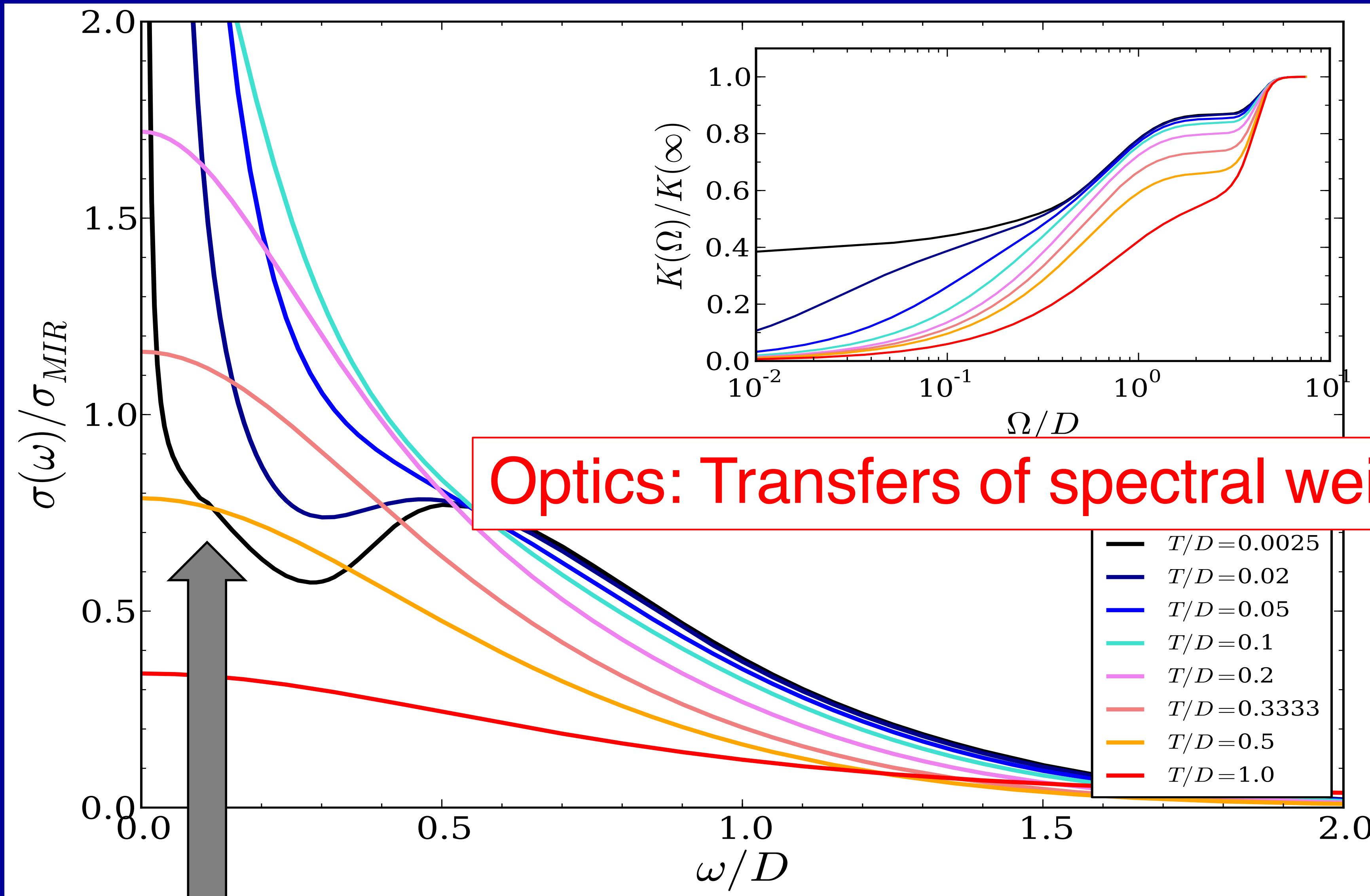
Deng et al. PRL 110 (2013) 086401 ; Xu et al. PRL 111 (2013) 036401

Quasiparticles SURVIVE all the way to T_{MIR}

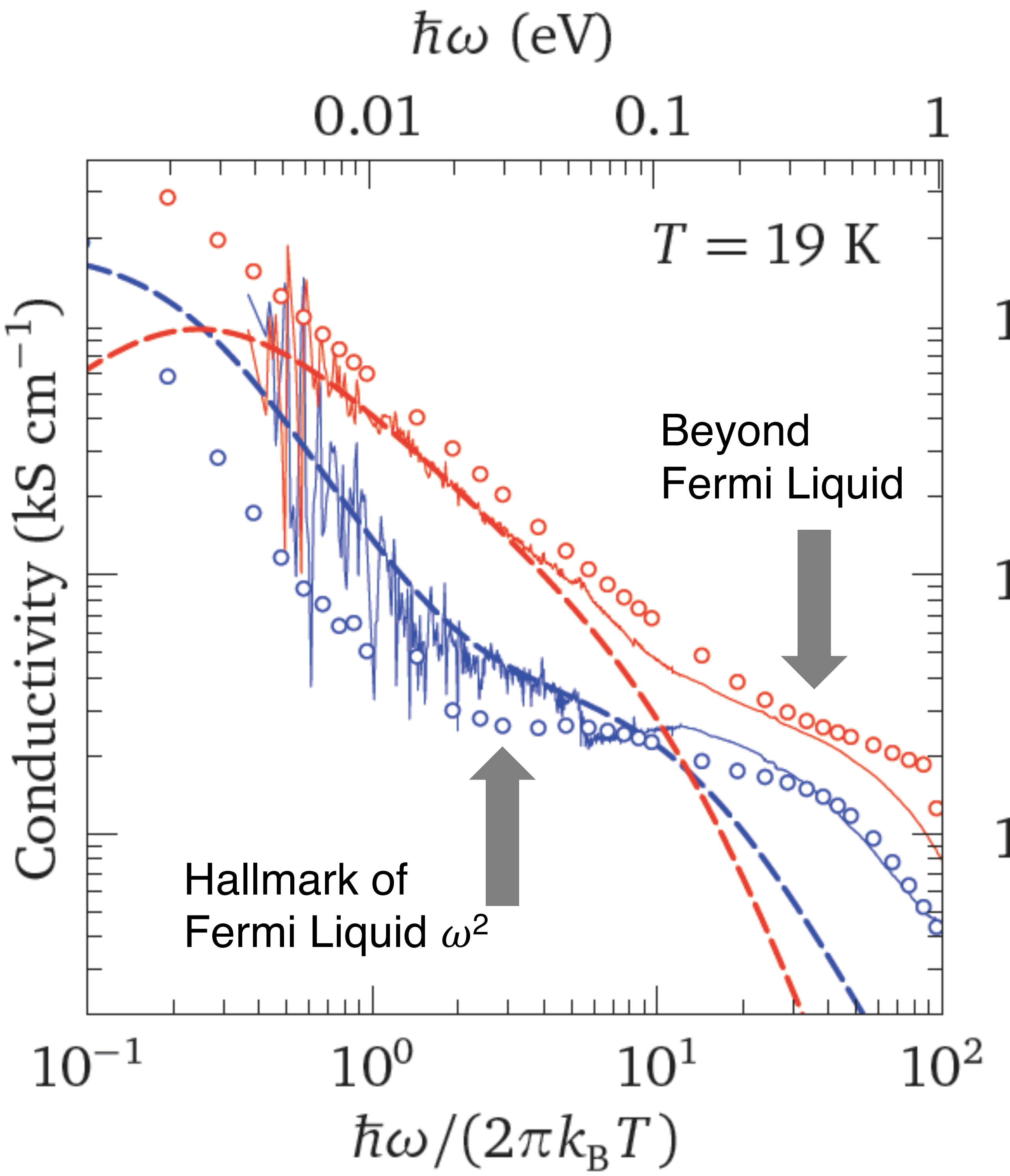
[Here, on the ‘dark side’ ω>0 of the Fermi surface]



Optics: Transfers of spectral weight



This non-Drude ``foot'' is actually the signature of Landau's Fermi liquid (ω^2) in the optical spectrum



Sr_2RuO_4

Re σ(ω)

Im σ(ω)

Plain Lines:
Experiment

Dashed Line:
Fermi Liquid Theory

Dots:
Theoretical Calculation (LDA+DMFT)

D.Stricker et al.
PRL 113, 0874040 (2014)

Take-home messages from this decade-old study:

- Well-defined `resilient' QPs exist well above the range of validity of FL theory, all the way up to T_{MIR}
- They evolve as T is increased, and live increasingly far away from the T=0 Fermi surface
- Their scattering rate saturate at the Mott-Ioffe-Regel "limit", <u>not necessarily resistivity</u>
- Clear spectroscopic signatures of the existence of resilient QPs and of the MIR crossover

Conductivity from DMFT

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

From Kubo formula

Vertex corrections vanish because v_k is odd in k

Tr is over bands/orbitals (not spin)

Low-T state of Sr_2RuO_4: a Fermi Liquid

~ T^2 up to about T_{FL} ~ 20K

KEY OBSERVATION:
$\rho \ll \rho_{MIR}$ at T ~ T_{FL}
Hence large regime of T
with non-T^2 (non FL) transport
but still `good' metal

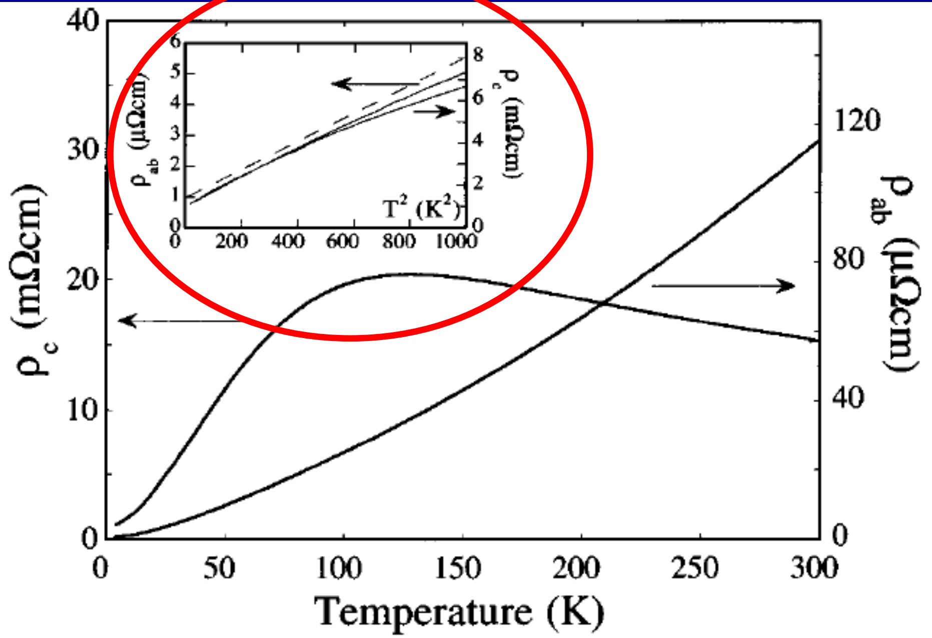
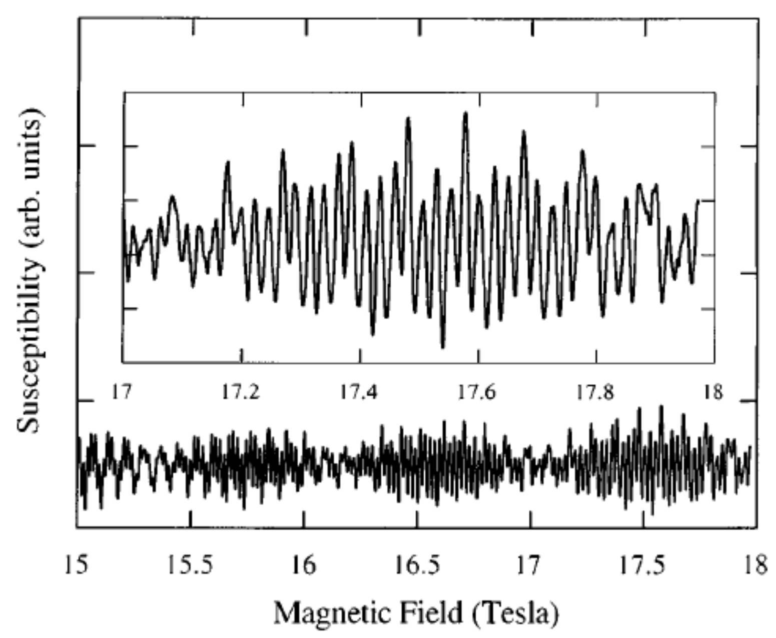


FIG. 1. Zero-field $\rho_{ab}(T)$ and $\rho_c(T)$ of Sr_2RuO_4. The inset shows $\rho_c(T)$ and $\rho_{ab}(T)$ below 32 K plotted against T^2. The dashed line is a guide to the eye.



Beautiful quantum oscillations

Shameless Advertising:
We can now calculate transport from DMFT highly accurately for real materials

7. arXiv:2412.16363 [pdf, other] cond-mat.mtrl-sci cond-mat.str-el

Fermi-Liquid T^2 Resistivity: Dynamical Mean-Field Theory Meets Experiment

Authors: Fabian B. Kugler, Jeremy Lee-Hand, Harrison LaBollita, Lorenzo Van Muñoz, Jason Kaye, Sophie Beck, Alexander Hampel, Antoine Georges, Cyrus E. Dreyer

3. arXiv:2505.04508 [pdf, ps, other] cond-mat.mtrl-sci cond-mat.str-el

Low-temperature transport in high-conductivity correlated metals: a density-functional plus dynamical mean-field study of cubic perovskites

Authors: Harrison LaBollita, Jeremy Lee-Hand, Fabian B. Kugler, Lorenzo Van Muñoz, Sophie Beck, Alexander Hampel, Jason Kaye, Antoine Georges, Cyrus E. Dreyer

1. arXiv:2506.10143 [pdf, ps, other] cond-mat.mtrl-sci cond-mat.str-el

Mechanisms for the ultralow room-temperature resistivity of $SrMoO_3$

Authors: Jennifer Coulter, Fabian B. Kugler, Harrison LaBollita, Antoine Georges, Cyrus E. Dreyer

PHYSICAL REVIEW MATERIALS **7**, 093801 (2023)

Editors' Suggestion

Combining electron-phonon and dynamical mean-field theory calculations of correlated materials: Transport in the correlated metal Sr_2RuO_4

David J. Abramovitch,[1,*] Jin-Jian Zhou,[2,*] Jernej Mravlje,[3] Antoine Georges,[4,5] and Marco Bernardi[1,6,†]

PHYSICAL REVIEW LETTERS **133**, 186501 (2024)

Respective Roles of Electron-Phonon and Electron-Electron Interactions in the Transport and Quasiparticle Properties of $SrVO_3$

David J. Abramovitch,[1,2] Jernej Mravlje,[3,4] Jin-Jian Zhou,[5] Antoine Georges,[6,2,7,8] and Marco Bernardi[1,*]

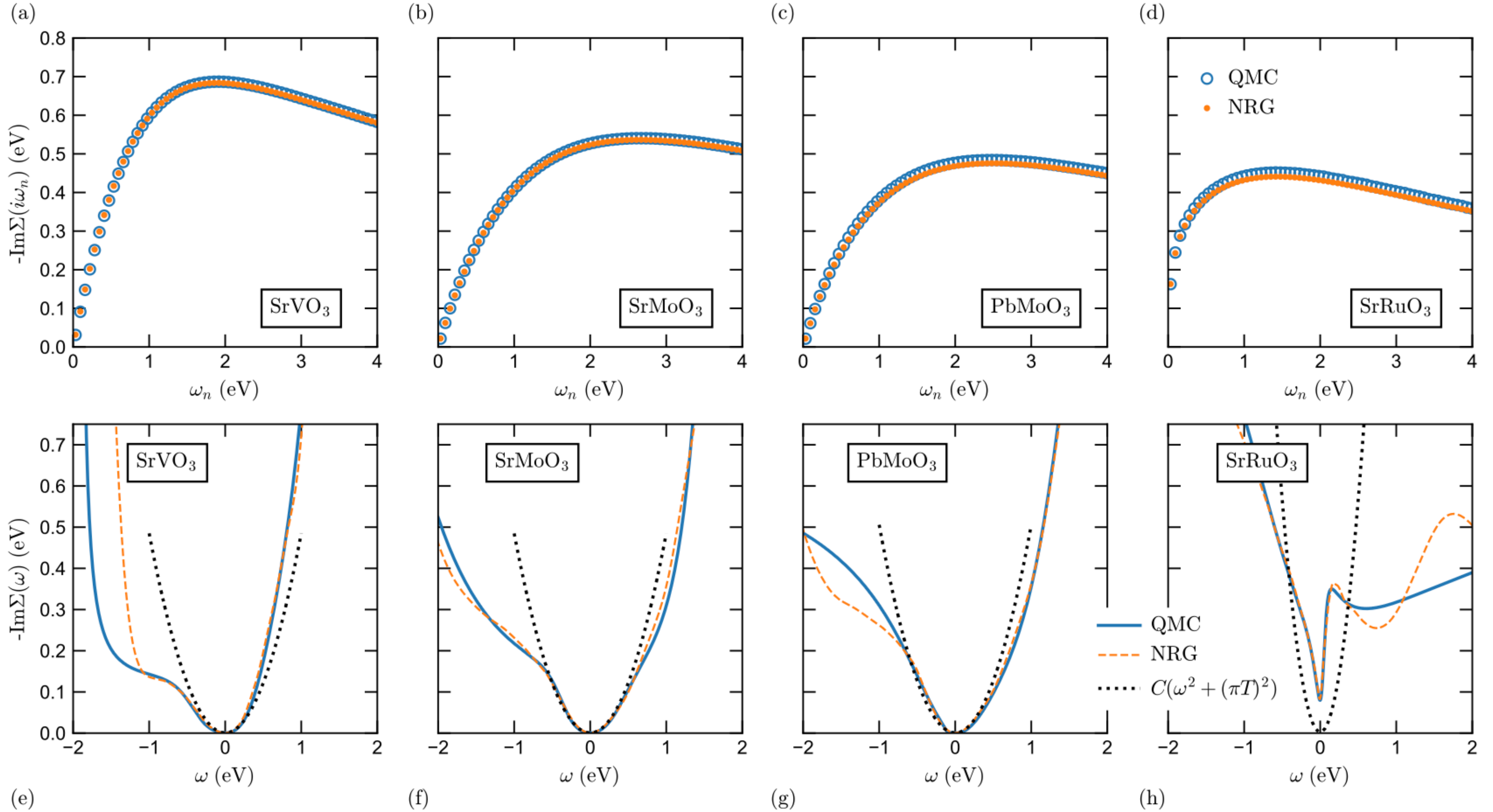


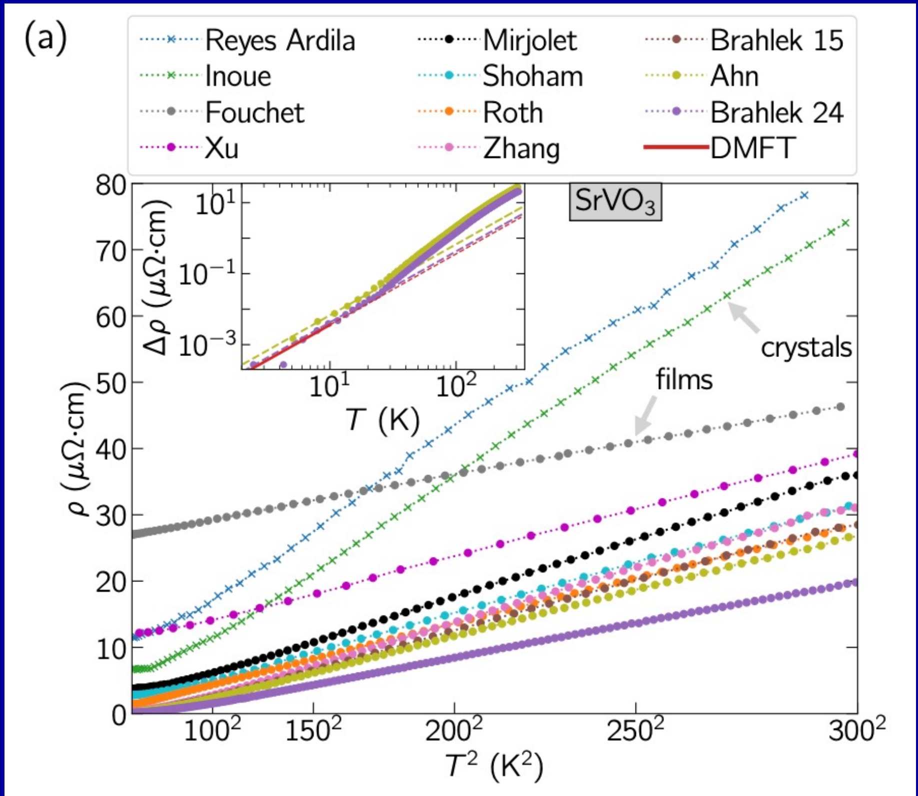
FIG. 4. QMC (blue) and NRG (orange) comparison of the DMFT self-energy on the Matsubara imaginary-frequency axis (top) and the real-frequency axis (bottom) for $SrVO_3$, $SrMoO_3$, $PbMoO_3$, and $SrRuO_3$ at $T = 116$ K ($\beta = 100$/eV). The dashed (black) lines indicate a fit of the real-frequency data to the Fermi-liquid form $C(\omega^2 + \pi^2 T^2)$. The Fermi-liquid fit to $SrRuO_3$ is clearly not successful. We note that increasing C to match $\mathrm{Im}\,\Sigma(0)$ does not lead to an overall better fit.

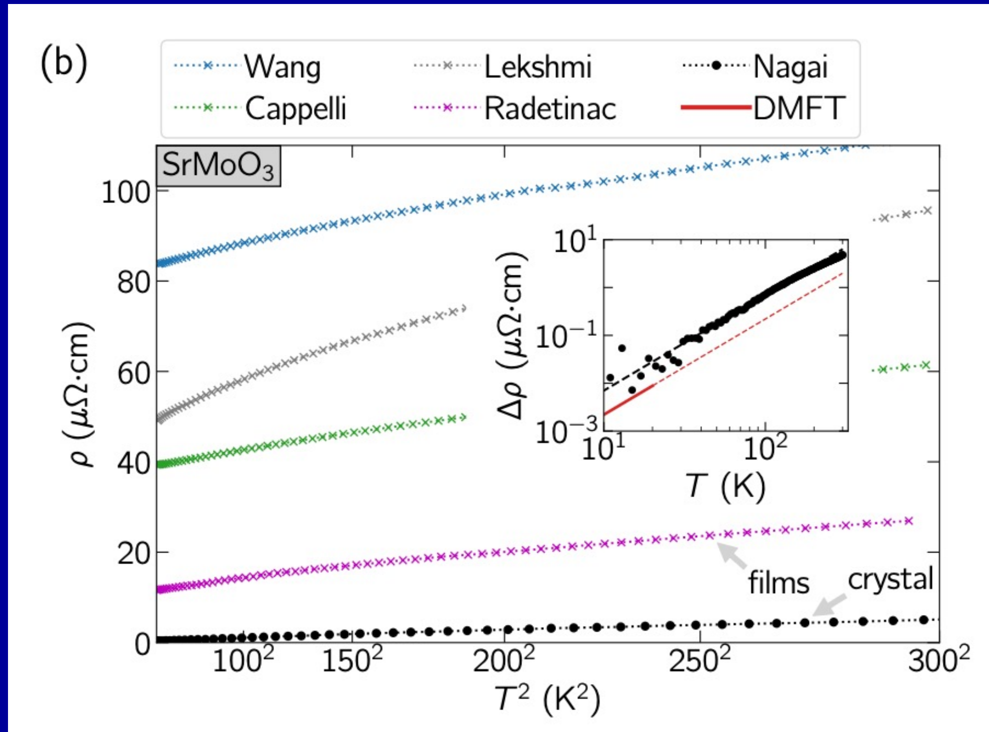
3. arXiv:2505.04508 [pdf, ps, other] cond-mat.mtrl-sci cond-mat.str-el

Low-temperature transport in high-conductivity correlated metals: a density-functional plus dynamical mean-field study of cubic perovskites

Authors: Harrison LaBollita, Jeremy Lee-Hand, Fabian B. Kugler, Lorenzo Van Muñoz, Sophie Beck, Alexander Hampel, Jason Kaye, Antoine Georges, Cyrus E. Dreyer

… but the experimental situation is a bit of a mess…





Beyond single-site DMFT:
Why?
How?

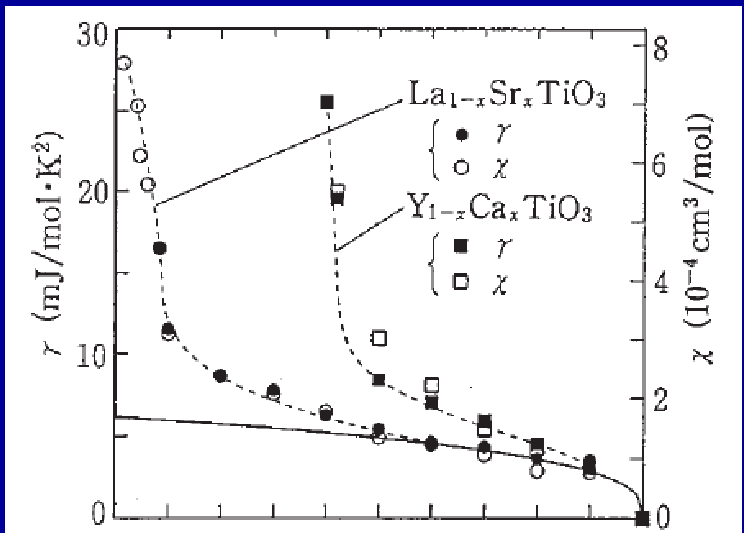
→Taking better account
of non-local spatial correlations

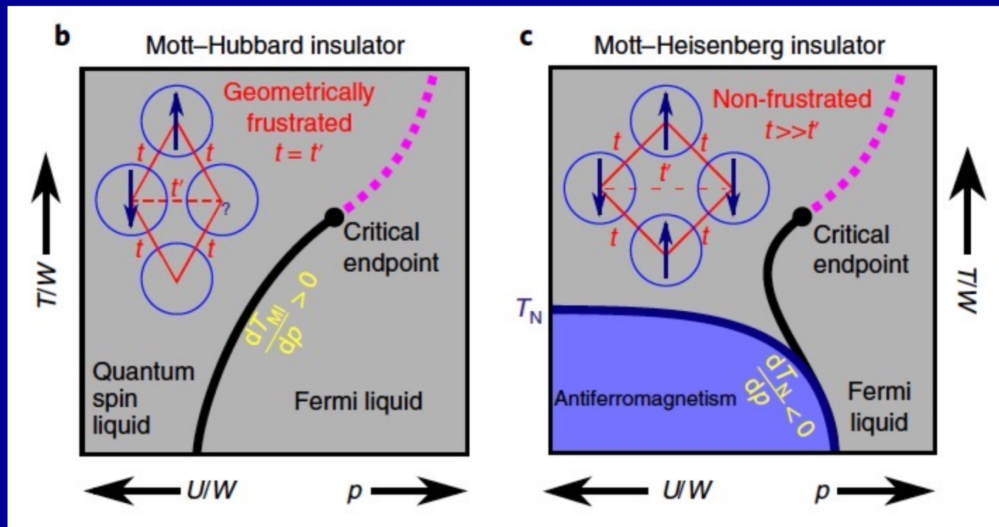
To what extent does DMFT take spatial correlations into account ?

- Key point: $$\boxed{J_{ij} = O(\frac{1}{d}) \ , \ \sum_j J_{ij} = O(1)}$$
- → Ordered Phases have Tc = O(1)
- 2-particle correlation functions know about ordering and critical behavior: non-trivial $\chi(\vec{Q}, \omega)$
- BUT NO FEEDBACK OF SPATIAL CORRELATIONS/FLUCTUATIONS INTO 1-PARTICLE PROPERTIES

We expect:

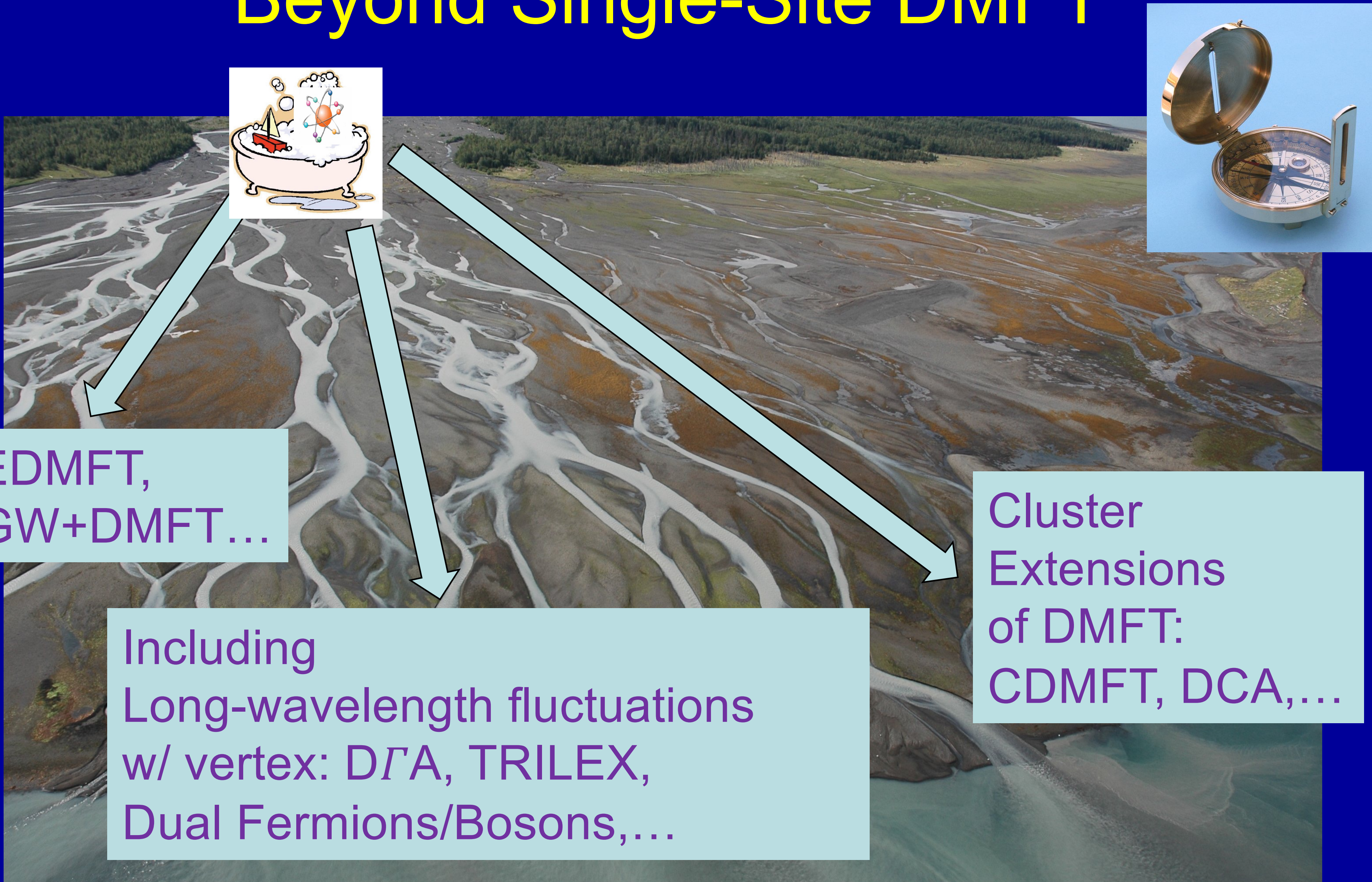
- The divergence of the effective mass to be cutoff by (spin) correlations
- e.g. large-N t-J: $Z \propto \delta \;\;,\;\; m^*/m \sim \left[\delta + \frac{J}{td}\right]^{-1}$
- cf. finite entropy of low-T insulator





Suppression of Pomeranchuk effect at low T

Including Spatial Fluctuations: Beyond Single-Site DMFT



EDMFT,
GW+DMFT…

Including
Long-wavelength fluctuations
w/ vertex: DΓA, TRILEX,
Dual Fermions/Bosons,…

Cluster
Extensions
of DMFT:
CDMFT, DCA,…

Embedding Methods Are Controlled

Cluster extensions of single-site DMFT

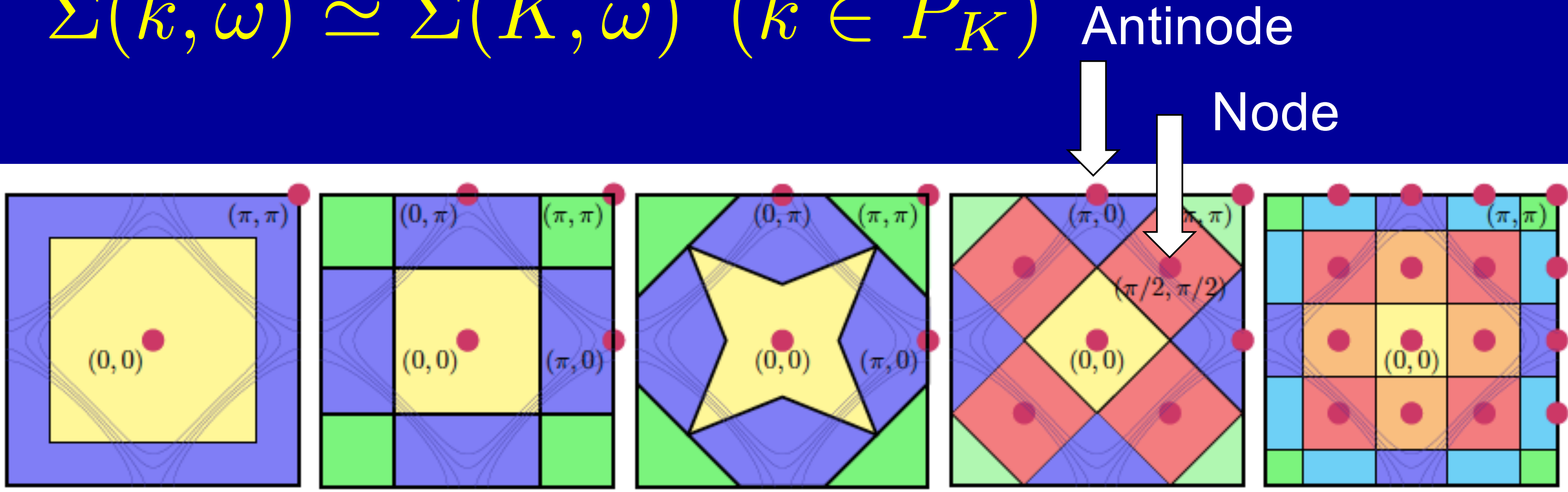
→ `Molecular' mean-field

(cf. Bethe-Peierls, Kikuchi)

Several flavors, e.g. DCA: Patching momentum-space, cluster used to calculate self-energy at cluster momenta.

Self-energy approximated as piecewise constant in momentum space:

$$\Sigma(k,\omega) \simeq \Sigma(K,\omega) \;\; (k \in P_K)$$



Numerous works by several groups in the last ~ 20 years

For reviews see:

[27] T. Maier, M. Jarrell, T. Pruschke, and M. H. Hettler, Rev. Mod. Phys. **77**, 1027 (2005).
[28] G. Kotliar, S. Y. Savrasov, K. Haule, V. S. Oudovenko, O. Parcollet, and C. A. Marianett, Rev. Mod. Phys. **78**, 865 (2006).
[29] A. M. S. Tremblay, B. Kyung, and D. Senechal, Low Temp. Phys. **32**, 424 (2006).

Cincinatti/Baton Rouge (Jarrell et al.), Rutgers (Kotliar, Haule et al.), Sherbrooke (Tremblay, Senechal et al., Kyung, Sordi), Columbia (Millis et al.)., Michigan (Gull et al.) Oak Ridge (Maier et al.), Tokyo (Imada, Sakai et al.) Hamburg(Lichtenstein et al.), Rome (Capone et al.) Paris/Saclay/Orsay (Parcollet, Ferrero, AG, Civelli et al.), Stuttgart (Gunnarsson) etc…

To quote only one achievement:

These approaches have established that the Pseudogap in the doped 2D Hubbard model is caused by spin correlations

(not pair or CDW fluctuations)

Many groups and authors 2005 → 2020

See e.g. PRX 8, 021048 for references

Recent `handshake':

- With Tensor Network Methods (MEETS)
  Wietek et al. PRX 11, 031007 (2021)
- With diagrammatic Mont Carlo (CDET)
  Wu et al. PRB 96, 041105R, 2017; Simkovic et al. arXiv:2209.09237

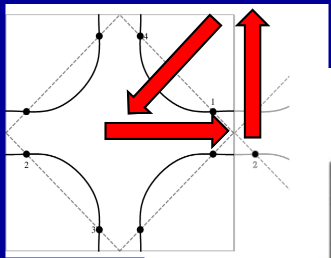
Controlled results, converged to infinite cluster size, are possible in part of the PG regime

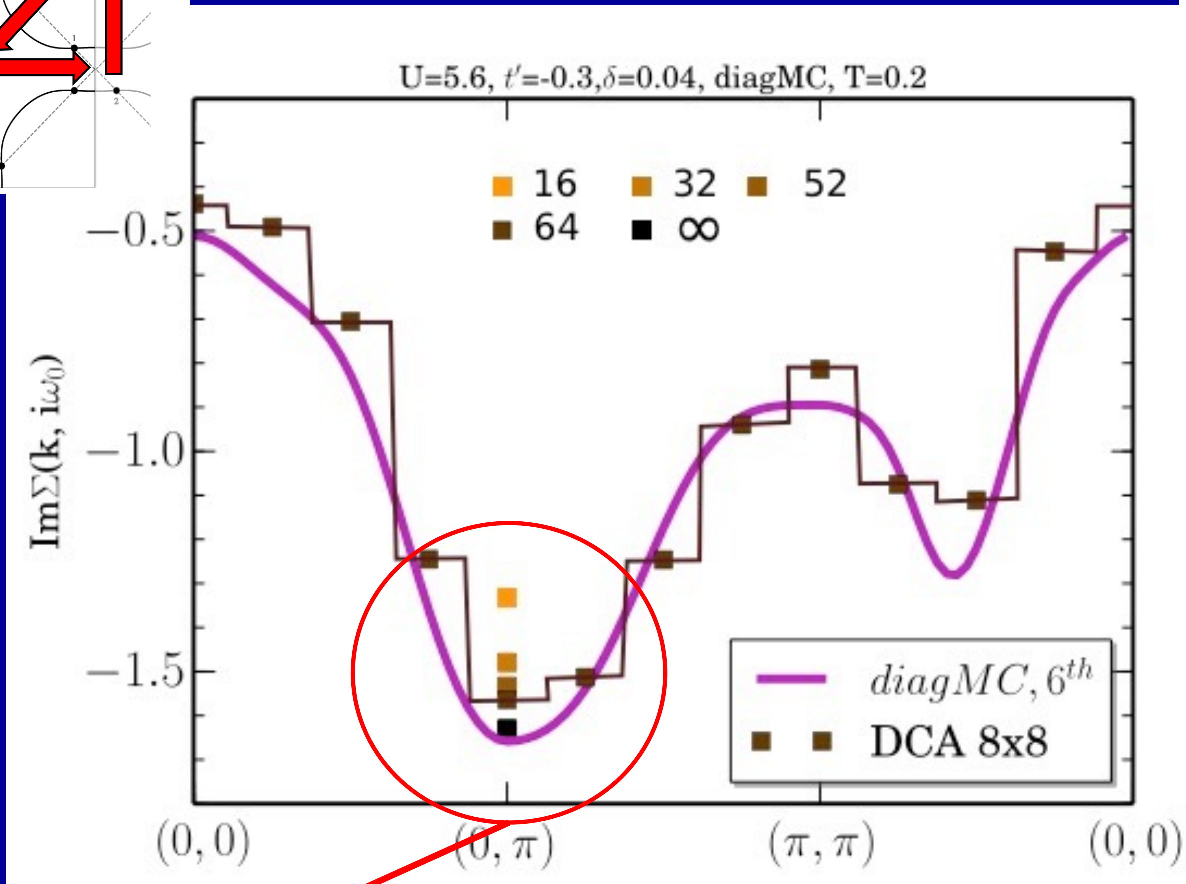
Wei Wu, Ferrero, AG, Kozik PRB 96, 041105R (2017)

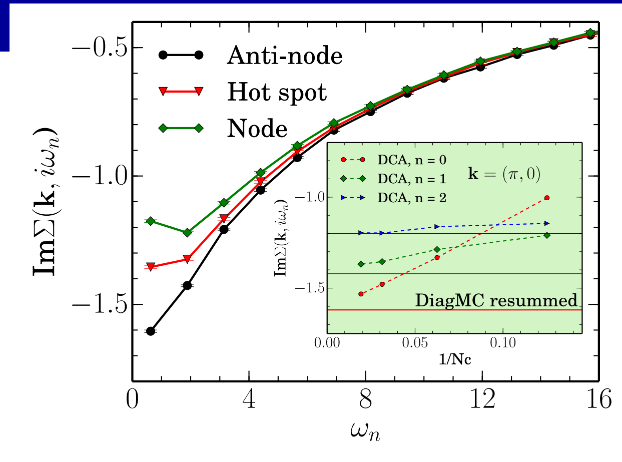
- For U/t=5.6 , t'/t=-0.3 and doping p=0.04 (reference `Wei point' ☺)
- CONVERGE the self energy at T=0.2t with two independent methods:
- DCA w/ convergence in cluster size
- Diagrammatic Monte Carlo on the Infinite Lattice
- Recently significant improvements to the DiagMC method (RDET) have allowed to reach T/t=0.1 Rossi,Simkovic, Ferrero EPL 132 (2020) 11001

DCA and DiagMC: quantitative agreement

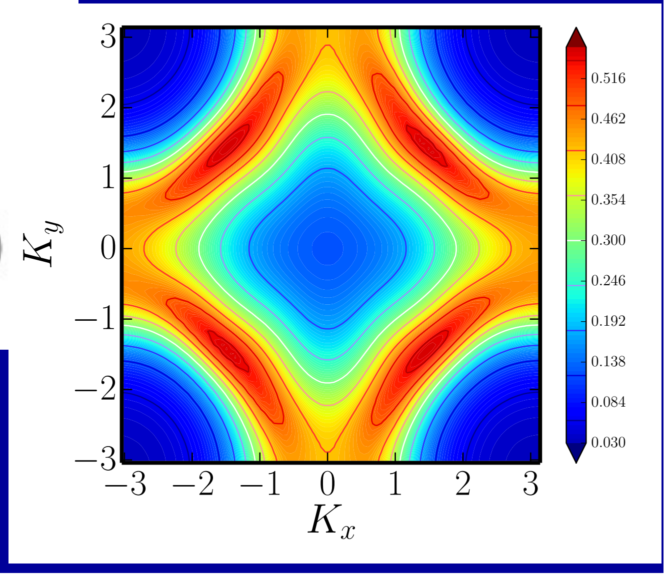
→ Computational solution of the 2D Hubbard model in this regime !







Nodal/Antinodal Dichotomy



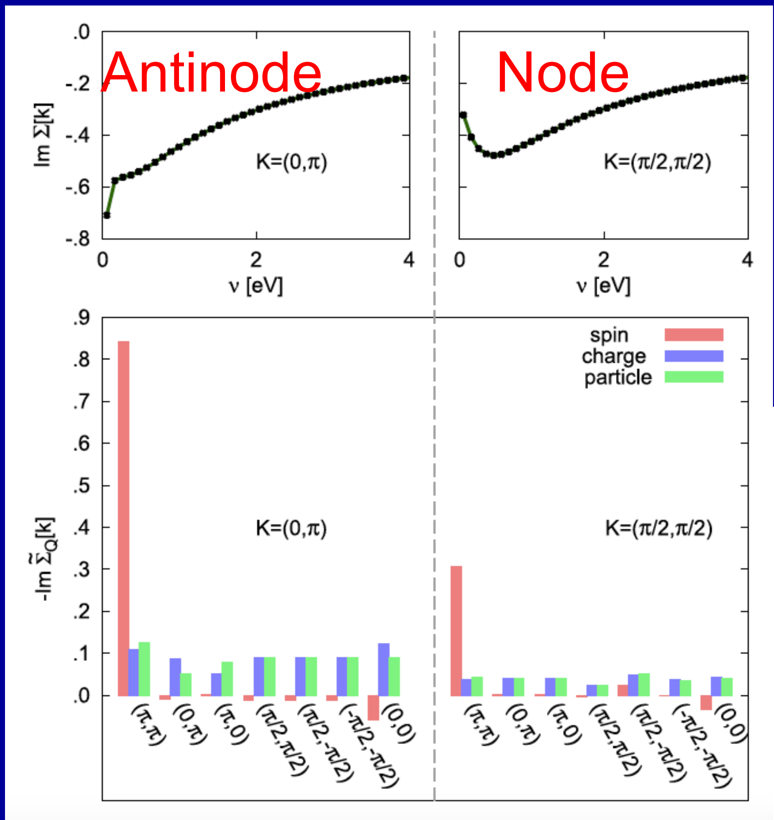
ImΣ becomes LARGE at antinode !

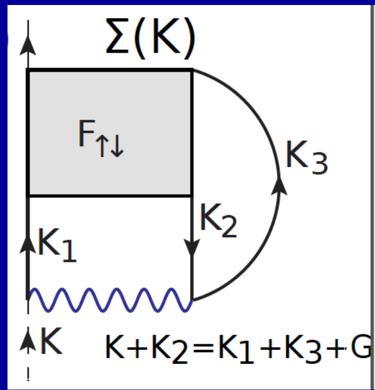
`Fluctuation Diagnostics’

PRL **114**, 236402 (2015) PHYSICAL REVIEW LETTERS week ending 12 JUNE 2015

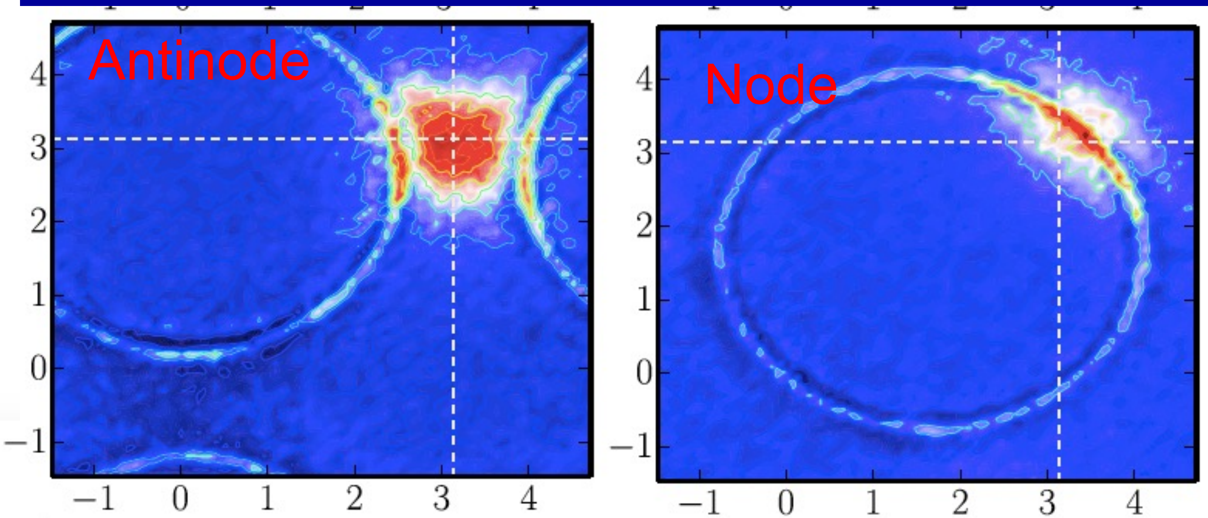
Fluctuation Diagnostics of the Electron Self-Energy: Origin of the Pseudogap Physics

O. Gunnarsson,[1] T. Schäfer,[2] J. P. F. LeBlanc,[3,4] E. Gull,[4] J. Merino,[5] G. Sangiovanni,[6] G. Rohringer,[2] and A. Toschi[2]





Wei et al. (2017) - DiagMC



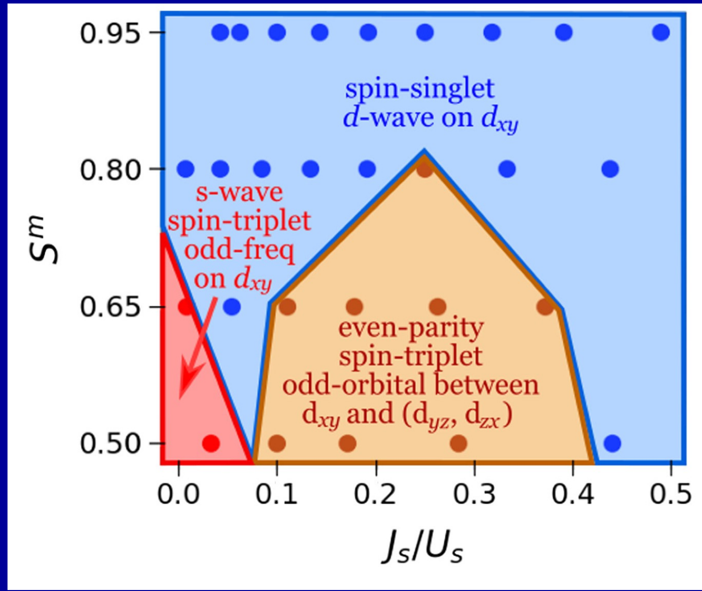
DCA Gunnarsson et al

Superconductivity with Quantum Embedding

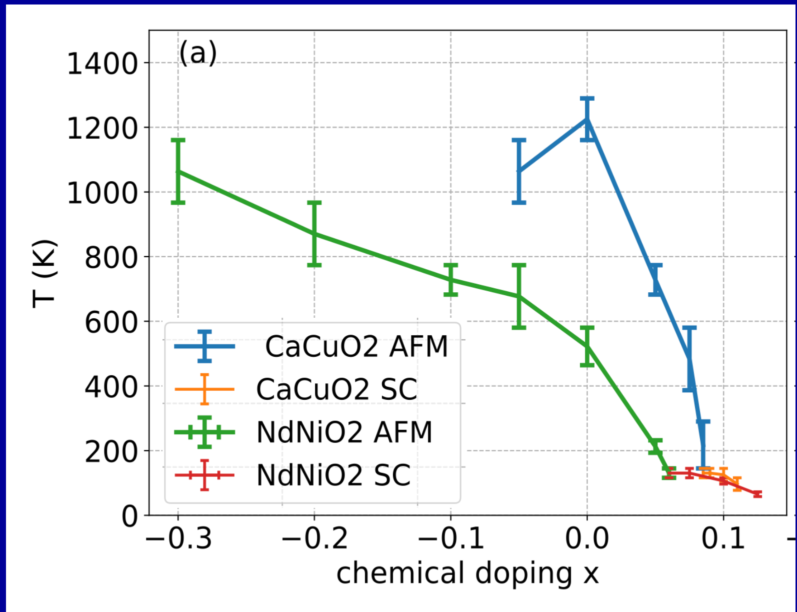
Sr_2RuO_4

FIG. 4. Phase diagram of the leading superconducting instabilities. A lower J_s/U_s implies more charge fluctuations, while the magnetic Stoner factor S^m quantifies the proximity to a magnetic instability.

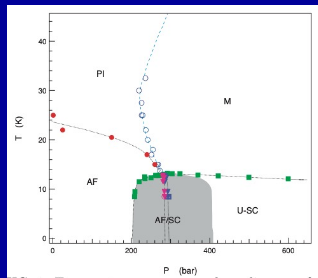
O.Gingras et al.,
PRL 123 217005 (2019)



Infinite-Layer Nickelates

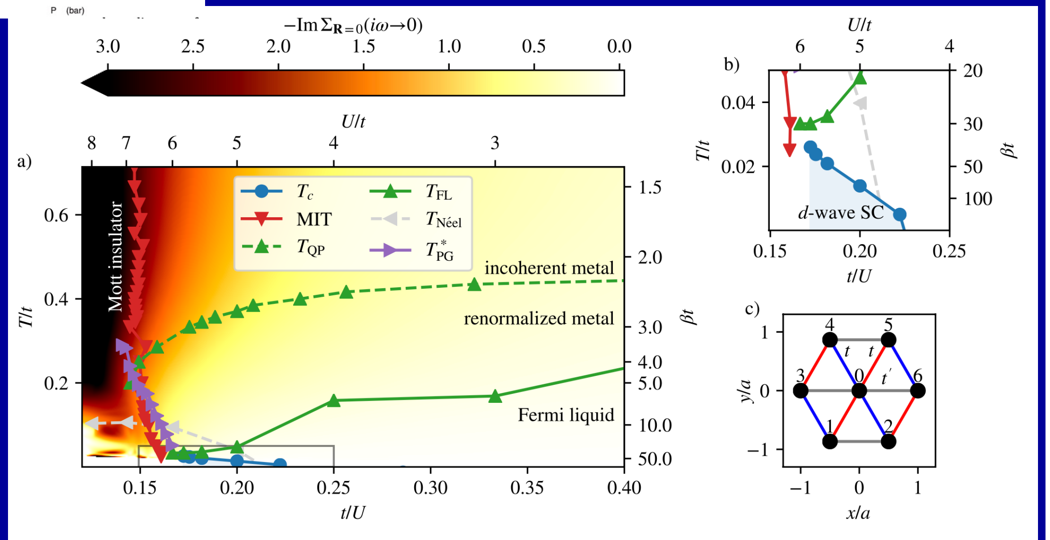


Karp, Hampel, Millis PRB 105 205131 2022



kappa-ET organic compounds

Menke, Schäfer, Ferrero et al. soon on arXiv



Conclusion

Outlook

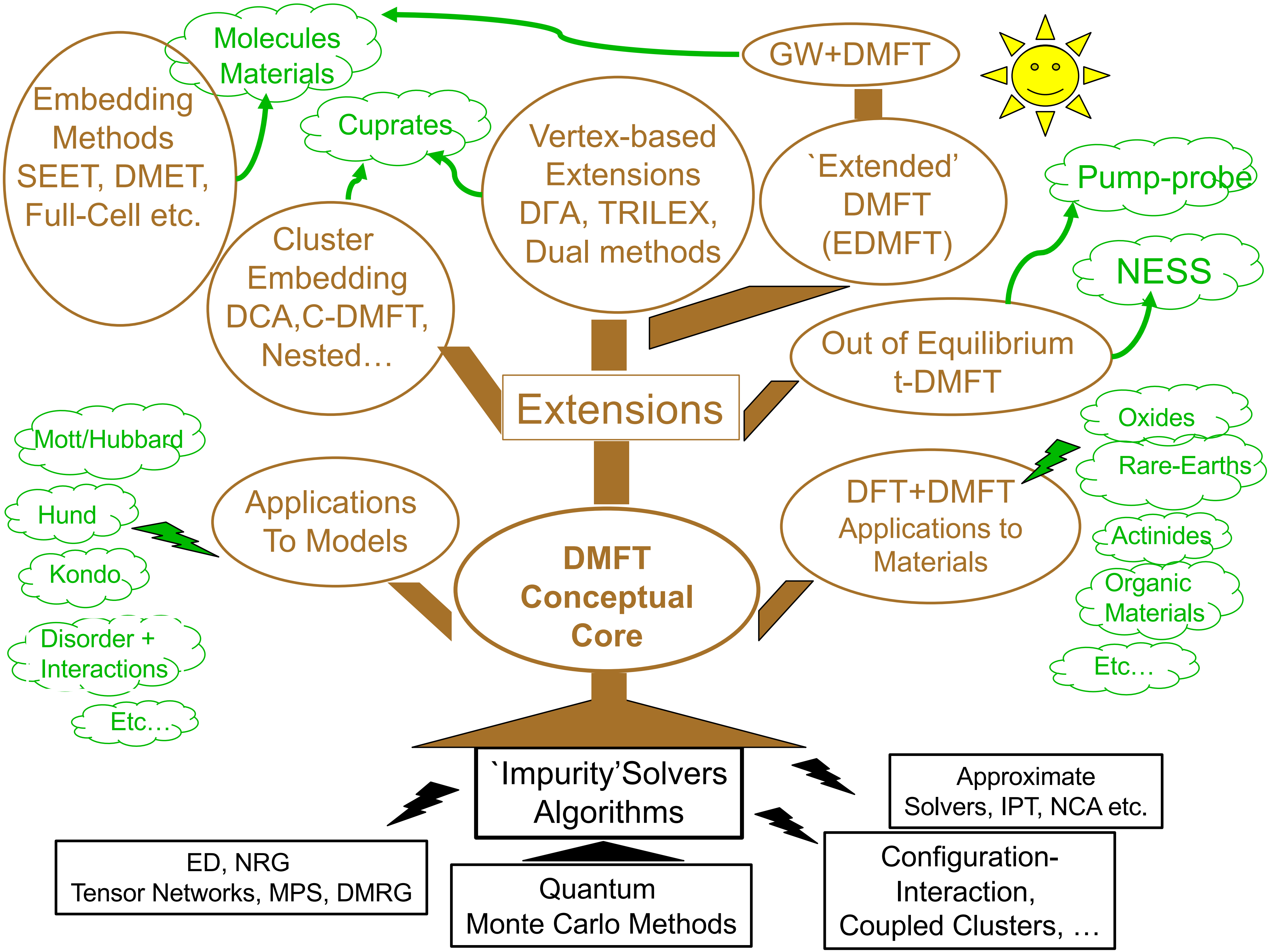
Perspectives

…

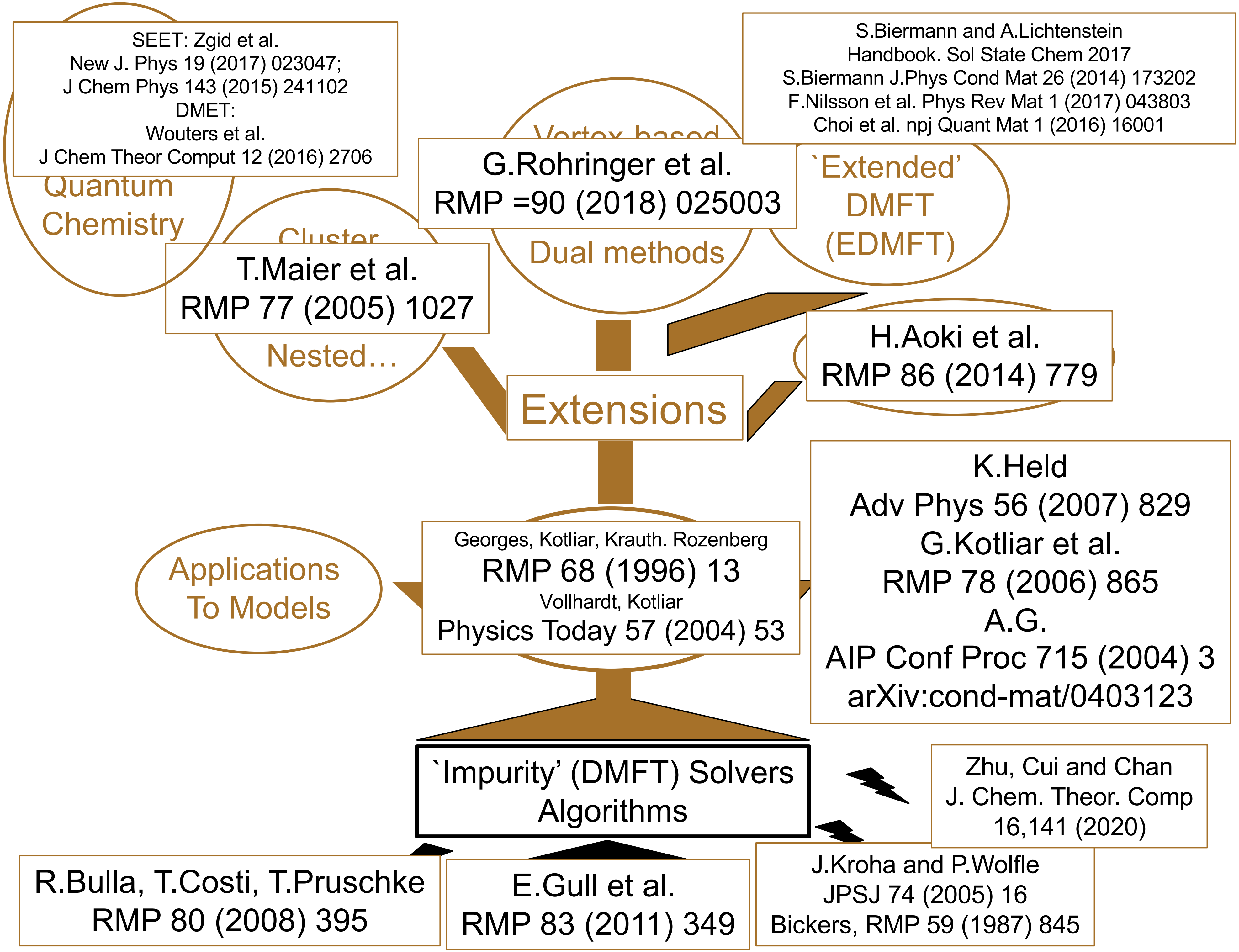
Take-Home Message

Dynamical Mean-Field Theory (DMFT),
and more broadly Quantum Embedding methods
combined with electronic structure,
has transformed our ability to
understand, calculate and predict
the properties of materials
with strong electronic correlations

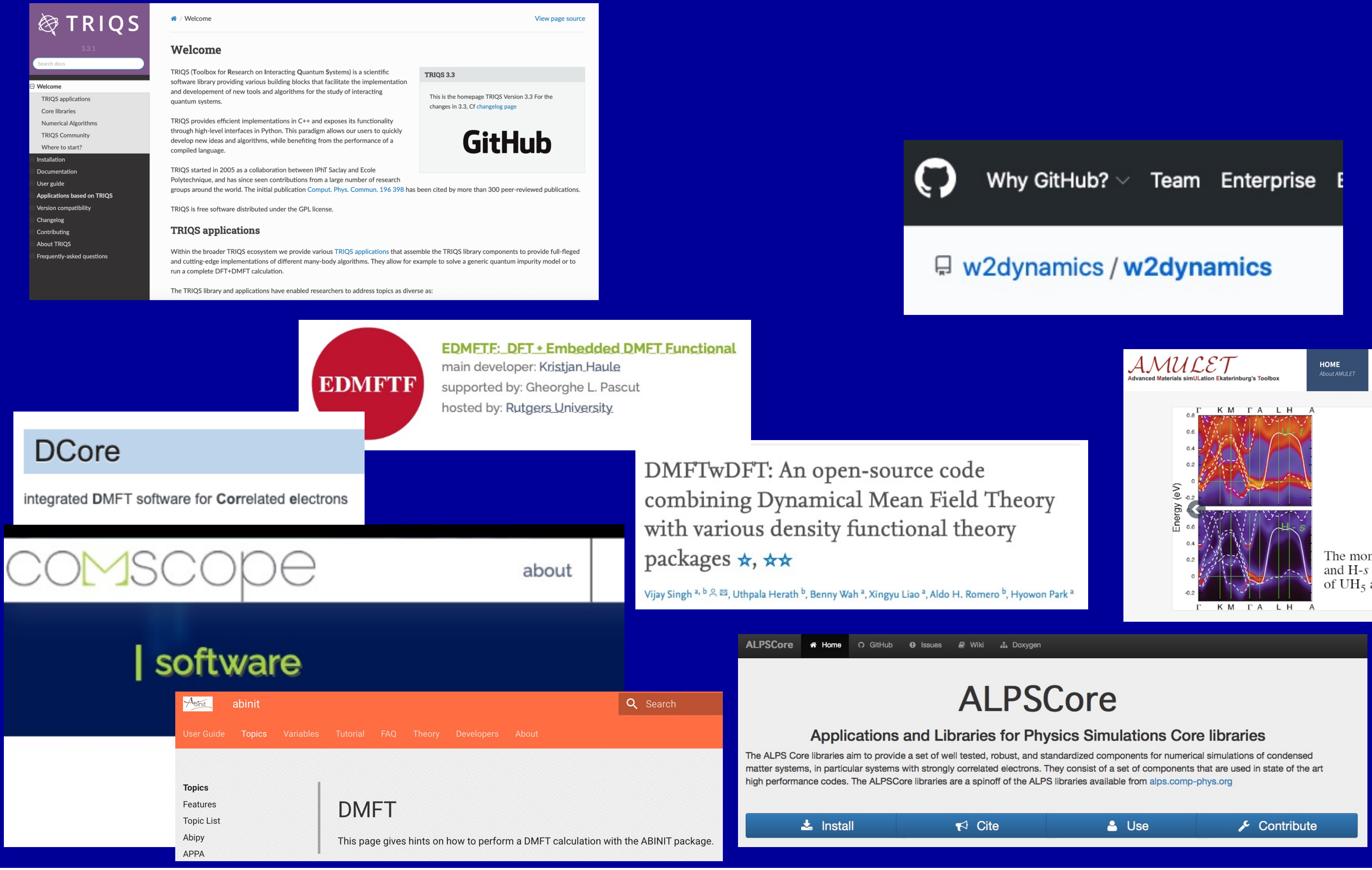
Numerous opportunities for further developments…



Molecules
Materials
GW+DMFT
Embedding Methods SEET, DMET, Full-Cell etc.
Cuprates
Vertex-based Extensions DΓA, TRILEX, Dual methods
`Extended' DMFT (EDMFT)
Pump-probe
NESS
Cluster Embedding DCA,C-DMFT, Nested…
Out of Equilibrium t-DMFT
Extensions
Oxides
Rare-Earths
Mott/Hubbard
Hund
Kondo
Disorder + Interactions
Etc…
Applications To Models
DMFT Conceptual Core
DFT+DMFT Applications to Materials
Actinides
Organic Materials
Etc…
`Impurity'Solvers Algorithms
Approximate Solvers, IPT, NCA etc.
ED, NRG Tensor Networks, MPS, DMRG
Quantum Monte Carlo Methods
Configuration-Interaction, Coupled Clusters, …

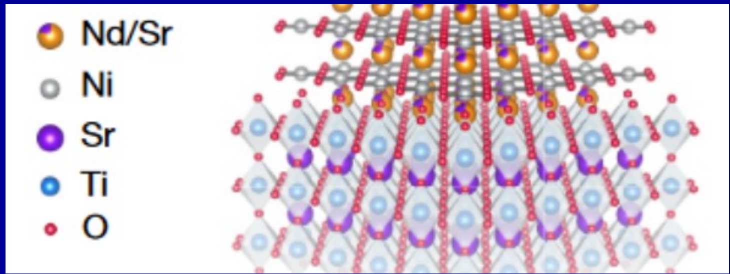

SEET: Zgid et al.
New J. Phys 19 (2017) 023047;
J Chem Phys 143 (2015) 241102
DMET:
Wouters et al.
J Chem Theor Comput 12 (2016) 2706
Quantum
Chemistry
G.Rohringer et al.
RMP =90 (2018) 025003
Dual methods
S.Biermann and A.Lichtenstein
Handbook. Sol State Chem 2017
S.Biermann J.Phys Cond Mat 26 (2014) 173202
F.Nilsson et al. Phys Rev Mat 1 (2017) 043803
Choi et al. npj Quant Mat 1 (2016) 16001
`Extended'
DMFT
(EDMFT)
Cluster
T.Maier et al.
RMP 77 (2005) 1027
Nested…
H.Aoki et al.
RMP 86 (2014) 779
Extensions
K.Held
Adv Phys 56 (2007) 829
G.Kotliar et al.
RMP 78 (2006) 865
A.G.
AIP Conf Proc 715 (2004) 3
arXiv:cond-mat/0403123
Applications
To Models
Georges, Kotliar, Krauth. Rozenberg
RMP 68 (1996) 13
Vollhardt, Kotliar
Physics Today 57 (2004) 53
`Impurity' (DMFT) Solvers
Algorithms
Zhu, Cui and Chan
J. Chem. Theor. Comp
16,141 (2020)
R.Bulla, T.Costi, T.Pruschke
RMP 80 (2008) 395
E.Gull et al.
RMP 83 (2011) 349
J.Kroha and P.Wolfle
JPSJ 74 (2005) 16
Bickers, RMP 59 (1987) 845

A Vital Community Endeavor: Efficient and Sustainable Open-Source Software Libraries



Among many applications of DMFT to materials of recent interest…

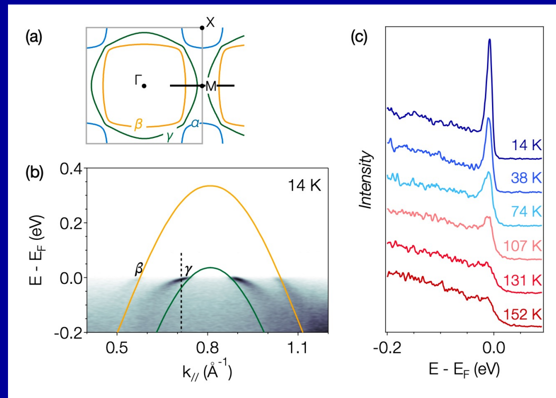
Infinite-Layer Nickelates

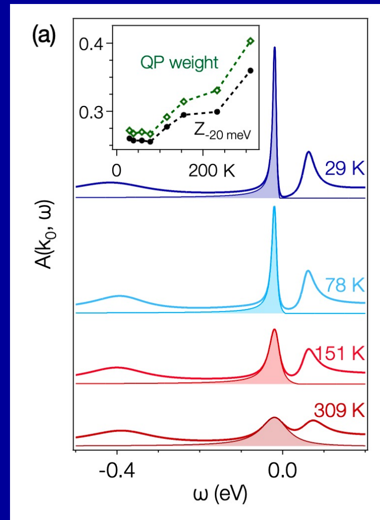


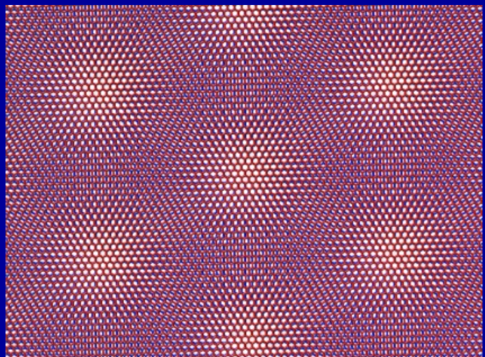
Many papers using DMFT – At CCQ:
J.Karp, A.Hampel, H. LaBollita, A.Millis

Sr_2RuO_4 arXiv:2308.02313

A.Hunter, Sophie Beck et al





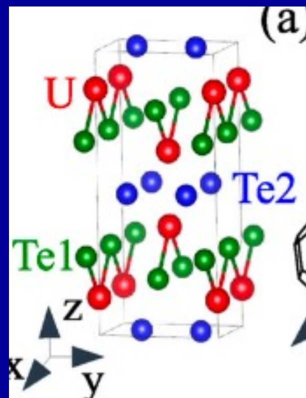


moiré:
TBLG
and
dichalcogenides

Dynamical Mean-Field Theory of Moiré Bilayer Transition Metal Dichalcogenides: Phase Diagram, Resistivity, and Quantum Criticality

Jiawei Zang,J.Wang, J.Cano, AG &AJ Millis
PRX 12, 021064 (2022)

UTe_2



Orbital selective Kondo effect in heavy fermion superconductor UTe_2

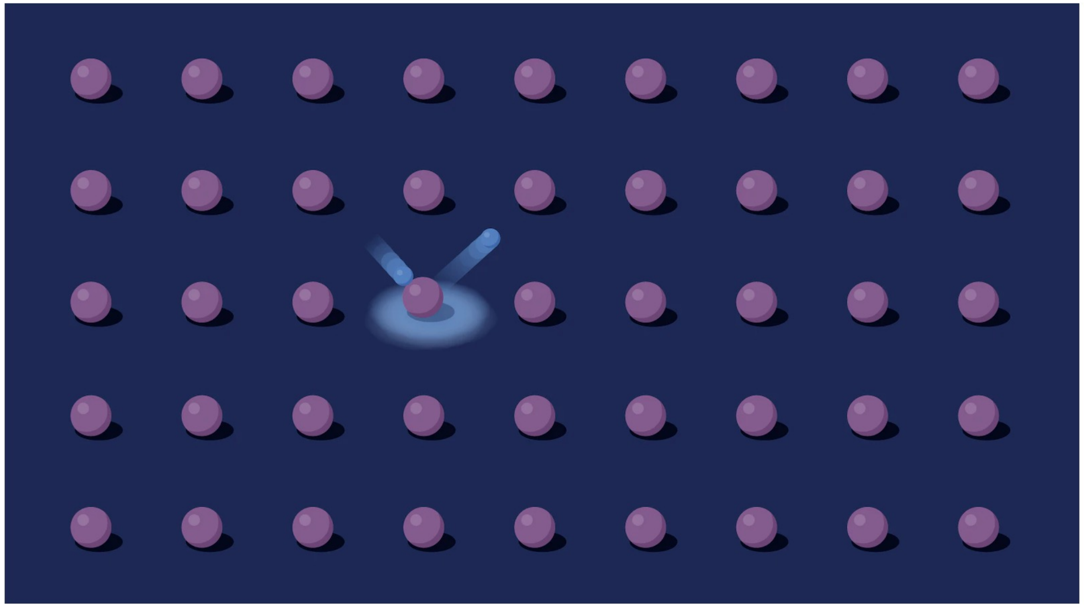
Byungkyun Kang[1,2], Sangkook Choi[2] and Hyunsoo Kim[3,4]

npj-qm, 2022

Looking Ahead…

- Looking forward to the next big advance on `impurity solvers'. Tensor Networ and METTS methods?
- Towards fully ab initio electronic structure for strong correlations: GW+DMFT (and beyond)
- Extensions of embedding schemes to include longer-range correlations; combination with diagMC?

DMFT-QE Symposium



2023 Schedule

Date	Speaker	Title	Speaker	Title
October 30, 2023 Recordings available via the link.	Philipp Werner	Nonequilibrium DMFT description of photo-doped Mott insulators	Anna Tamai	Temperature evolution of quasiparticles in Sr2RuO4: from a Fermi liquid to a bad metal state
November 27th, 2023	Karsten Held	Nickelate superconductors calculated by dynamical vertex approximation	Giorgio Sangiovanni	Mott insulators with boundary zeros
January 8, 2024				
February 5, 2024				
March 11, 2024				
April 15, 2024				

Collège de France Lectures
Spring 2019
devoted to DMFT (2019)

Website:

https://www.college-de-france.fr/site/antoine-georges/index.htm

Lectures (in French) are video recorded
PDF and Audio of lectures also available for all years
PDF for (almost) all seminars

Shakespeare's anticipation of DMFT: Correlation effects `in a nutshell'

"O God! I could be <u>bounded in a nutshell</u>,

and count myself <u>king of infinite space</u>,

were it not that I have bad dreams !"

William Shakespeare (in: Hamlet)

P.W. Anderson on DMFT:

In theory, the big news is the DMFT (dynamic mean-field theory) which gives us a systematic way to deal with the major effects of strong correlations.
After nearly 50 years, we are finally able to understand the Mott transition, for instance, at least in three dimensions, and to model the Kondo volume collapse in cerium.

In: ``The Future lies ahead'' Proc. Intl. Conf on ``Recent Progress in Many-Body Theories'' Santa Fe, 2004 (World Scientific 2006) Reprinted in ``More and different. Notes from a thoughtful curmudgeon''

A heartfelt 'THANK YOU!' to collaborators and friends over the years, and especially to:

Igor Abrikosov, Markus Aichhorn, Oscar Akerlund, Bernard Amadon, Ole K. Andersen, Ryotaro Arita, Ferdi Aryasetiawan, Dmitri Basov, Felix Baumberger, Sophie Beck, Jean-Sebastien Bernier, Christophe Berthod, Silke Biermann, Jean-Philippe Brantut, Stuart Brown, Sebastien Burdin, Massimo Capone, Iacopo Carusotto, Sara Catalano, Andrea Cavalleri, Maximilien Cazayous, Peter Cha, Johan Chang, Shubhayu Chatterjee, Marcello Civelli, Dorothee Colson, Pablo Cornaglia, Theo Costi, Luca de'Medici, Tung-Lam Dao, Jean Dalibard, Lorenzo De Leo, Xiaoyu Deng, Claribel Dominguez, Philipp Dumitrescu, Martin Eckstein, Claude Ederer, Olle Eriksson, Michel Ferrero, Matthew Fishman, Serge Florens, Jennifer Fowlie, Atsushi Fujimori, Yann Gallais, Alexandru Georgescu, Thierry Giamarchi, Marta Gibert, Daniel Grempel, Marco Grioni, Charles Grenier, Paco Guinea, Emanuel Gull, Alexander Hampel, Philipp Hansmann, Syed Hassan, Kristjan Haule, Karsten Held, Masatoshi Imada, Didier Jaccard, Dieter Jaksch, Denis Jerome, Mikhail Katsnelson, Eun-Ah Kim, Minjae Kim, Michael Köhl, Corinna Kollath, Gabriel Kotliar, Evgeny Kozik, Werner Krauth, Hulikal Krishnamurthy, Fabian Kugler, Mathieu Le Tacon, Giacomo Mazza, Andy Millis, Jernej Mravlje, Laurent Laloux, Frank Lechermann, Ivan Leonov, Sasha Lichtenstein, Peter Lunts, Andy Mackenzie, Roman Mankowsky, Yigal Meir, Takashi Miyake,Jocienne Nelson, Yusuke Nomura, Olivier Parcollet, Indranil Paul, Eva Pavarini, Oleg Peil, Luca Perfetti, Lode Pollet, Dario Poletti, Sasha Poteryaev, Leonid Pourovskii, Cyril Proust, Malte Rösner, Javier Robledo-Moreno, Marcelo Rozenberg, Angel Rubio, Alexander Rubtsov, Subir Sachdev, Alain Sacuto, Tanusri Saha-Dasgupta, Shiro Sakai, Christophe Salomon, Vito Scarola, Thomas Schäfer, Mathias Scheurer, Darrell Schlom, Anirvan Sengupta, Michael Sentef, Sriram Shastry, Kyle Shen, Qimiao Si, Nicola Spaldin, Tudor Stanescu, Miles Stoudenmire, Hugo Strand, Damien Stricker, Alaska Subedi, Louis Taillefer, Anna Tamai, Ciro Taranto, Jeremie Teyssier, Jan Tomczak, Yoshi Tokura, Alessandro Toschi, André-Marie Tremblay, Jean-Marc Triscone, Alexei Tsvelik, Veronica Vildosola, Dirk van der Marel, Jan von Delft, Cedric Weber, Tim Wehling, Nils Wentzell, Felix Werner, Philipp Werner, Alexander Wietek, Steve White, Wei Wu, Pavel Wzietek, Manuel Zingl, Rok Žitko

Apologies to those I didn't to mention for lack of space or by mistake…!