Spin freezing in unconventional superconductors

Philipp Werner

University of Fribourg

Beijing, August 2018

Spin freezing in unconventional superconductors

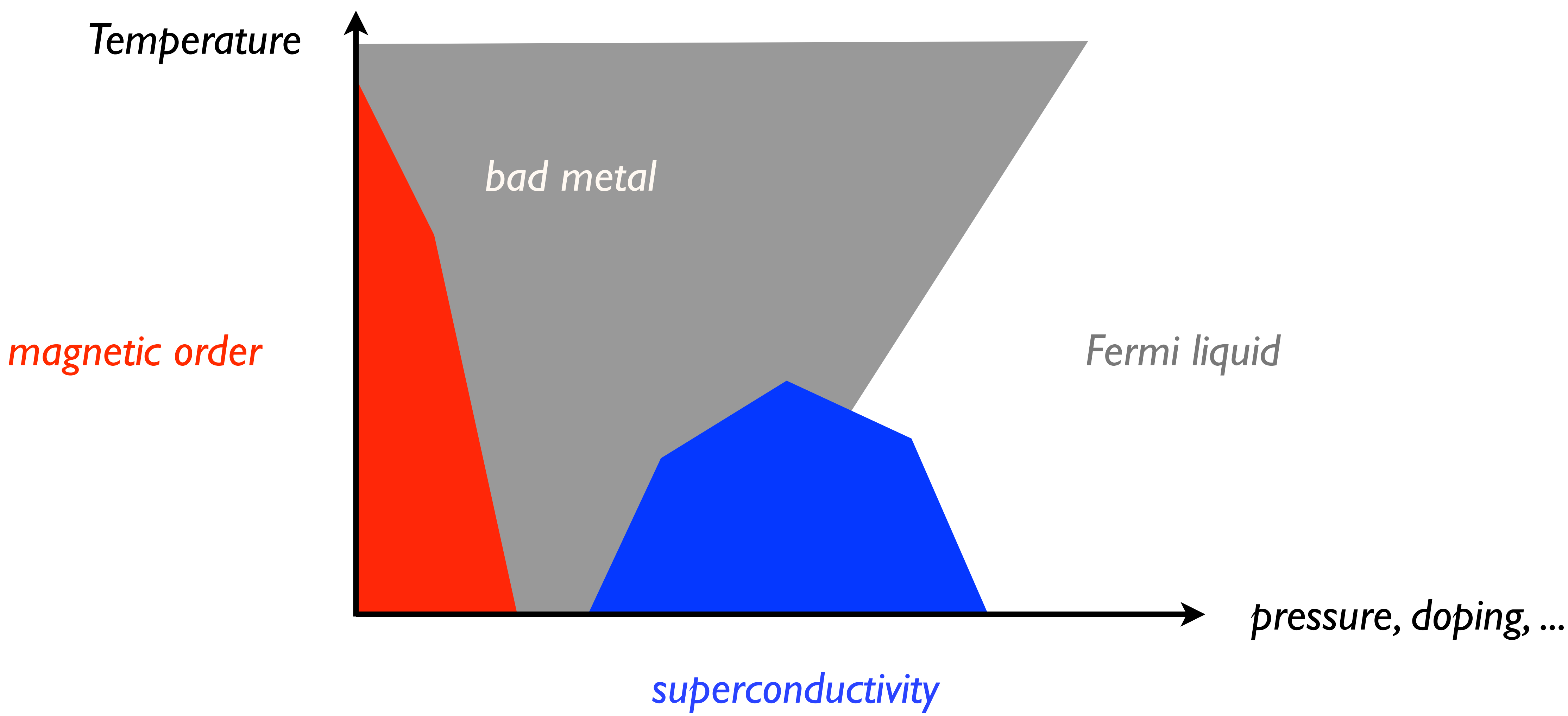
In collaboration with:

Shintaro Hoshino (Saitama)
Hiroshi Shinaoka (Saitama)
Aaram Kim (London)
Naoto Tsuji (RIKEN)

Beijing, August 2018

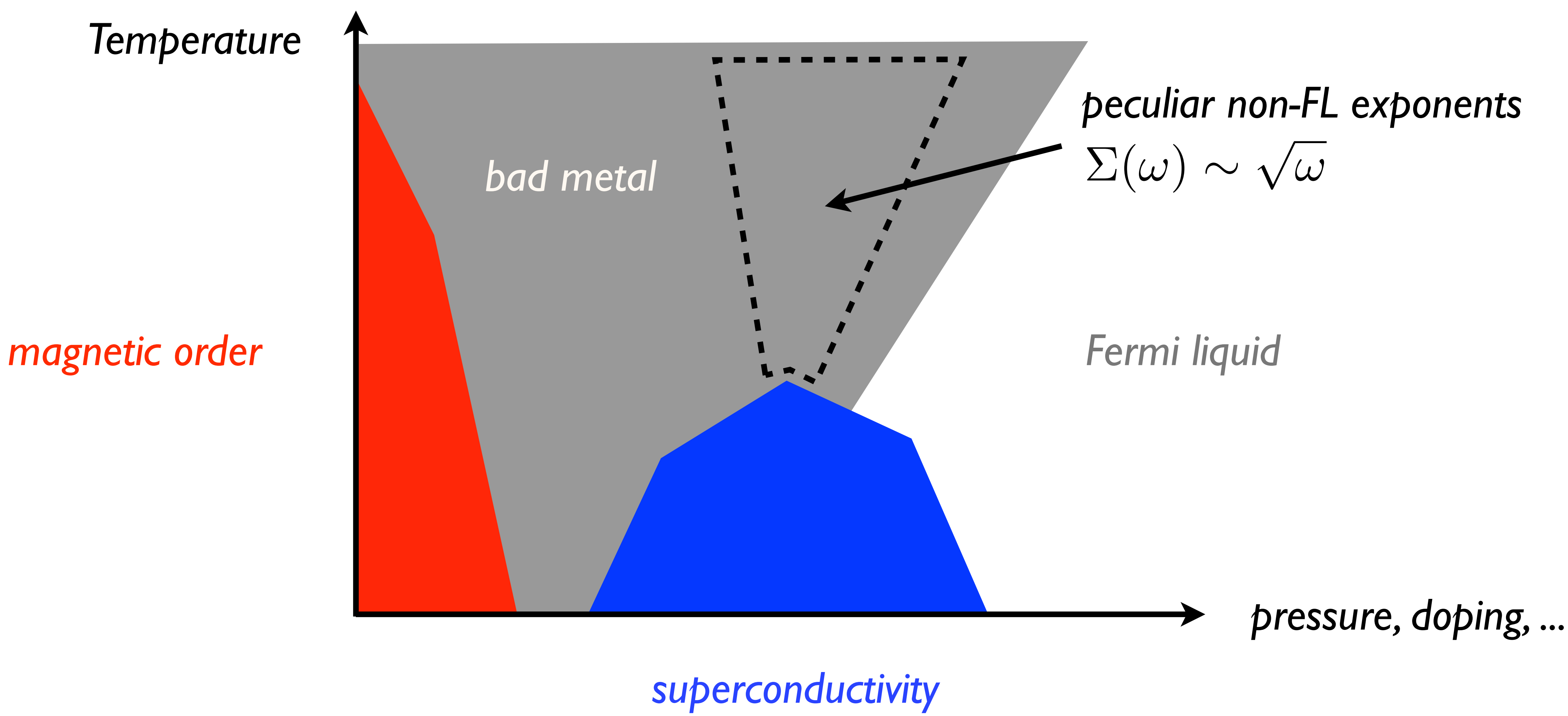
Introduction

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



Introduction

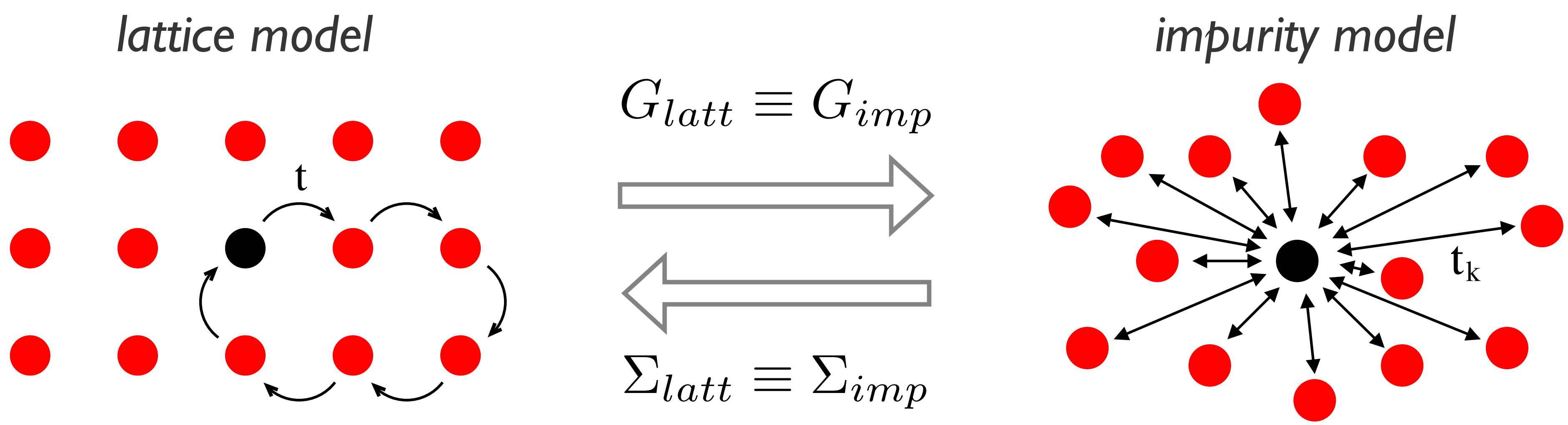
- Connection between spin-freezing and Sachdev-Ye model
  - Sachdev-Ye model as an effective model describing the spin-freezing crossover regime
  - Behavior of out-of-time-order correlation functions



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 et al., PRL (2006)

- CT-QMC solvers allow efficient simulation of multiorbital models

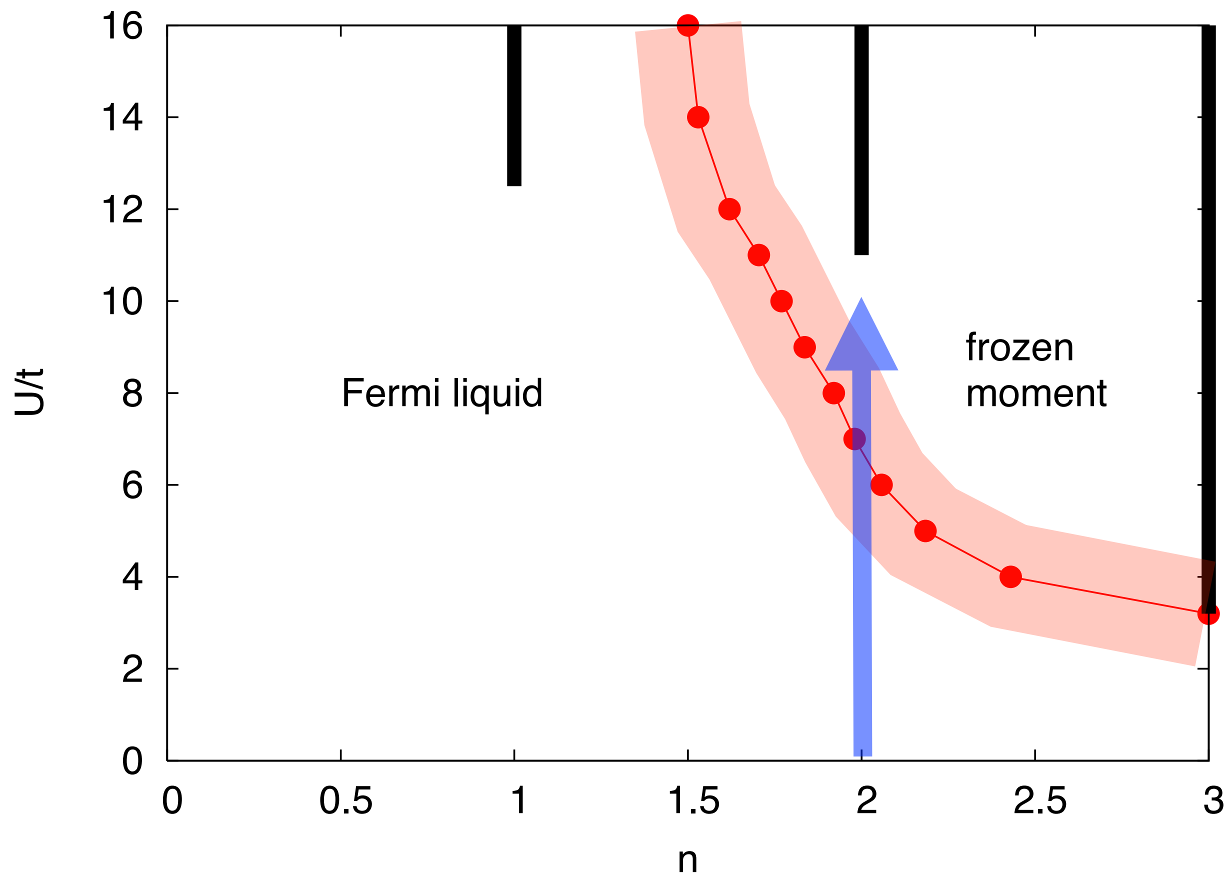
$$H_{\mathrm{loc}} = -\sum_{\alpha,\sigma} \mu n_{\alpha,\sigma} + \sum_{\alpha} U n_{\alpha,\uparrow} n_{\alpha,\downarrow}$$
$$+ \sum_{\alpha>\beta,\sigma} U' n_{\alpha,\sigma} n_{\beta,-\sigma} + (U' - J) n_{\alpha,\sigma} n_{\beta,\sigma}$$
$$- \sum_{\alpha\neq\beta} J(\psi^\dagger_{\alpha,\downarrow}\psi^\dagger_{\beta,\uparrow}\psi_{\beta,\downarrow}\psi_{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

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



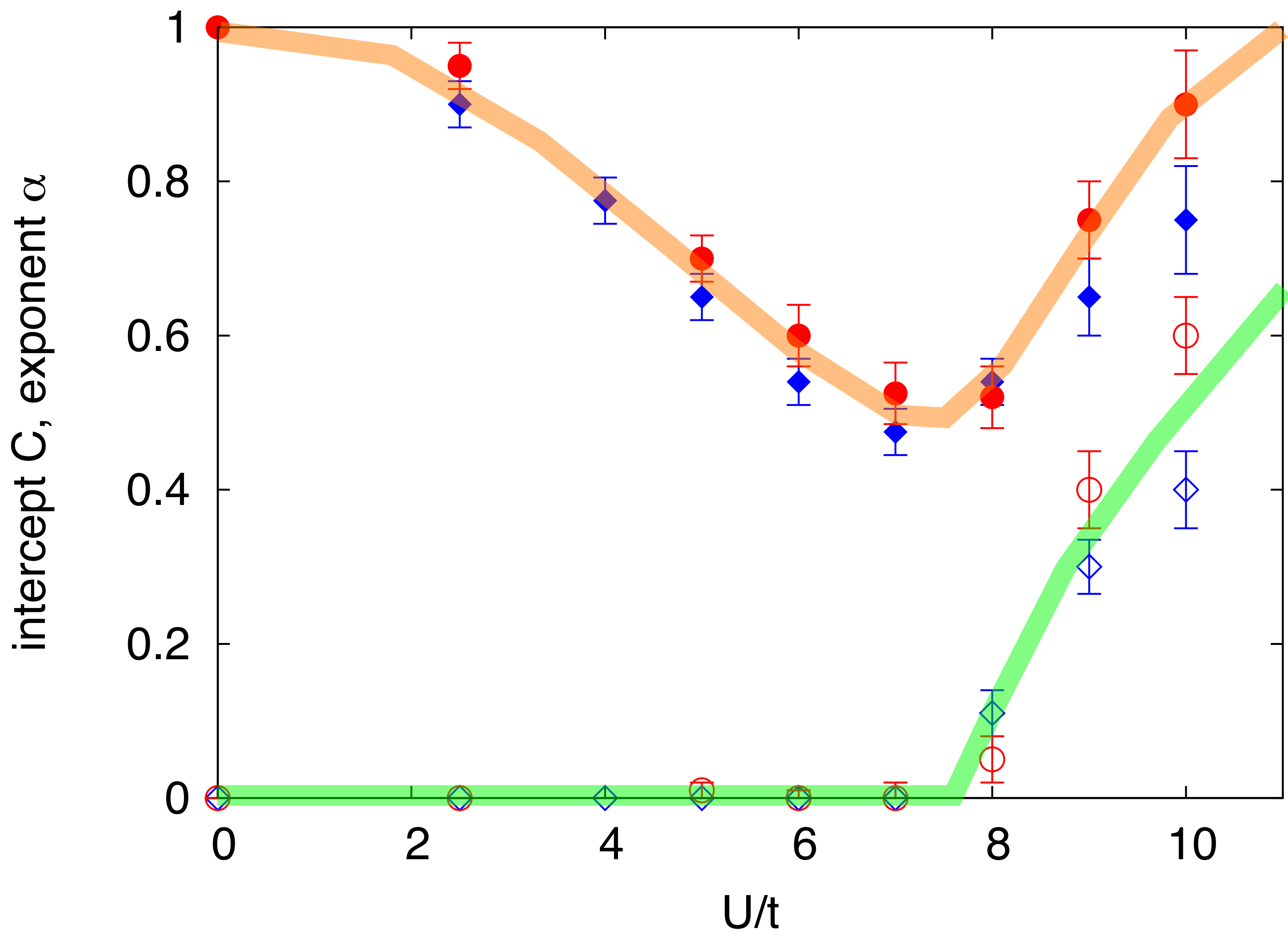
- Metallic phase: "transition" from Fermi liquid to spin-glass
- Narrow crossover regime with self-energy

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

3-orbital model

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

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



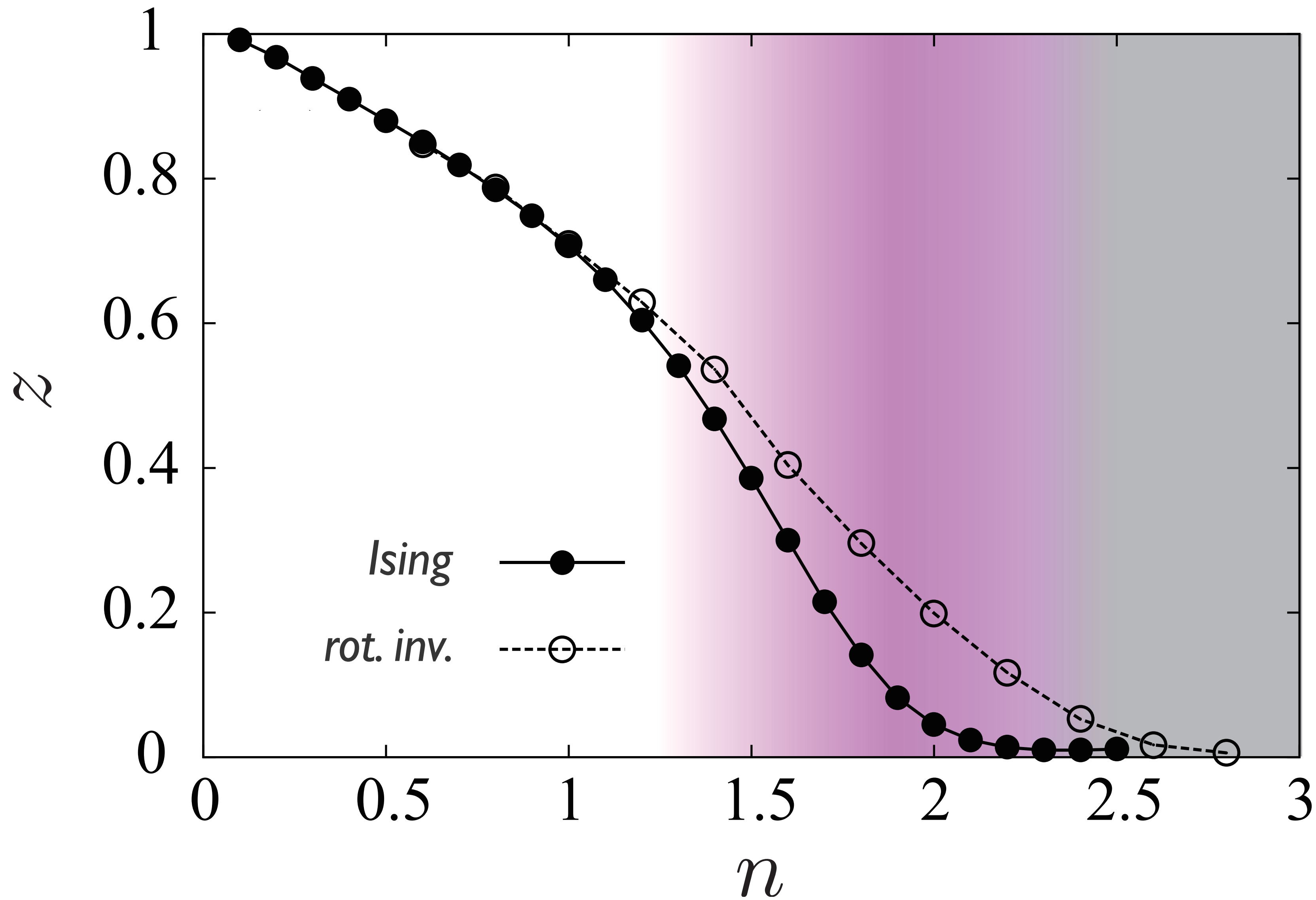
- Square-root self-energy coincides with on-set of frozen moments

3-orbital model

Hoshino & Werner
PRL 115, 247001 (2015)

- Spin-freezing leads to a small "quasi-particle weight" z

$$z \approx 1/(1 - \mathrm{Im}\Sigma(i\omega_0)/\omega_0)$$

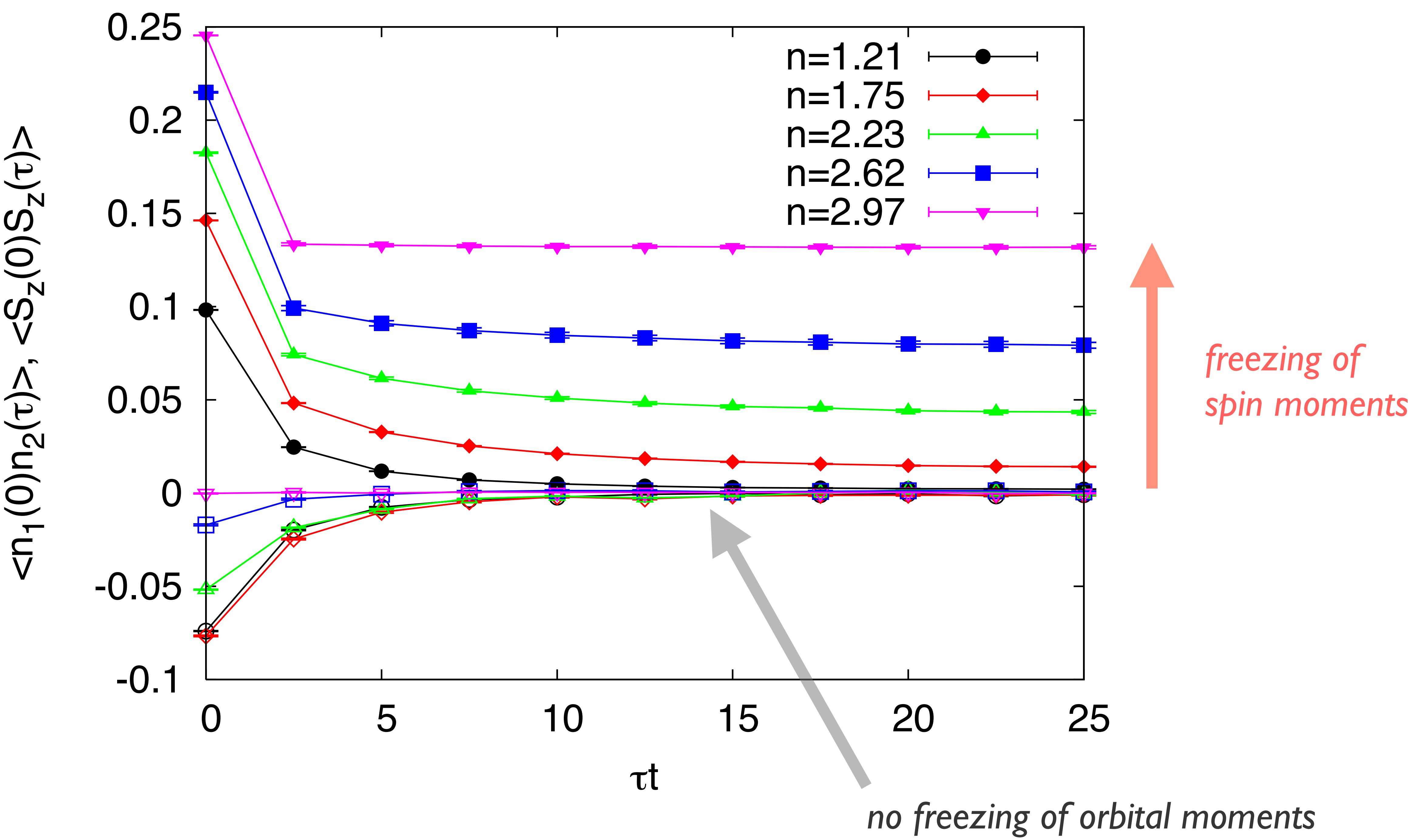


no quasi-particles in spin-frozen regime

3-orbital model

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

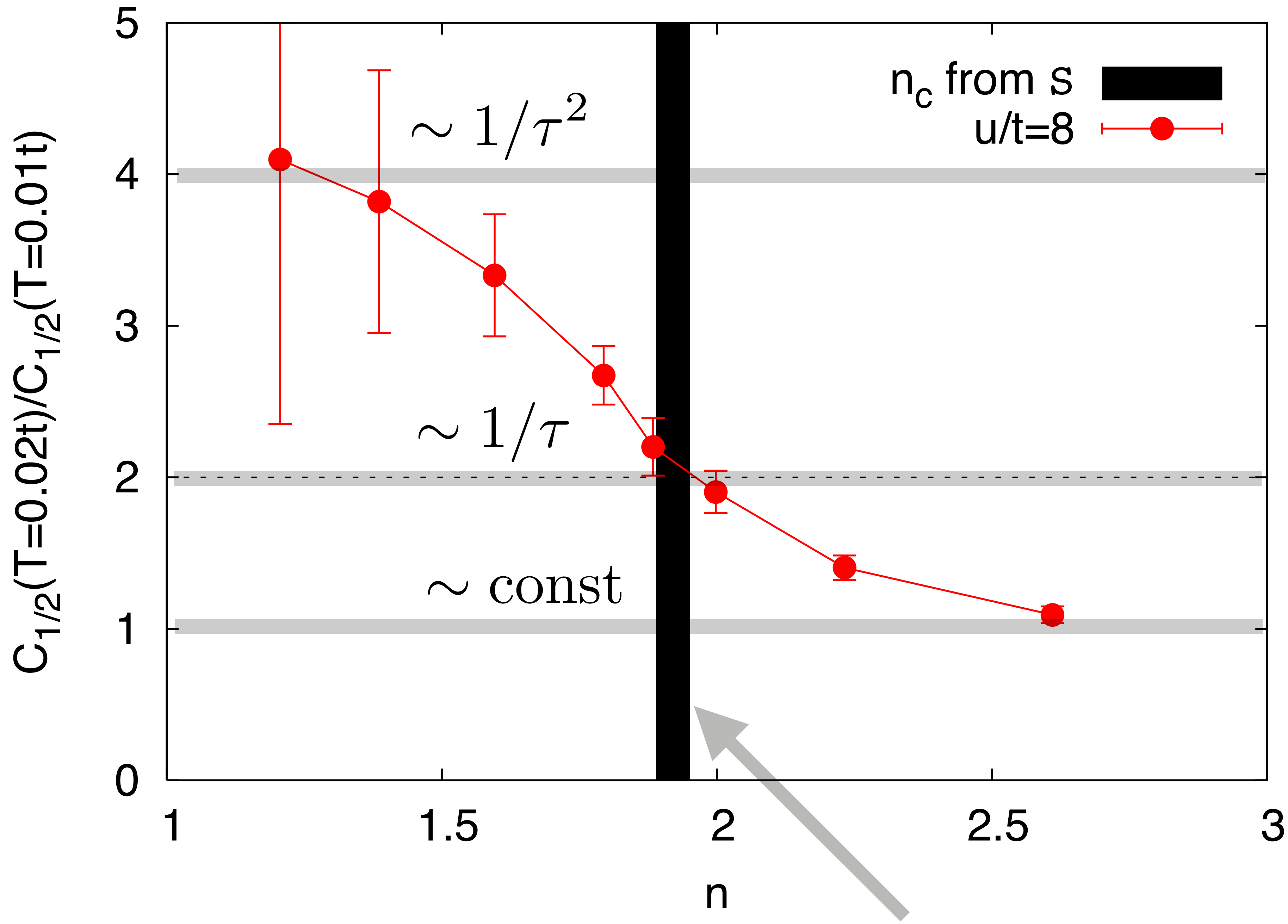
- Spin-spin and orbital-orbital correlation functions



3-orbital model

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

- Decay of spin correlations



Fermi liquid

$$C_{1/2}(\beta) = \langle S^z S^z \rangle (\tau = \beta/2)$$

frozen spins

spin-freezing crossover

3-orbital model

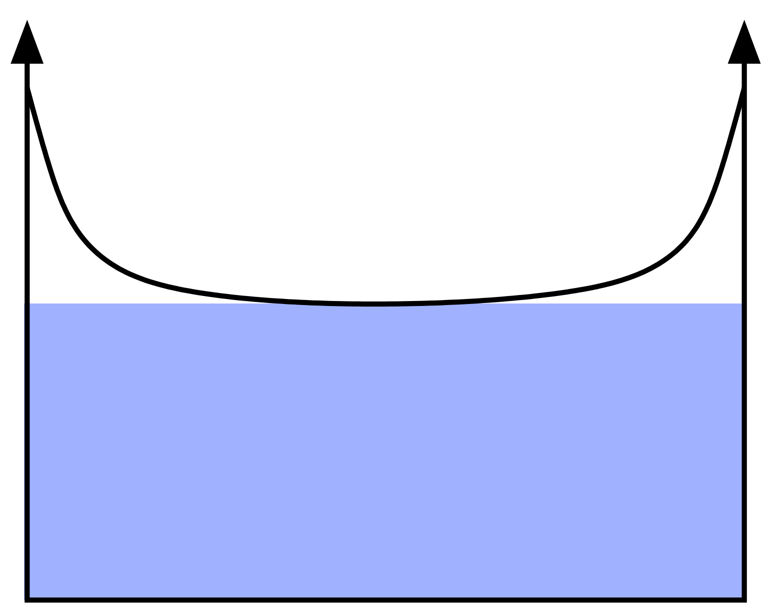
Hoshino & Werner
PRL 115, 247001 (2015)

- Consider the local susceptibility

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

and its dynamic contribution

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

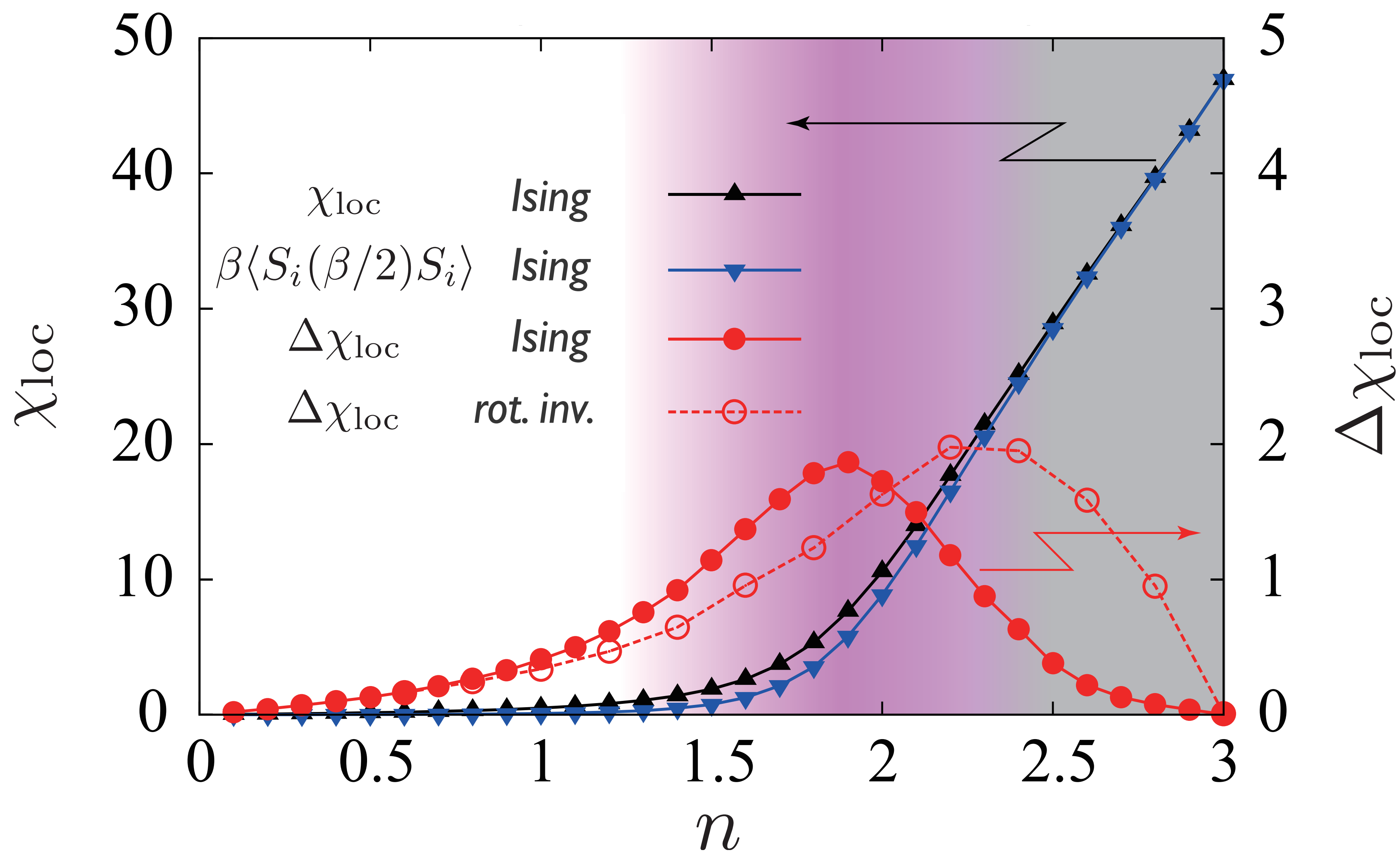


subtract the (frozen) long-time value

3-orbital model

Hoshino & Werner
PRL 115, 247001 (2015)

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

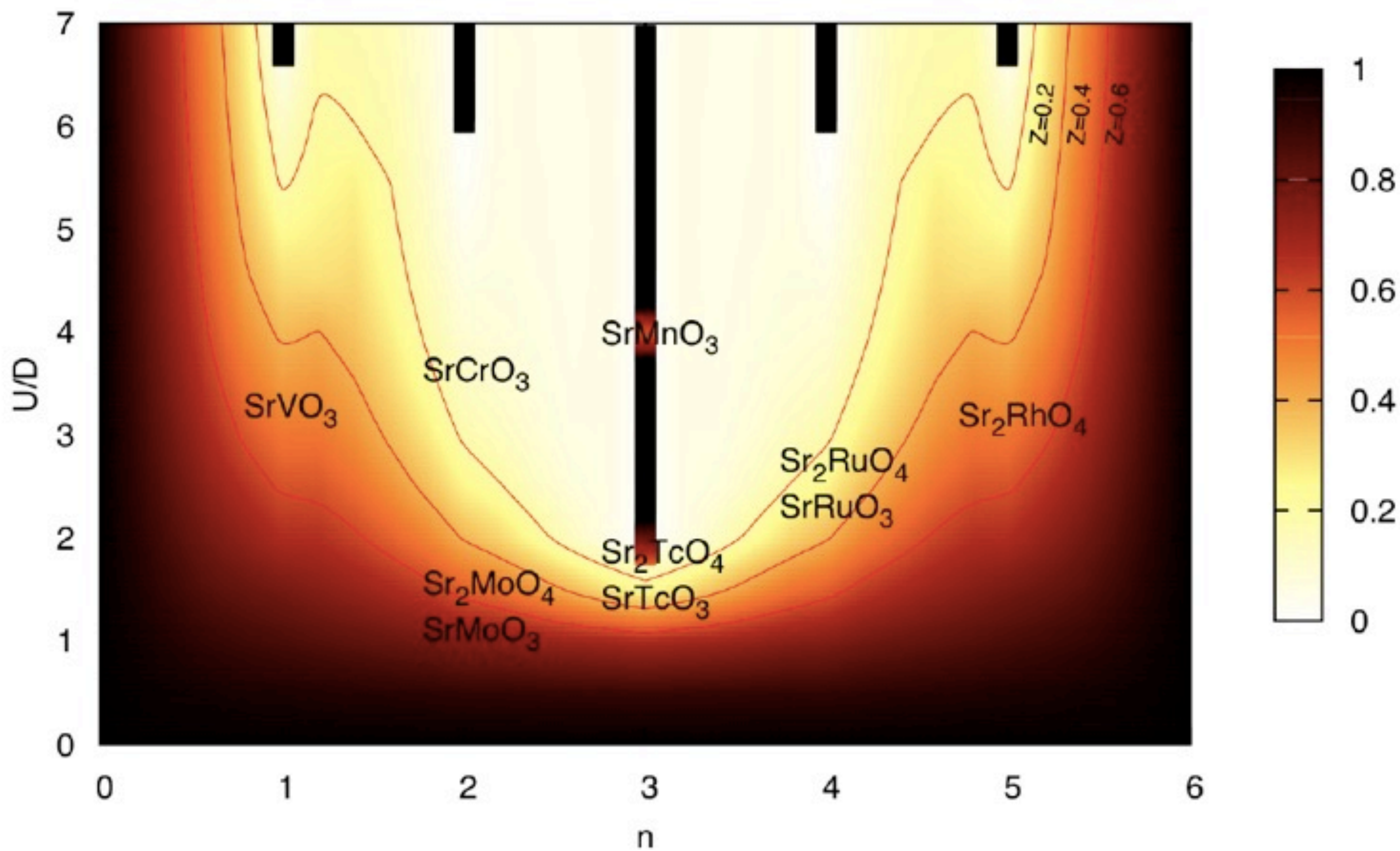


- Crossover regime is characterized by large local moment fluctuations

3-orbital model

- "quasi-particle weight" *z*

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



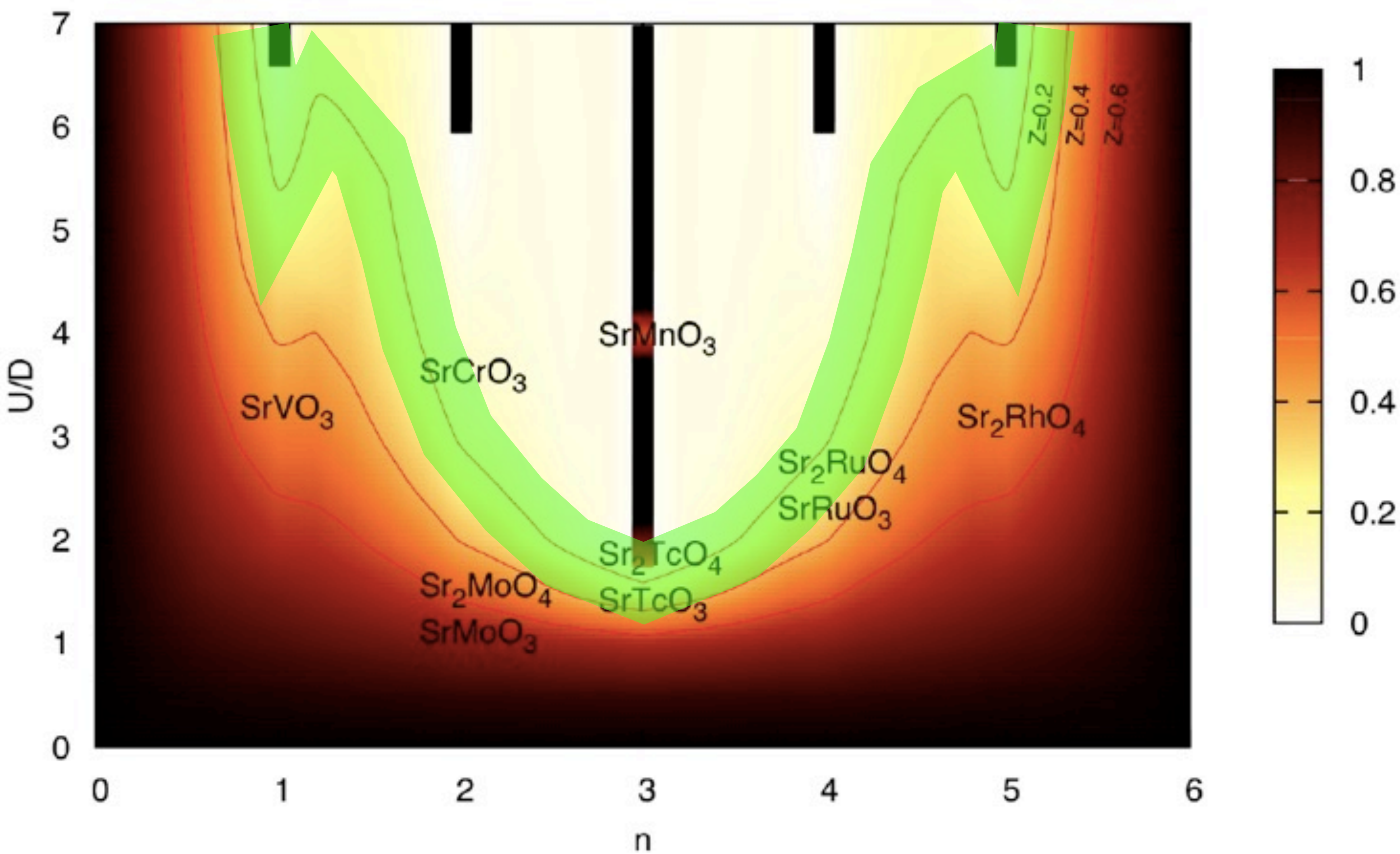
- Hund coupling *J*: Strongly correlated metal far from the Mott transition

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

Strontium Ruthenates

- 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

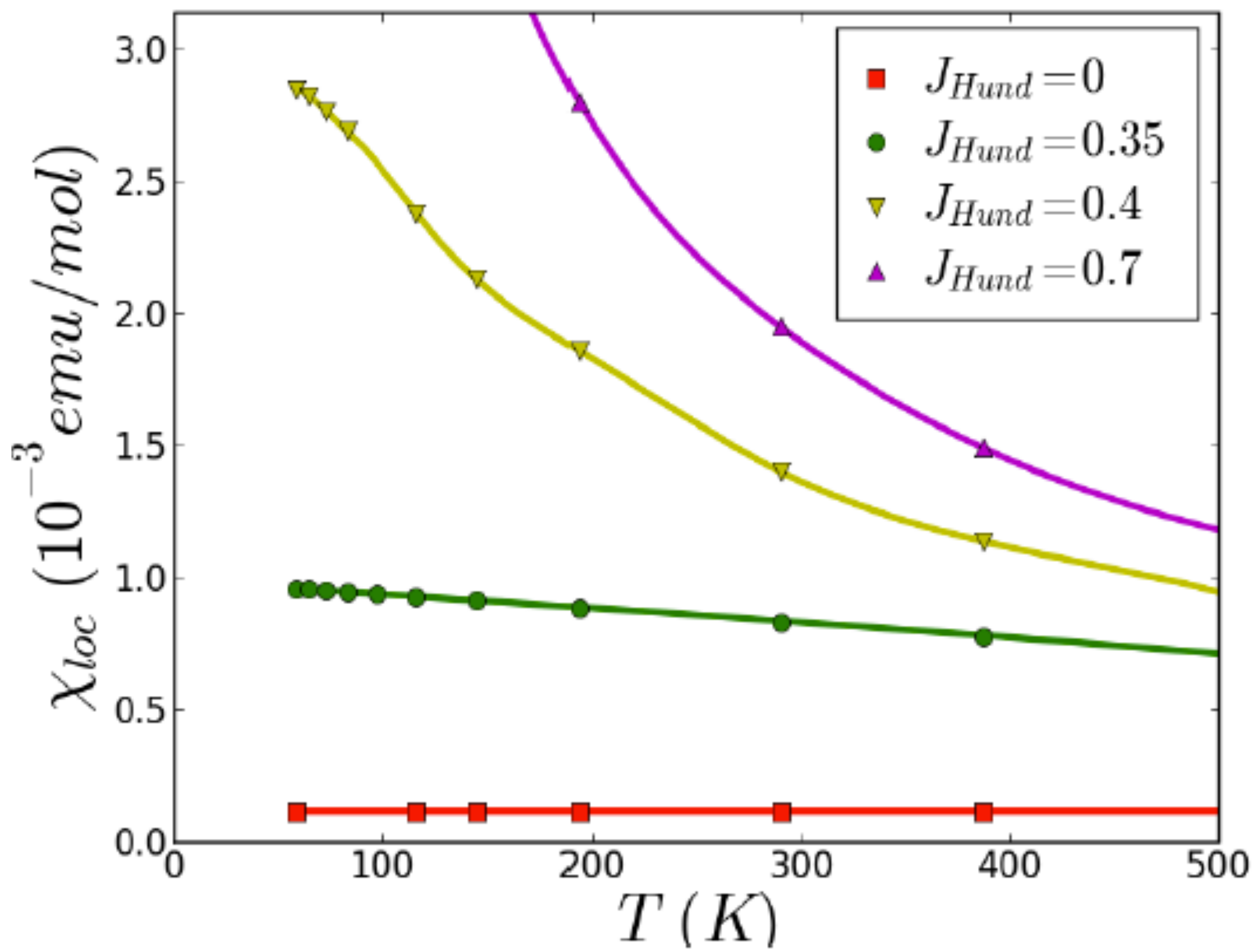
P. Kostic, Y. Okada,* N. C. Collins, and Z. Schlesinger
Department of Physics, University of California, Santa Cruz, California 95064

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.

Pnictides

- Strongly correlated despite moderate *U*



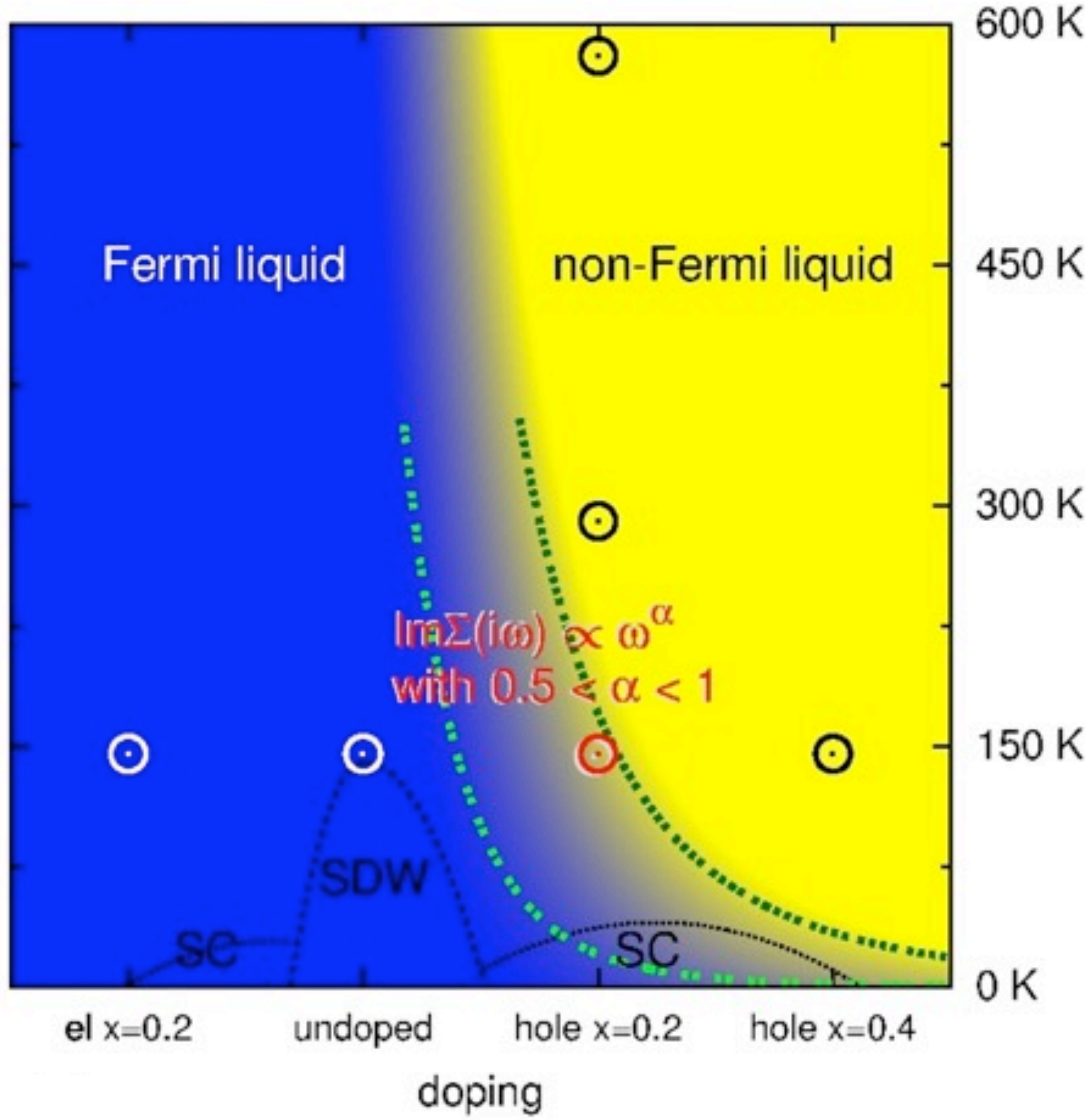
incoherent metal state resulting from Hund's coupling

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

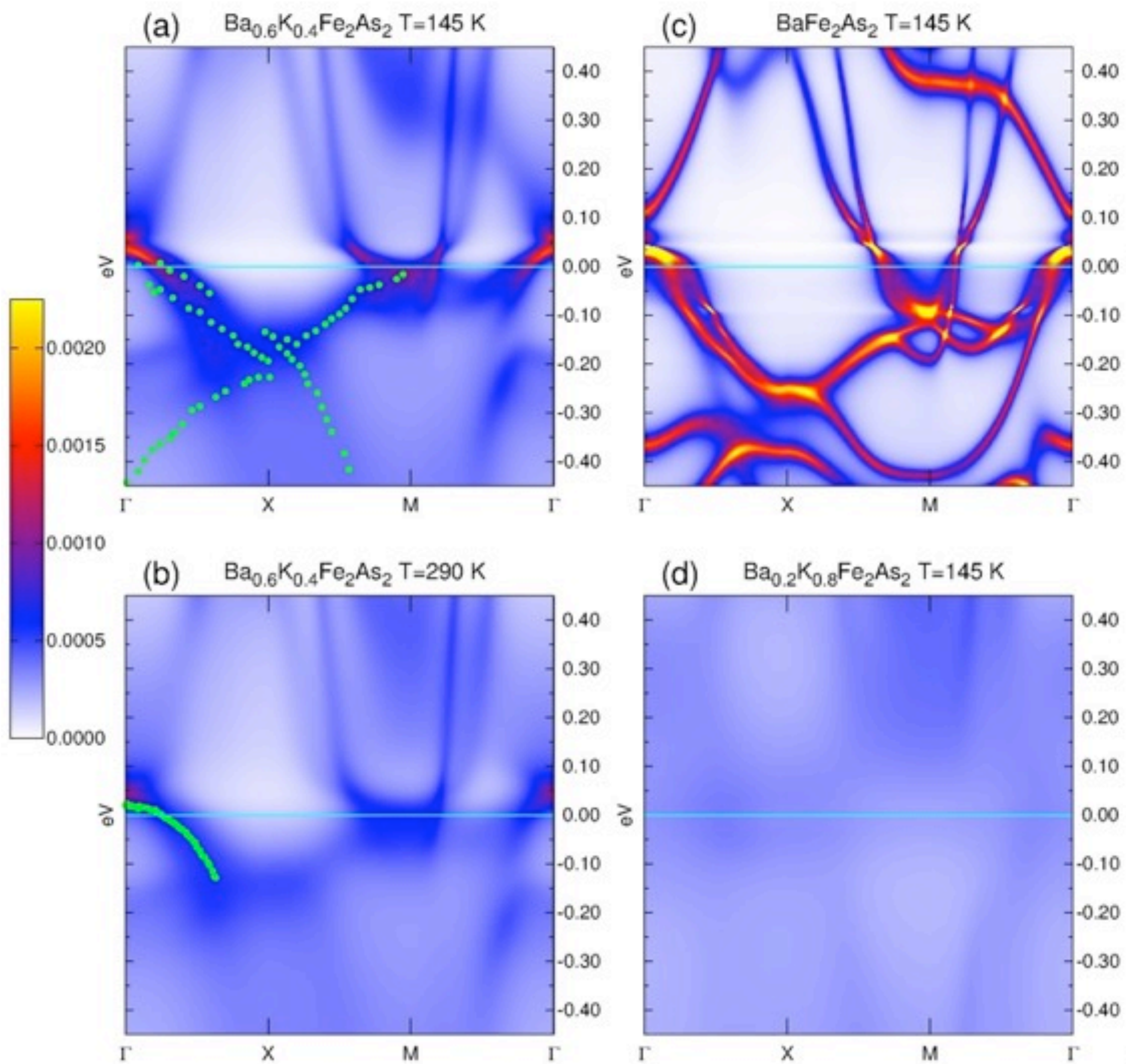
non-FL properties near optimal doping

incoherent metal in the overdoped regime

Pnictides

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

- Strong doping and temperature dependence of electronic structure



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:

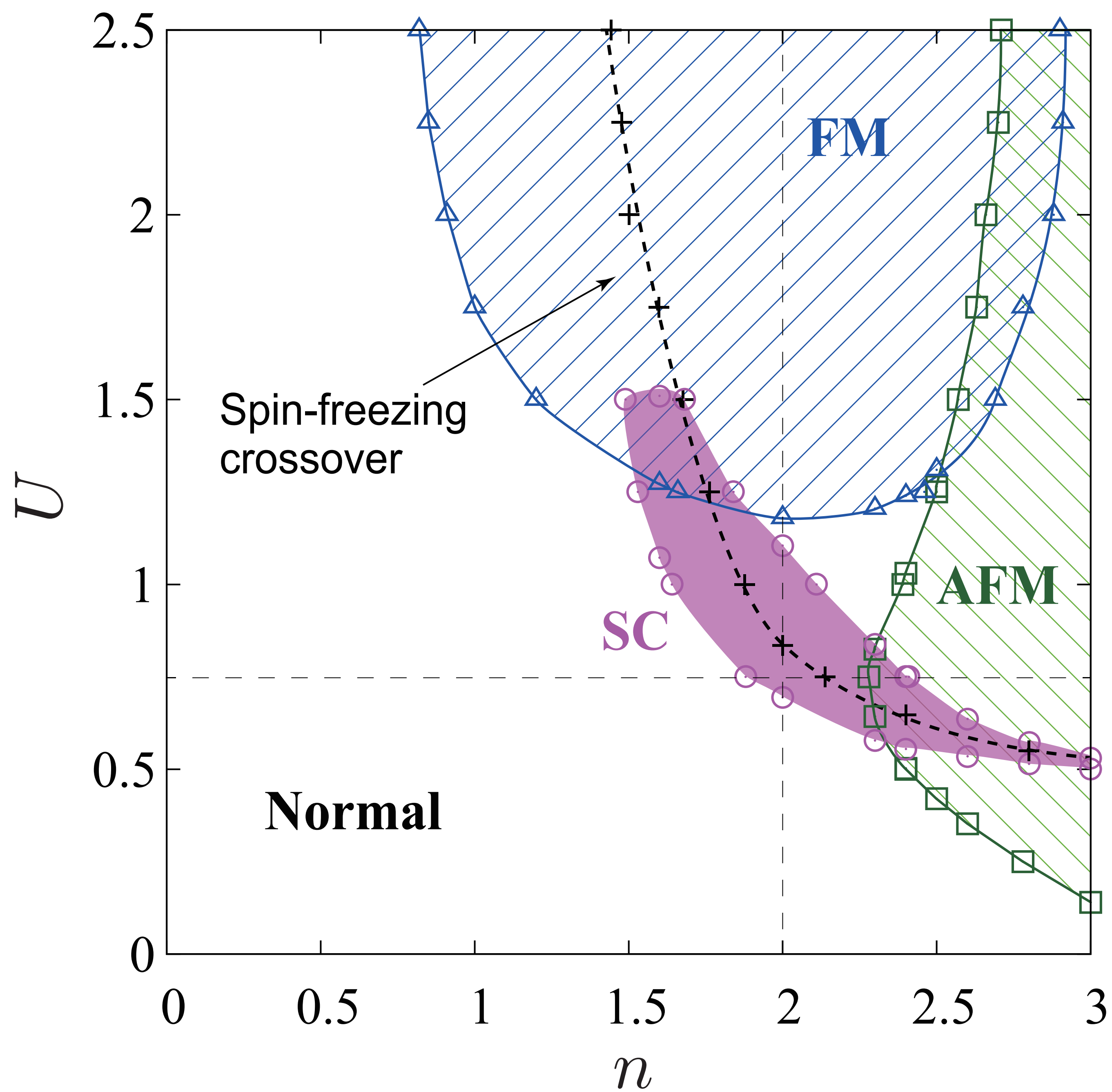
    charge, spin, orbital, spin-orbital
  - off-diagonal orders:

    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

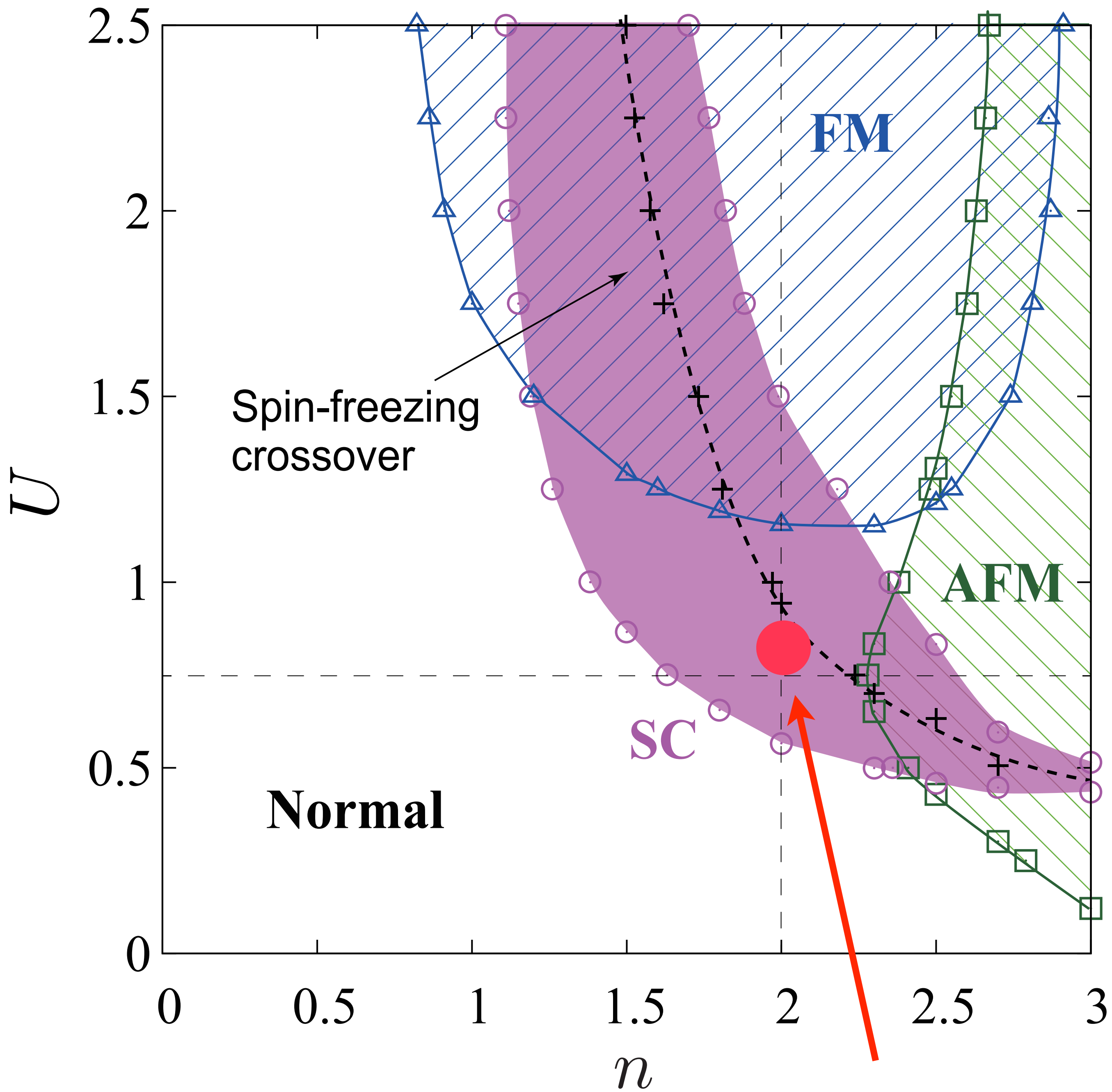
FM at large U away from half-filling

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

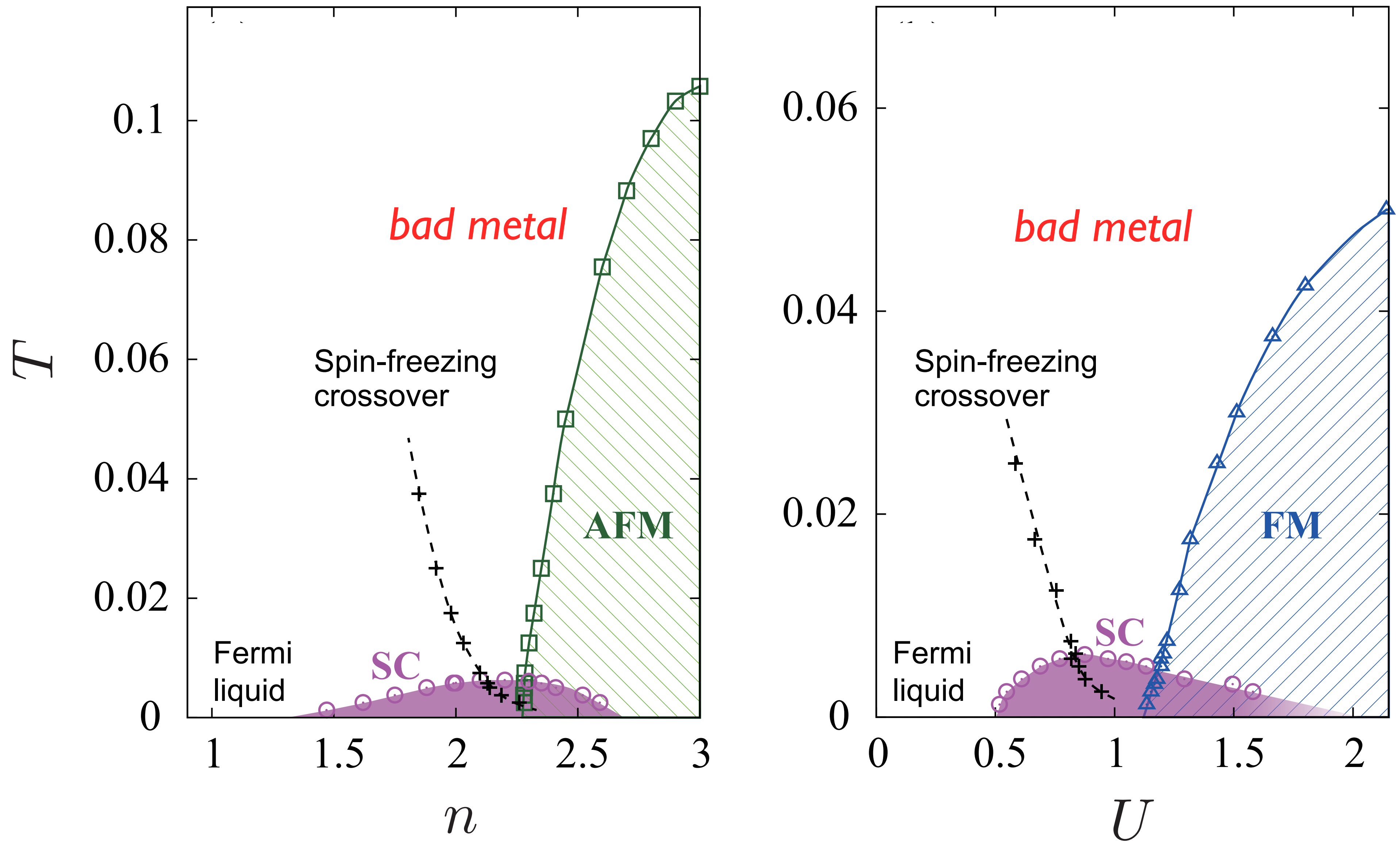
spin-triplet superconductivity in the spin-freezing crossover region

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

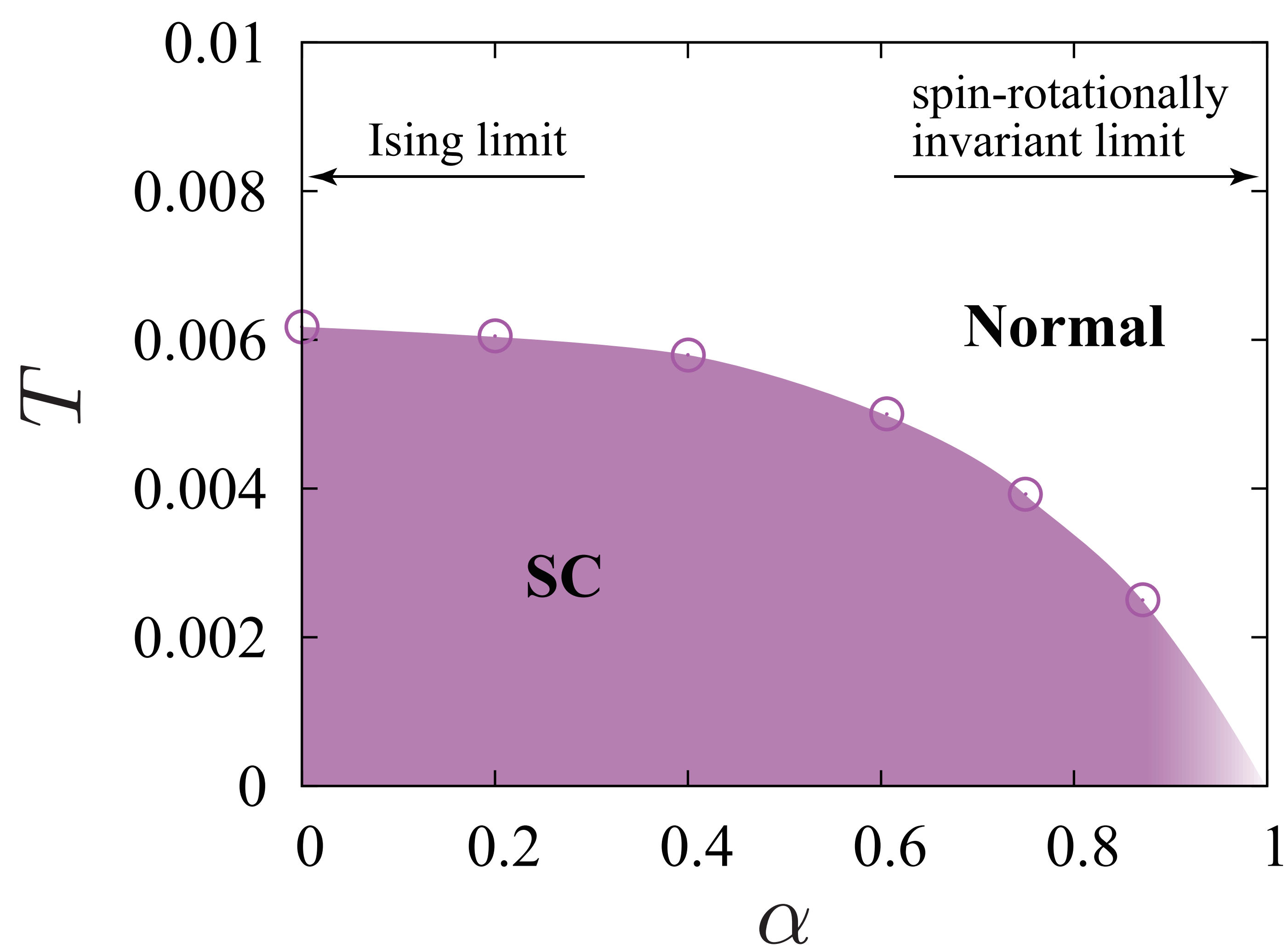


- Generic phasediagram of unconventional SC without QCP!

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

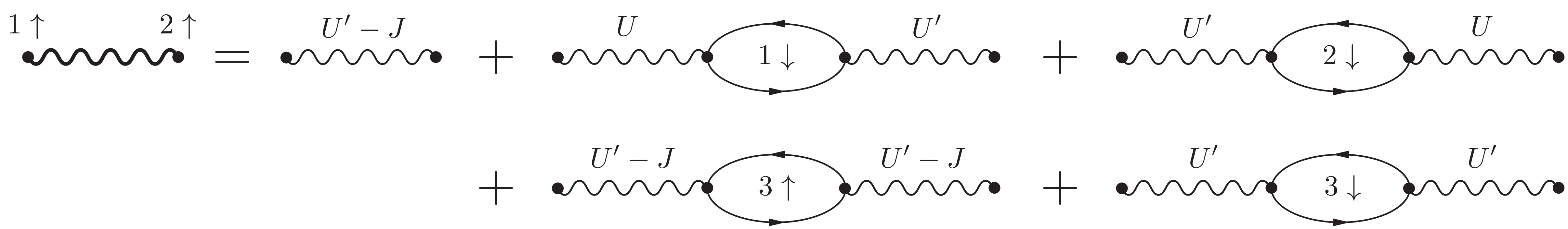
Hoshino & Werner
PRL 115, 247001 (2015)

- 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

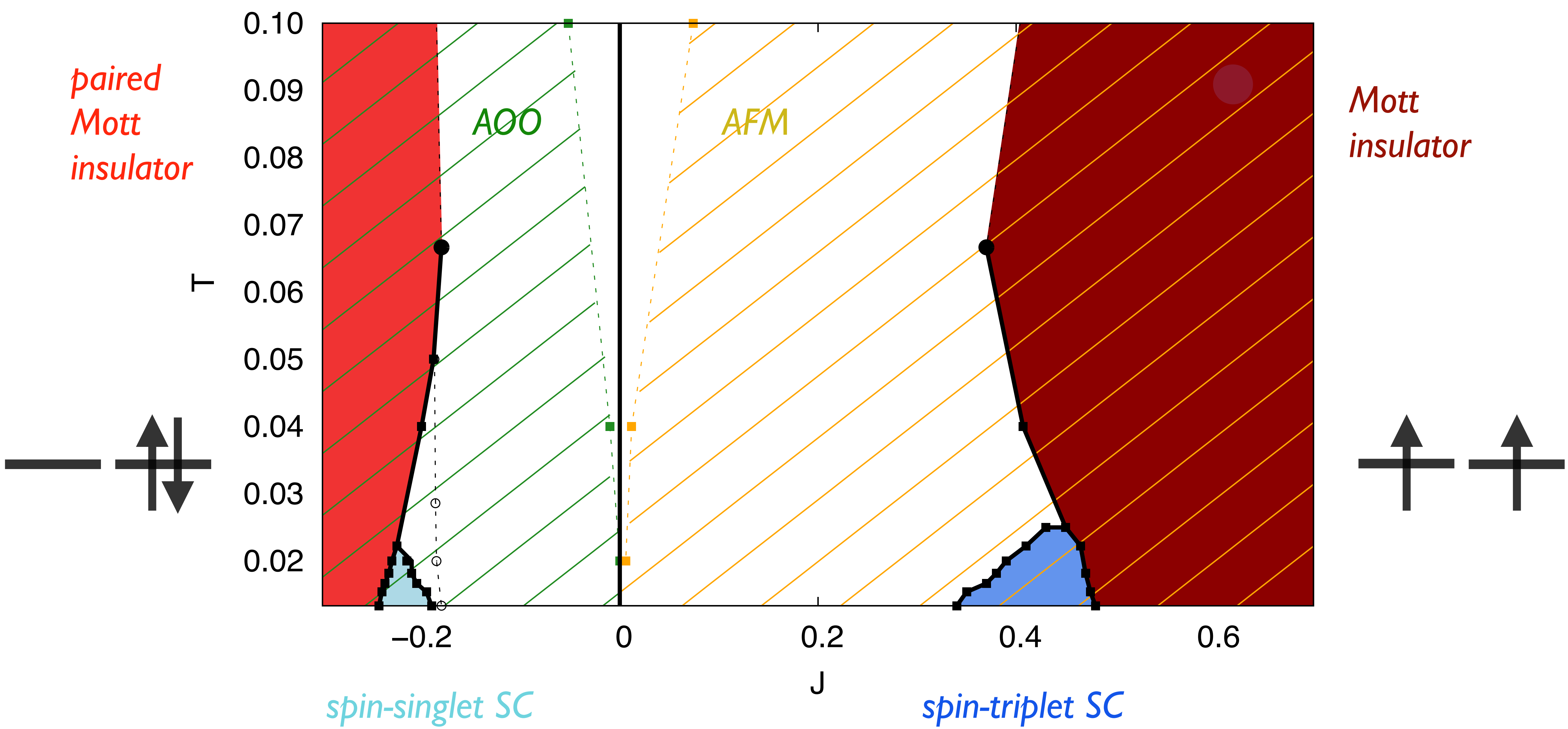
$$\tilde{U}_{1\uparrow,2\uparrow}(0) = U' - J - [2UU' + (U'-J)^2 + U'^2]\chi_{\mathrm{loc}}$$

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)

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

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

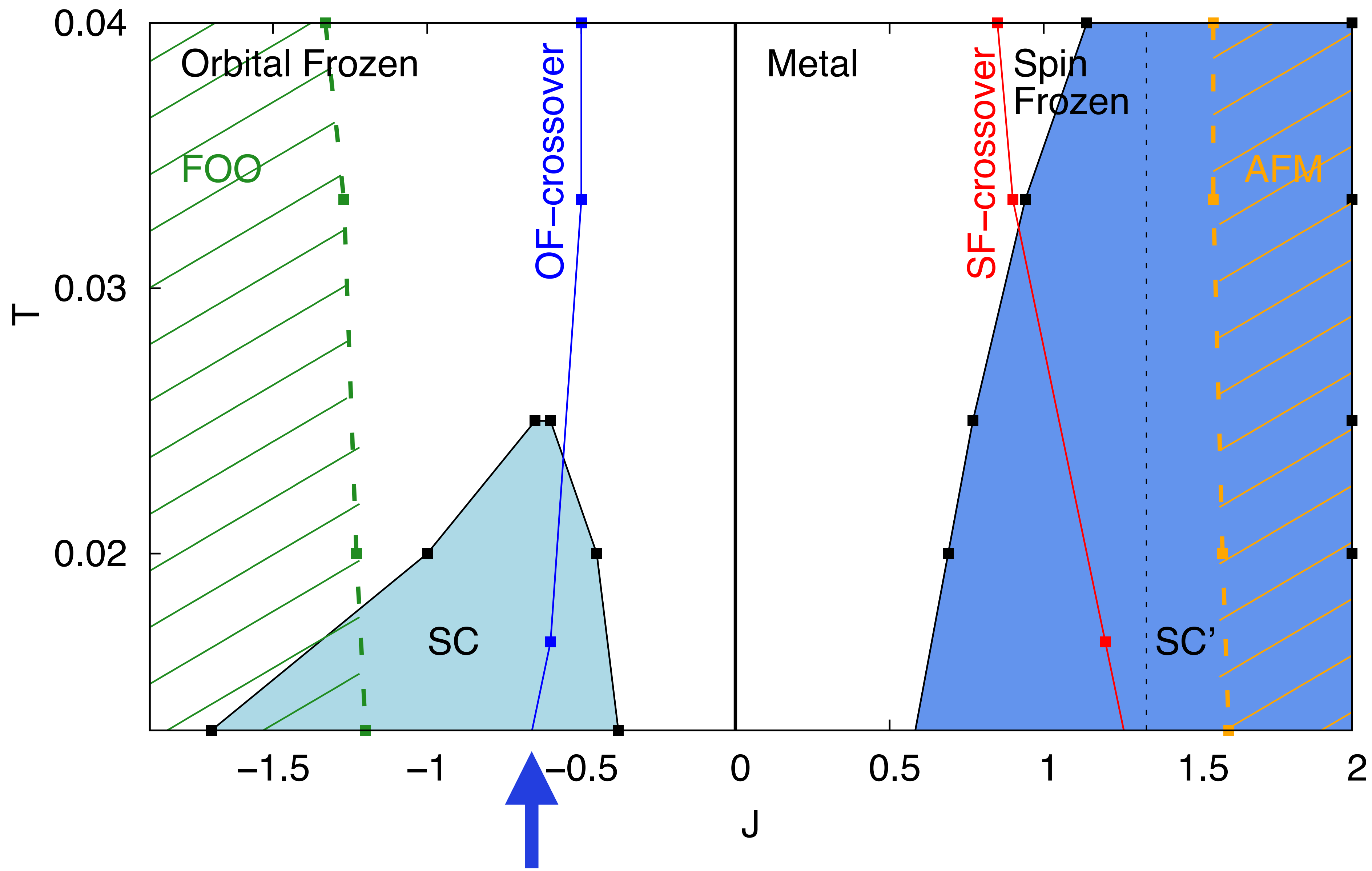
$$\begin{pmatrix} d_{i,1\downarrow} \\ d_{i,2\uparrow} \end{pmatrix} \longrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} d_{i,1\downarrow} \\ d_{i,2\uparrow} \end{pmatrix}$$

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

Negative J and orbital freezing

Steiner et al.
PRB 94, 075107 (2016)

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



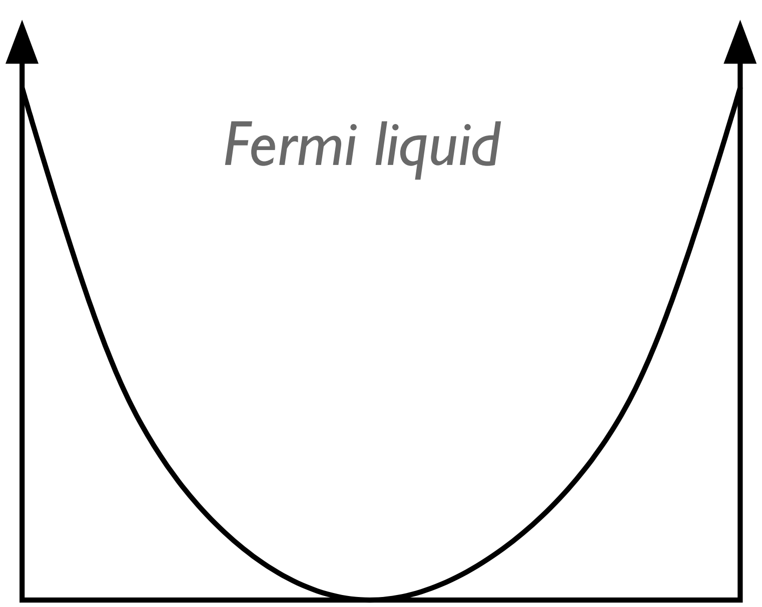
line of maximum orbital fluctuations

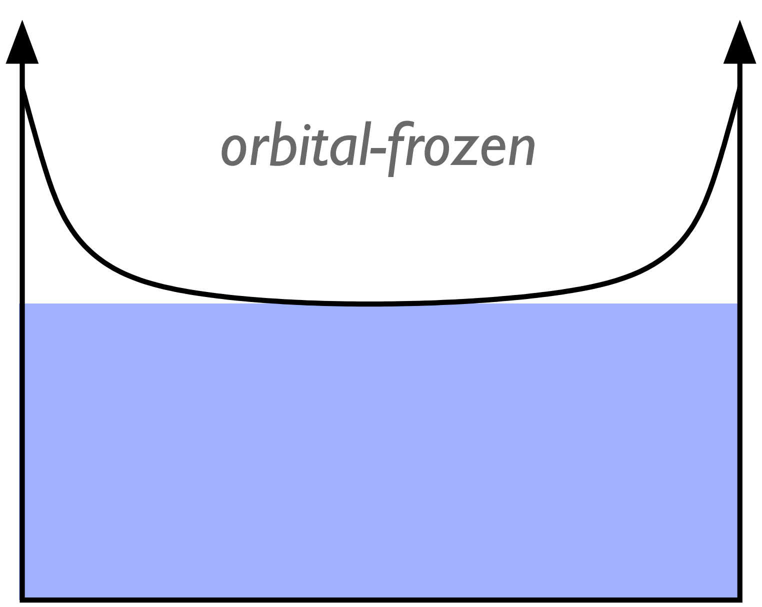
Negative J and orbital freezing

Steiner et al.
PRB 94, 075107 (2016)

- Orbital freezing seen in the decay of the (imaginary-time) orbital-orbital correlation function $\langle o(\tau)o(0)\rangle,\ o = n_1 - n_2$
  - fermi liquid metal: $\langle o(\tau)o(0)\rangle \sim 1/\tau^2 \ \ (\tau \text{ large})$
  - orbital-frozen metal: $\langle o(\tau)o(0)\rangle \sim \text{const} > 0$
- Orbital freezing crossover line: maximum of orbital fluctuations

$$\Delta\chi_{\rm orb} \equiv \int_0^\beta d\tau[\langle o(\tau)o(0)\rangle - \langle o(\beta/2)o(0)\rangle]$$





Negative J and orbital freezing

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  - orbital-frozen metal: $\langle o(\tau)o(0)\rangle \sim \text{const} > 0$
- Orbital freezing crossover line: maximum of orbital fluctuations

$$\Delta\chi_{\rm orb} \equiv \int_0^\beta d\tau [\langle o(\tau)o(0)\rangle - \langle o(\beta/2)o(0)\rangle]$$

- Orbital fluctuations induce attractive interaction for on-site pairs
  - Effective interaction which includes bubble diagrams:

analogous to: Inaba & Suga, PRL (2012)

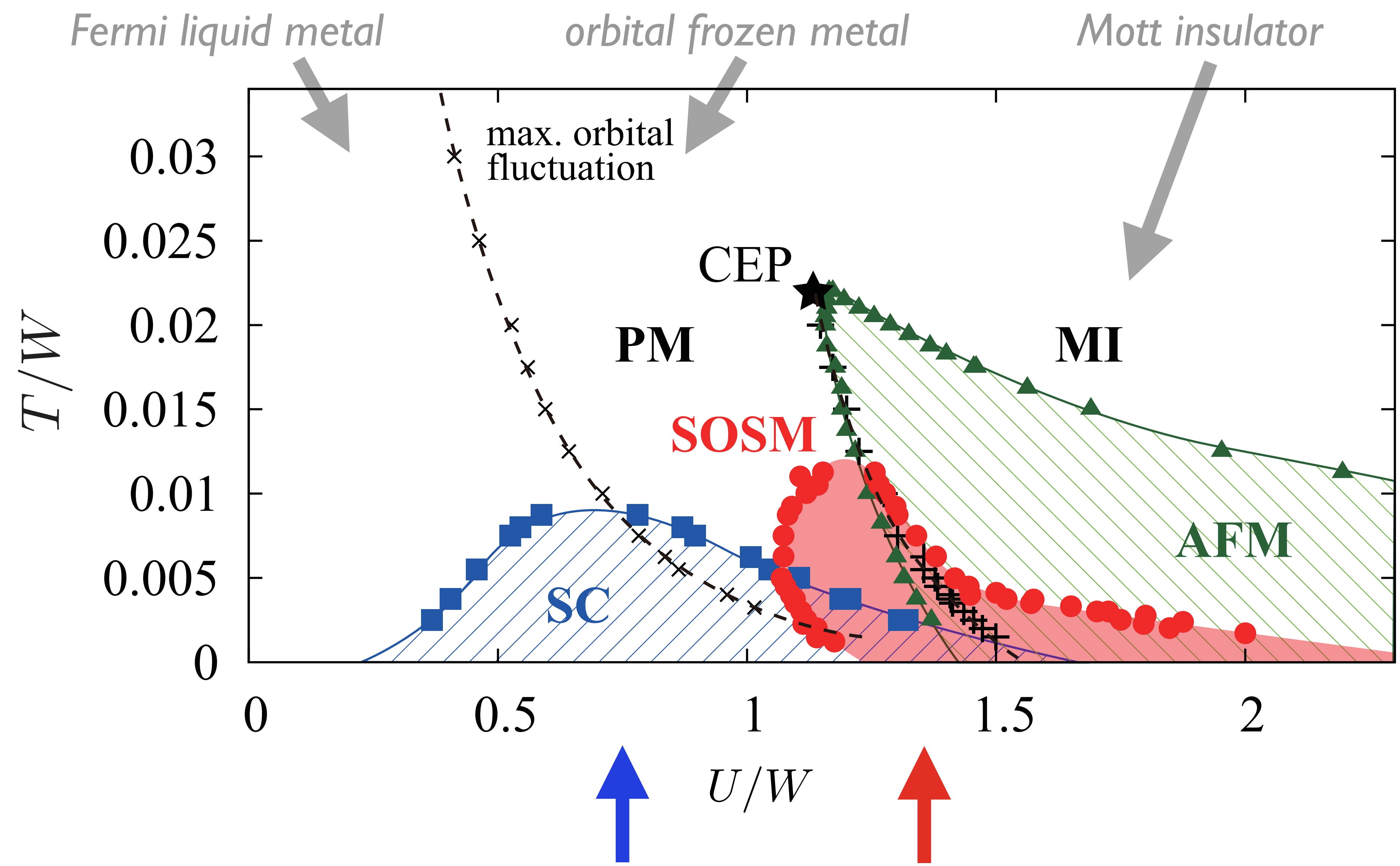
$$\tilde{U}_{\alpha\beta}(q) = U_{\alpha\beta} - \sum_\gamma U_{\alpha\gamma}\chi_\gamma(q)\tilde{U}_{\gamma\beta}(q)$$

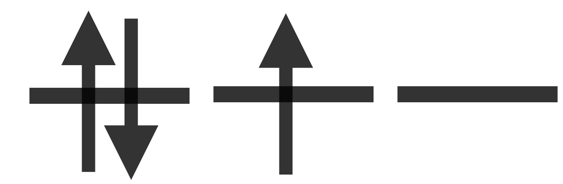
$$\Rightarrow \quad \tilde{U} = U - 4U'[U' + |J|]\Delta\chi_{\rm orb} + O(U^3)$$

Negative J and orbital freezing

Hoshino & Werner
PRL 118, 177002 (2017)

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





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)

- Unconventional SC in the spin-freezing regime
  - Strontium ruthenates
  - Uranium-based SC
  - Pnictides
  - CrAs, MnP
  - ...

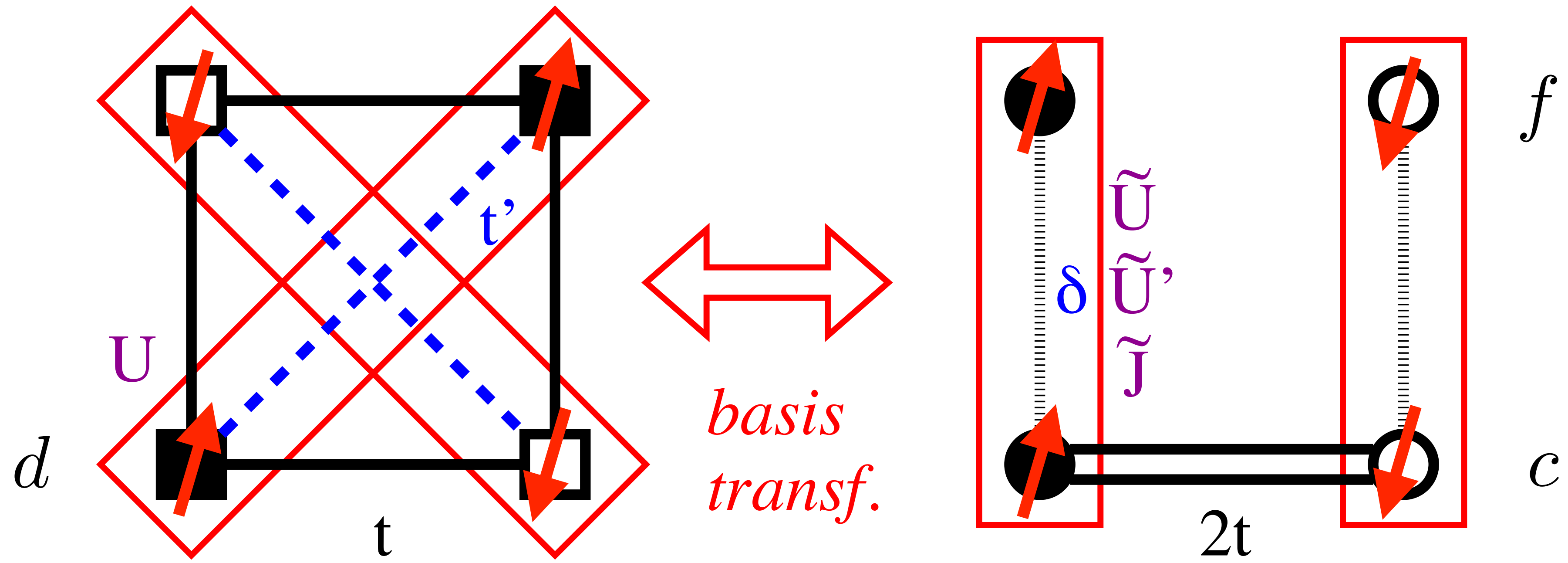
- Unconventional SC in the orbital-freezing regime
  - Alkali-doped fullerides

- What about cuprates? Can spin-freezing play any role in a single-band 2D Hubbard model?
  - naive answer: NO, correct answer: YES

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 $\delta = 2t'$

Cuprates

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

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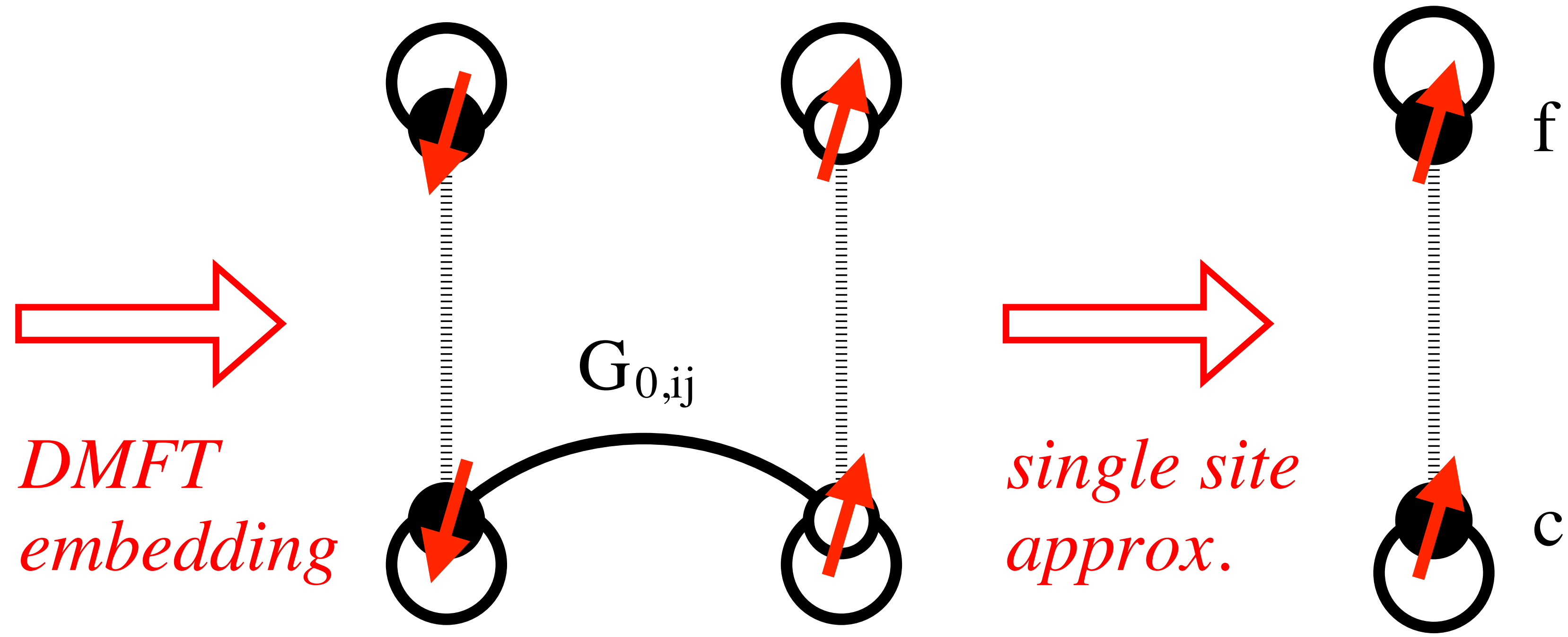

$$c_1 = \frac{1}{\sqrt{2}}(d_1 + d_3) \quad c_2 = \frac{1}{\sqrt{2}}(d_2 + d_4)$$

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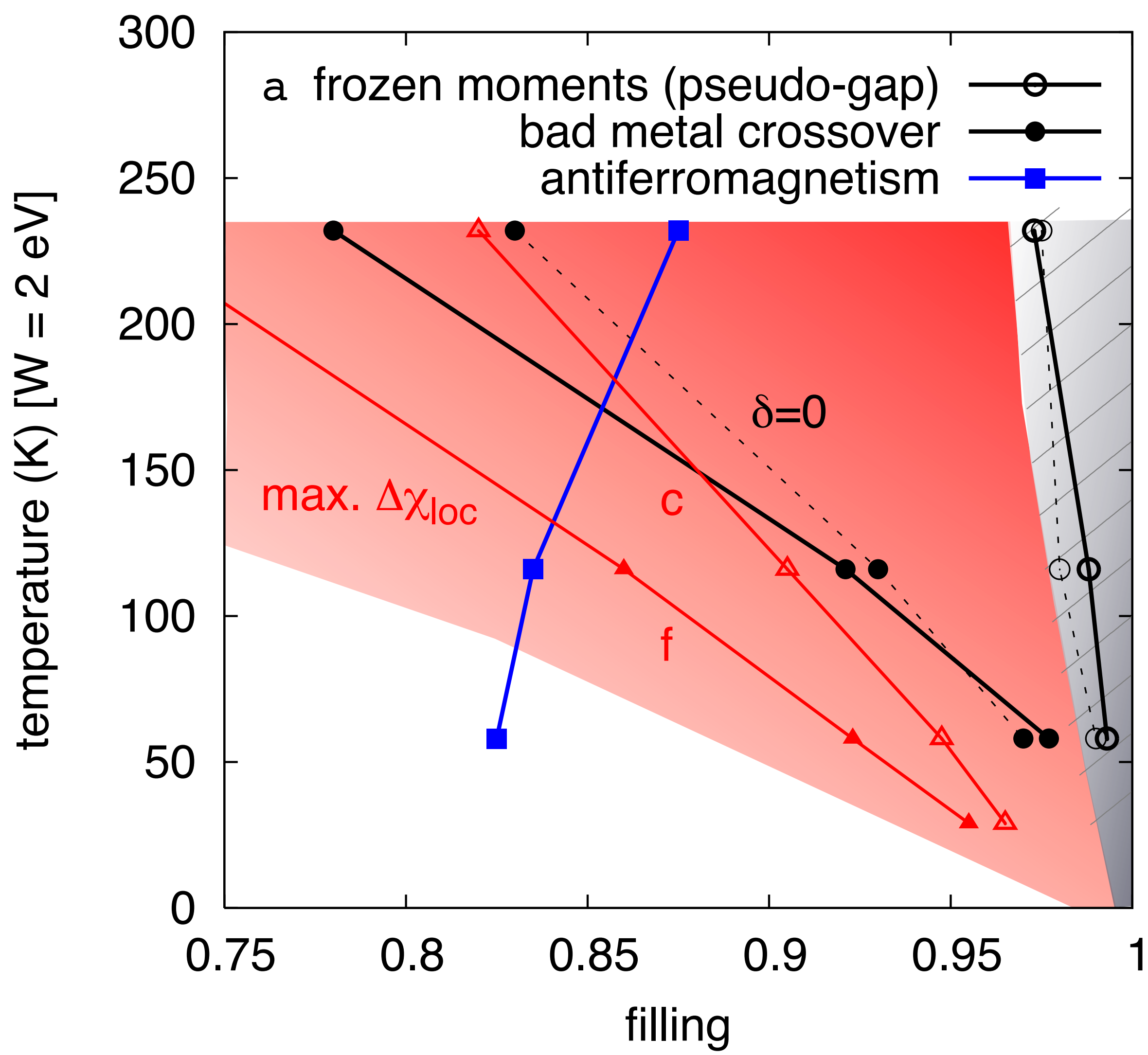
Cuprates

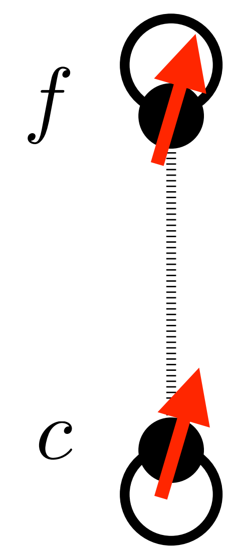
Werner, Hoshino & Shinaoka
PRB 94, 245134 (2016)

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

emerging (fluctuating) local moments = bad metal regime



frozen moments =pseudo-gap phase

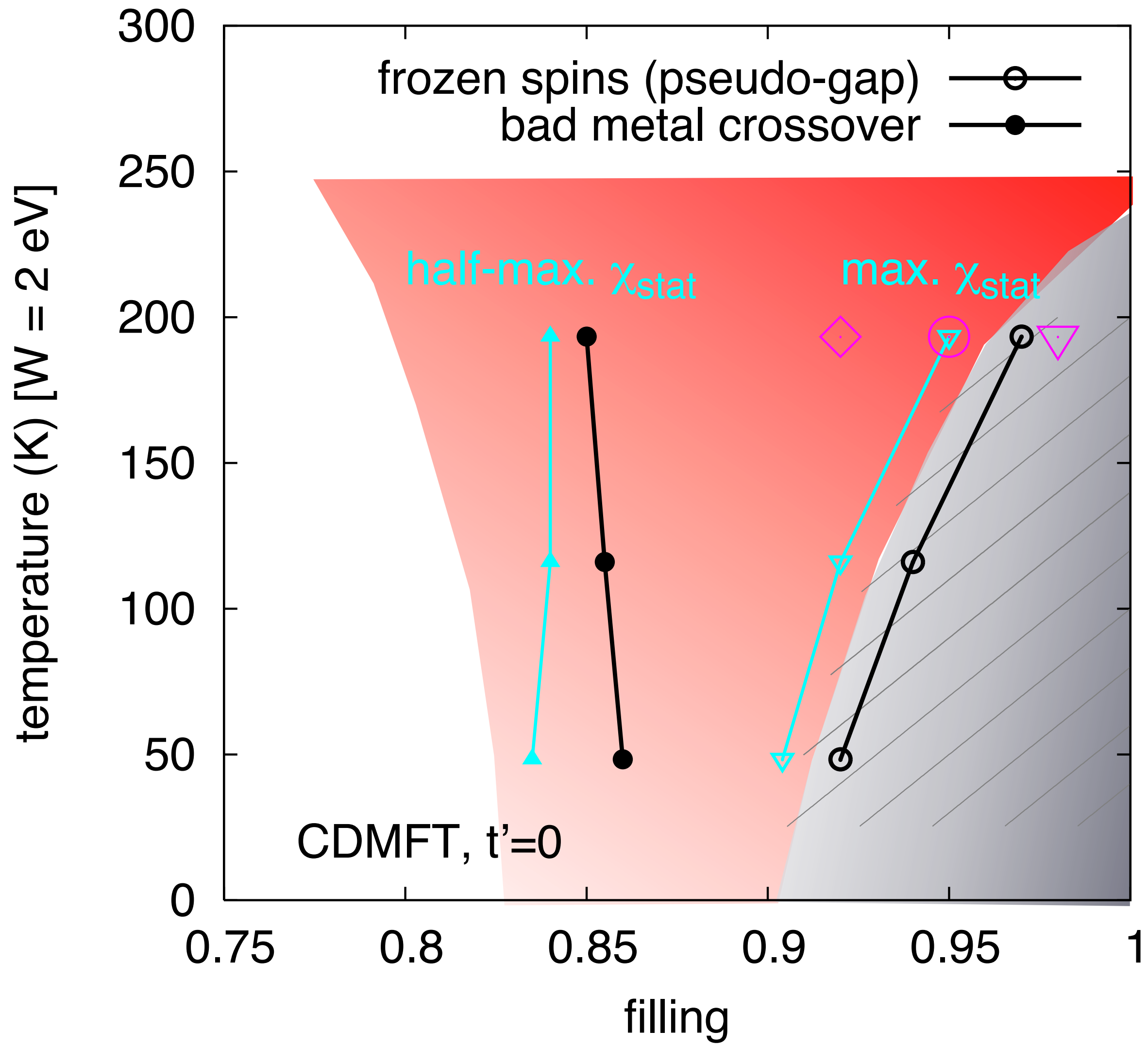


Cuprates

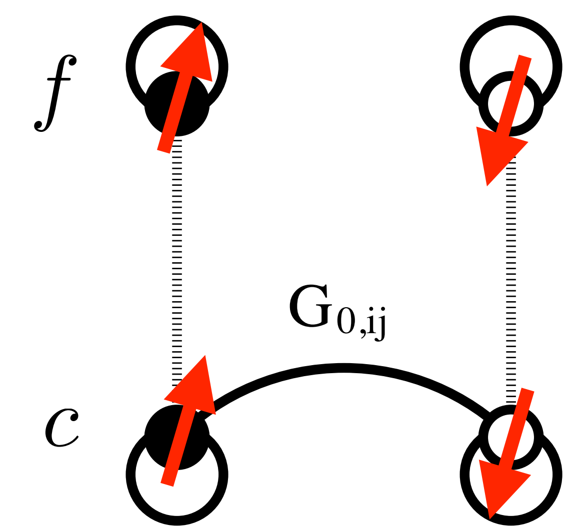
Werner, Hoshino & Shinaoka
PRB 94, 245134 (2016)

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

emerging (fluctuating) local moments = bad metal regime



frozen moments =pseudo-gap phase



Cuprates

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

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

emerging (fluctuating)
local moments
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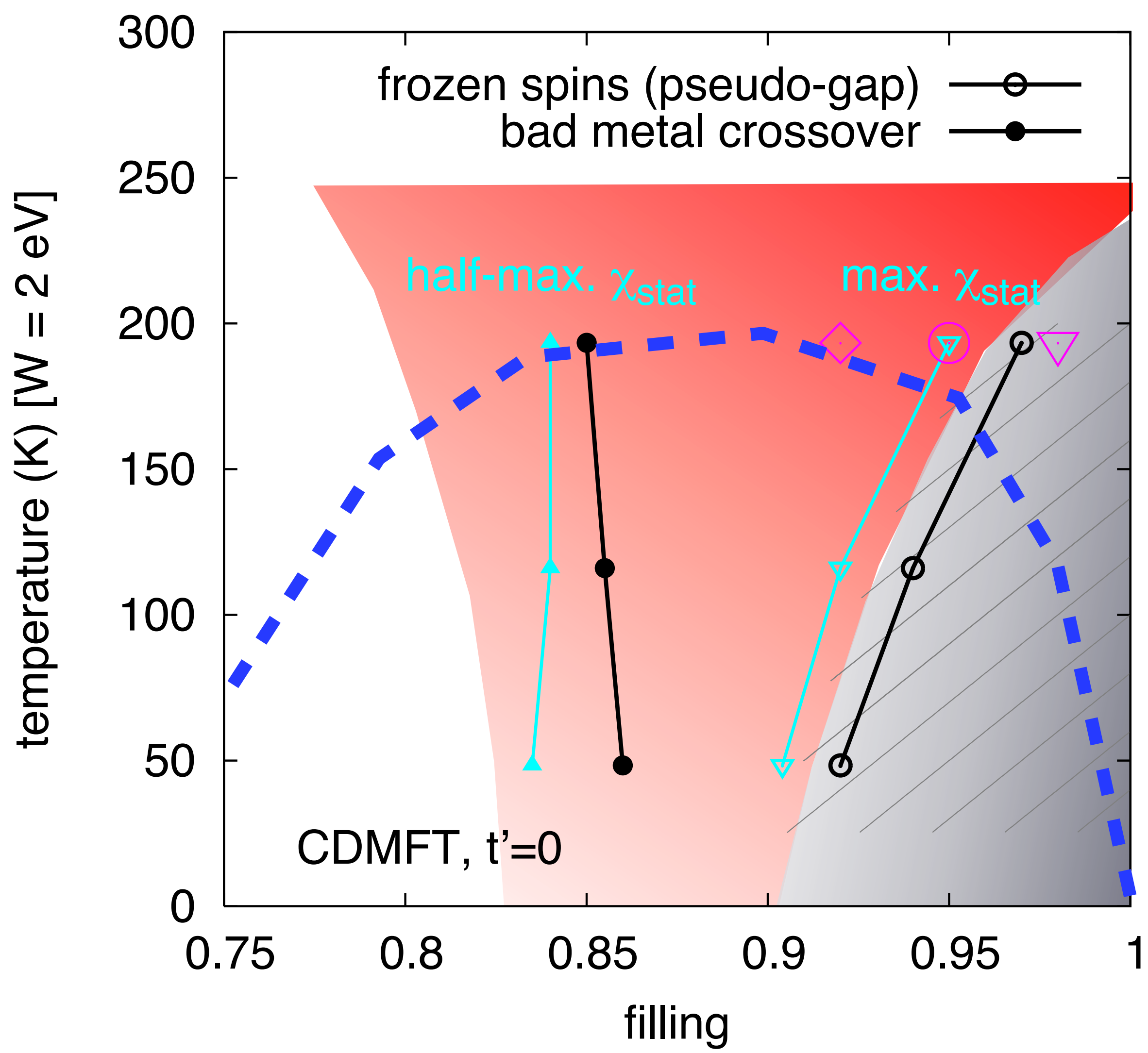


frozen moments
=pseudo-gap phase

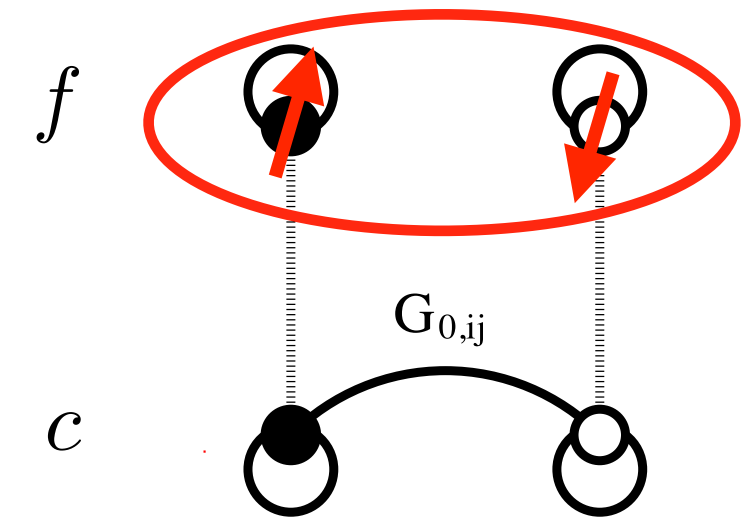
SC dome [4-site cluster DMFT, Maier et al, (2005)]
induced by fluctuating local moments?

Cuprates

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

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

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

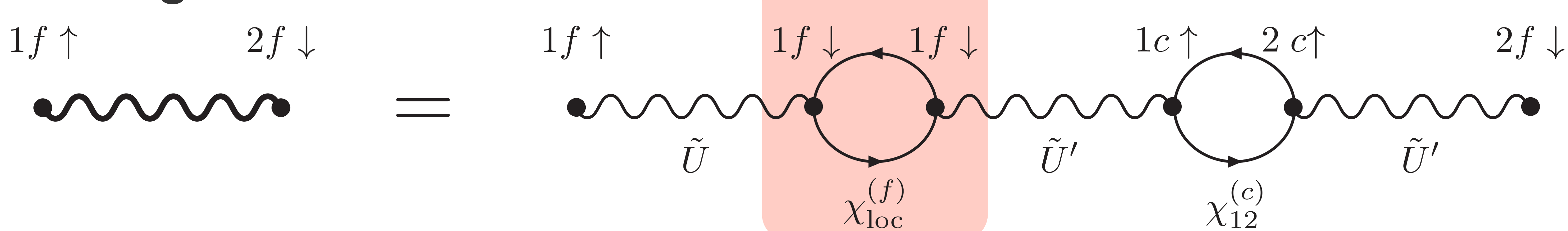


- Effective attractive interaction:

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

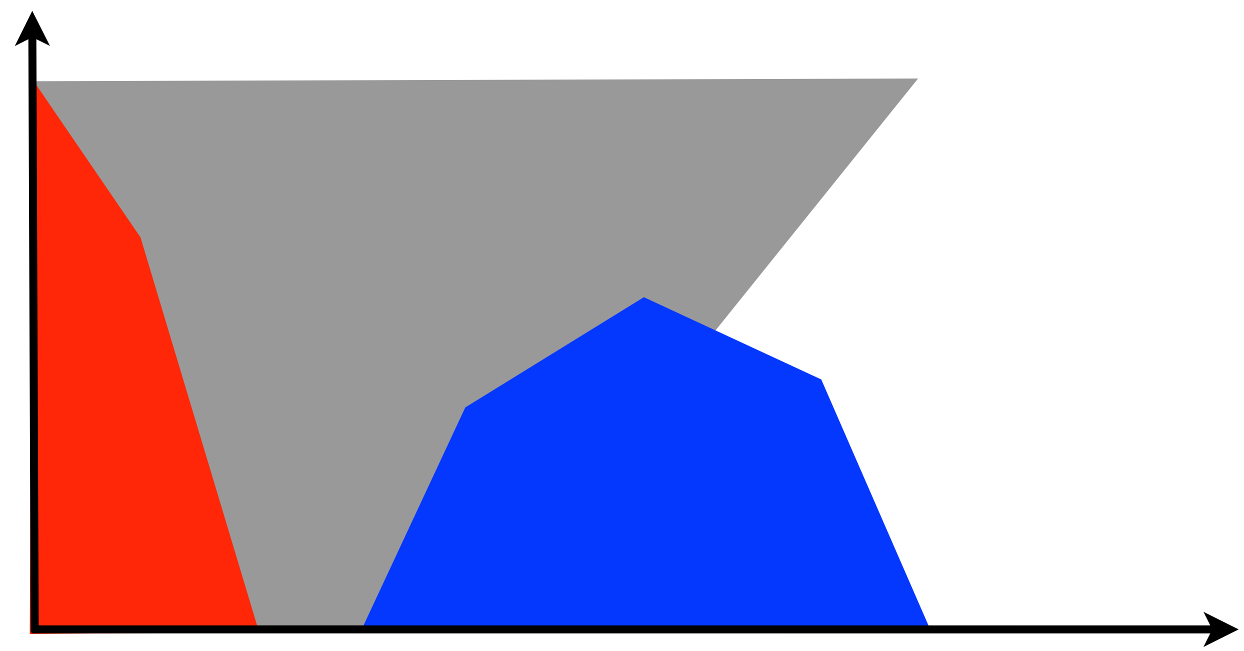
local spin fluctuations (needed because U'-J=0)

- Leading contribution:



Summary I

- 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

Connection to Sachdev-Ye model

- Sachdev-Ye model

  Spin-*S* quantum Heisenberg model with infinite-range Gaussian-random interactions *Sachdev & Ye, PRL (1993)*

$$H = \frac{1}{\sqrt{NM}} \sum_{i>j} J_{ij} S_i \cdot S_j$$

$$P(J_{ij}) \sim \exp[-J_{ij}^2/(2J^2)]$$

$$N \to \infty : \ \text{number of sites}$$

$$S : SU(M) \text{ spin operator } (M \text{ large})$$

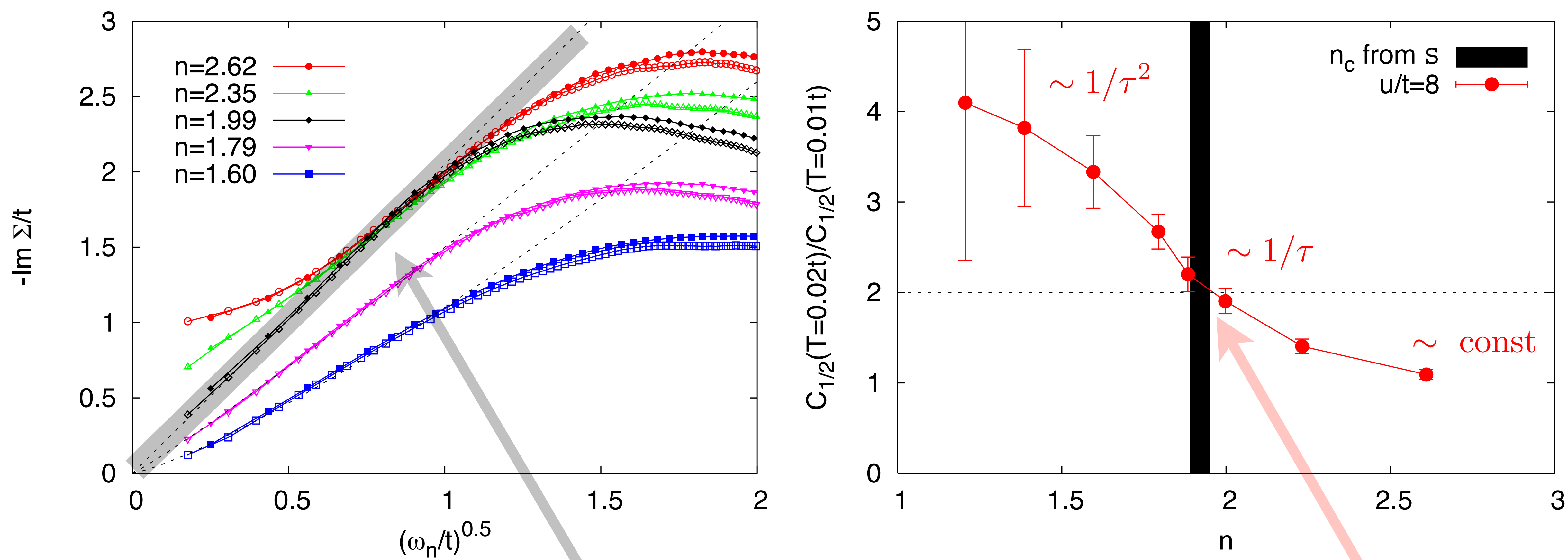
Fermionize spins, calculate saddle-point solution in the large-*M* limit

$$G^{-1}(i\omega_n) = i\omega_n - \Sigma(i\omega_n), \quad \Sigma(\tau) = -J^2 G(\tau) G(-\tau) G(\tau)$$

$$\Longrightarrow \quad G(i\omega) \sim 1/\sqrt{\omega_n}, \quad \Sigma(i\omega_n) \sim i\sqrt{\omega_n}, \quad \langle S_i^a(\tau) S_i^a(0)\rangle \sim 1/\tau$$

Connection to Sachdev-Ye model

- Sachdev-Ye model



Same non-Fermi liquid exponents as in the spin-freezing crossover region *Werner et al., PRL (2008)*

$$G(i\omega) \sim 1/\sqrt{\omega_n}, \quad \Sigma(i\omega_n) \sim i\sqrt{\omega_n}, \quad \langle S_i^a(\tau)S_i^a(0)\rangle \sim 1/\tau$$

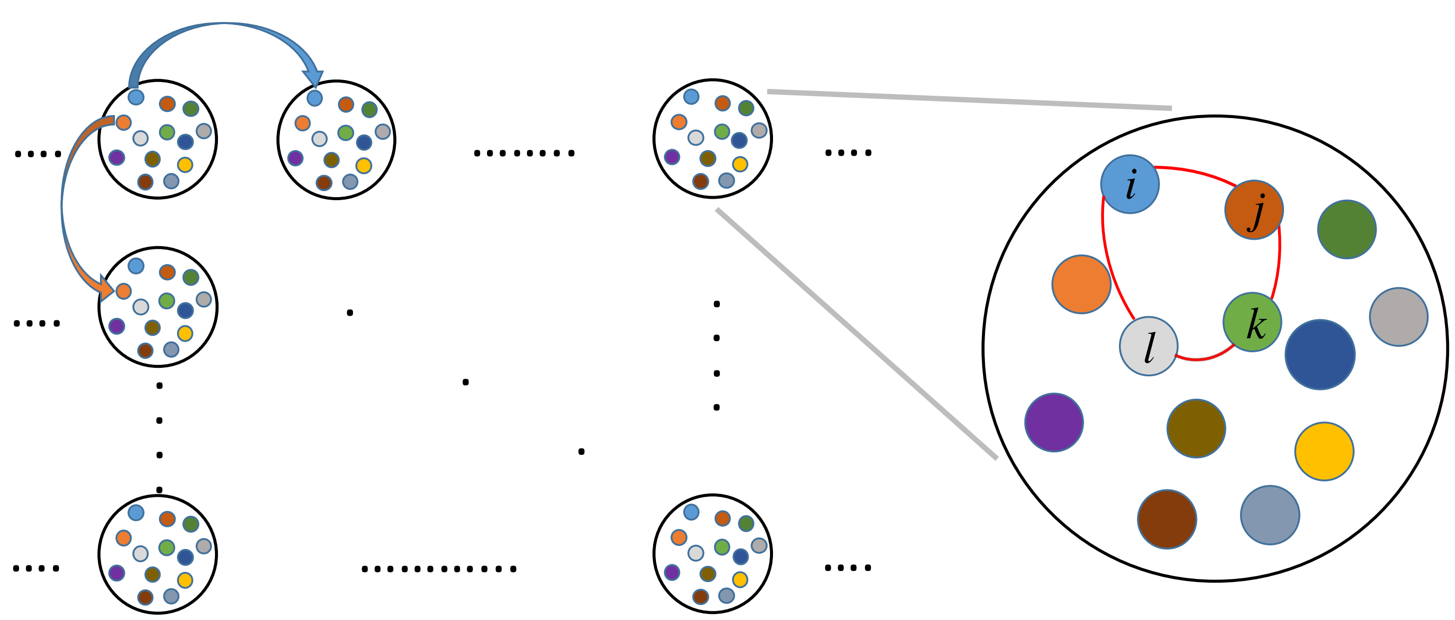
Connection to Sachdev-Ye model

- Sachdev-Ye model: recent extensions
- Sachdev-Ye-Kitaev (SYK) model: Fermionic version with Gaussian-random interaction tensor (same saddle point equations)

$$H^{\mathrm{SYK}} = \frac{1}{(2M)^{3/2}} \sum_{ijkl} U_{ijkl} c_i^\dagger c_j^\dagger c_k c_l, \qquad M = \text{ number or orbitals}$$

- Lattice of "SYK atoms": $H^{\mathrm{lattice}} = \sum_{r,r',l} t_{r,r'} c^\dagger_{r',l} c_{r,l} + \sum_r H_r^{\mathrm{SYK}}$

  Chowdhury et al, arxiv:1801.06178



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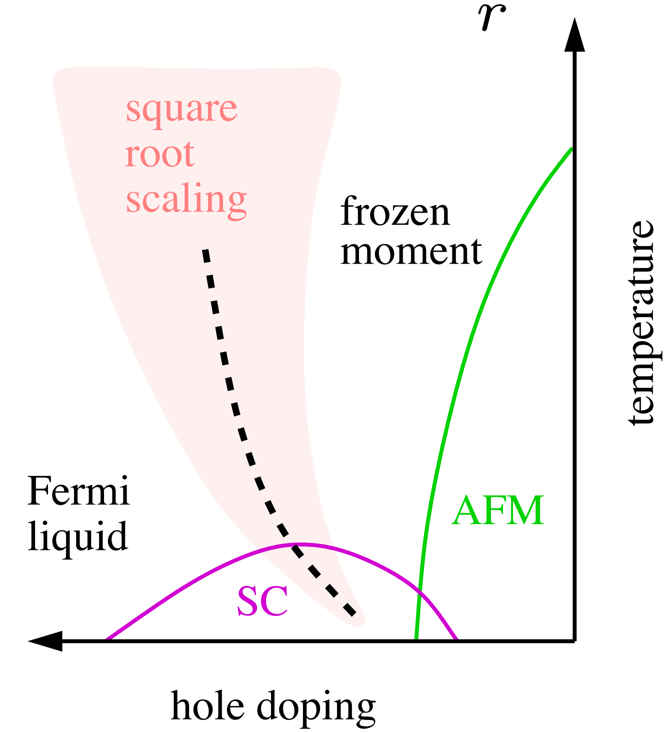
high *T*: local physics dominates

→ same as SYK

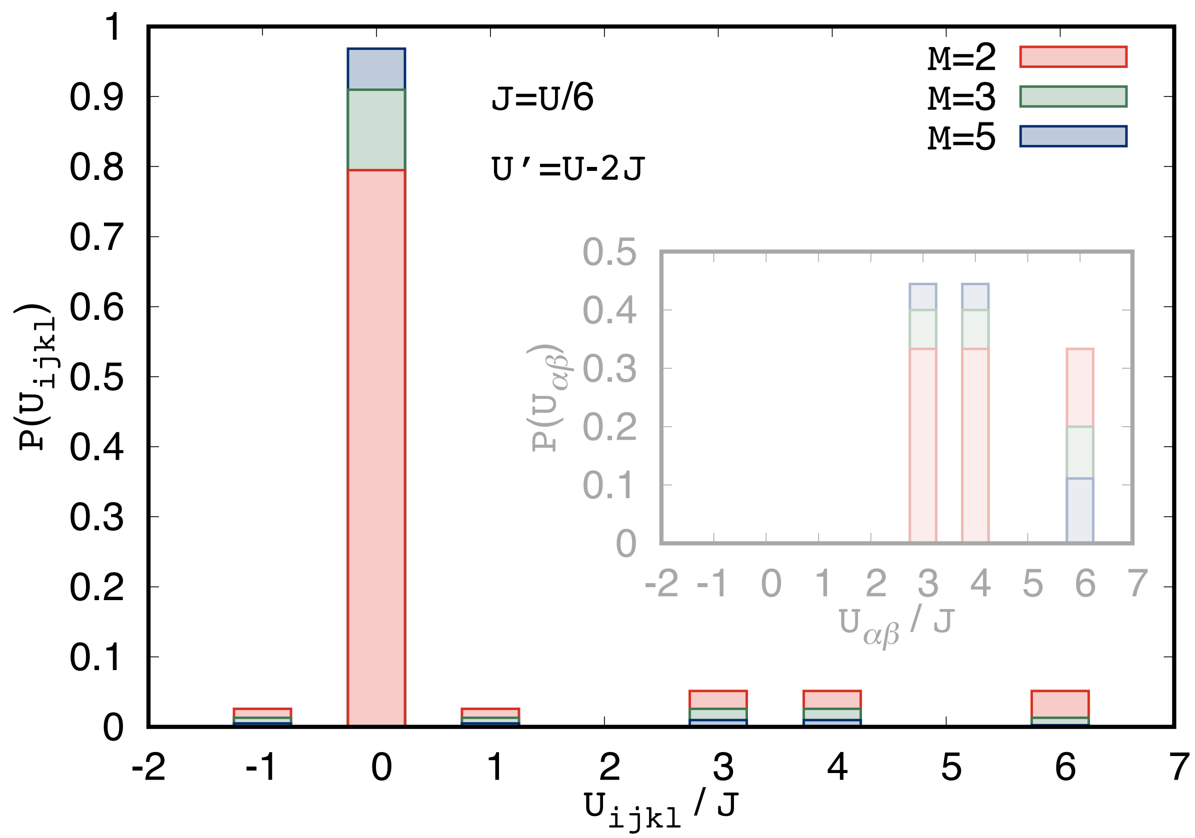
low *T*: Fermi-liquid metal



Connection to Sachdev-Ye model

Werner, Kim & Hoshino
arxiv:1805.04102

- Interaction tensor
- Gaussian-random interaction tensor is unphysical
- U_{ijkl} for a Slater-Kanamori interaction with *M*=2,3,5 orbitals



Switch to density-density interactions $\sum_{\alpha,\beta} U_{\alpha\beta} n_\alpha n_\beta$ and focus on inter-orbital terms ($O(M^2)$ terms)

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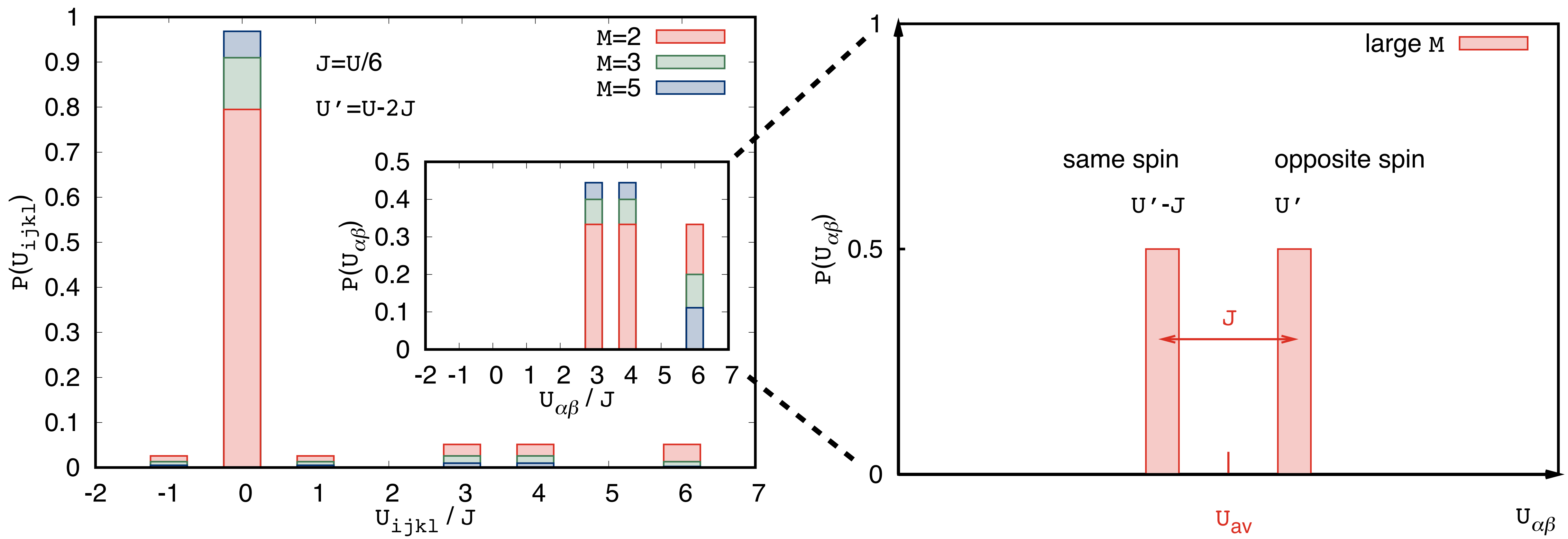

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Connection to Sachdev-Ye model

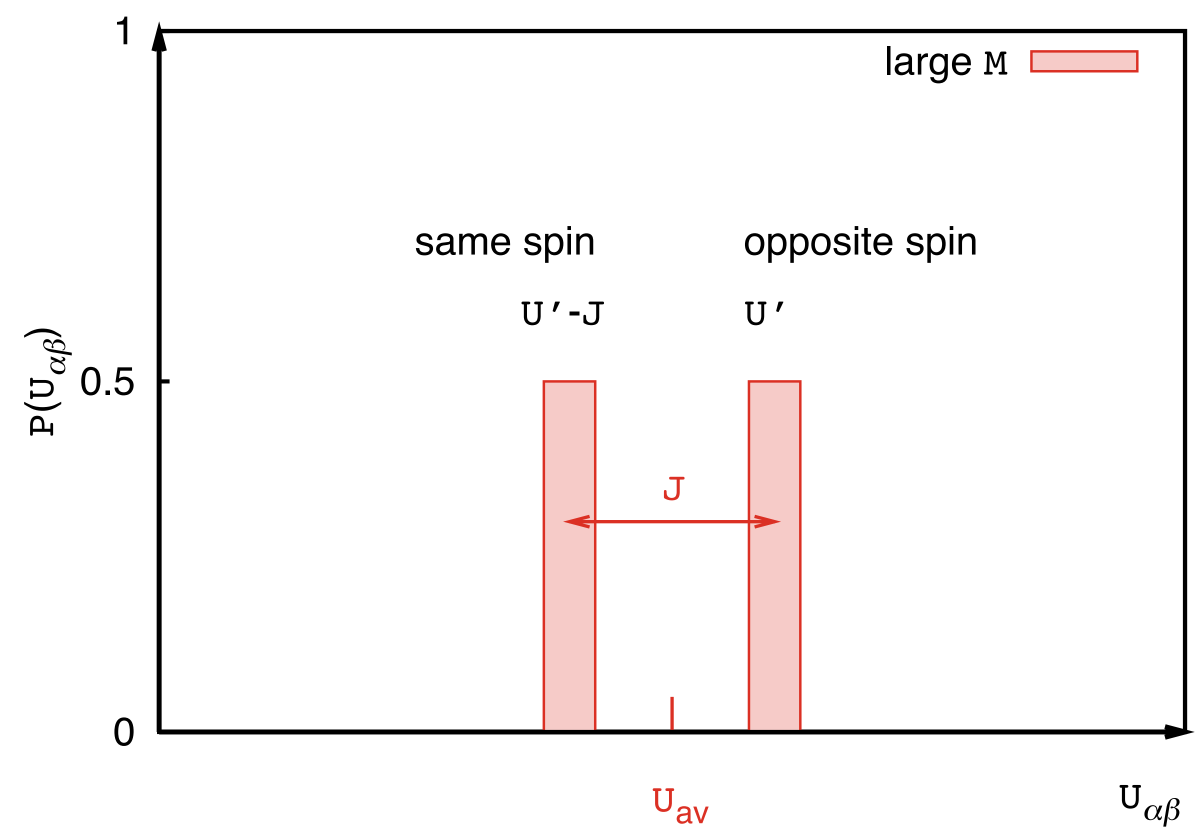
Werner, Kim & Hoshino
arxiv:1805.04102

- Interaction tensor
- Gaussian-random interaction tensor is unphysical
- Physically meaningful and much simpler model:

Density-density interactions with random-bimodal distribution

average interaction is the "Hubbard *U*"

difference between the two interactions is the Hund coupling



- This model has the same saddle point equations as the SY(K) model

Connection to Sachdev-Ye model

Werner, Kim & Hoshino
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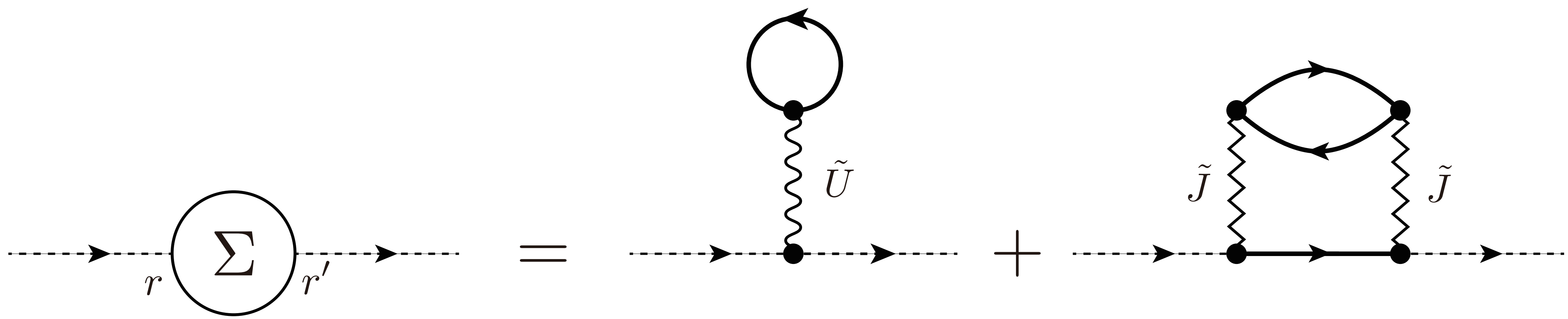
- Important point: interaction vertex in the second order diagram is Hund coupling



Hartree diagram: monopole interaction

2nd order diagram: Hund coupling effect

Consequence: no Hund coupling, no interesting non-FL properties

- Same equations as for the SYK lattice model ⟶ same physics:

  non-FL properties ($\Sigma(i\omega_n) \sim \sqrt{\omega_n},\ \langle S^z(\tau) S^z(0)\rangle \sim 1/\tau$) at high T

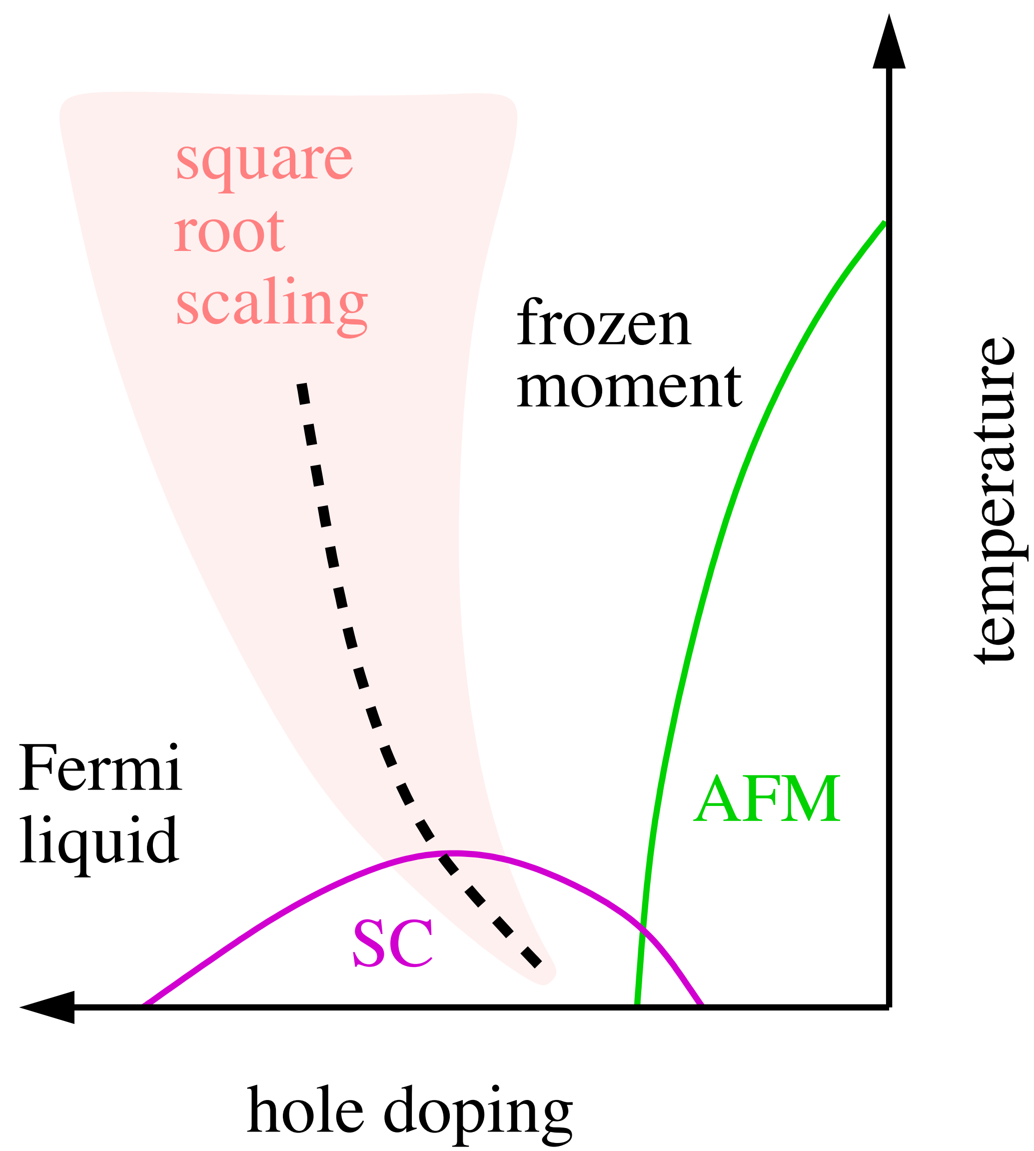
  FL metal at low T

Connection to Sachdev-Ye model

Werner, Kim & Hoshino
arxiv:1805.04102

- Interpretation of the generic DMFT phase diagram

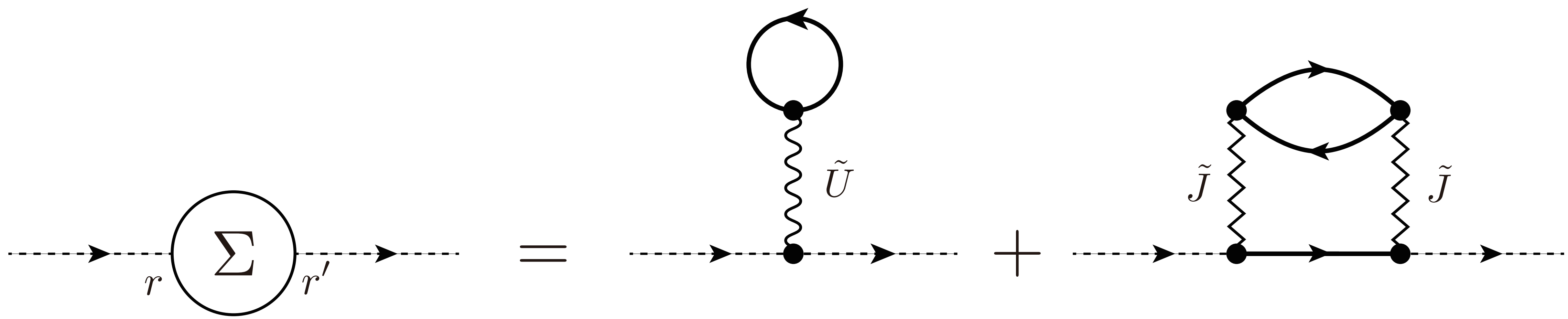
- As filling increases, local moments appear due to effect of Hund coupling
- As these moments form, the "Kondo screening temperature" drops, resulting in a bad metal with frozen moments
- The SY equations describe the spin-freezing crossover regime characterized by fluctuating moments
- The SY equations also naturally explain the connection to superconductivity



Connection to Sachdev-Ye model

Werner, Kim & Hoshino
arxiv:1805.04102

- Connnection to superconductivity



- Effective interaction which takes account of "polarization bubble":

$$U_{\text{eff}}(i\omega_n) = \tilde{U} + \tilde{J}P(i\omega_n)\tilde{J}, \quad P(\tau) = G(\tau)G(-\tau)$$

From $G(i\omega_n) \sim 1/\sqrt{\omega_n}$ follows $P(\tau) \sim 1/\tau$ and thus

$$P(i\omega_n) = -\frac{1}{\sqrt{2\pi\tilde{J}}}\log(\tilde{J}/\omega_n) \quad \Rightarrow \quad U_{\text{eff}}(\omega \to 0) \to -\infty$$

Outlook

Tsuji & Werner
in preparation

- Out-of-time-order correlation functions

$$\mathrm{OTOC}(t,t') = \langle A(t)B(t')A(t)B(t')\rangle$$

probes chaotic nature of quantum systems *Larkin & Ovchinnikov, JETP (1969)*

- Conjecture: universal bound on growth rate of OTOCs
Maldacena, Shenker, Stanford, J. High Energy Phys. (2016)

$$\mathrm{OTOC}(t,t') = c_0 + c_1 \exp[\lambda(t-t')] + \dots, \qquad \lambda \le 2\pi\beta$$

- SYK model saturates this bound on chaos

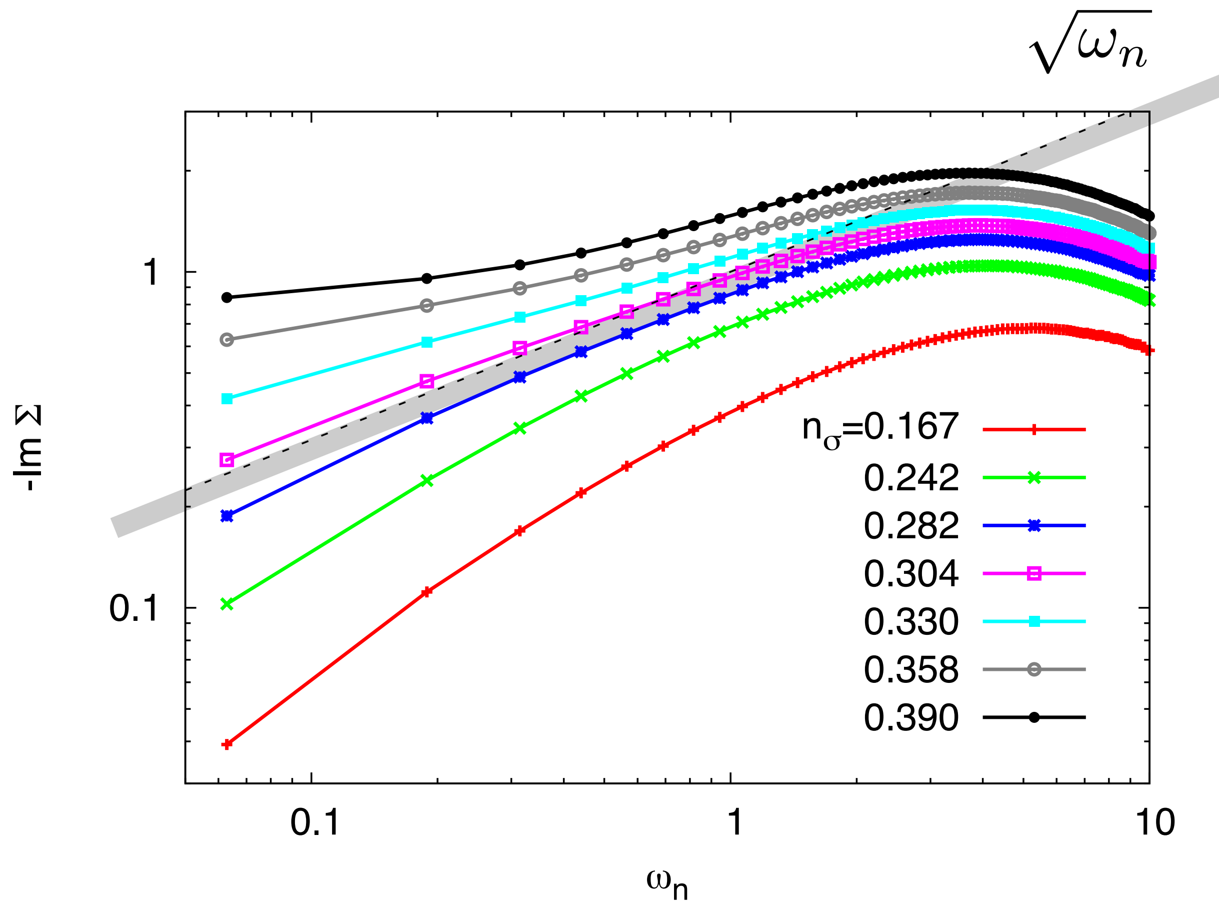
- Question: nontrivial behavior of OTOCs in the spin-freezing crossover regime of multi-orbital Hubbard models?

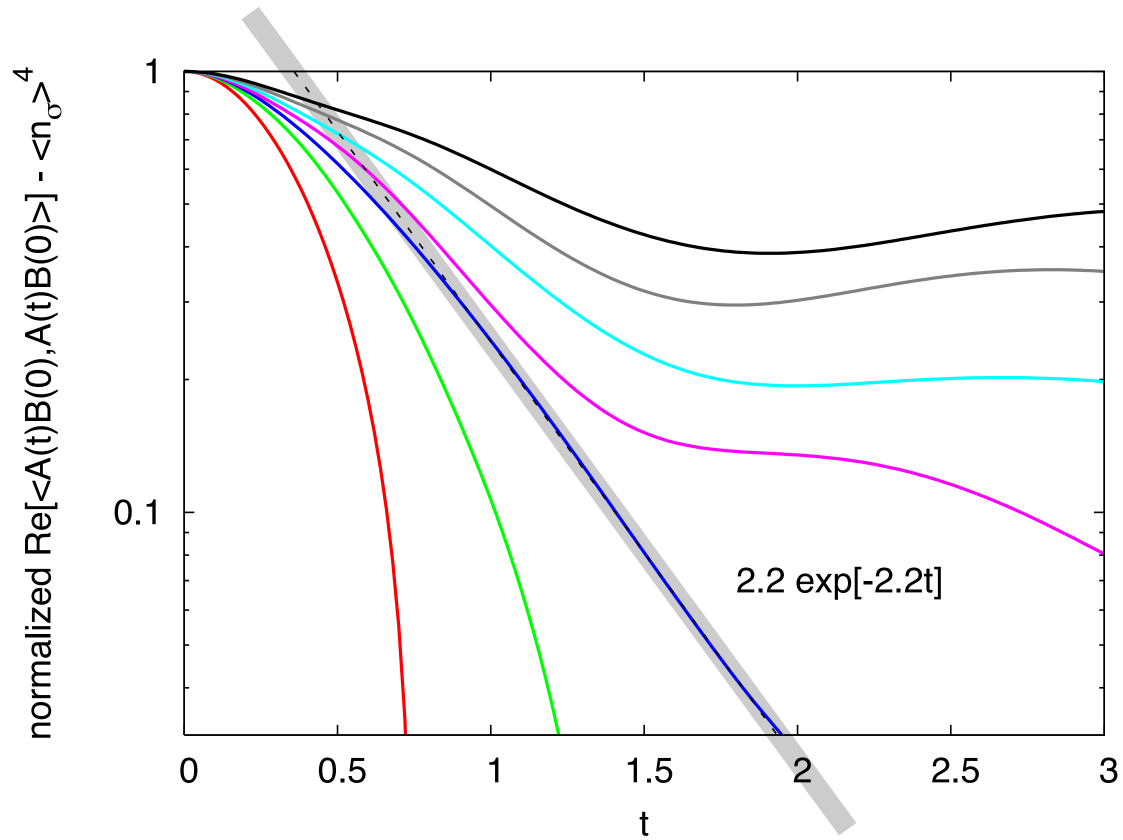
Outlook

Tsuji & Werner
in preparation

- Out-of-time-order correlation functions

$$\mathrm{OTOC}(t,t') = \langle A(t)B(t')A(t)B(t')\rangle \qquad A = B = n_{1\sigma}$$





- Exponential decay of OTOC in the spin-freezing crossover regime
- Similar to ED results for finite-*M* SYK model *Fu & Sachdev, PRB (2016)*

Summary II

- SY equations can be derived from M-orbital Hubbard model with bimodal-distributed density-density interactions

- SY equations describe the spin-freezing crossover regime and the superconductivity at low T

- Non-Fermi liquid behavior arises from Hund coupling

- Spin-OTOC exhibits exponential decay in the fluctuating moment regime (similar to finite-M SY model)

Spin-freezing: P. Werner, E. Gull, M. Troyer and A. Millis, *PRL 101, 166405 (2008)*
Connection to superconductivity: S. Hoshino and P. Werner, *PRL 115, 247001 (2015)*
Connection to A3C60: K. Steiner, S. Hoshino, Y. Nomura and P. Werner, *PRB 94, 075107 (2016)*
Connection to cuprates: P. Werner, S. Hoshino and S. Shinaoka, *PRB 94, 245134 (2016)*
Connection to Sachdev-Ye model: P. Werner, A. Kim and S. Hoshino, *arxiv:1805.04102*