Spin freezing and unconventional superconductivity

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Aspen, March 2020

Spin freezing and unconventional superconductivity

In collaboration with:

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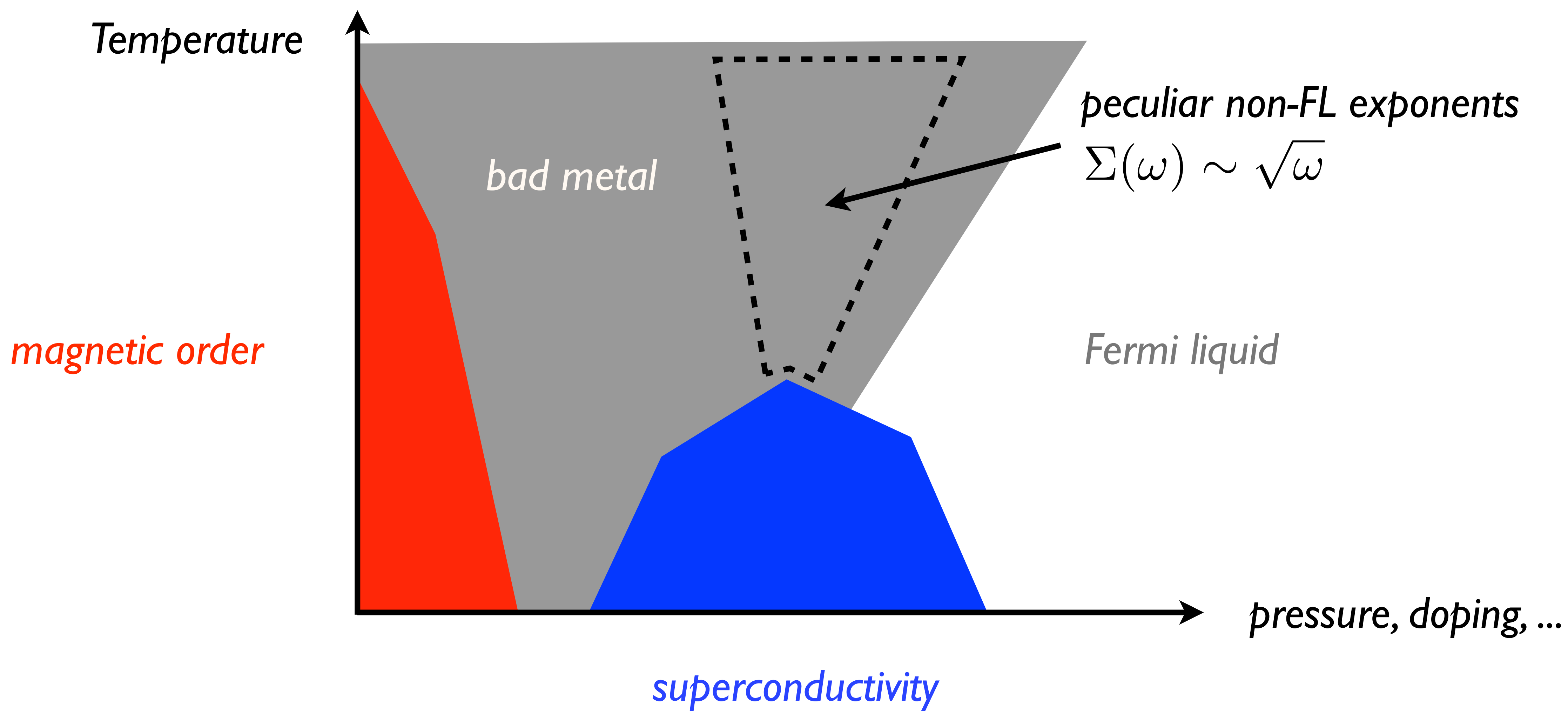
Aspen, March 2020

Introduction

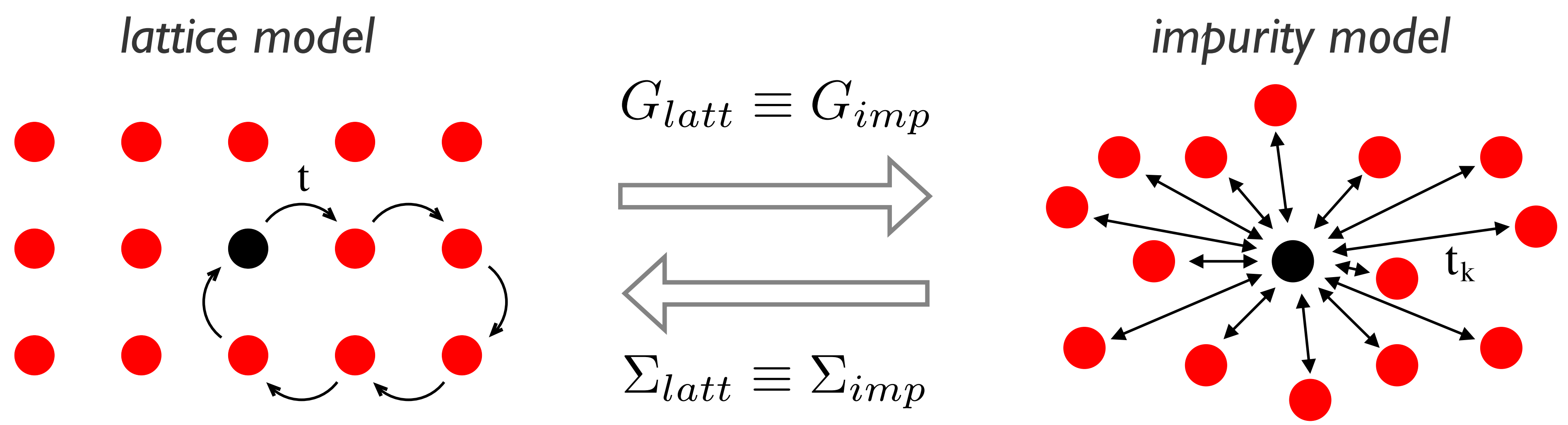
- Generic phase diagram of unconventional superconductors
  - Superconducting dome next to a magnetically ordered phase
  - Non-Fermi liquid metal above the superconducting dome



Method

Georges and Kotliar, PRB (1992)

- Dynamical mean field theory DMFT: mapping to an impurity problem



- Impurity solver: computes the Green's function of the correlated site

- Bath parameters = "mean field": optimized in such a way that the bath mimics the lattice environment

Method

Werner & Millis, PRB 74, 155107 (2006)

- CT-QMC solvers allow efficient simulation of multiorbital models

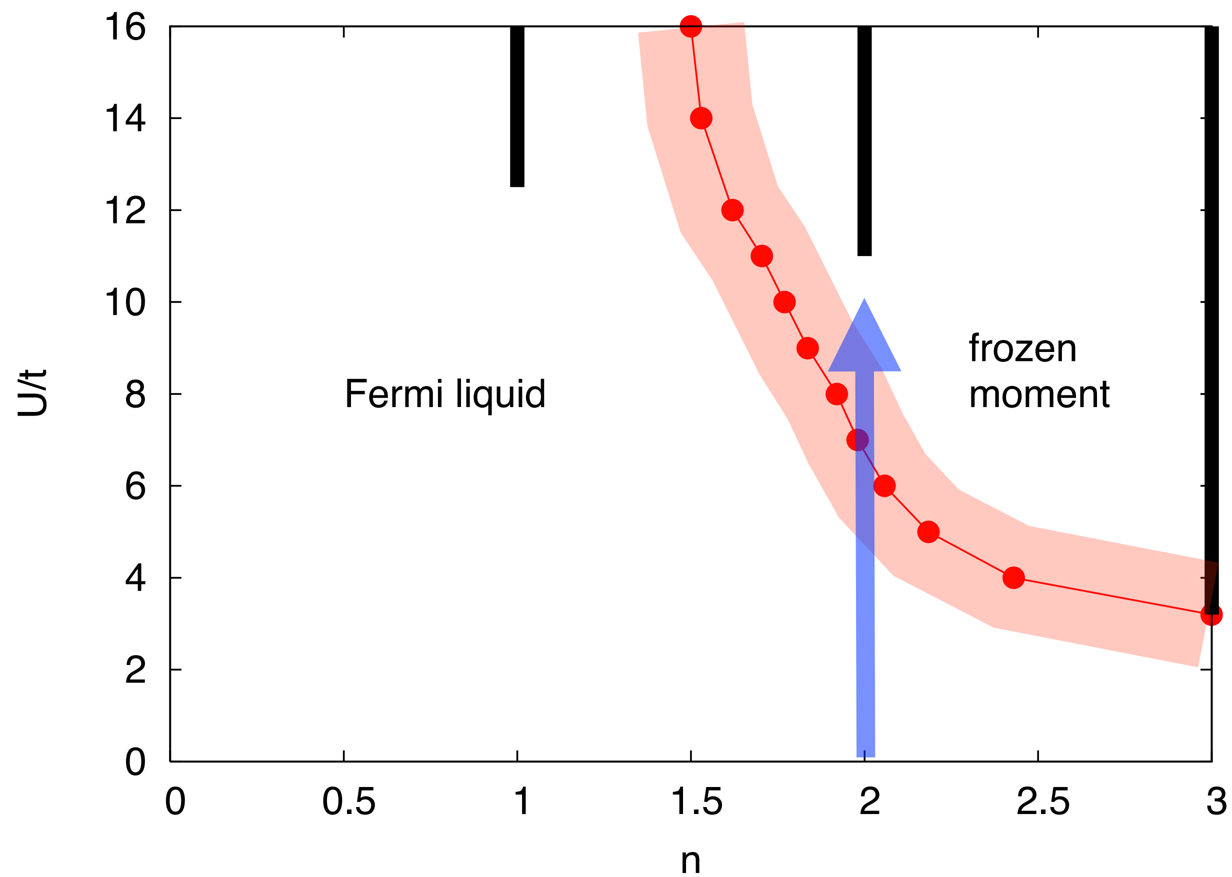
$$H_{\text{loc}} = -\sum_{\alpha,\sigma} \mu n_{\alpha,\sigma} + \sum_{\alpha} U n_{\alpha,\uparrow} n_{\alpha,\downarrow}$$
$$+ \sum_{\alpha>\beta,\sigma} U' n_{\alpha,\sigma} n_{\beta,-\sigma} + (U'-J) n_{\alpha,\sigma} n_{\beta,\sigma}$$
$$- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{\alpha,\uparrow} + \psi^\dagger_{\beta,\uparrow}\psi^\dagger_{\beta,\downarrow}\psi_{\alpha,\uparrow}\psi_{\alpha,\downarrow} + h.c.)$$

- Relevant cases:
  - 4 electrons in 3 orbitals: Sr_2RuO_4
  - 3 electrons in 3 orbitals, $J<0$: A_3C_{60}
  - 6 electrons in 5 orbitals: *Fe*-pnictides

3-orbital model

Werner, Gull, Troyer & Millis
PRL 101, 166405 (2008)

- Phase diagram for $U' = U - 2J, J/U = 1/6, \beta = 50$



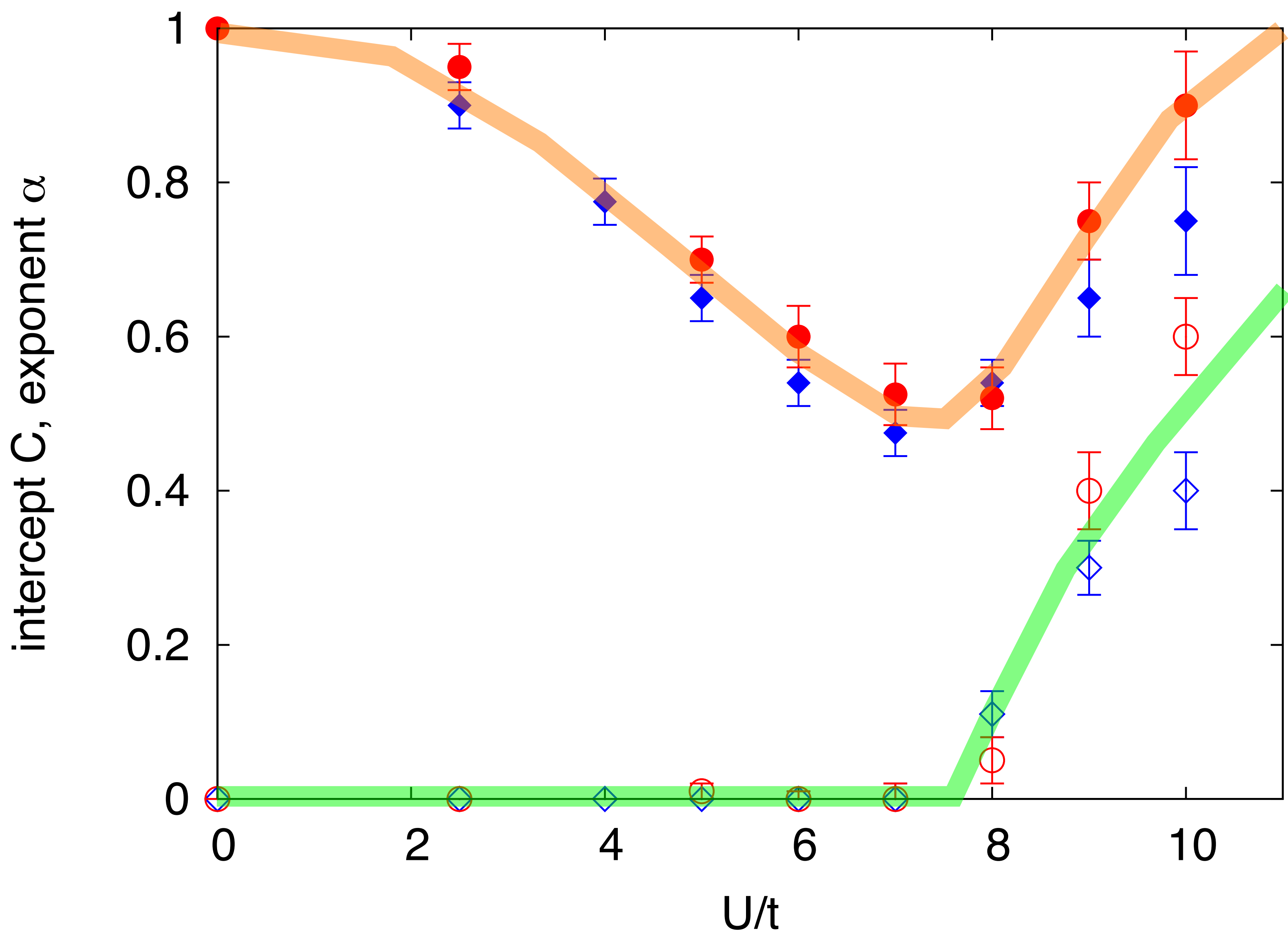
- Metallic phase: "transition" from Fermi liquid to incoherent metal
- Narrow crossover regime with self-energy

$$\mathrm{Im}\Sigma/t \sim (i\omega_n/t)^\alpha, \ \alpha \approx 0.5$$

3-orbital model

Werner, Gull, Troyer & Millis
PRL 101, 166405 (2008)

- Fit self-energy by $-\mathrm{Im}\Sigma(i\omega_n) = \boxed{C} + A(\omega_n)^{\boxed{\alpha}}$



- Square-root self-energy coincides with on-set of frozen moments

Strontium Ruthenates

Werner, Gull, Troyer & Millis
PRL 101, 166405 (2008)

- A self-energy with frequency dependence $\Sigma(\omega) \sim \omega^{1/2}$ implies an optical conductivity $\sigma(\omega) \sim 1/\omega^{1/2}$

VOLUME 81, NUMBER 12 PHYSICAL REVIEW LETTERS 21 SEPTEMBER 1998

Non-Fermi-Liquid Behavior of $SrRuO_3$: Evidence from Infrared Conductivity

P. Kostic, Y. Okada,* N. C. Collins, and Z. Schlesinger
Department of Physics, University of California, Santa Cruz, California 95064

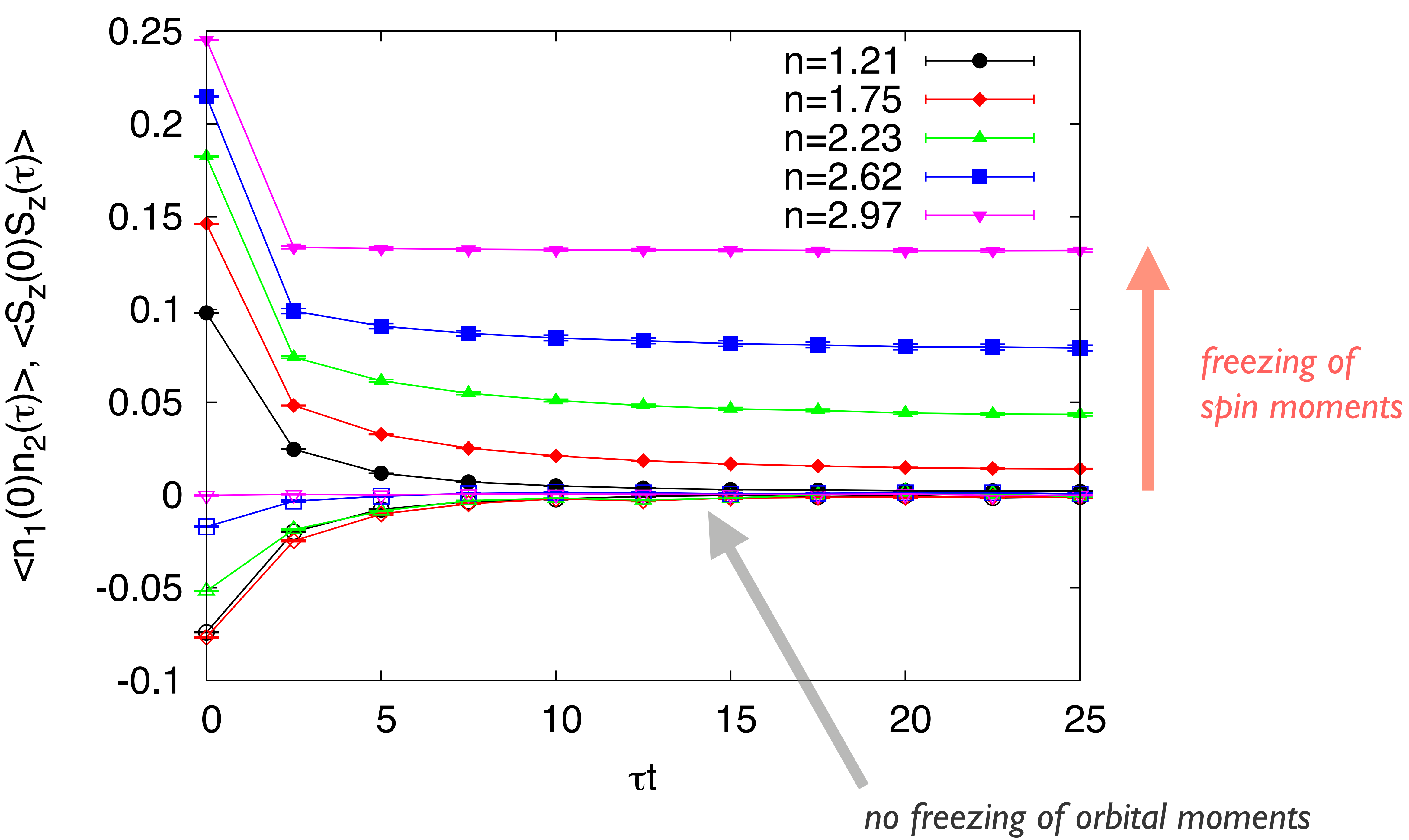
J. W. Reiner, L. Klein,† A. Kapitulnik, T. H. Geballe, and M. R. Beasley
Edward L. Ginzton Laboratories, Stanford University, Stanford, California 94305
(Received 13 March 1998)

The reflectivity of the itinerant ferromagnet $SrRuO_3$ has been measured between 50 and 25 000 cm^{-1} at temperatures ranging from 40 to 300 K, and used to obtain conductivity, scattering rate, and effective mass as a function of frequency and temperature. We find that at low temperatures the conductivity falls unusually slowly as a function of frequency (proportional to $1/\omega^{1/2}$), and at high temperatures it even appears to increase as a function of frequency in the far-infrared limit. The data suggest that the charge dynamics of $SrRuO_3$ are substantially different from those of Fermi-liquid metals.

Spin freezing

Werner, Gull, Troyer & Millis
PRL 101, 166405 (2008)

- Spin-spin and orbital-orbital correlation functions



Spin freezing

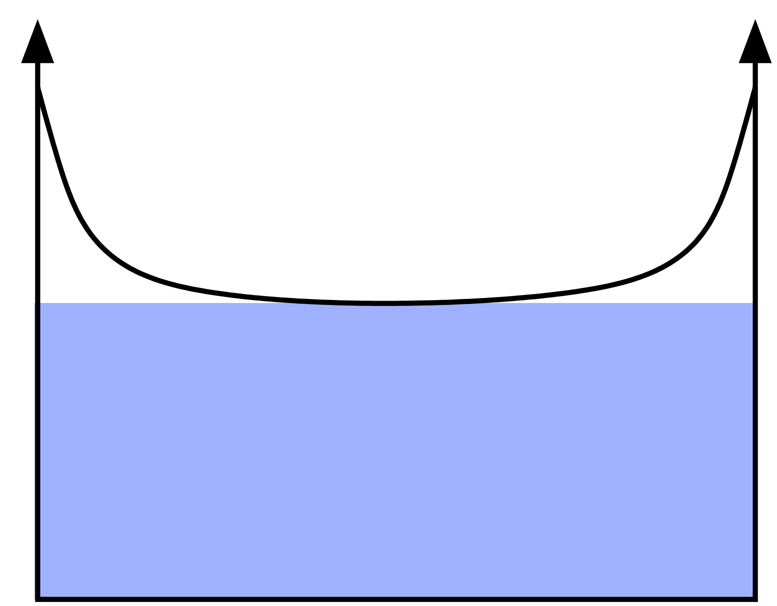
Hoshino & Werner
PRL 115, 247001 (2015)

- Consider the local susceptibility

$$\chi_{\mathrm{loc}} = \int_0^\beta d\tau \langle S_z(\tau) S_z(0) \rangle$$

and its dynamic contribution

$$\Delta\chi_{\mathrm{loc}} = \int_0^\beta d\tau [\langle S_z(\tau) S_z(0) \rangle - \langle S_z(\beta/2) S_z(0) \rangle]$$

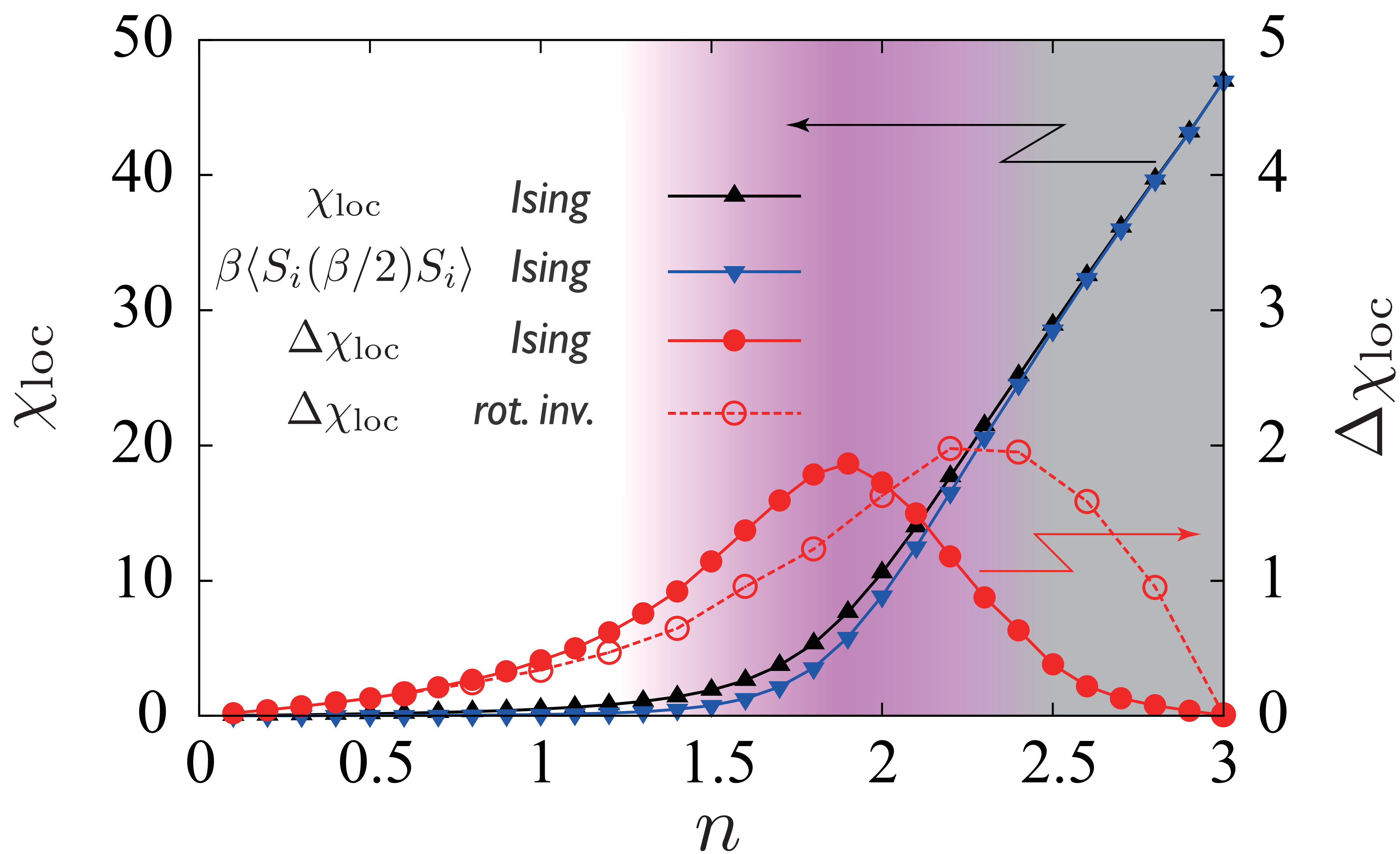


subtract the (frozen) long-time value

Spin freezing

Hoshino & Werner
PRL 115, 247001 (2015)

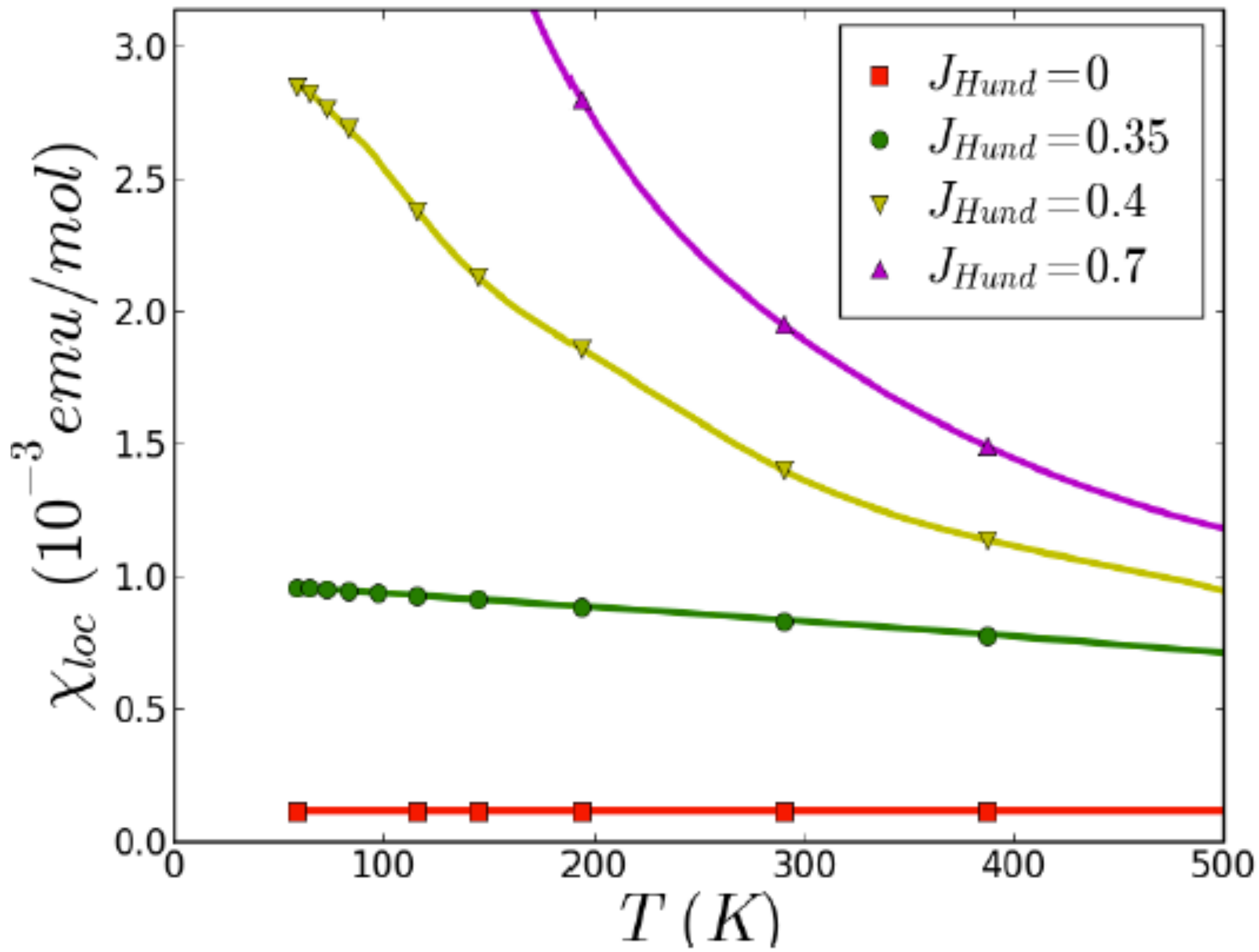
- Consider the local susceptibility χ_{loc} and its dynamic contribution $\Delta\chi_{\mathrm{loc}}$



- Crossover regime is characterized by large local moment fluctuations

Pnictides

- Strongly correlated despite moderate *U*



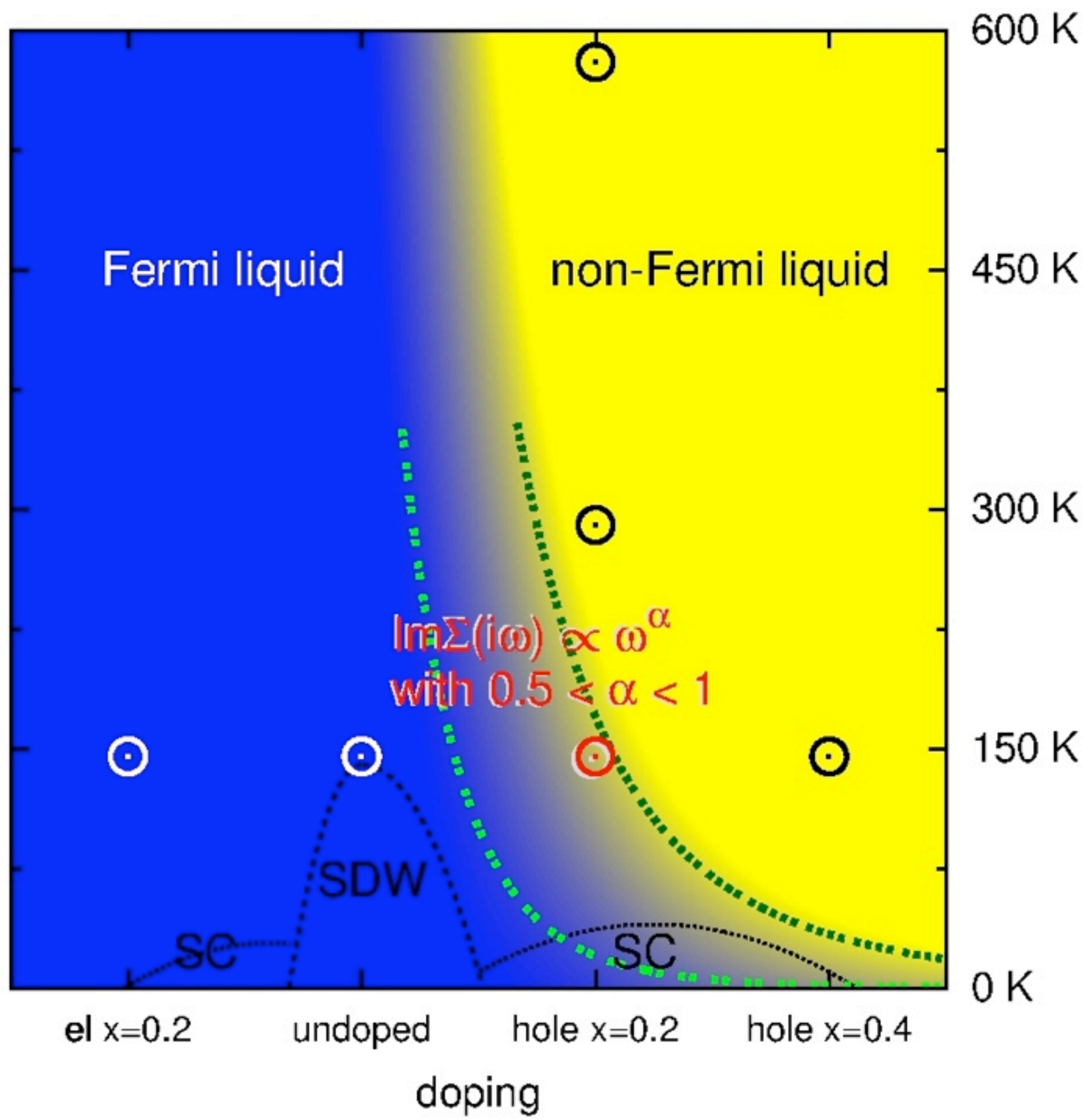
incoherent metal state resulting from Hund's coupling

Haule & Kotliar, NJP (2009)

Pnictides

Werner *et al.*
Nature Phys. 8, 331 (2012)

- Strong doping and temperature dependence of electronic structure



$BaFe_2As_2$:

conventional FL metal in the underdoped regime

non-FL properties near optimal doping

incoherent metal in the overdoped regime

Long-range order

Hoshino & Werner
PRL 115, 247001 (2015)

- Identify ordering instabilities by divergent lattice susceptibilities
  - Calculate local vertex from impurity problem
  - Approximate vertex of the lattice problem by this local vertex
  - Solve Bethe-Salpeter equation to obtain lattice susceptibility

- The following orders (staggered and uniform) are considered:
  - diagonal orders:

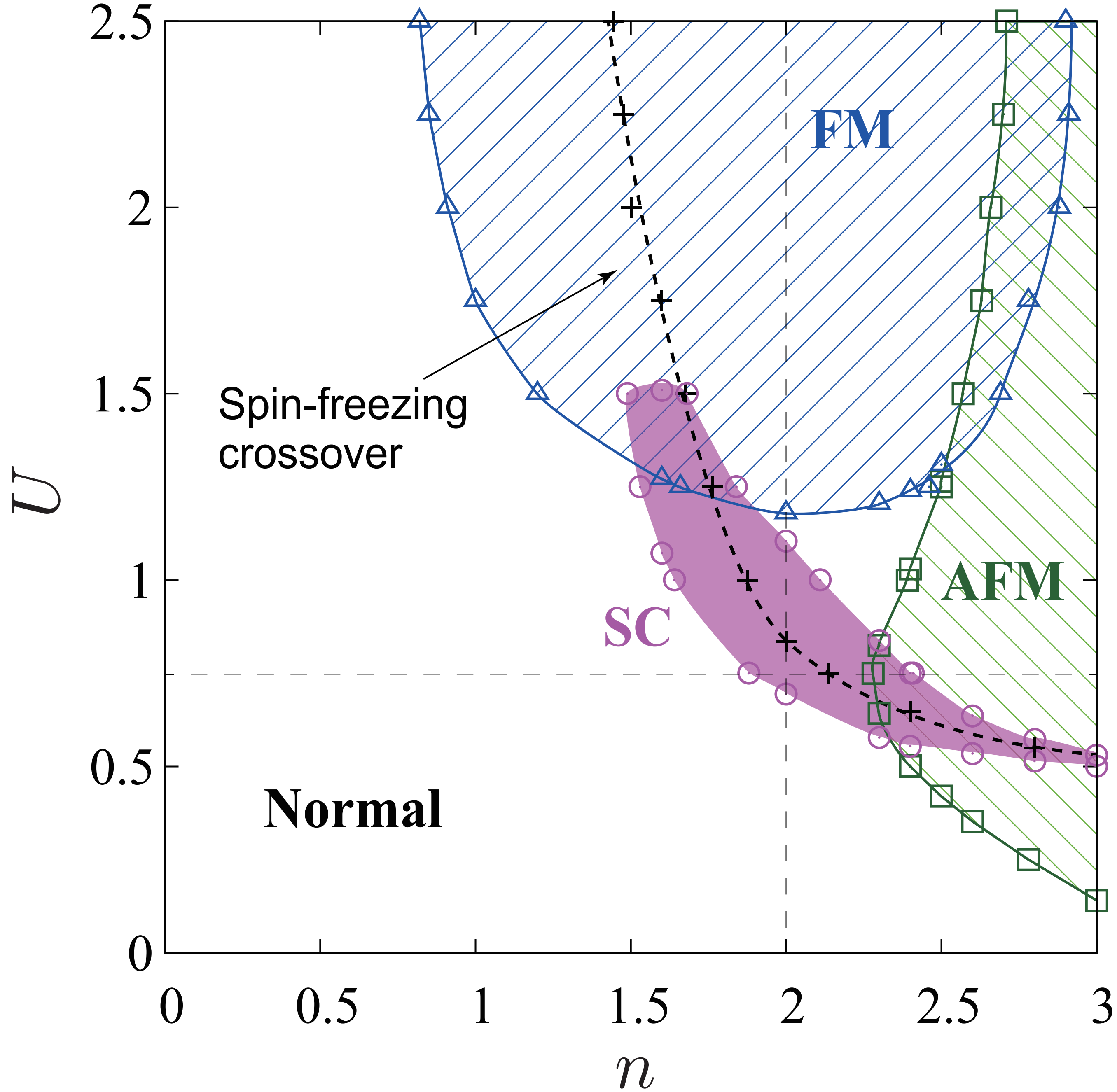
    charge, spin, orbital, spin-orbital
  - off-diagonal orders:

    orbital-singlet-spin-triplet SC, orbital-triplet-spin-singlet SC

Long-range order

Hoshino & Werner
PRL 115, 247001 (2015)

- 3-orbital model, Ising interactions



AFM near half-filling

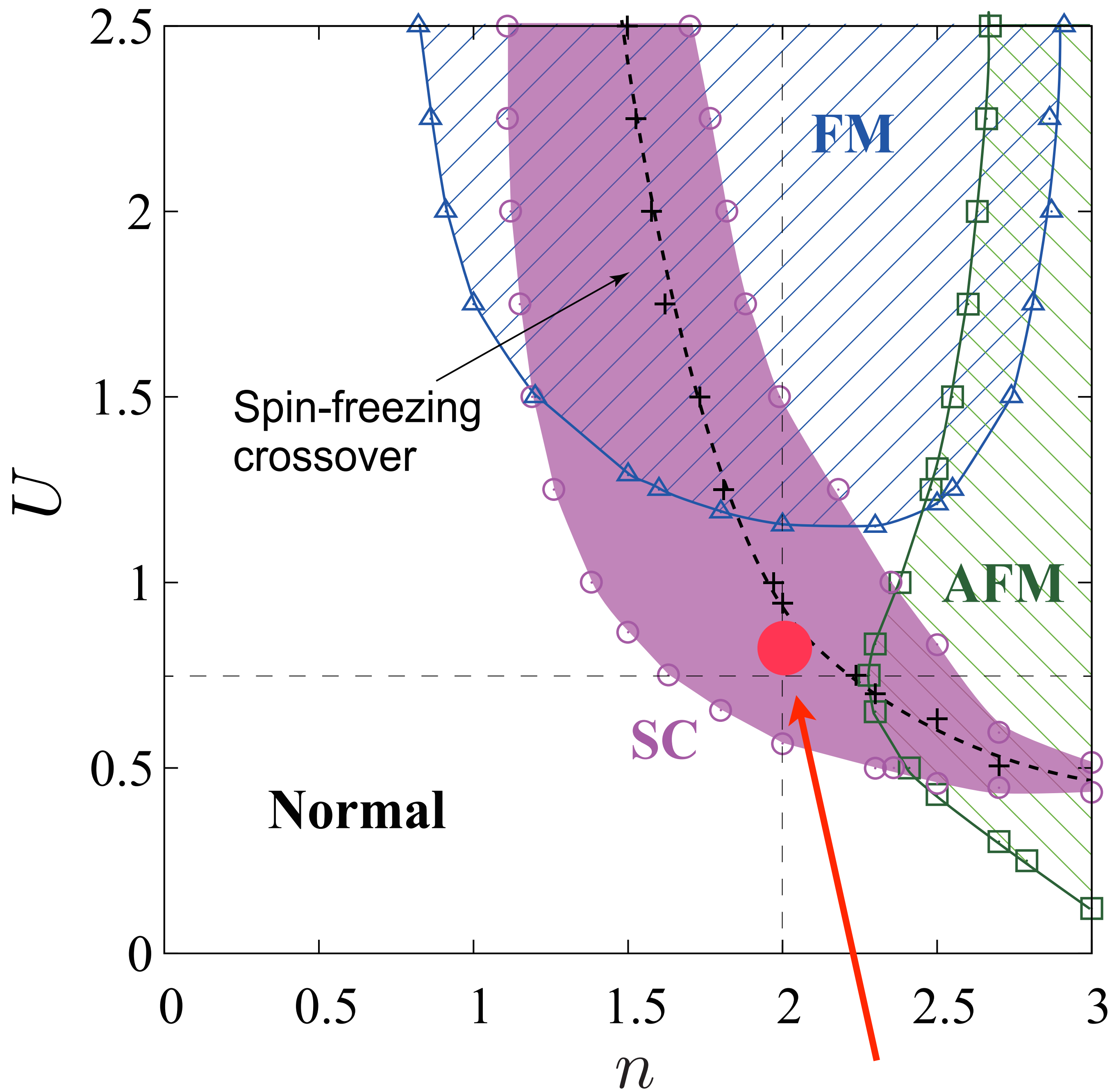
FM at large U away from half-filling

spin-triplet superconductivity in the spin-freezing crossover region

Long-range order

Hoshino & Werner
PRL 115, 247001 (2015)

- 3-orbital model, Ising interactions (lower temperature)



AFM near half-filling

FM at large U away from half-filling

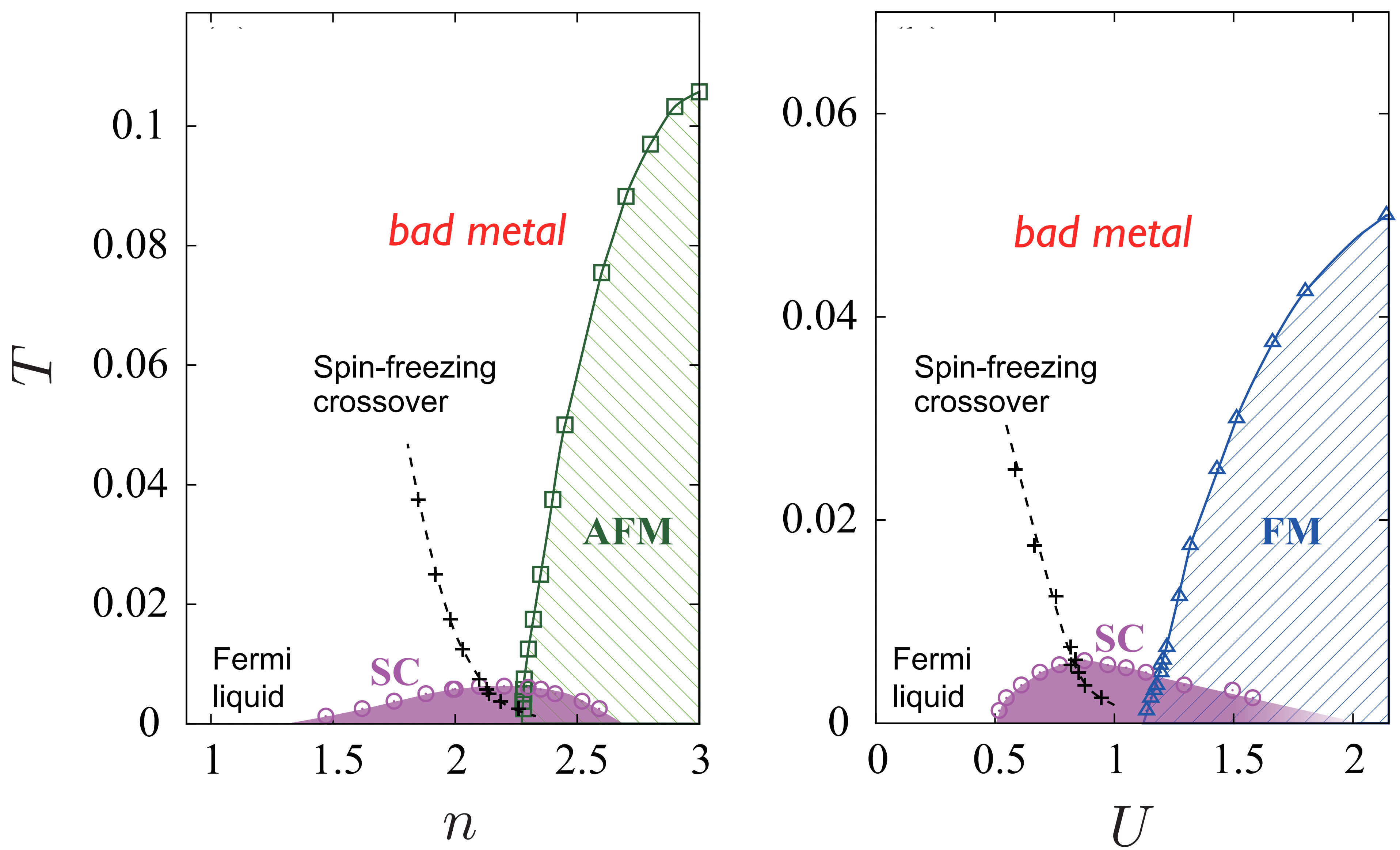
spin-triplet superconductivity in the spin-freezing crossover region

parameter regime relevant for Sr_2RuO_4

Long-range order

Hoshino & Werner
PRL 115, 247001 (2015)

- T_c dome and non-FL metal phase next to magnetic order

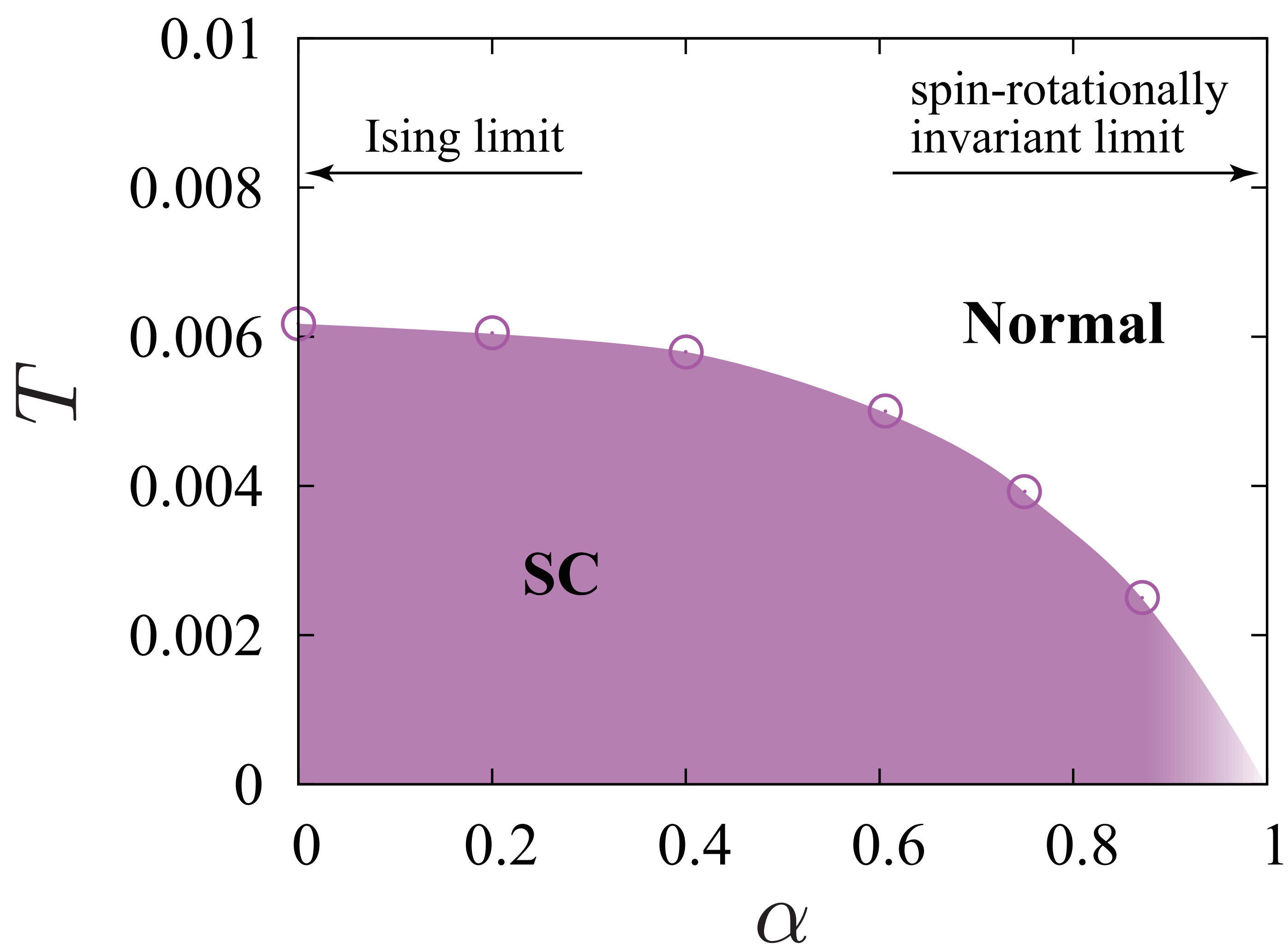


- Generic phasediagram of unconventional SC without QCP!

Long-range order

Hoshino & Werner
PRL 115, 247001 (2015)

- T_c dome and non-FL metal phase next to magnetic order



- Need spin-anisotropy (SO coupling) for high T_c

  probably relevant for: Sr_2RuO_4, UGe_2, URhGe, UCoGe, ...

Long-range order

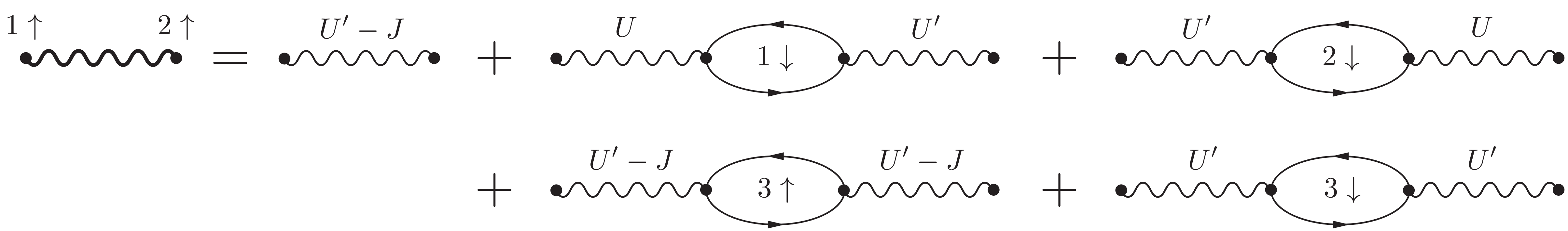
Hoshino & Werner
PRL 115, 247001 (2015)

- Pairing induced by local spin fluctuations

  Weak-coupling argument inspired by Inaba & Suga, PRL (2012)

- Effective interaction which includes bubble diagrams:

$$\tilde{U}_{\alpha\beta}(q) = U_{\alpha\beta} - \sum_{\gamma} U_{\alpha\gamma}\chi_{\gamma}(q)\tilde{U}_{\gamma\beta}(q)$$



- Effective inter-orbital same-spin interaction

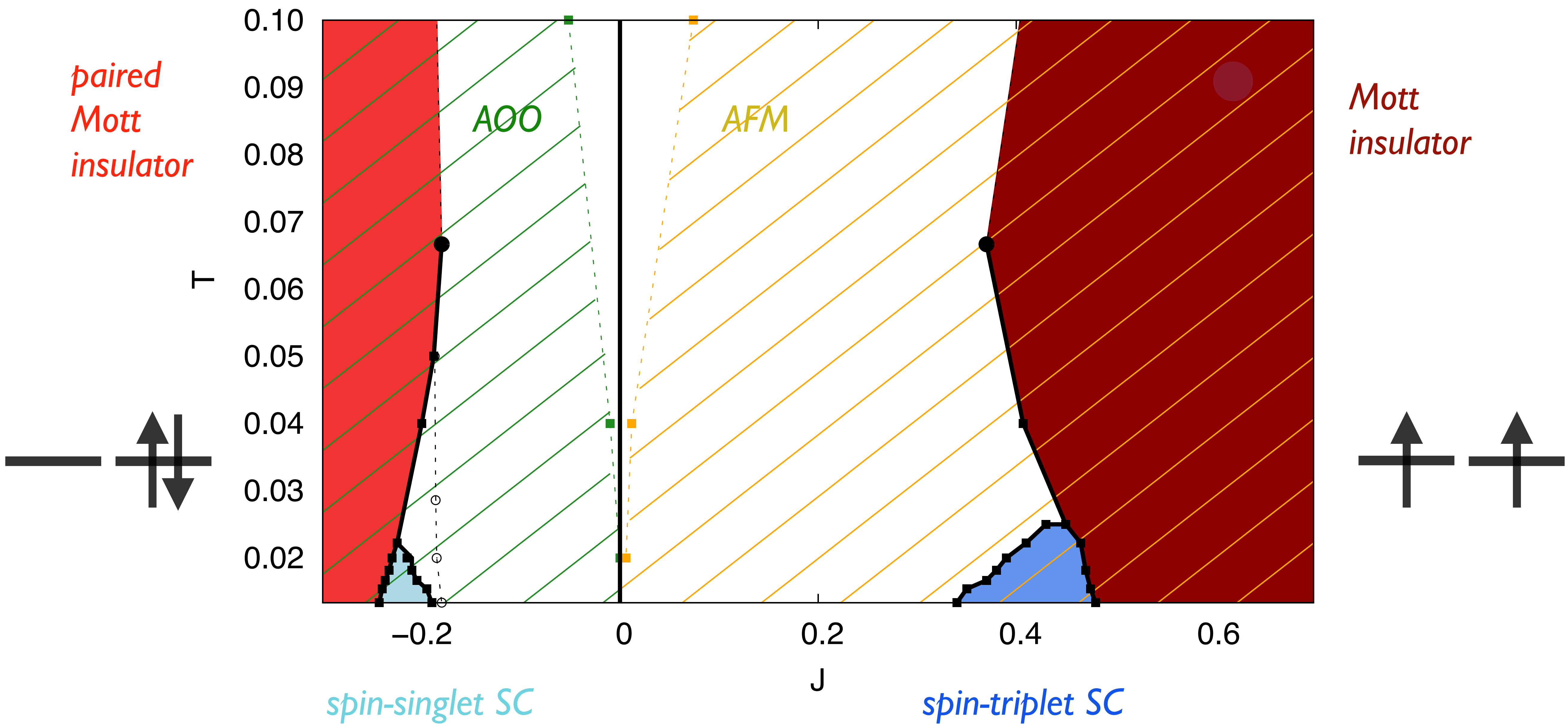
$$\tilde{U}_{1\uparrow,2\uparrow}(0) = U' - J - [2UU' + (U'-J)^2 + U'^2]\chi_{\mathrm{loc}}$$

in the weak-coupling regime: $\chi_{\mathrm{loc}} = \Delta\chi_{\mathrm{loc}}$

Negative J and orbital freezing

Steiner et al.
PRB 94, 075107 (2016)

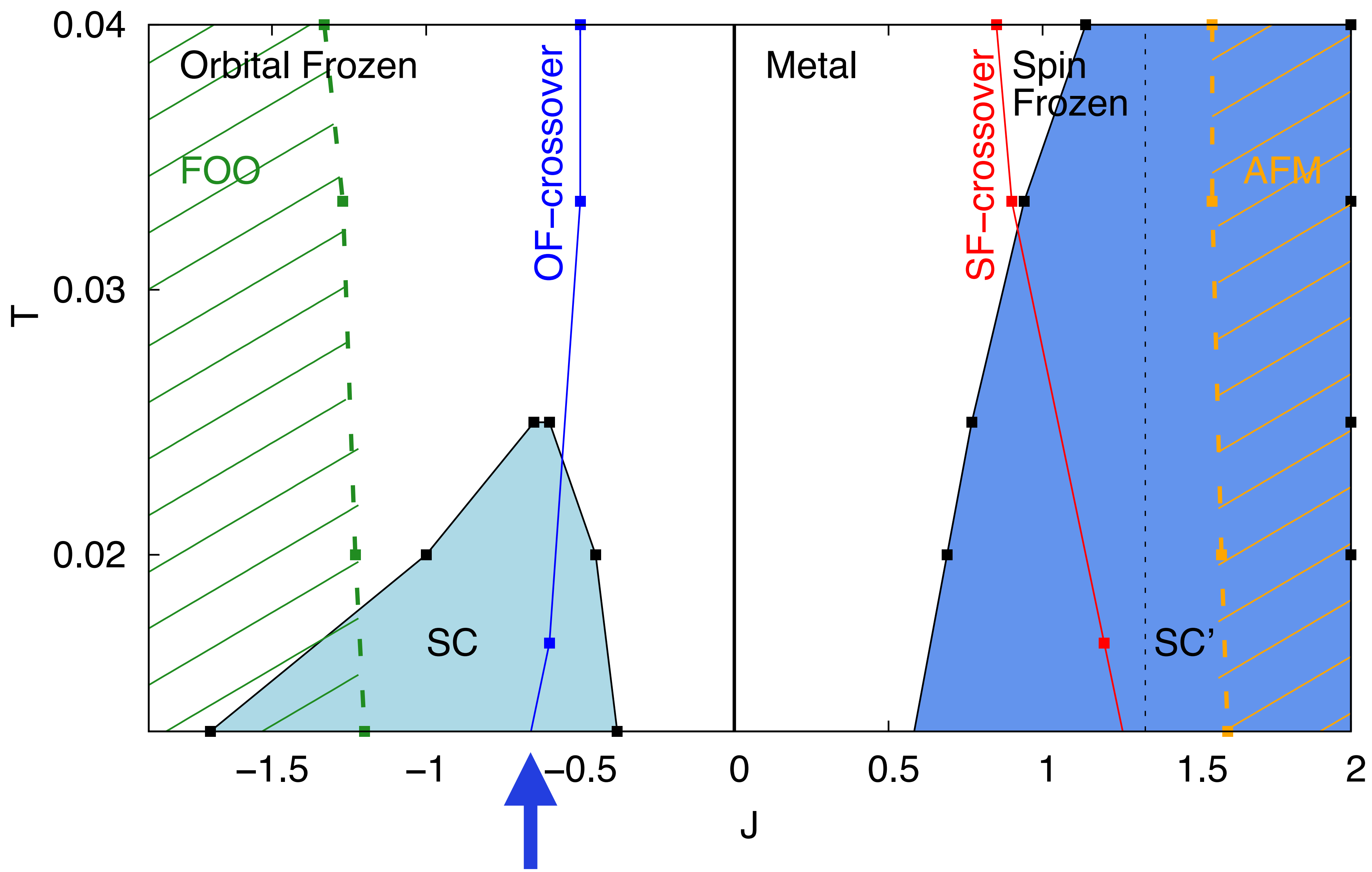
- 2-orbital model (U=bandwidth=4)



Negative J and orbital freezing

Steiner et al.
PRB 94, 075107 (2016)

- Away from half-filling: SC dome peaks near orbital freezing line



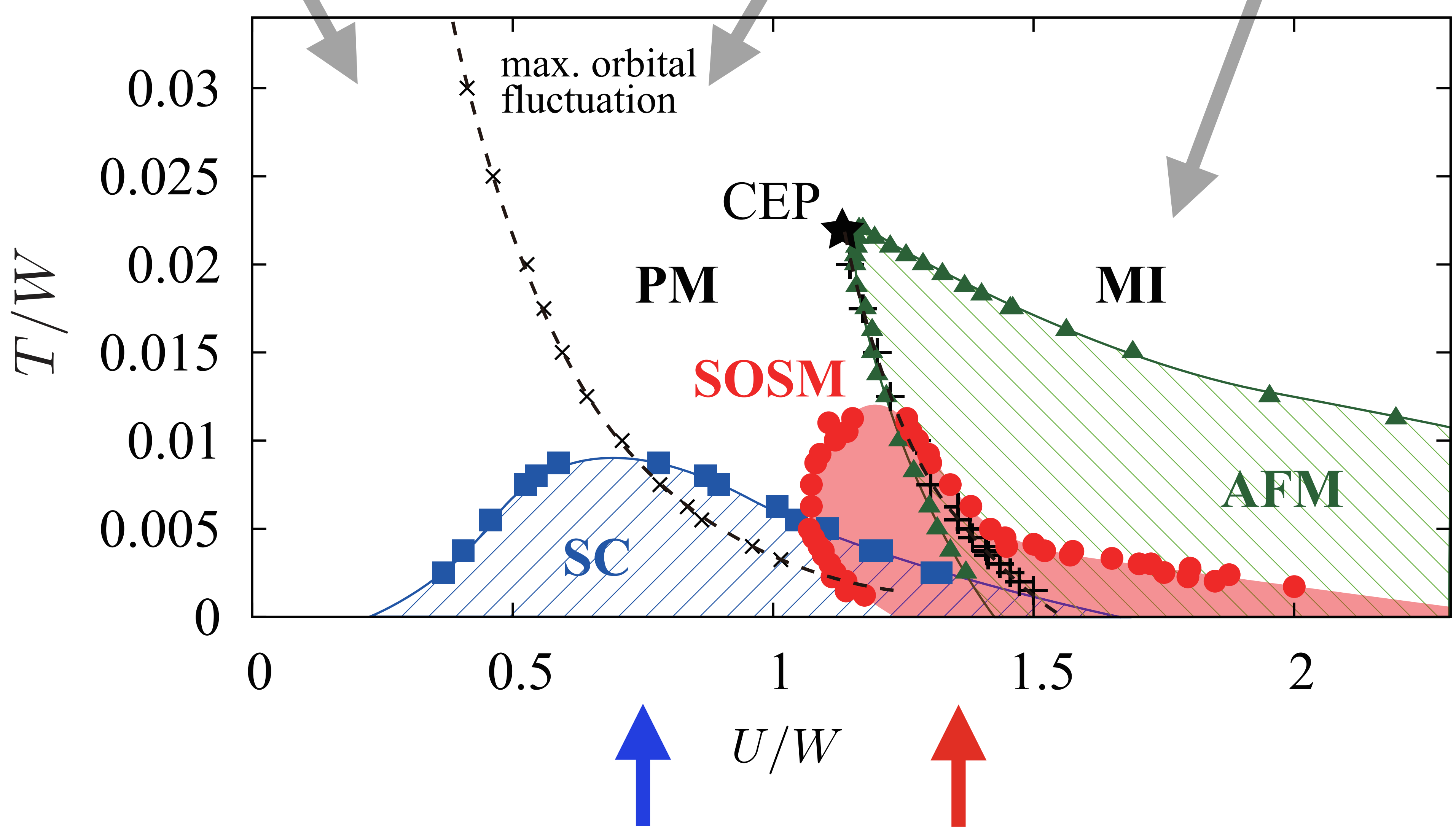
line of maximum orbital fluctuations

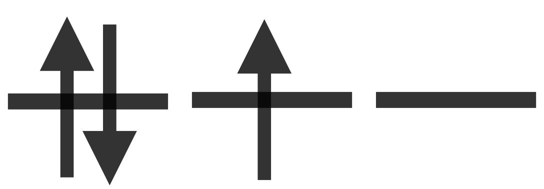
Negative J and orbital freezing

Hoshino & Werner
PRL 118, 177002 (2017)

- Half-filled 3-orbital model with J<0 (A_3C_{60})

Fermi liquid metal *orbital frozen metal* *Mott insulator*





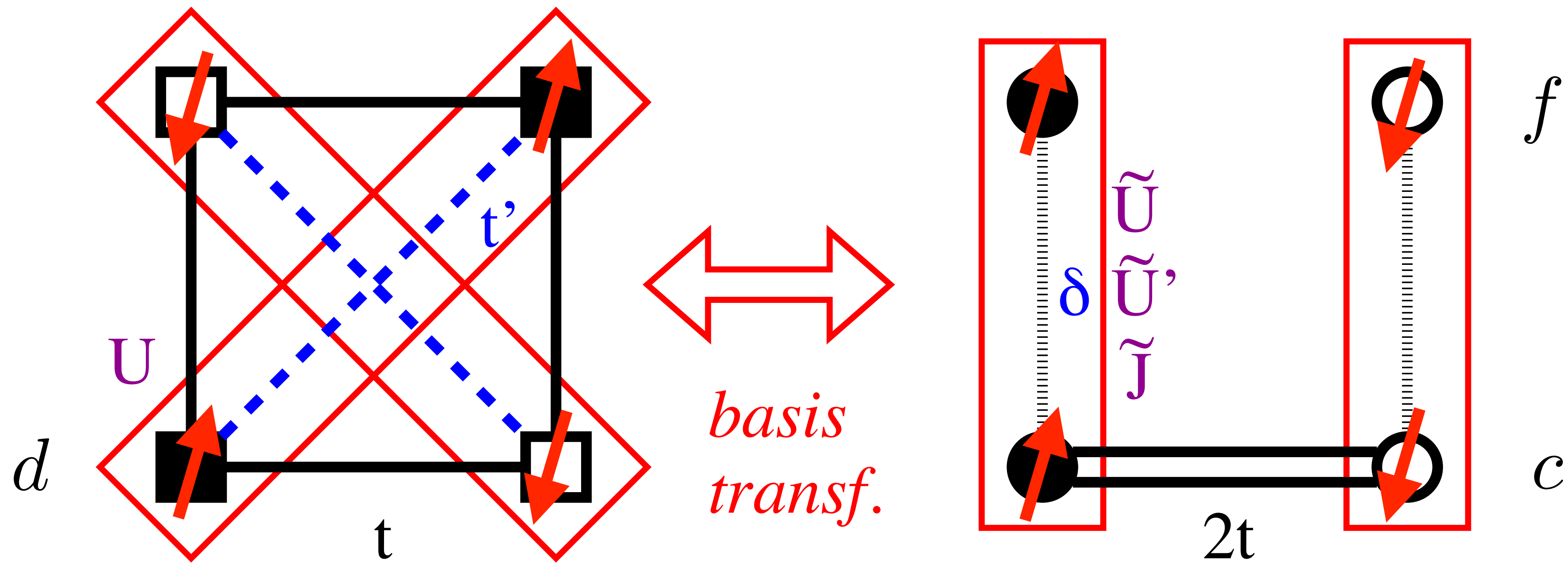
SC dome peaks in the region of maximum orbital fluctuations

spontaneous symmetry breaking into an orbital selective Mott phase ("Jahn-Teller metal")

Cuprates

Werner, Hoshino & Shinaoka
PRB 94, 245134 (2016)

- Mapping to an effective two-orbital model:



$$c_1 = \frac{1}{\sqrt{2}}(d_1 + d_3) \quad c_2 = \frac{1}{\sqrt{2}}(d_2 + d_4)$$
$$f_1 = \frac{1}{\sqrt{2}}(d_1 - d_3) \quad f_2 = \frac{1}{\sqrt{2}}(d_2 - d_4)$$

- Slater-Kanamori interaction with $\tilde{U} = \tilde{U}' = \tilde{J} = U/2$
  nnn hopping translates into a crystal-field splitting $\delta = 2t'$

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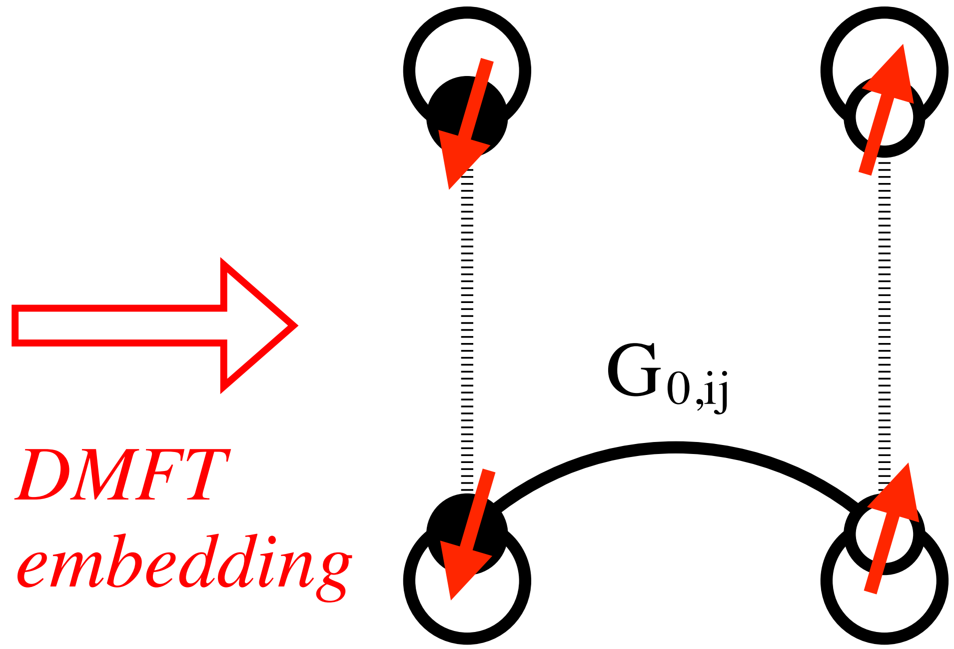

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Cuprates

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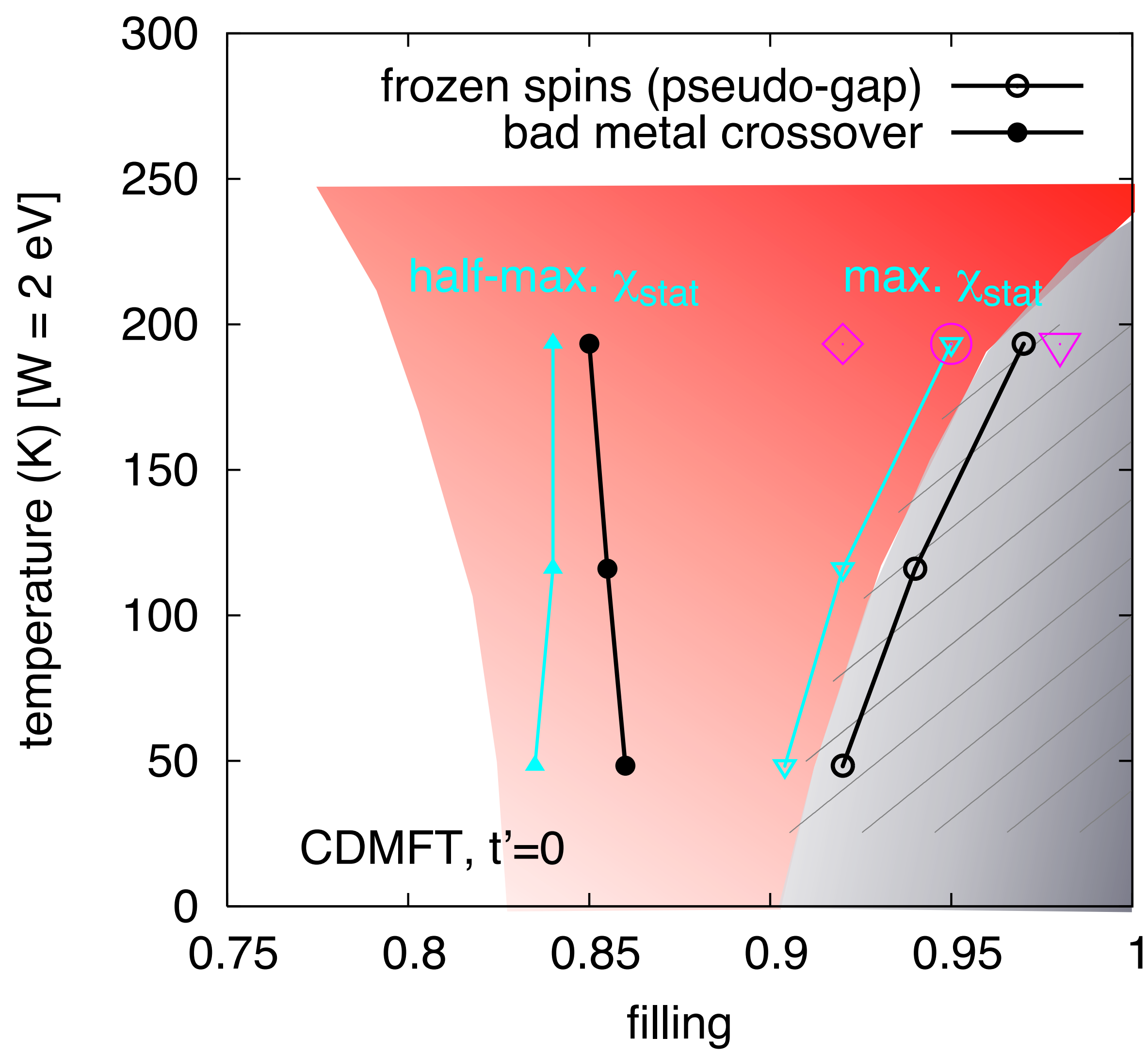
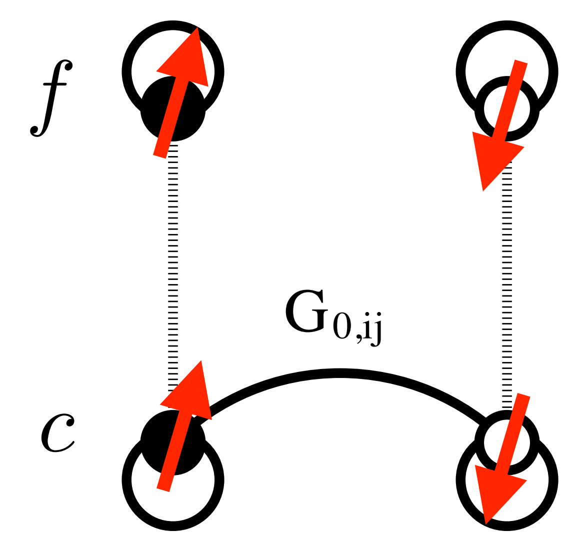
PRB 94, 245134 (2016)

- Phasediagram (2-site/2-orbital cluster DMFT)

emerging (fluctuating) local moments = bad metal regime



frozen moments =pseudo-gap phase



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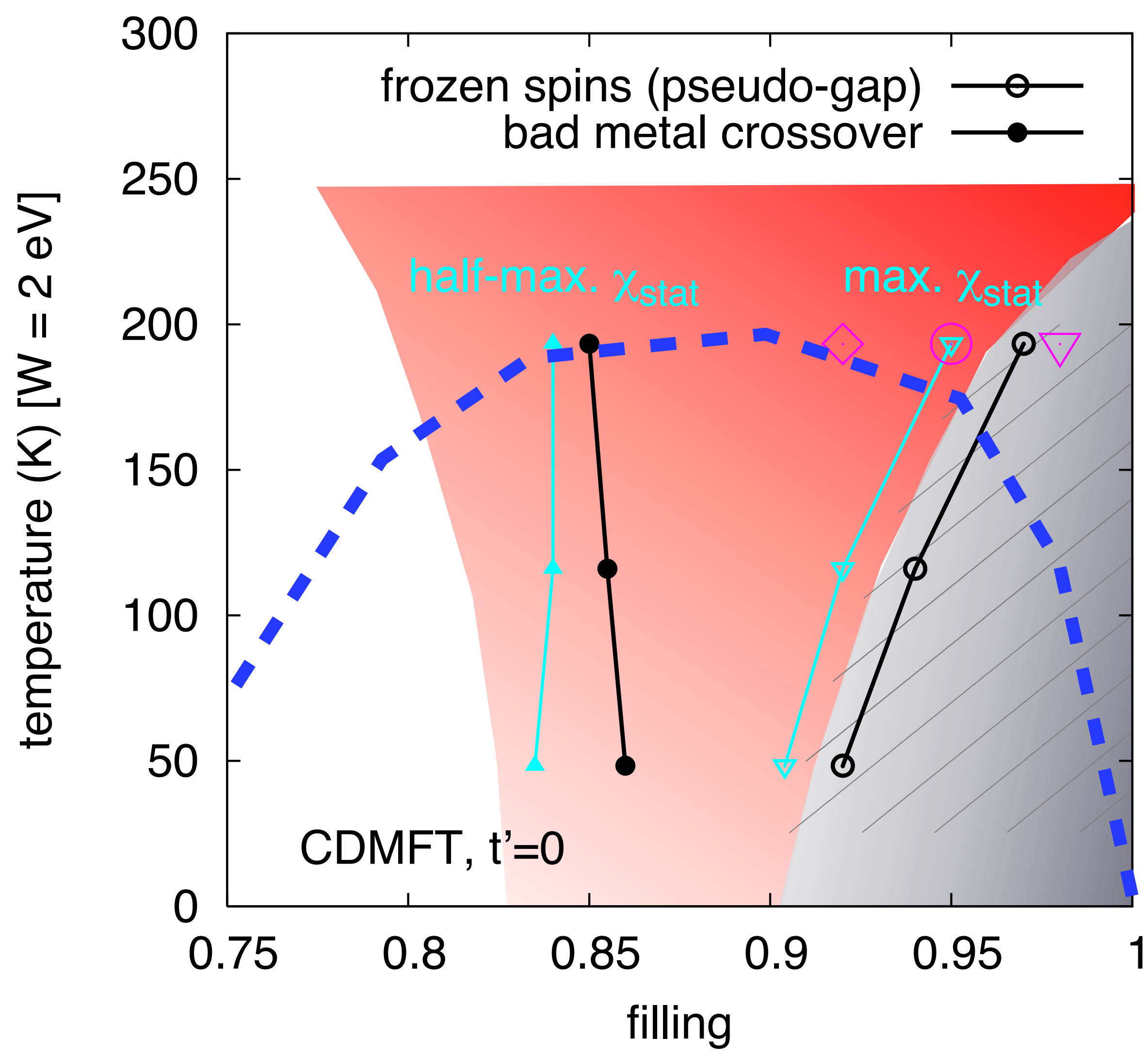


frozen moments =pseudo-gap phase

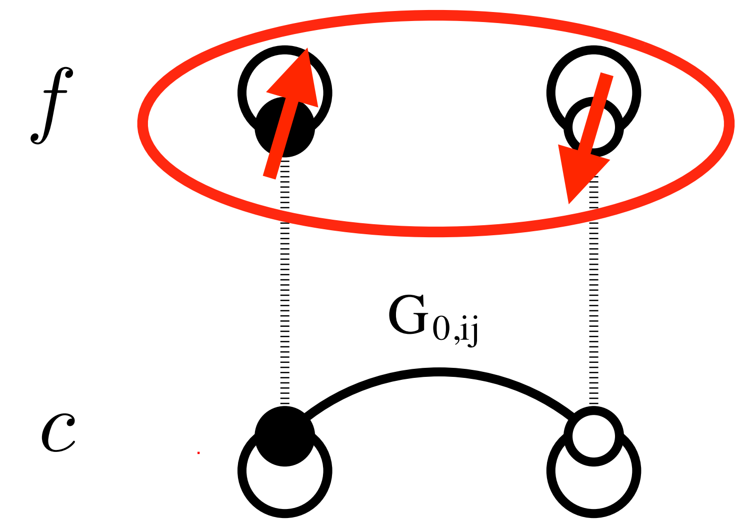
SC dome [4-site cluster DMFT, Maier et al, (2005)] induced by fluctuating local moments?

Cuprates

Werner, Hoshino & Shinaoka
PRB 94, 245134 (2016)

- d-wave SC induced by local spin fluctuations
- Transformation of the d-wave order parameter:

$$
\begin{aligned}
&(d^\dagger_{1\uparrow}d^\dagger_{2\downarrow} - d^\dagger_{1\downarrow}d^\dagger_{2\uparrow}) - (d^\dagger_{2\uparrow}d^\dagger_{3\downarrow} - d^\dagger_{2\downarrow}d^\dagger_{3\uparrow}) \\
+&(d^\dagger_{3\uparrow}d^\dagger_{4\downarrow} - d^\dagger_{3\downarrow}d^\dagger_{4\uparrow}) - (d^\dagger_{4\uparrow}d^\dagger_{1\downarrow} - d^\dagger_{4\downarrow}d^\dagger_{1\uparrow})
\end{aligned}
\quad \longrightarrow \quad 2(f^\dagger_{1\uparrow}f^\dagger_{2\downarrow} - f^\dagger_{1\downarrow}f^\dagger_{2\uparrow})
$$

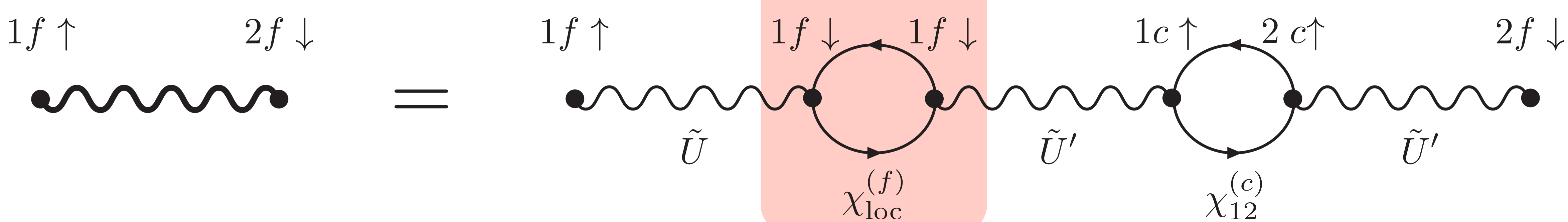


- Effective attractive interaction:

$$
\tilde{U}^{\mathrm{eff}}_{(1,f,\uparrow),(2,f,\downarrow)} = 2\tilde{U}^3\chi^{(f)}_{\mathrm{loc}}\chi^{(c)}_{12} + O(\tilde{U}^5)
$$

local spin fluctuations (needed because U'-J=0)

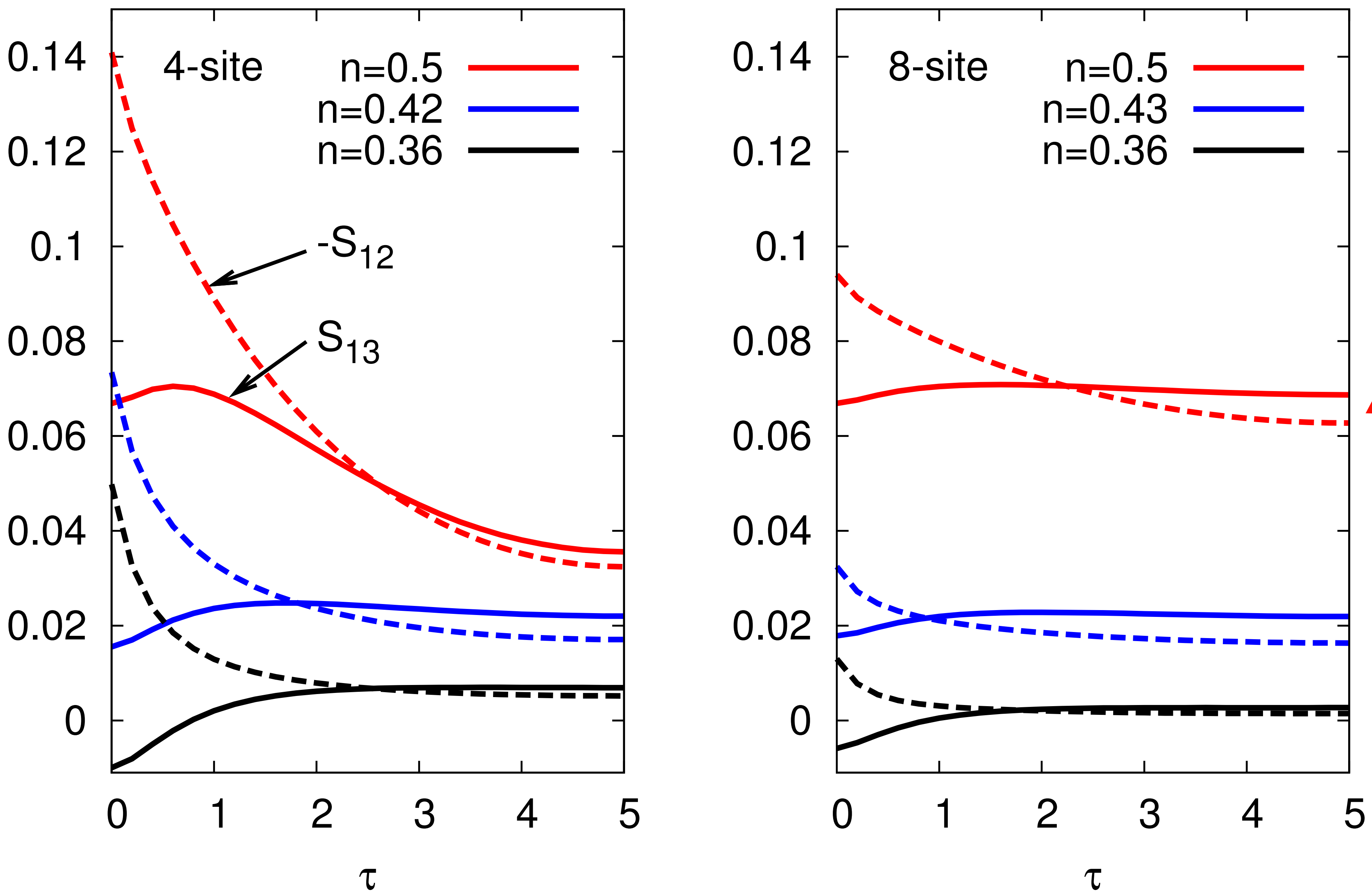
- Leading contribution:

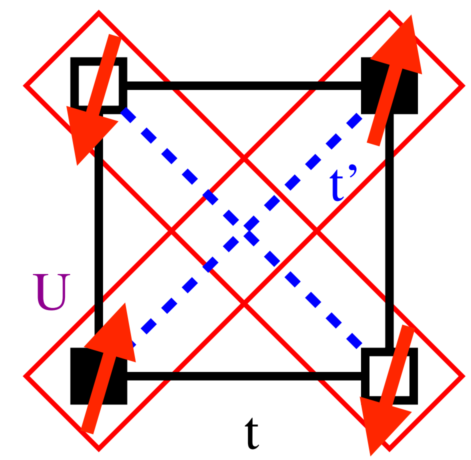


Further evidence

Werner, Xi & Gull
arxiv:1912.01260 (2019)

- Spin correlations in the 2D Hubbard model (DCA results)
- Compare nearest neighbor correlations (S_{12}) to diagonal next-nearest neighbor correlations (S_{13})



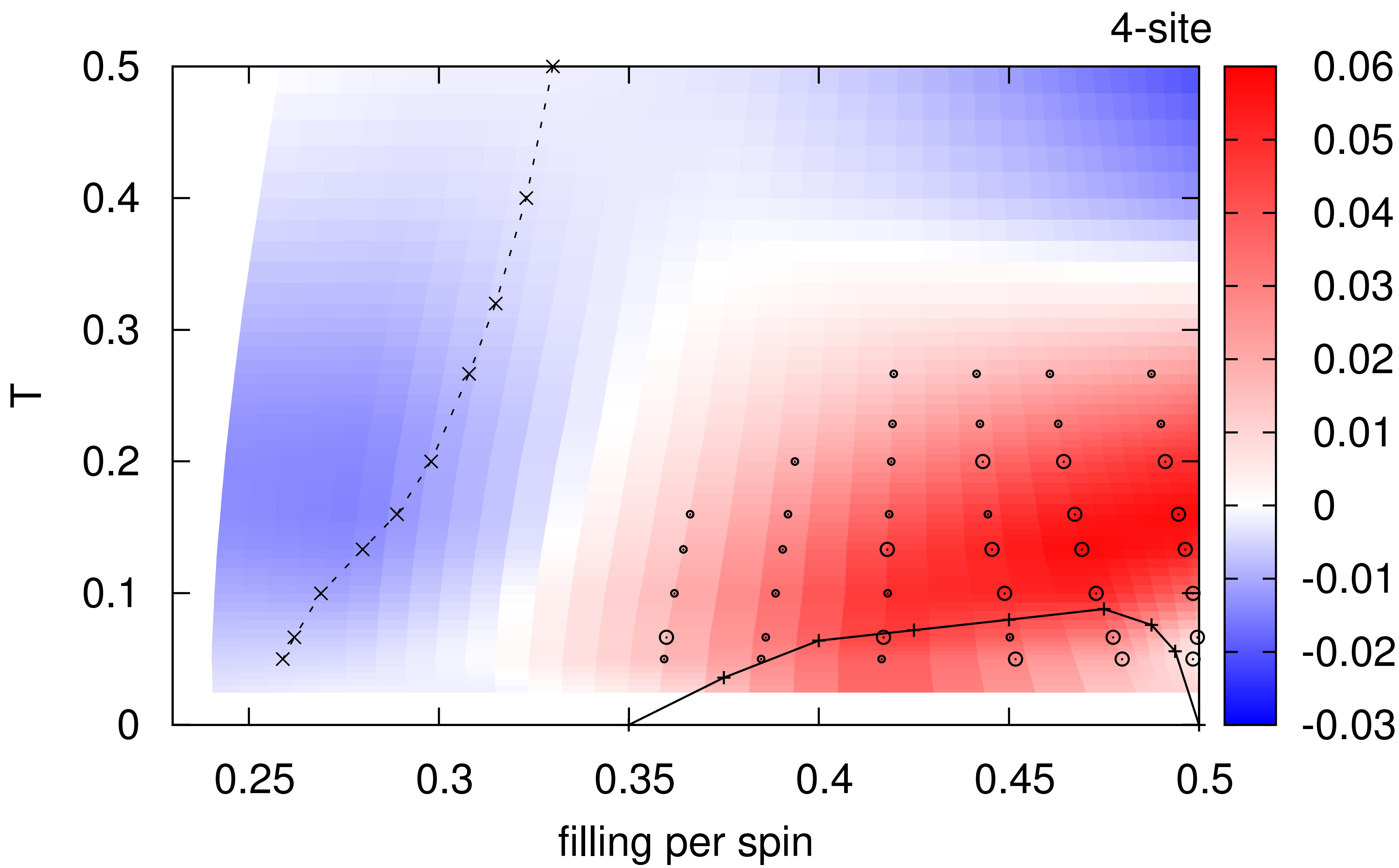


FM correlations dominate at long imaginary times

Further evidence

Werner, Xi & Gull
arxiv:1912.01260 (2019)

- Spin correlations in the 2D Hubbard model (DCA results)
- Plot $\beta[S_{13} - (-S_{12})]$ as a function of temperature and filling



robust FM correlations (formation of composite spin-1)

Further evidence

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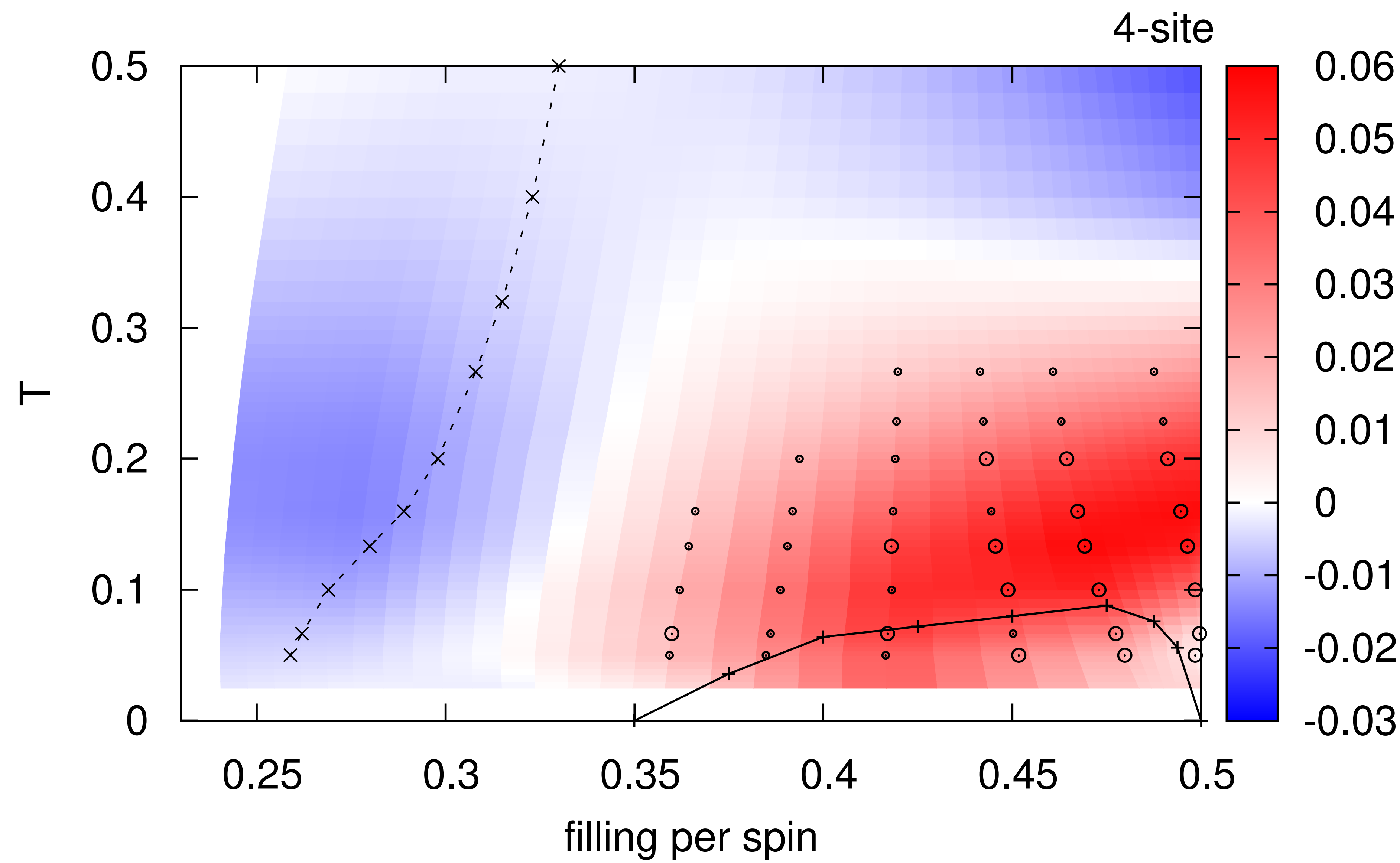


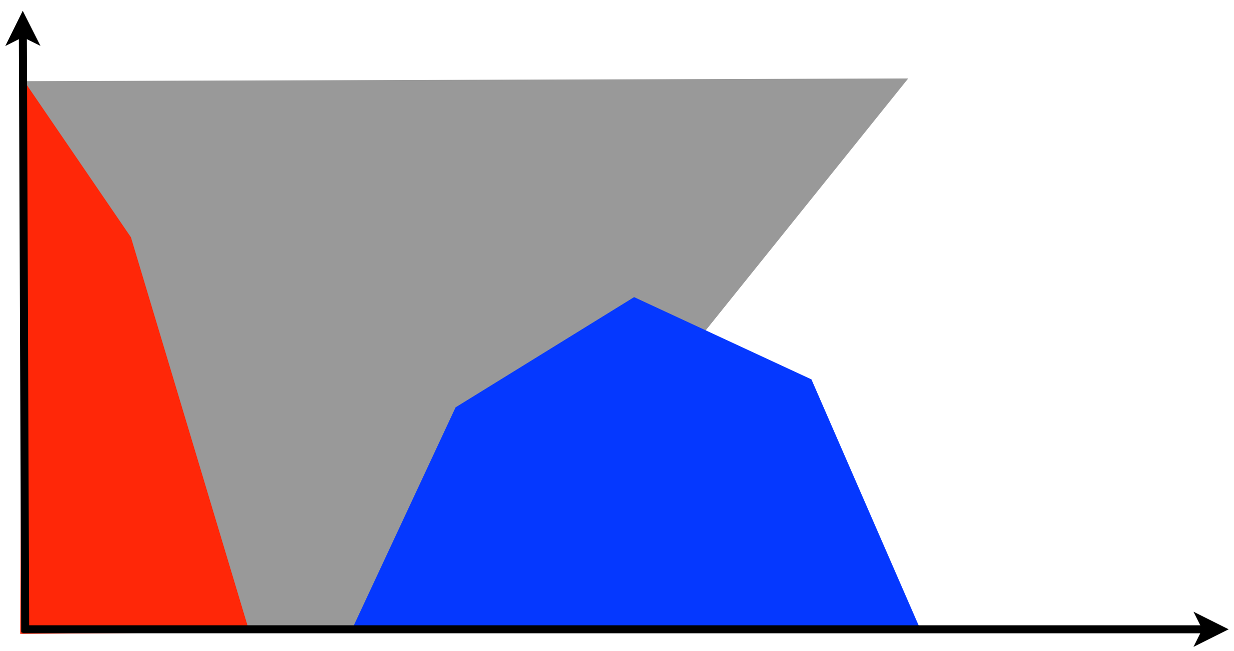
robust FM correlations (formation of composite spin-1)

black dots: pseudo gap at anti-node

- Appearance of composite spin-1 as origin of the pseudo-gap

Summary

- Spin/orbital freezing as a universal phenomenon in unconventional superconductors
  - Strontium ruthenates
  - Uranium-based SC
  - Pnictides
  - Fulleride compounds
  - Cuprates
  - ...



- Pairing induced by <u>local</u> spin or orbital fluctuations

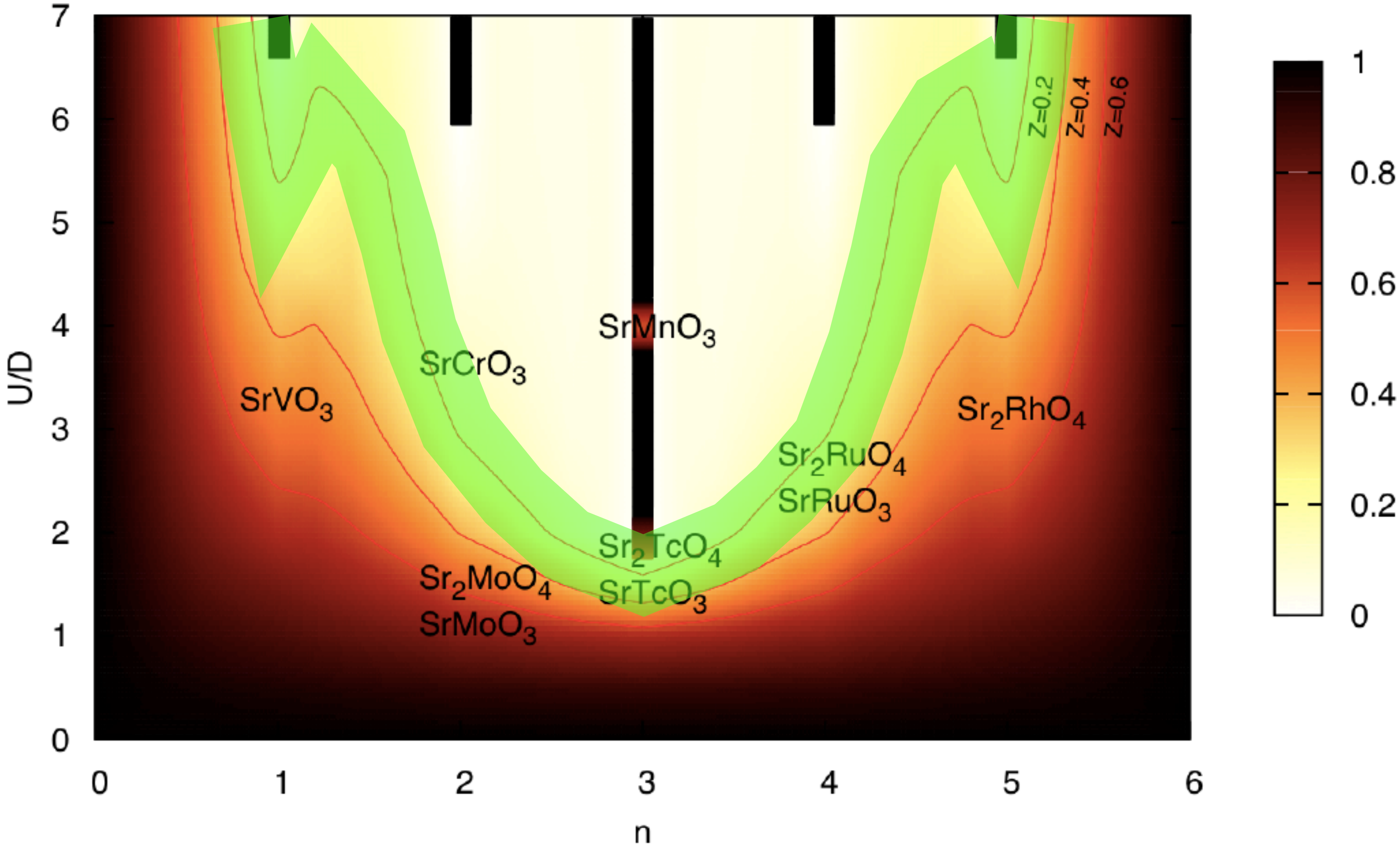
- Bad metal physics originates from fluctuating/frozen moments

3-orbital model

- "quasi-particle weight" *z*

from De' Medici, Mravlje & Georges, PRL (2011)

large local moment fluctuations

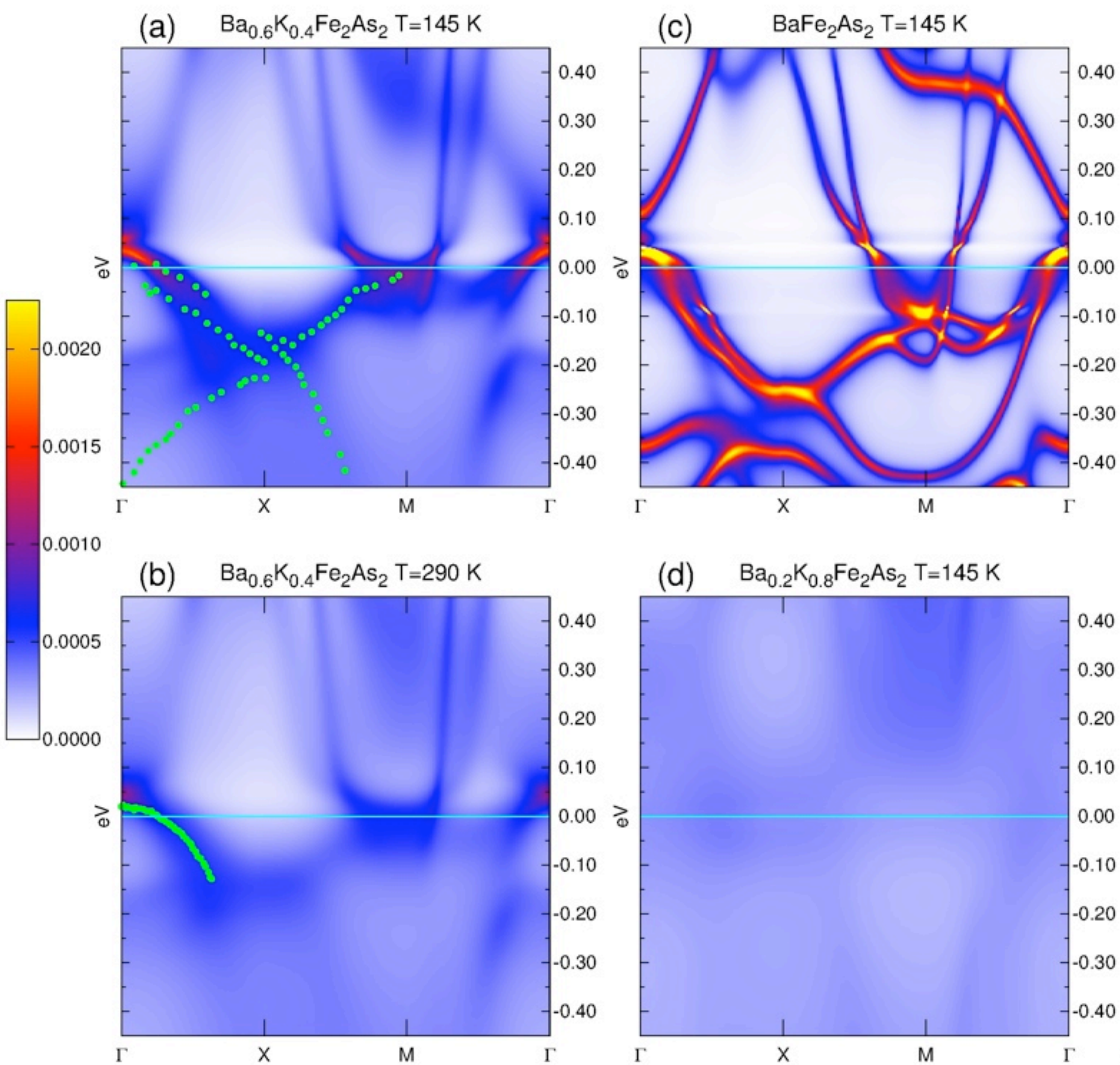


- Hund coupling *J*: Strongly correlated metal far from the Mott transition

Pnictides

Werner *et al.*
Nature Phys. 8, 331 (2012)

- Strong doping and temperature dependence of electronic structure



Negative J and orbital freezing

Steiner et al.
PRB 94, 075107 (2016)

- 2-orbital model (*U*=bandwidth=4)

- Mapping between *J*<0 and *J*>0:

$$\begin{pmatrix} d_{i,1\downarrow} \\ d_{i,2\uparrow} \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} d_{i,1\downarrow} \\ d_{i,2\uparrow} \end{pmatrix}$$

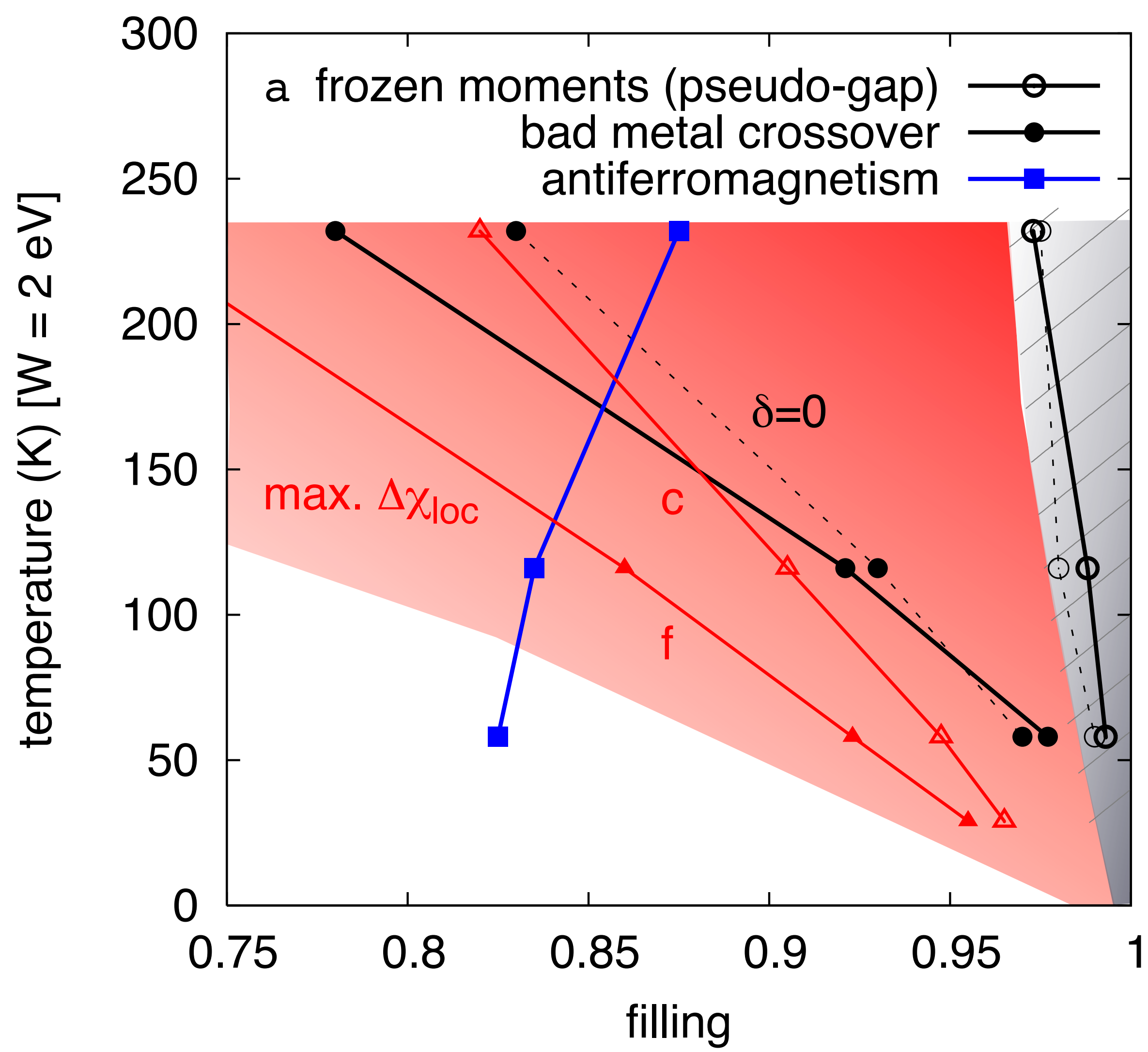
J<0:		*J*>0:
spin-singlet SC	$\longrightarrow$	spin-triplet SC
antiferro OO	$\longrightarrow$	AFM
ferro OO	$\longrightarrow$	FM
orbital freezing	$\longrightarrow$	spin freezing

Cuprates

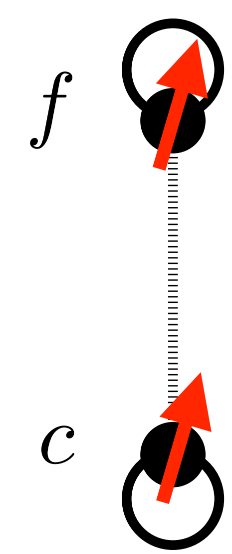
Werner, Hoshino & Shinaoka
PRB 94, 245134 (2016)

- Phasediagram (1-site/2-orbital DMFT)

emerging (fluctuating) local moments = bad metal regime



frozen moments =pseudo-gap phase



Further evidence

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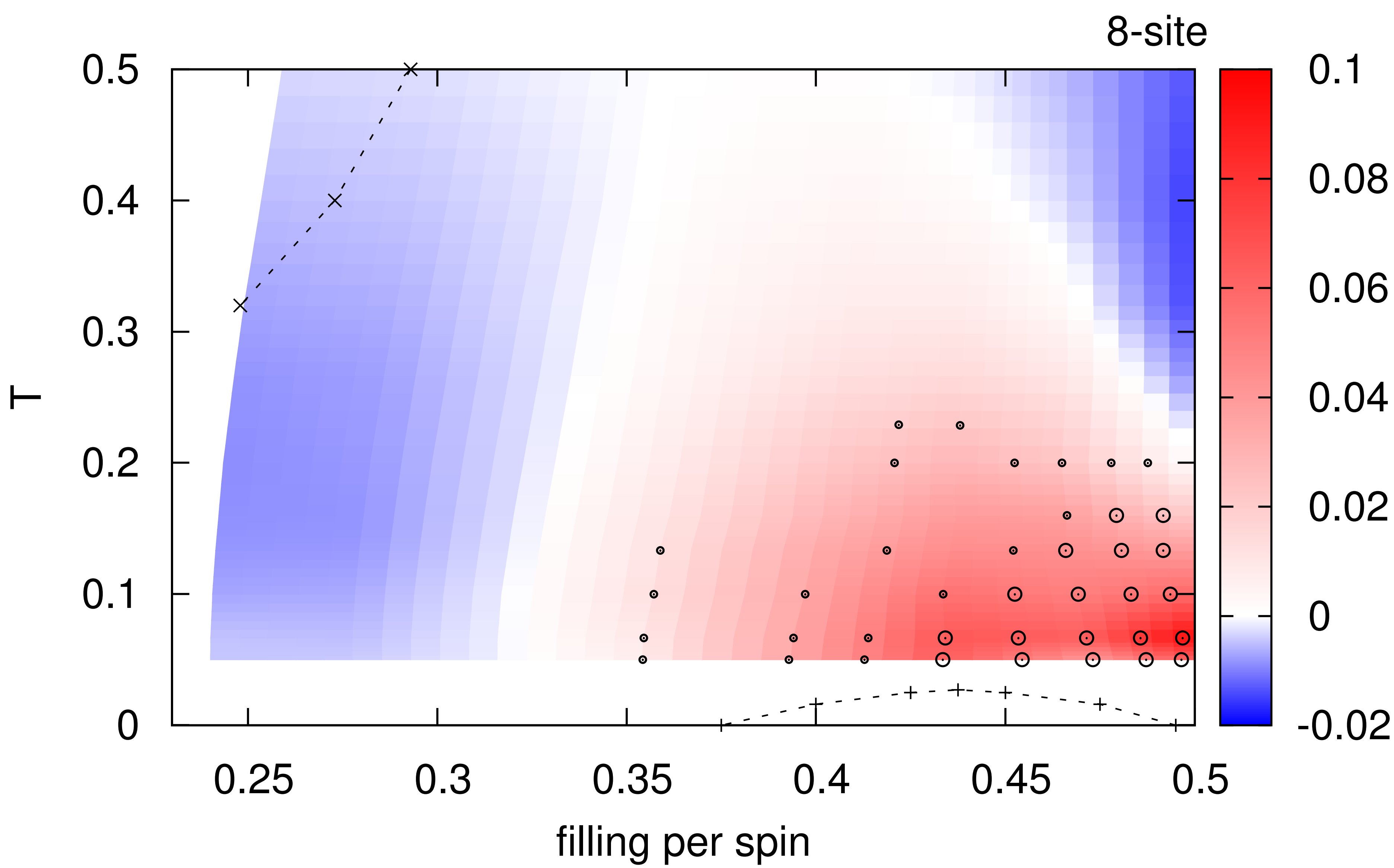

robust FM correlations (formation of composite spin-1)

- Appearance of composite spin-1 as origin of the pseudo-gap

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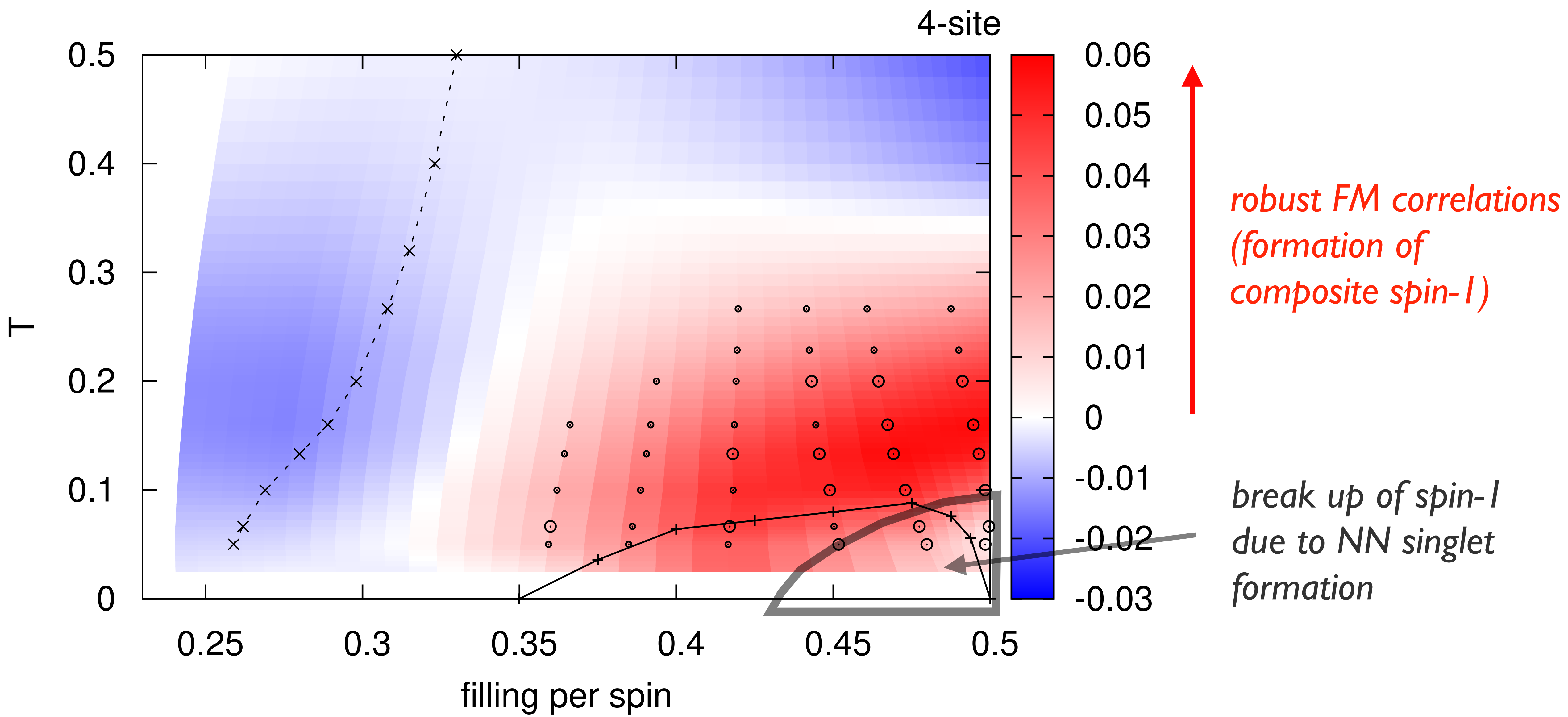

- Appearance of composite spin-1 as origin of the pseudo-gap