ORBITAL-SELECTIVE METAL-INSULATOR TRANSITIONS IN THE PRESENCE OF STRONG MAGNETIC FLUCTUATIONS

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ORBITAL-SELECTIVE METAL-INSULATOR TRANSITIONS

$Ca_{2-x}Sr_xRuO_4$ (0.2 < x < 0.5): metallic phase with “magnetic” behaviour

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Quasi-Two-Dimensional Mott Transition System $\mathbf{Ca_{2-x}Sr_xRuO_4}$

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(Received 28 December 1998)

We have revealed the phase diagram of $Ca_{2-x}Sr_xRuO_4$: the quasi-two-dimensional Mott transition system that connects the Mott insulator Ca_2RuO_4 with the spin-triplet superconductor Sr_2RuO_4. Adjacent to the metal/nonmetal transition at $x \simeq 0.2$, we found an antiferromagnetically correlated metallic region where non-Fermi-liquid behavior in resistivity is observed. Besides this, the critical enhancement of susceptibility toward the region boundary at $x_c \simeq 0.5$ suggests the crossover of magnetic correlation to a nearly ferromagnetic state, which evolves into the spin-triplet superconductor Sr_2RuO_4.

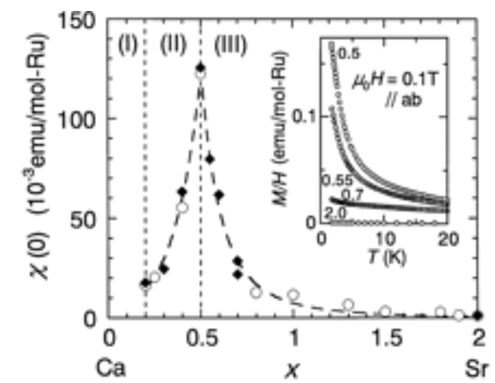

FIG. 4. $\chi(0)$: the susceptibility at 2.0 K against the Sr concentration x in the metallic regions II and III. The values for the polycrystalline samples are indicated by open circles, while for the single crystals, the solid diamonds represent the mean values $\chi_m(0)$ determined by the relation: $\chi_m(0) = \{\chi_a(0) + \chi_b(0) + \chi_c(0)\}/3$. The broken lines are guides to the eye. The inset displays $\chi(T)$ curves for region III under a field of 0.1 T parallel to the ab plane. Field-cooled and zero-field-cooled curves agree very well.

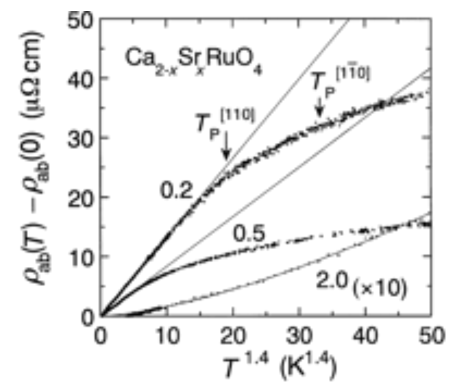

FIG. 5. Temperature dependence of the in-plane resistivity $\rho_{ab}(T)$ for $x = 0.2$, 0.5, and 2. Solid lines indicate fits with T^2 ($x = 2$), and $T^{1.4}$ ($x = 0.2$ and 0.5) dependence. The peak temperatures of the susceptibilities are indicated for $x = 0.2$.

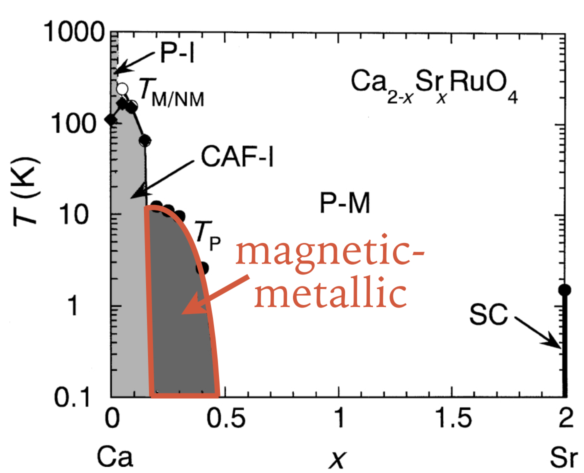

FIG. 1. Phase diagram of $Ca_{2-x}Sr_xRuO_4$ with the abbreviations: P for paramagnetic, CAF for canted antiferromagnetic, M for magnetic, SC for superconducting phase, -M for metallic phase, and -I for insulating phase. The solid circle, the open circle, and the solid diamond represent the peak temperature T_P of the susceptibility for the [001] component, the metal/nonmetal transition temperature $T_{M/NM}$, and the CAF transition temperature T_{CAF}, respectively.

Possible explanation:

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EDP Sciences

Orbital-selective Mott-insulator transition in $Ca_{2-x}Sr_xRuO_4$

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[2] Theoretische Physik , ETH-Hönggerberg 8093 Zürich, Switzerland
[3] Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan

Eur. Phys. J. B **25**, 191–201 (2002)
DOI: 10.1140/epjb/e20020021

Abstract. The electronic structures of the metallic and insulating phases of the alloy series $Ca_{2-x}Sr_xRuO_4$ ($0 \le x \le 2$) are calculated using LDA, LDA+U and Dynamical Mean-Field Approximation methods. In the end members the groundstate respectively is an orbitally non-degenerate antiferromagnetic insulator ($x = 0$) and a good metal ($x = 2$). For $x > 0.5$ the observed Curie-Weiss paramagnetic metallic state which possesses a local moment with the unexpected spin $S = 1/2$, is explained by the coexistence of localized and itinerant Ru-4d-orbitals. For $0.2 < x < 0.5$ we propose a state with partial orbital and spin ordering. An effective model for the localized orbital and spin degrees of freedom is discussed. The metal-insulator transition at $x = 0.2$ is attributed to a switch in the orbital occupation associated with a structural change of the crystal.

THEORETICAL APPROACHES TO OSMIT

Majority of studies - *local approximations to electronic correlations*

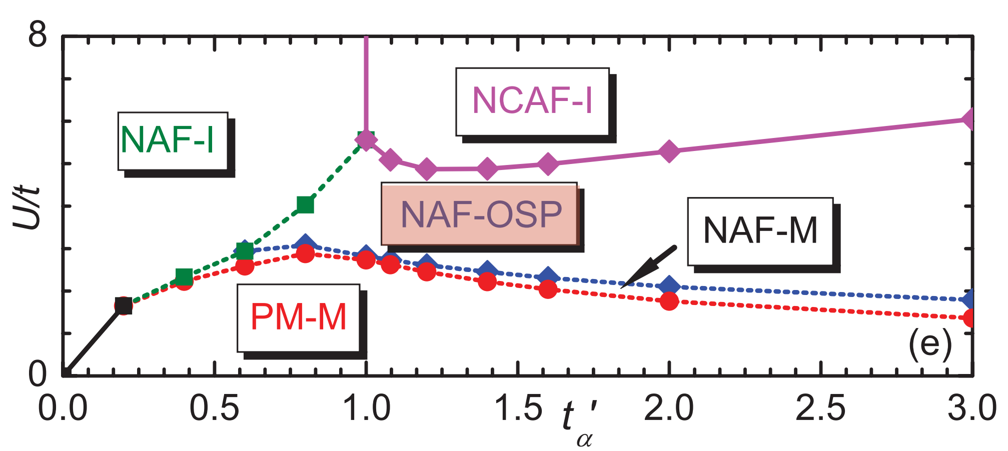
- Slave-spin approach or dynamical mean-field theory (DMFT)

⇒ Orbital-selective Mott transition (OSMT) - *no symmetry breaking, no magnetic fluctuations* ?

"Magnetic" OSMIT - *transition to the ordered magnetic phase*

- "Double-exchange" or "Hubbard-Heisenberg" models - *explicit inclusion of the local magnetic moment*
- Cluster mean-field or dynamical cluster approximation (DCA) - *local or short-range correlation effects*

[*Phys. Rev. B* **81**, 220506(**R**) (2010); *Phys. Rev. B* **84**, 020401(**R**) (2011); *Phys. Rev. B* **85**, 035123 (2012)]



(OSP - orbital-selective phase)

Phase diagram in U/t-t'_α at $t_\alpha = 1$, $t_\beta = 1$, $t'_\beta = 0$. Here $J/U = 0.25$ and filling is 1/2. Regions of different phases are indicated by the abbreviations defined in the text. M, metal; I, insulator. Solid and dotted lines represent first- and second-order phase transitions, respectively.

[*Phys. Rev. B* **85**, 035123 (2012)]

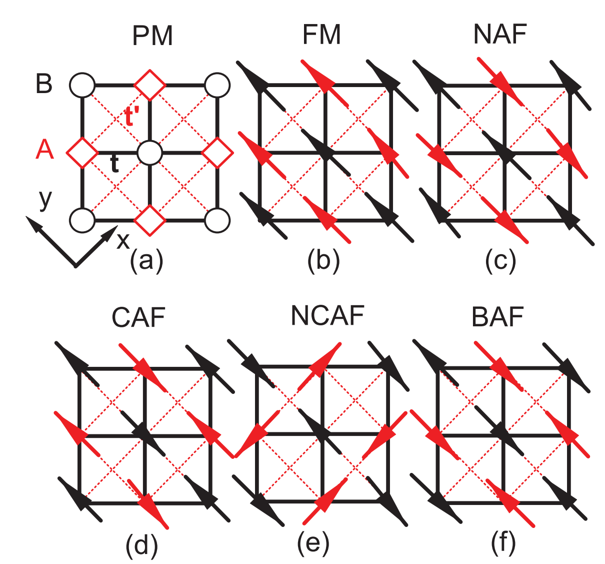


FIG. 1. (Color online) Schemes for the different magnetically ordered states we use in our calculations. (a) Paramagnetic state. Choices of sublattice and coordinate system are shown. (b) Ferromagnetic, (c) Néel, (d) collinear, (e) noncollinear, and (f) bicollinear antiferromagnetic states.

Conclusion: "OSPT is not sensitive to the strength of Hund's rule coupling. Orbitals with distinct band dispersions are crucial for the OSPT, while different bandwidths alone will not support the existence of OSPT when magnetic order is considered."

DUAL TRILEX APPROACH

E.A.S. *et al.*, *PRB* **100**, 205115 (2019)

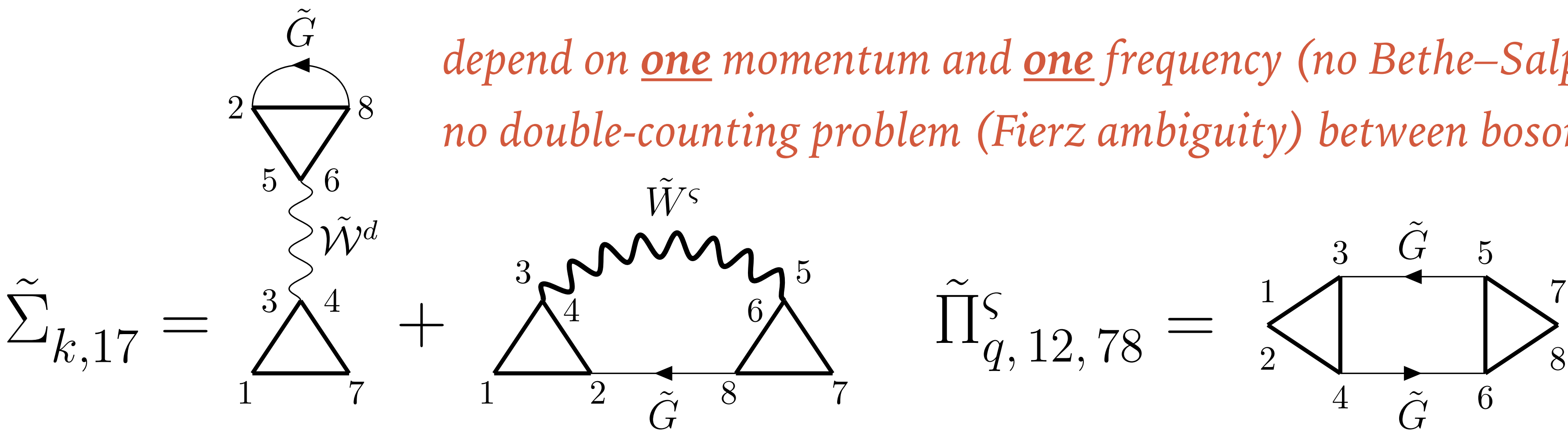
V. Harkov *et al.*, *PRB* **103**, 245123 (2021); M. Vandelli *et al.*, *SciPost Phys. 13, 0366* (2022)

For TRILEX see: T. Ayral & O. Parcollet / *PRB* **92**, *115109 (2015), PRB* **93**, *235124 (2016)*

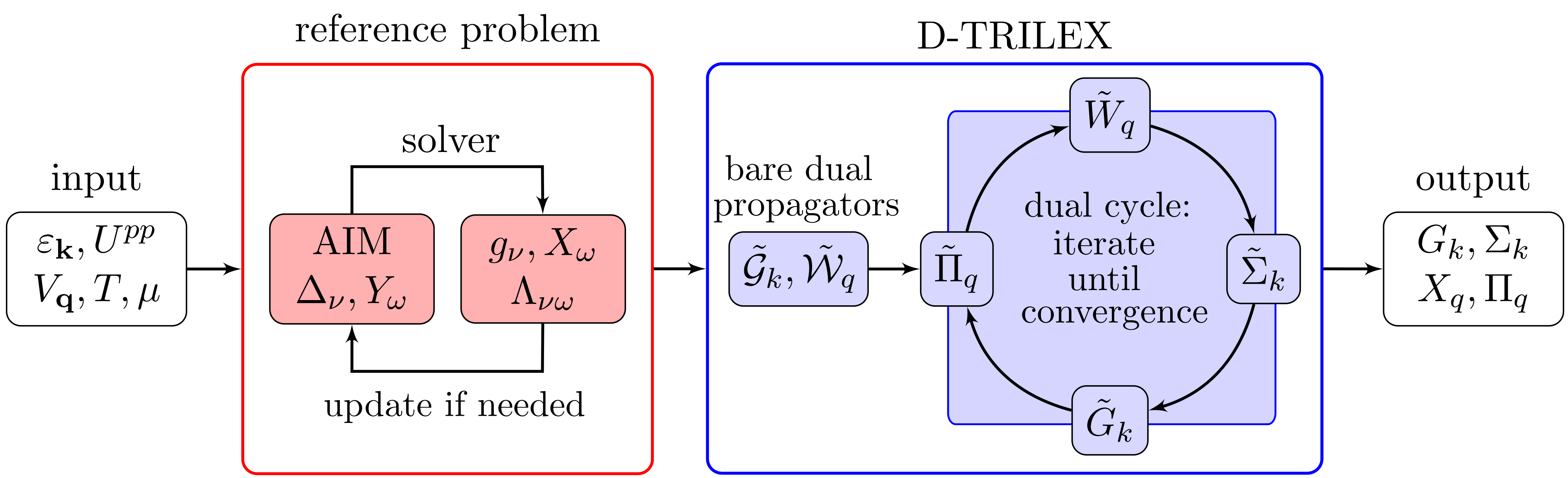
D-TRILEX self-energy and polarization operator beyond (E)DMFT:

*depend on **one** momentum and **one** frequency (no Bethe–Salpeter eq.)*

no double-counting problem (Fierz ambiguity) between bosonic channels



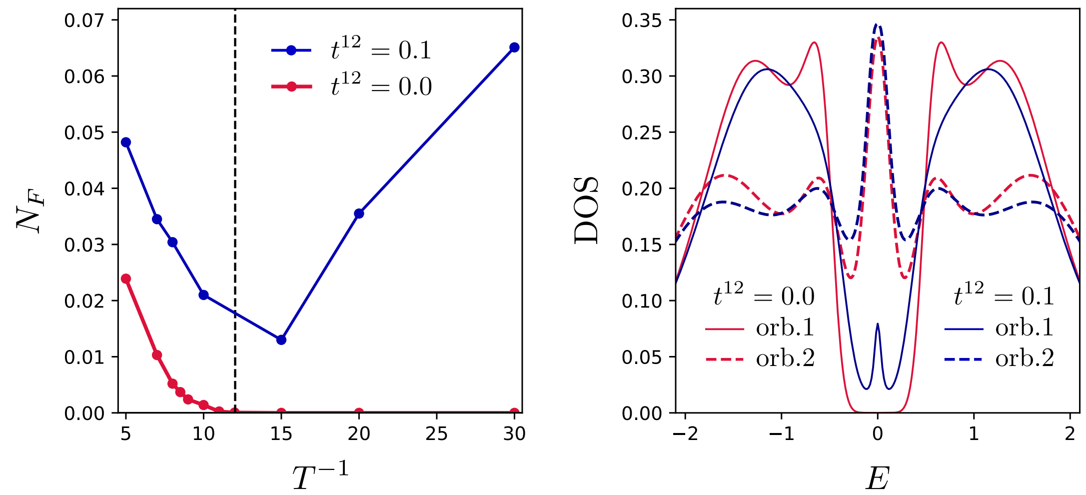
Computational workflow:



ORBITAL-SELECTIVE MOTT TRANSITION VS STRONG MAGNETIC FLUCTUATIONS

DMFT: F. B. Kugler and G. Kotliar, *PRL* **129**, 096403 (2022)

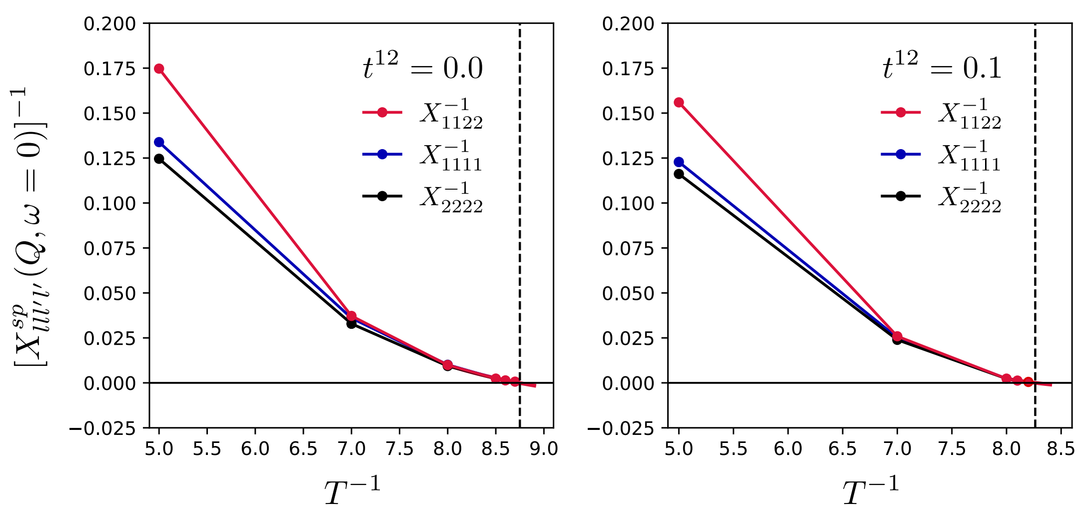
Density at Fermi energy for narrow orb., and DOS:



$t^{12} = 0$, $\beta_{OSMT} = 12$; $t^{12} \neq 0$ - no OSMT

[*PRL* **95**, 066402 (2005)]: $t^{12}_{\text{local}} \neq 0$ - no OSMT

Inverse of magnetic susceptibility at Q=(π, π, π):



$t^{12} = 0$, $\beta_{AFM} = 8.75$; $t^{12} = 0.1$, $\beta_{AFM} = 8.25$

D-TRILEX: E.A.S., *PRL* **129**, 096404 (2022)

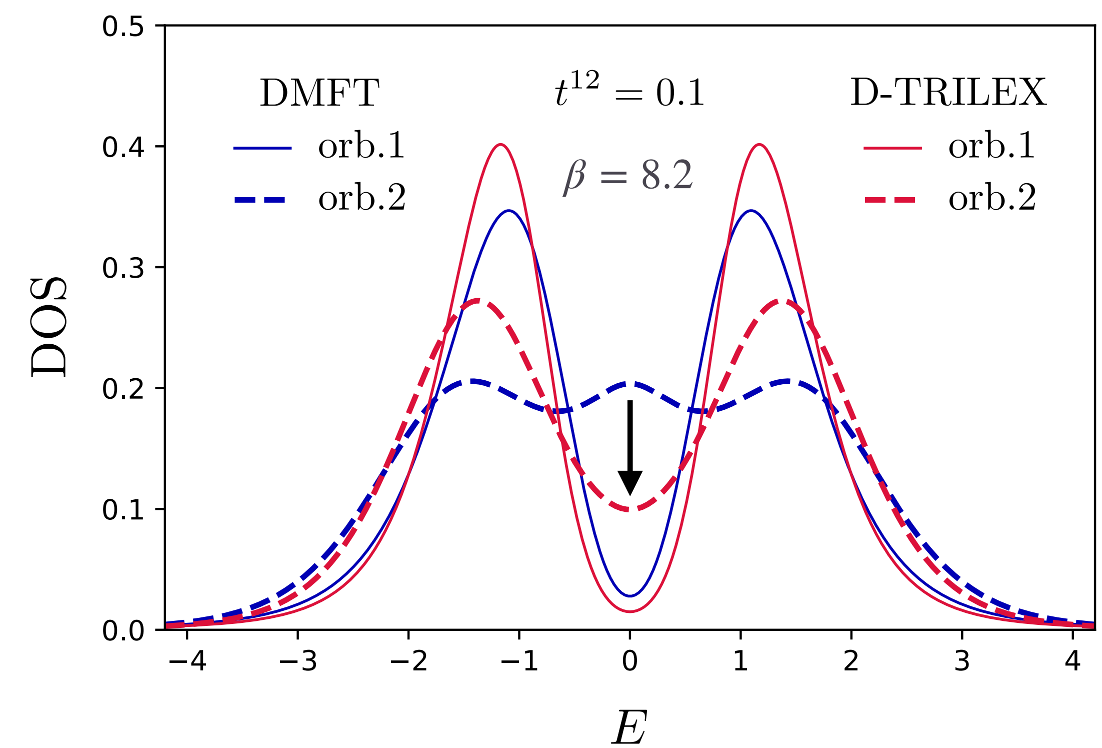
Hubbard model on a cubic lattice:

$t^{11} = 1/6$, $t^{22} = 1/3$ *different bandwidths*

$t^{12} = 0.0$ *or* 0.1 *interorbital hopping*

$U = 2.4$, $J = 0.4$ *Kanamori interaction*

DOS close to the Néel transition:



Effect of strong magnetic fluctuations:

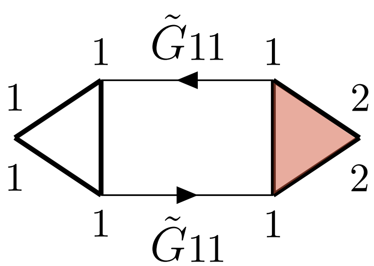
OSMT → Néel transition

No orbital selectivity in the Néel transition !

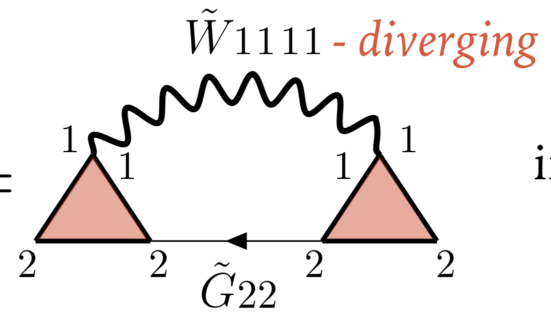
ORBITAL-SELECTIVE MOTT TRANSITION VS STRONG MAGNETIC FLUCTUATIONS

Mechanism of the Néel transition:

(if Hund's exchange coupling $J \neq 0$)

$\tilde{\Pi}_{11,22} =$ 

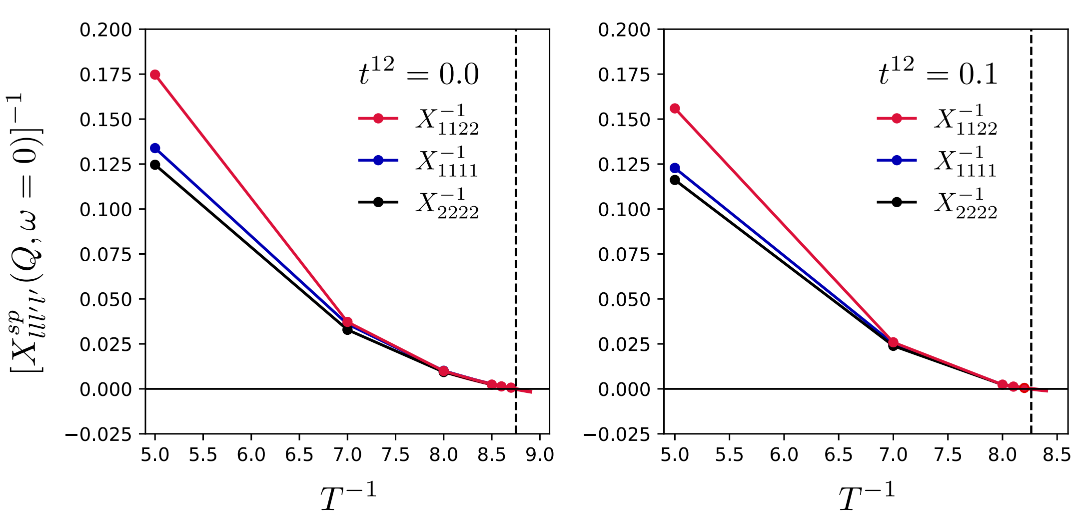
mixes orbital contributions to the spin susceptibility/W

$\tilde{\Sigma}_{22} =$ 

couples diverging interaction to electrons of the metallic orbital

Inter-orbital vertex corrections are important !

Inverse of magnetic susceptibility at $Q=(\pi,\pi,\pi)$:



$t^{12}=0,\ \beta_{AFM}=8.75;\ \ t^{12}=0.1,\ \beta_{AFM}=8.25$

D-TRILEX: E.A.S., *PRL* **129**, 096404 (2022)

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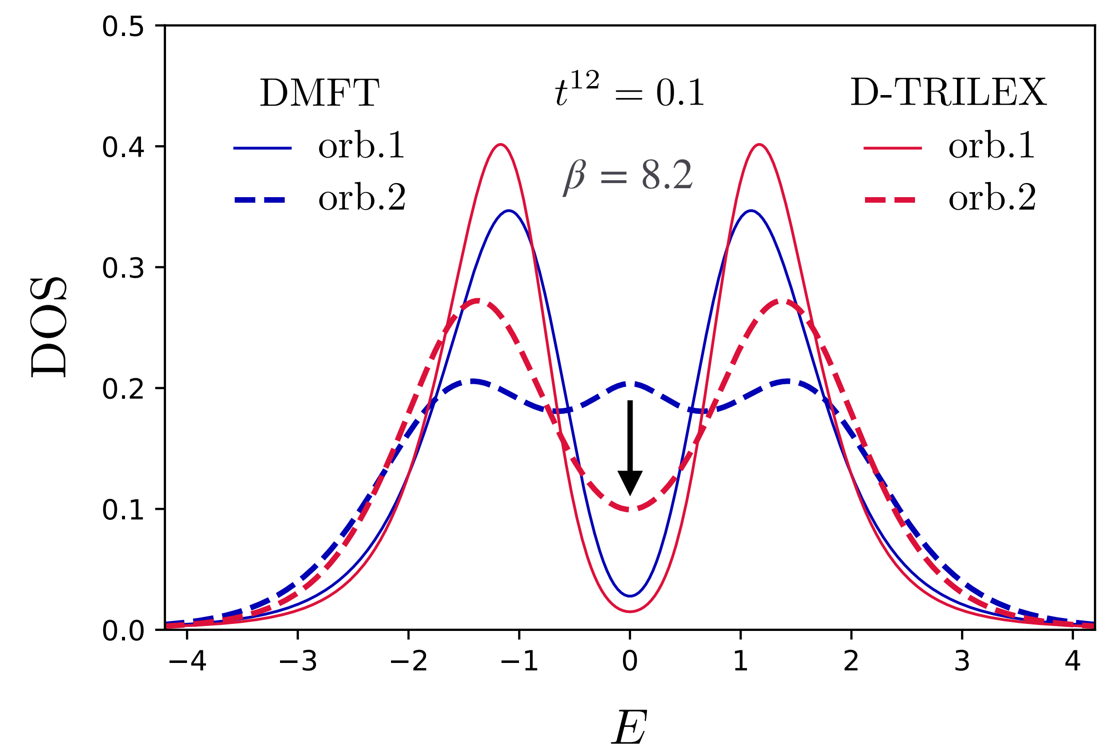

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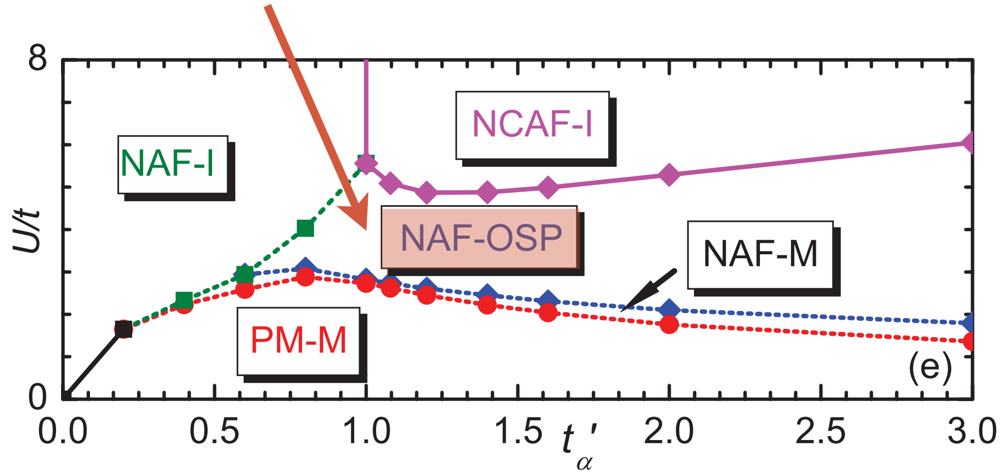
ORBITAL-SELECTIVE NÉEL TRANSITION

Hund's coupling J:

* Acts as a band decoupler [Luca de' Medici, *PRB* **83**, 205112 (2011)] *(for single-particle quantities !)*
* Couples collective electronic excitations [**E.A.S.**, *PRL* **129**, 096404 (2022)]

No OSMIT found in our calculations !



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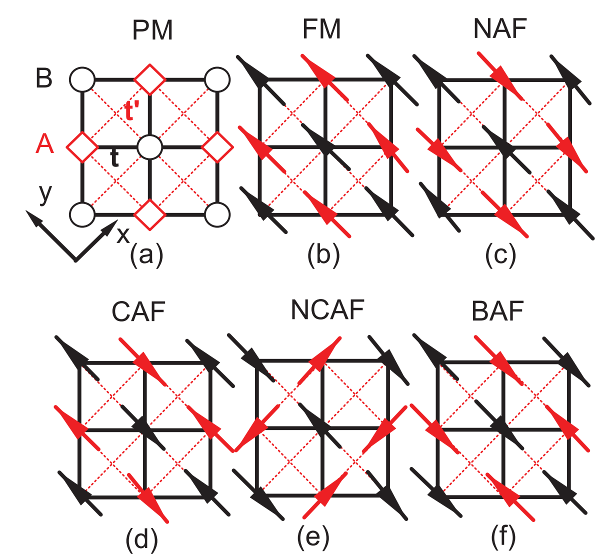

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ORBITAL-SELECTIVE NÉEL TRANSITION

E.A.S. & S. Biermann, *arXiv:2305.16730* (2023)

Hund's coupling *J*:

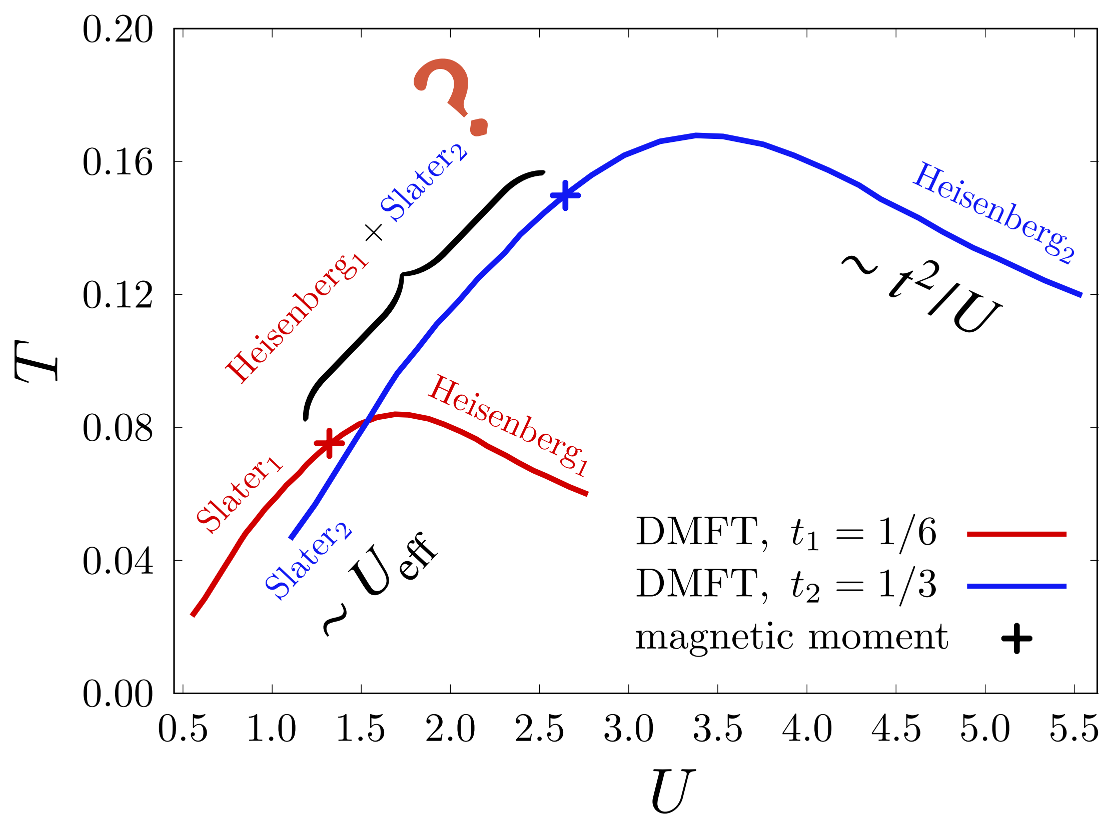
* Acts as a band decoupler [Luca de' Medici, *PRB* **83**, 205112 (2011)] *(for single-particle quantities !)*

* Couples collective electronic excitations [E.A.S., *PRL* **129**, 096404 (2022)]

* $J=0$ *decouples magnetic fluctuations in different orbitals*

Hubbard model on a cubic lattice with $t_1=1/6$, $t_2=1/3$ *(different bandwidths)*

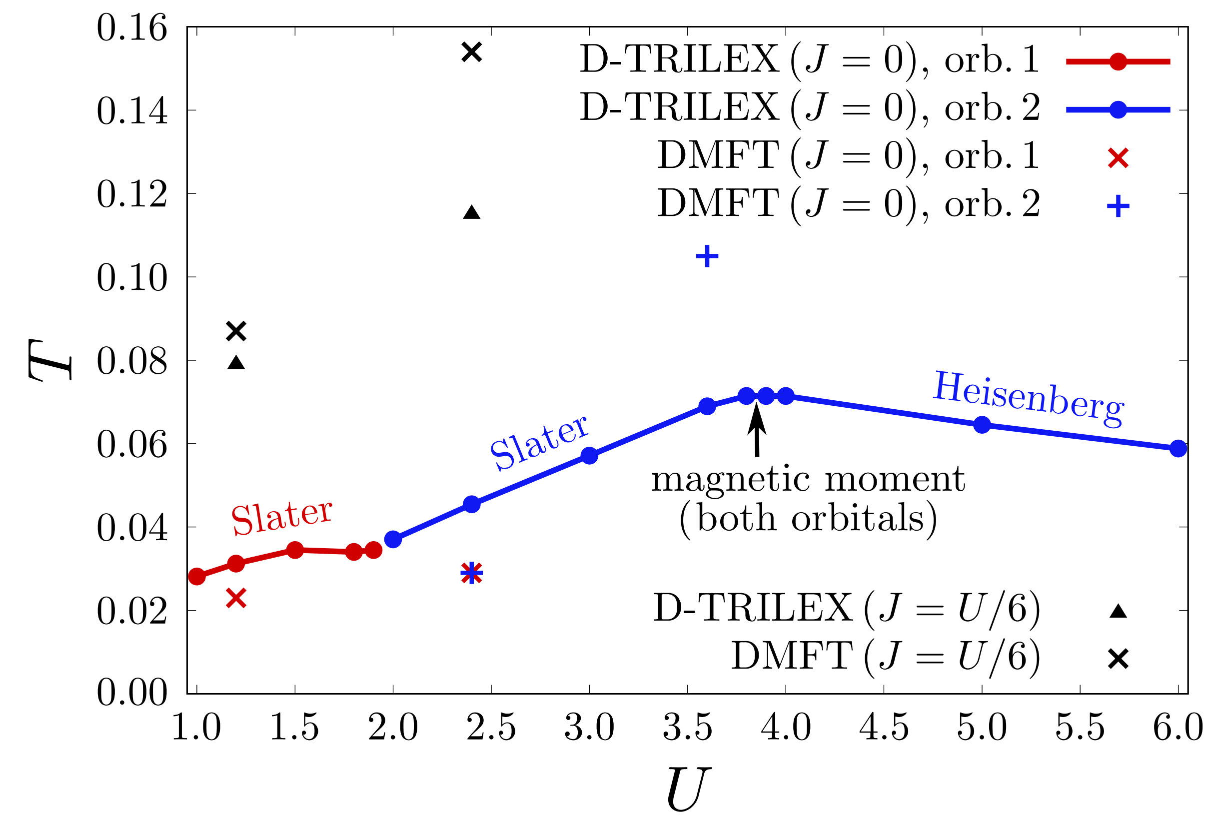
OSNT, expectation from a single band picture:



T_N DMFT: D. Hirschmeier *et al.*, *PRB* **92**, 144409 (2015)

Magnetic moment: E.A.S. *et al.*, *PRB* **105**, 155151 (2022)

D-TRILEX picture:



Even though magnetic fluctuations in different orbitals are decoupled, the local magnetic moment in **narrow** orbital can be Kondo screened by electrons from **wide** orbital !

THANK YOU FOR YOUR ATTENTION !

Conclusions:

- Strong magnetic fluctuations suppress the orbital-selective Mott transition and result in the non-orbital-selective Néel transition
- Hund's exchange J couples magnetic fluctuations from different orbitals that are efficiently mixed via inter-orbital vertex corrections
- For $J = 0$ a multi-orbital system with different bandwidths experiences the orbital-selective Néel transition for any value of the interaction
- The local magnetic moment is formed simultaneously on different orbitals

In collaboration with:

Matteo Vandelli, Alexander Lichtenstein (Universität Hamburg)

Viktor Harkov, Silke Biermann (École Polytechnique, IP Paris)