Uncovering non-Fermi-liquid behaviour in Hund metals

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Phys. Rev. Lett. **115**, 136401 (2015)

Ann. Phys. **405**, 365-409 (2018)

Nature Comm. **10**, 2721 (2019)

arXiv:1908:04362

arXiv:1910.13643 (to appear in PRL)

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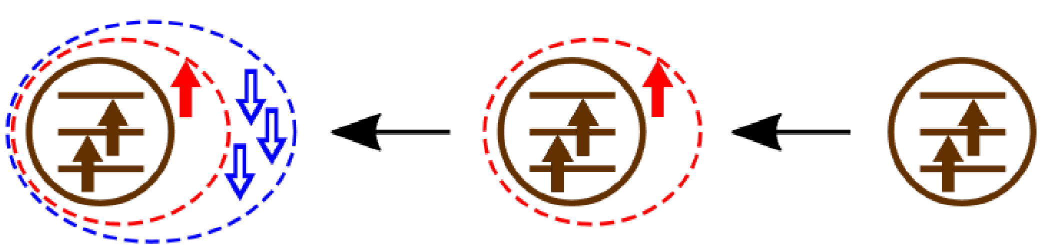

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Hund metals

- Multi-orbital systems with Hund coupling

- Correlations driven by Hund J_H rather than Hubbard U

  pnictides: Haule, Kotliar, arXiv:0805.0722, New J. Phys. 11, 025021 (2009)
  ruthenates: Werner, Gull, Troyer, Millis, arXiv:0806.2621, PRL **101**, 166405 (2008).

- Non-trivial interplay between orbital and spin degrees of freedom

  “three bands are different from one”

- Incoherent (bad metal) transport behavior at large temperatures

- Very low Fermi-liquid coherence scales

- Collective name for these properties: “Hund metals”

  Yin, Haule, Kotliar, arXiv:1104.3454, Nat. Mater. 10, 932 - 935 (2011).

Questions addressed in this talk

- Experiments observe coherence-incoherence crossover –

  what is its nature?

- Many DMFT computations observe fractional power laws –

  what is their origin?

- The Fermi-liquid scale is very small –

  can it be tuned to zero? what happens then?

Strategy:

- analyze minimal models

- detune them from ‘physical’ regime into ‘clarifying’ regime

Minimal model for Hund metals: 3-band Hubbard-Hund model

Werner, Gull, Troyer, Millis, PRL 2008
de' Medici, Mravlje, Georges, PRL 2011
Yin, Haule, Kotliar, PRB 2012
Stadler, Yin, JvD, Kotliar, Weichsebaum, PRL 2015

3-band Hubbard model with Hund's coupling:

$$\hat{H}_{\mathrm{HHM}} = \sum_i \left(-\mu \hat{N}_i + \hat{H}_{\mathrm{int}}[\hat{d}^\dagger_{im\sigma}]\right) + \sum_{\langle ij\rangle m\sigma} t\, \hat{d}^\dagger_{im\sigma} \hat{d}_{jm\sigma}$$

$$\hat{N}_i = \sum_{m\sigma} \hat{d}^\dagger_{im\sigma} \hat{d}_{im\sigma}$$

energy unit: t = 1

$$\hat{H}_{\mathrm{int}}[\hat{d}^\dagger_{im\sigma}] = \tfrac{3}{4} J_H \hat{N}_i + \tfrac{1}{2}(U - \tfrac{1}{2} J_H)\hat{N}_i(\hat{N}_i - 1) - J_H \hat{\mathbf{S}}_i^2$$

the 3 orbitals are degenerate

$$\hat{S}_i^\alpha = \tfrac{1}{2} \sum_{m\sigma\sigma'} \hat{d}^\dagger_{im\sigma} \sigma^\alpha_{\sigma\sigma'} \hat{d}_{im\sigma} \qquad \mathrm{Tr}[\sigma^\alpha \sigma^\beta] = 2\delta_{\alpha\beta}$$

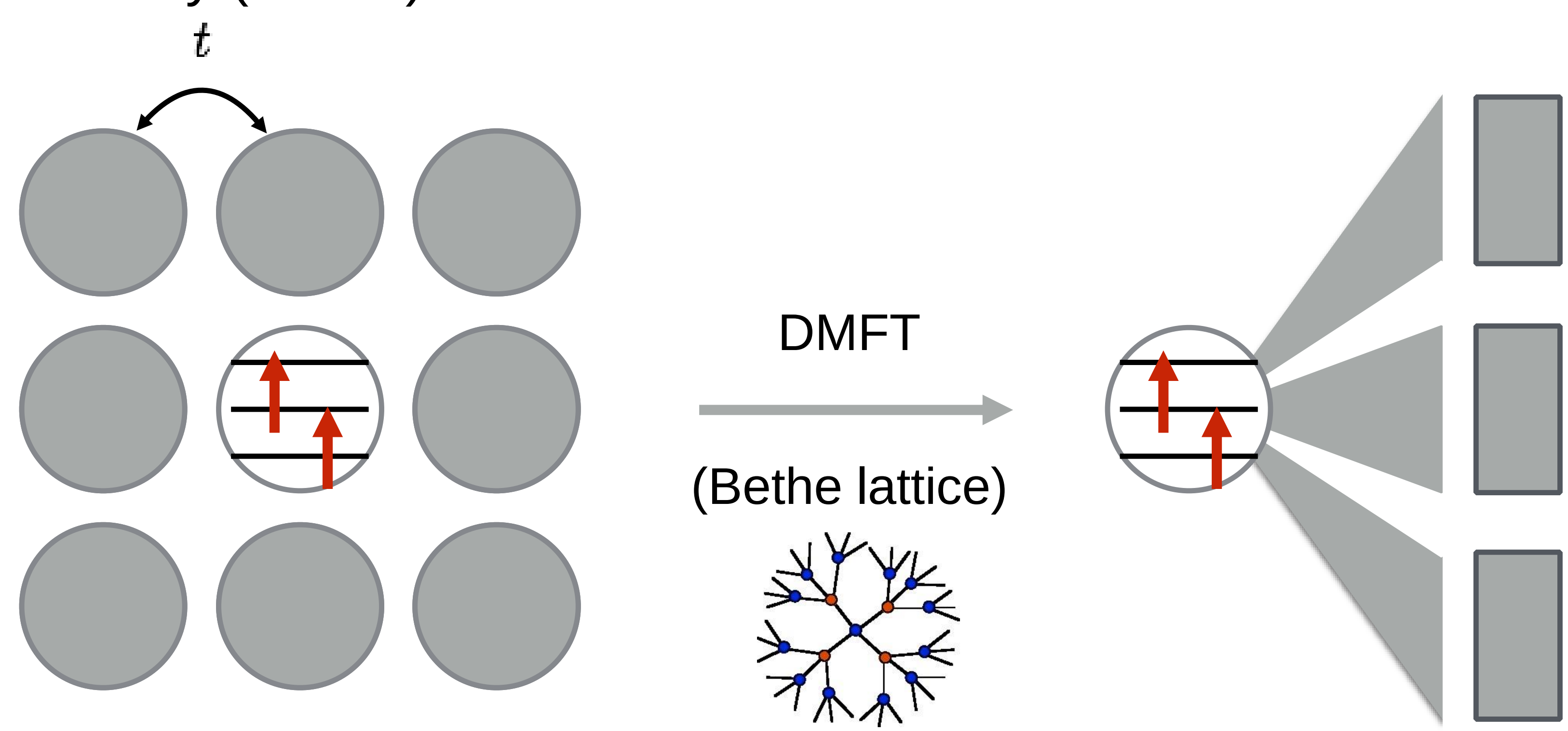
symmetry: $U(1)_{ch} \times SU(2)_{sp} \times SU(3)_{orb}$

Dynamical mean-field theory (DMFT): treat environment as self-consistent bath: $\Sigma(\mathbf{k}, \omega) \simeq \Sigma(\omega)$

$n_d = \langle \hat{N}_i \rangle \simeq 2$

$m = 1, 2, 3$

$\sigma \in \{\uparrow, \downarrow\}$



self-consistent 3-band Anderson-Hund model (3AHM)

treat with NRG

Numerical Renormalization Group (NRG)

Needed: real-frequency “quantum impurity solvers”

that can treat 3-band models at very low temperatures!

+ high spectral resolution at arbitrarily low energies

+ real-frequency data

+ arbitrary temperatures

+ no sign problem

- costs increase exponentially with number of bands

for multi-band models

+ exploiting abelian and non-abelian symmetries:

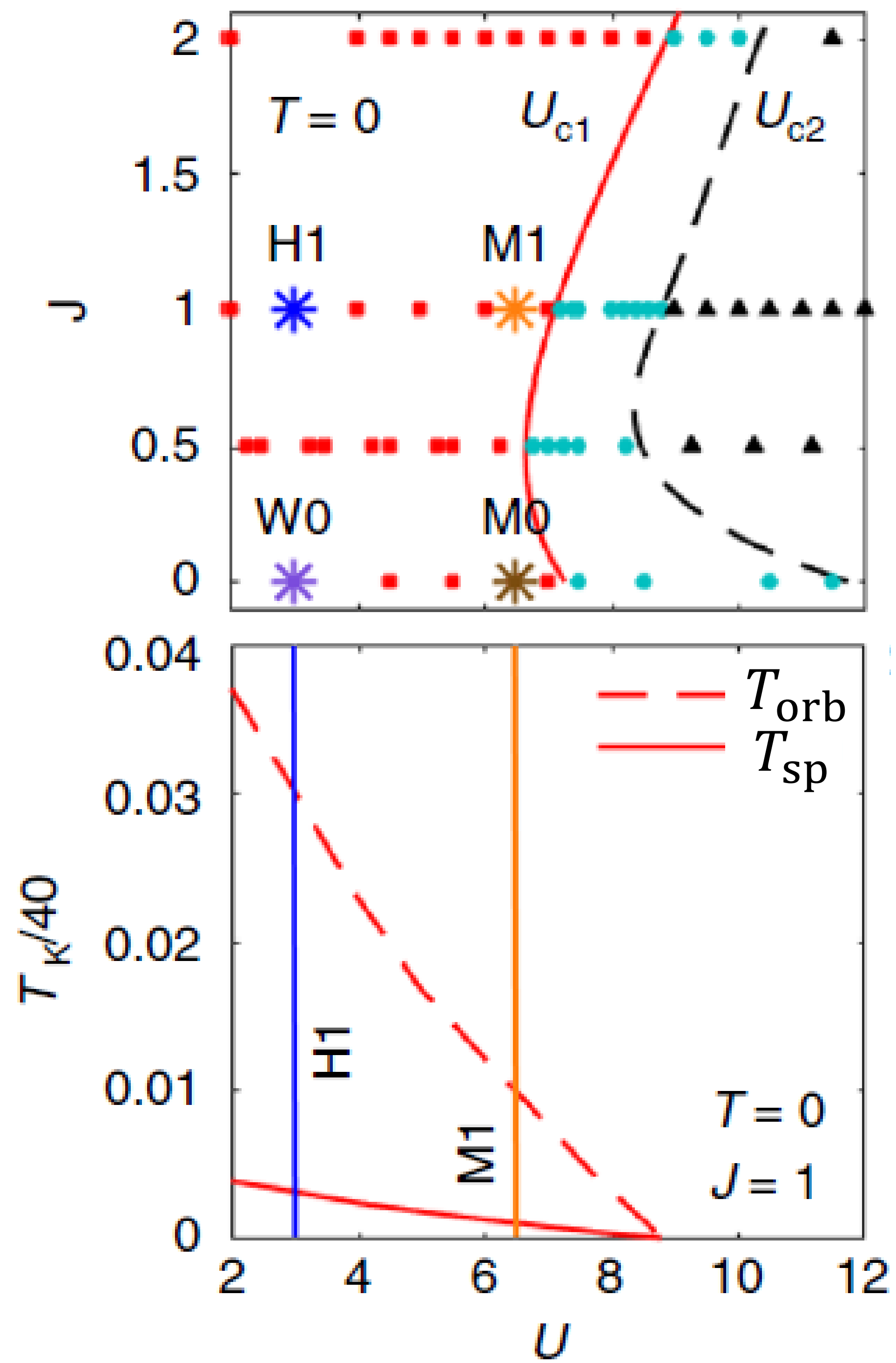
+ interleaved NRG for non-symmetric models

Anders, Schiller, PRL 95 (2005), PRB 74 (2006)
Weichselbaum, Verstraete, Schollwöck, Cirac, von Delft, cond-mat/0504305 (2005); Weichselbaum, PRB,86 (2012)
Peters, Pruschke, Anders, PRB 74 (2006); Weichselbaum, von Delft, PRL 99 (2007)
Zitko, Computer Phys. Comm. 180 (2009); Zitko, Pruschke, PRB 79 (2009)
Toth, Moca, Legeza, Zarand, PRB 78 (2008); Weichselbaum, Ann. Phys. 327 (2012)
Mitchell, Galpin, Wilson-Fletcher, Logan, Bulla, PRB 89 (2014)
Stadler, Mitchell, von Delft, Weichselbaum, PRB, 93 (2016)
Lee, Weichselbaum, PRB 94 (2016).

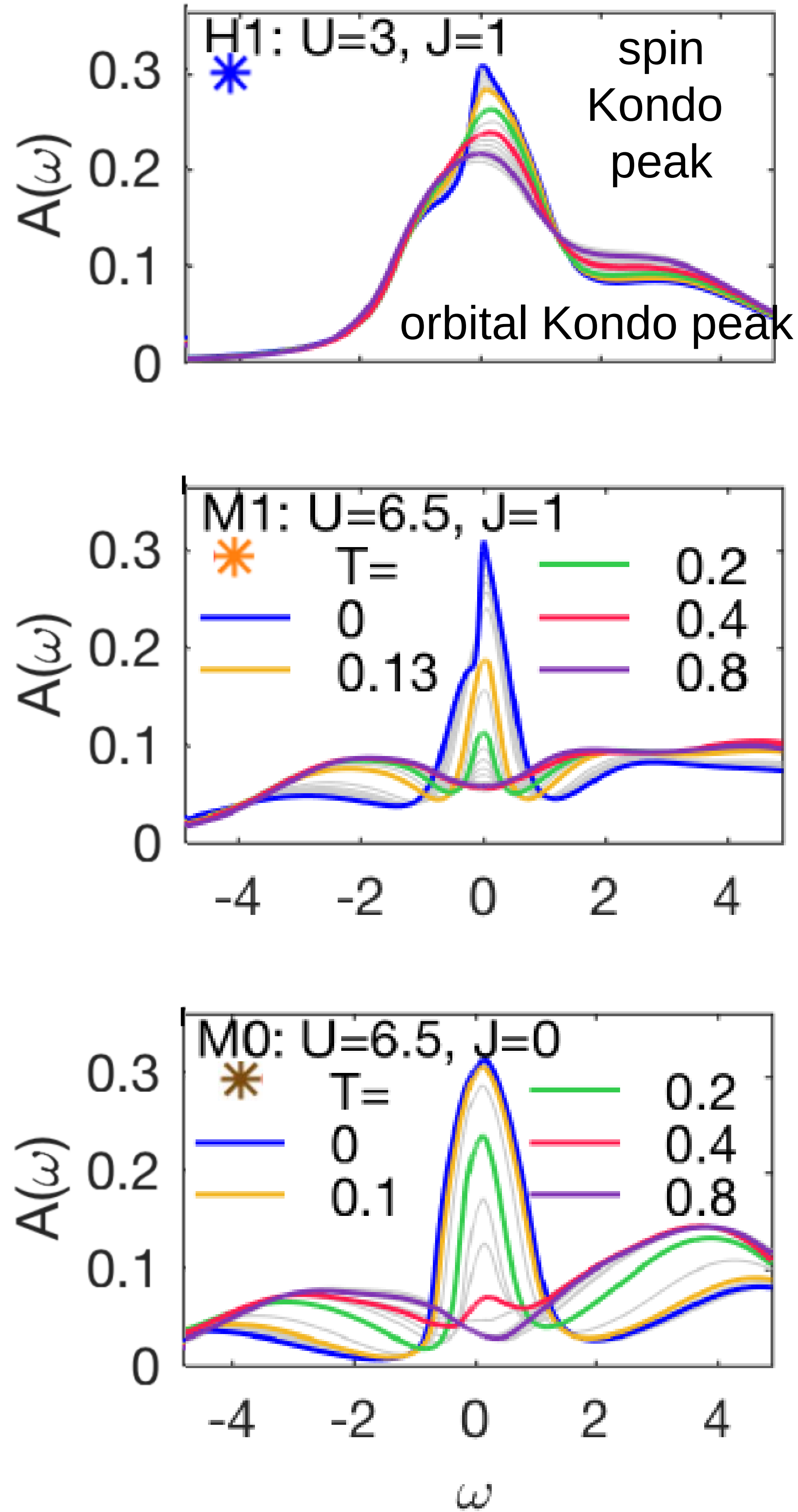
Andreas Weichselbaum

U, J phase diagram at T=0

Deng, Stadler, Haule, Weichselbaum, von Delft, Kotliar, Nature Comm. 2019



Spectral functions at finite T



no Mott transition
two-tier peak shape
needle: spin Kondo peak
hump: orbital Kondo peak
spin-orbital separation

“Hund system”
(e.g. Sr_2RuO_4)

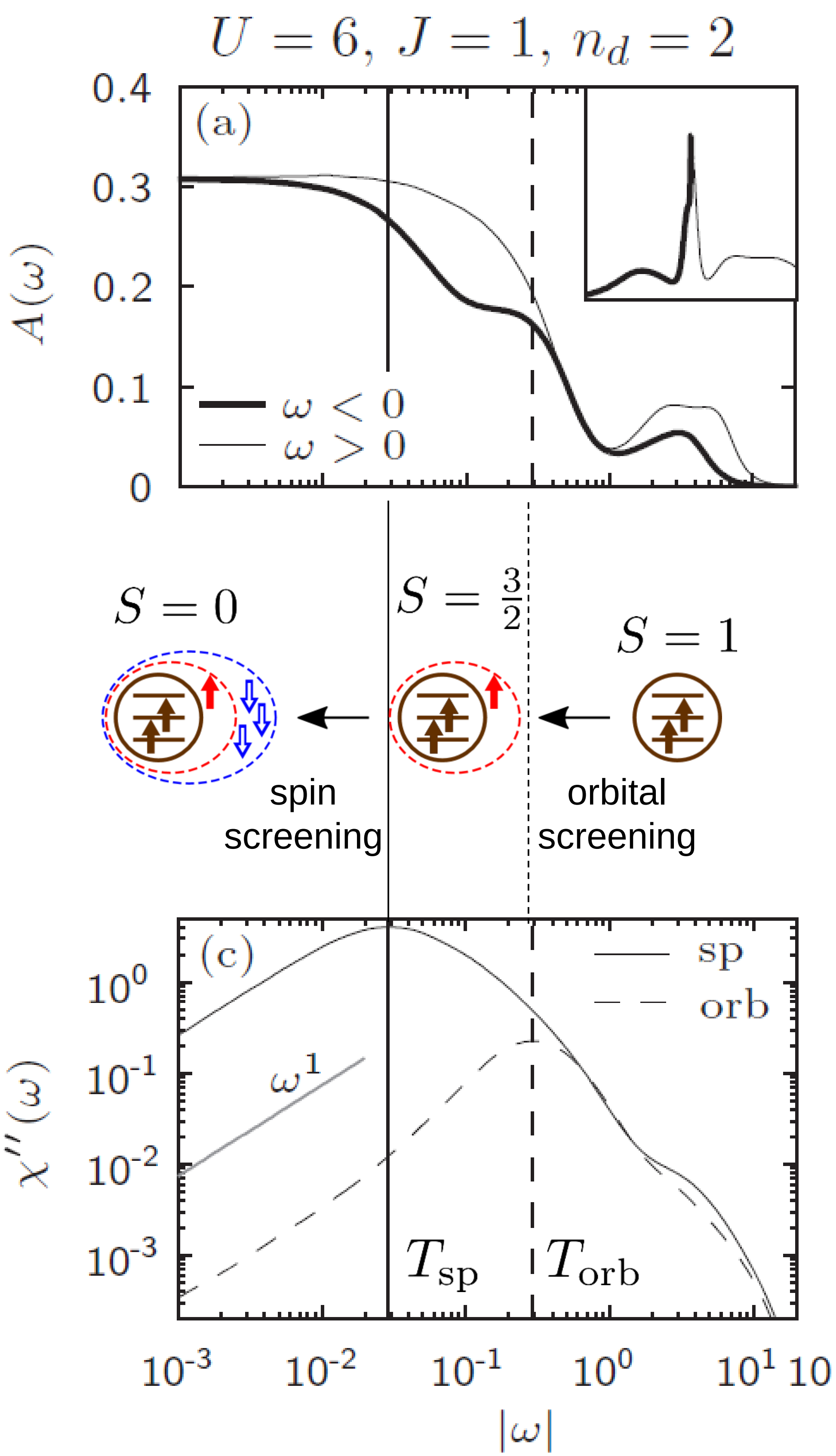
strongly correlations
Mott transition
Hund substructure

“Mott system with
spin-orbital separation”
(e.g. V_2O_3)

strong correlatons
Mott transition

“Mott system”

Spin-orbital separation



Stadler, et al. PRL 2015

Spin and orbital susceptibilities:

$$\chi_{\mathrm{sp}}(\omega) = \sum_{\alpha} \langle \hat{S}^{\alpha} \| \hat{S}^{\alpha} \rangle_{\omega} \qquad \hat{S}^{\alpha}_{i} = \tfrac{1}{2} \sum_{m\sigma\sigma'} \hat{d}^{\dagger}_{im\sigma} \sigma^{\alpha}_{\sigma\sigma'} \hat{d}_{im\sigma} \qquad \mathrm{Tr}[\sigma^{\alpha}\sigma^{\beta}] = 2\delta_{\alpha\beta}$$

$$\chi_{\mathrm{orb}}(\omega) = \sum_{a} \langle \hat{T}^{a} \| \hat{T}^{a} \rangle_{\omega} \qquad T^{a} = \tfrac{1}{2} \sum_{\sigma m m'} \hat{d}^{\dagger}_{m\sigma} \tau^{a}_{mm'} \hat{d}_{m'\sigma} \qquad \mathrm{Tr}[\tau^{a}\tau^{b}] = 2\delta_{ab}$$

- maximum of χ''_{sp} defines T_{sp}
- maximum of χ''_{orb} defines T_{orb}
- $T_{\mathrm{sp}} \ll T_{\mathrm{orb}} \quad \Rightarrow$ “spin-orbital separation”:

- as temperature is decreased, first orbital degrees of freedom get screened, then spin degrees of freedom [anticipated by Okada & Yosida, 1973]
- $T_{\mathrm{sp}} < \omega < T_{\mathrm{orb}}$: incoherent intermediate regime
- dominated by slow fluctuations of large local moments (orbital degrees of freedom are already screened)
- alternative nomenclature: “spin freezing”

Werner, Gull, Troyer, Millis, PRL 2008.

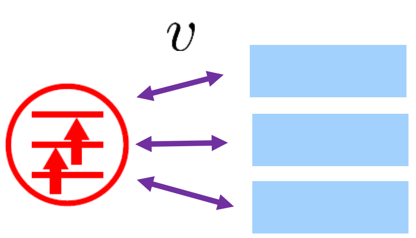
spin dynamics seems to slow down
(since spin screening scale T_{sp} is very small)

Can we uncover NFL behavior by suppressing T_{sp} ?

Strategy: don't insist on DMFT self-consistency. Instead:

- consider 3-orbital Anderson-Hund (3oAH) model

  without self-consistency, $H_{3\mathrm{oAH}}(U, J_{\mathrm{H}}, \Gamma)$



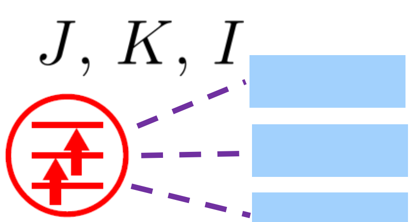
- 3oAH model exhibits orbital overscreening (NFL regime),

  but has $T_{sp} \neq 0$, Fermi-liquid ground state.

- 3oAH model can be mapped onto a 3-band spin-orbital Kondo (3soK) model,

  $H_{3\mathrm{soK}}(J_0, K_0, I_0)$

  Aron, Kotliar, PRL (2015), Horvat, Zitko, Mravlje PRB 2016, arXiv:1907.07100



- treat its exchange couplings as independent parameters

- tune them such that $T_{\mathrm{sp}} \to 0$

- then a large NFL regime opens up between $0 \simeq T_{\mathrm{sp}} < \omega \ll T_{\mathrm{orb}}$

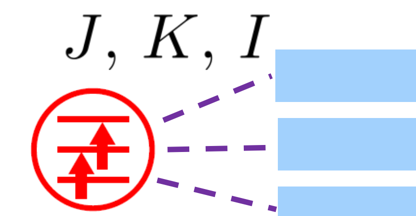
- analyze this NFL regime using NRG and conformal field theory (CFT)

Affleck, Ludwig, 1990-1994

3-channel spin-orbital Kondo model: weak-coupling analysis

Aron, Kotliar, PRL (2015)

$$H_{3\mathrm{soK}} = \sum_{k\sigma} \sum_{m=1,2,3} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + J_0\, \mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}} + K_0\, \mathbf{T}\cdot\mathbf{J}_{\mathrm{orb}} + I_0\, \mathbf{S}\cdot\mathbf{J}_{\text{sp-orb}}\cdot\mathbf{T}.$$



$$(S,\lambda)_{\mathrm{imp}} = (1, \square)$$

$$J^\alpha_{\mathrm{sp}} = \sum_{kk'} c^\dagger_{k\sigma m} \sigma^\alpha_{\sigma\sigma'} c_{k'\sigma' m} \qquad J^a_{\mathrm{orb}} = \sum_{kk'} c^\dagger_{k\sigma m} \tau^a_{mm'} c_{k'\sigma m'} \qquad J^a_{\text{sp-orb}} = \sum_{kk'} c^\dagger_{k\sigma m} \sigma^\alpha_{\sigma\sigma'} \tau^a_{mm'} c_{k'\sigma' m'}$$

spin current — orbital current — mixed current

symmetry: U(1) x SU(2)$_{\mathrm{sp}}$ x SU(3)$_{\mathrm{orb}}$

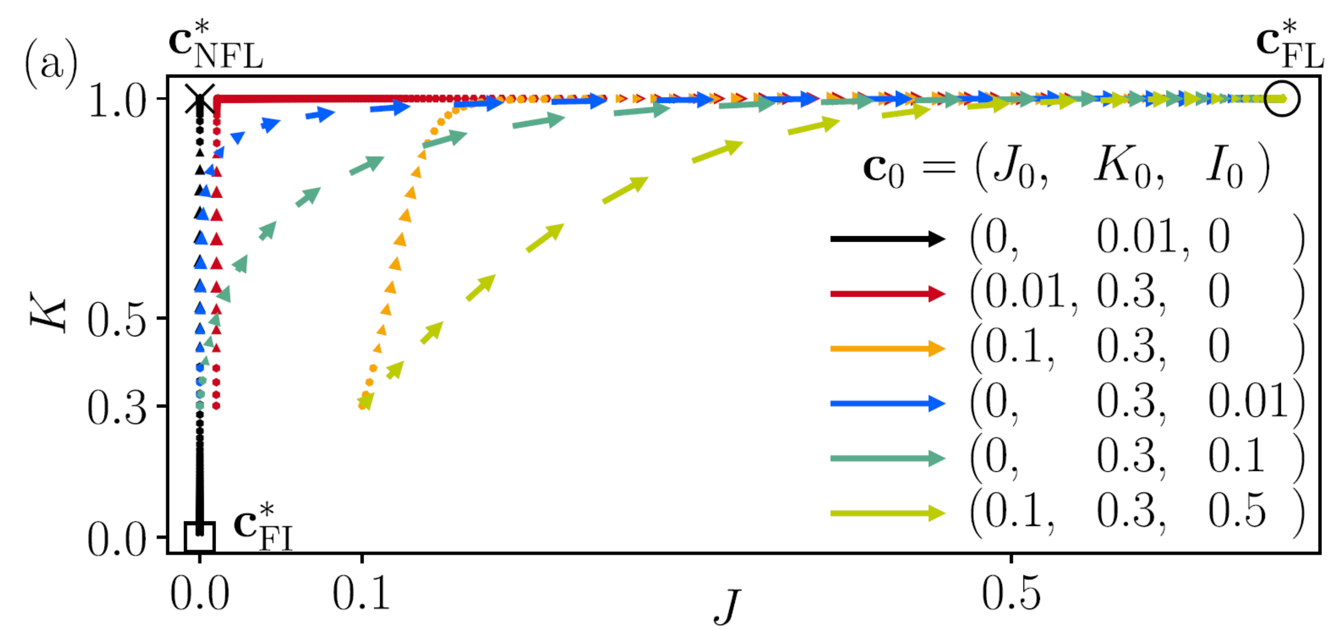
NFL fixed point is reached for

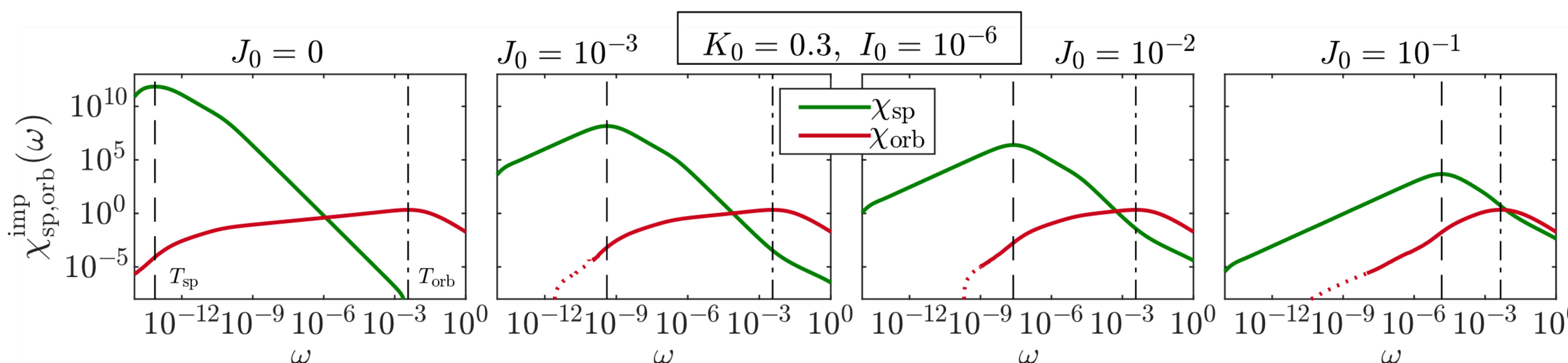
$$I_0 = 0,\ K_0 > 0,\ I_0 = 0$$

Relevant perturbations: $J_0 \neq 0,\ I_0 \neq 0$

drive system to FL fixed point.

weak-coupling RG flow, projected to J-K plane

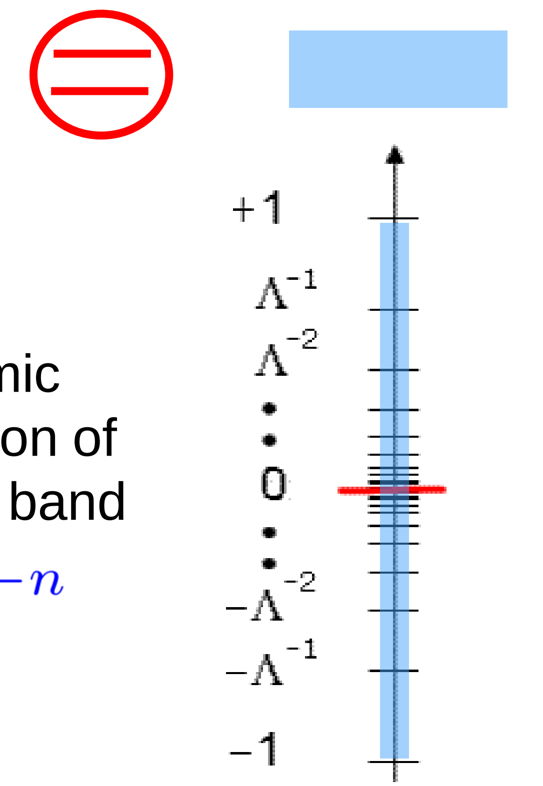




NRG primer: logarithmic discretization, Wilson chain

[Wilson, 1975]

$$H = H_0(d^\dagger, \underset{\substack{|||\\ f_0}}{d}) + \sum_k \varepsilon_k c_k^\dagger c_k + d^\dagger \underset{f_1}{\underbrace{v \sum_k c_k}} + v \sum_k c_k^\dagger d$$



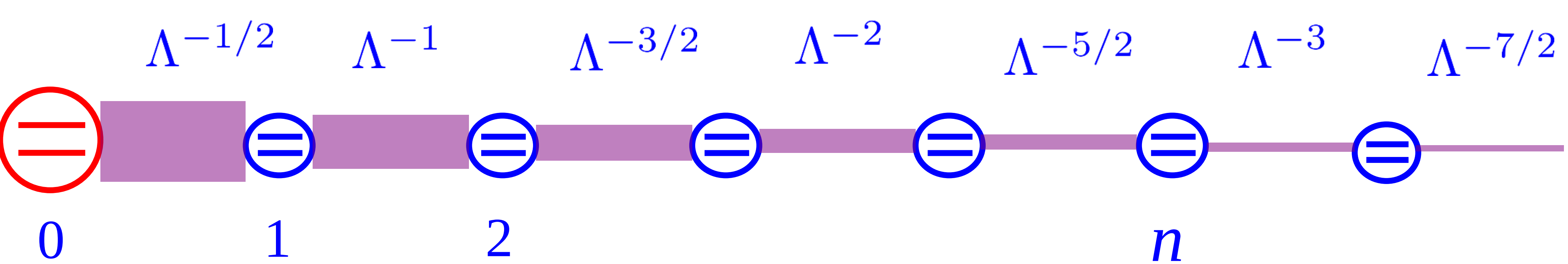
logarithmic discretization of conduction band

$$\xi_n \sim \Lambda^{-n}$$

$$\Lambda > 1$$

$$H = H_0(f_0^\dagger, f_0) + \sum_{n=1}^{\infty} t_n (f_n^\dagger f_{n-1} + f_{n-1}^\dagger f_n)$$

$$t_n \sim \Lambda^{-n/2}$$



Wilson chain

Diagonalize chain iteratively, discard high-energy states

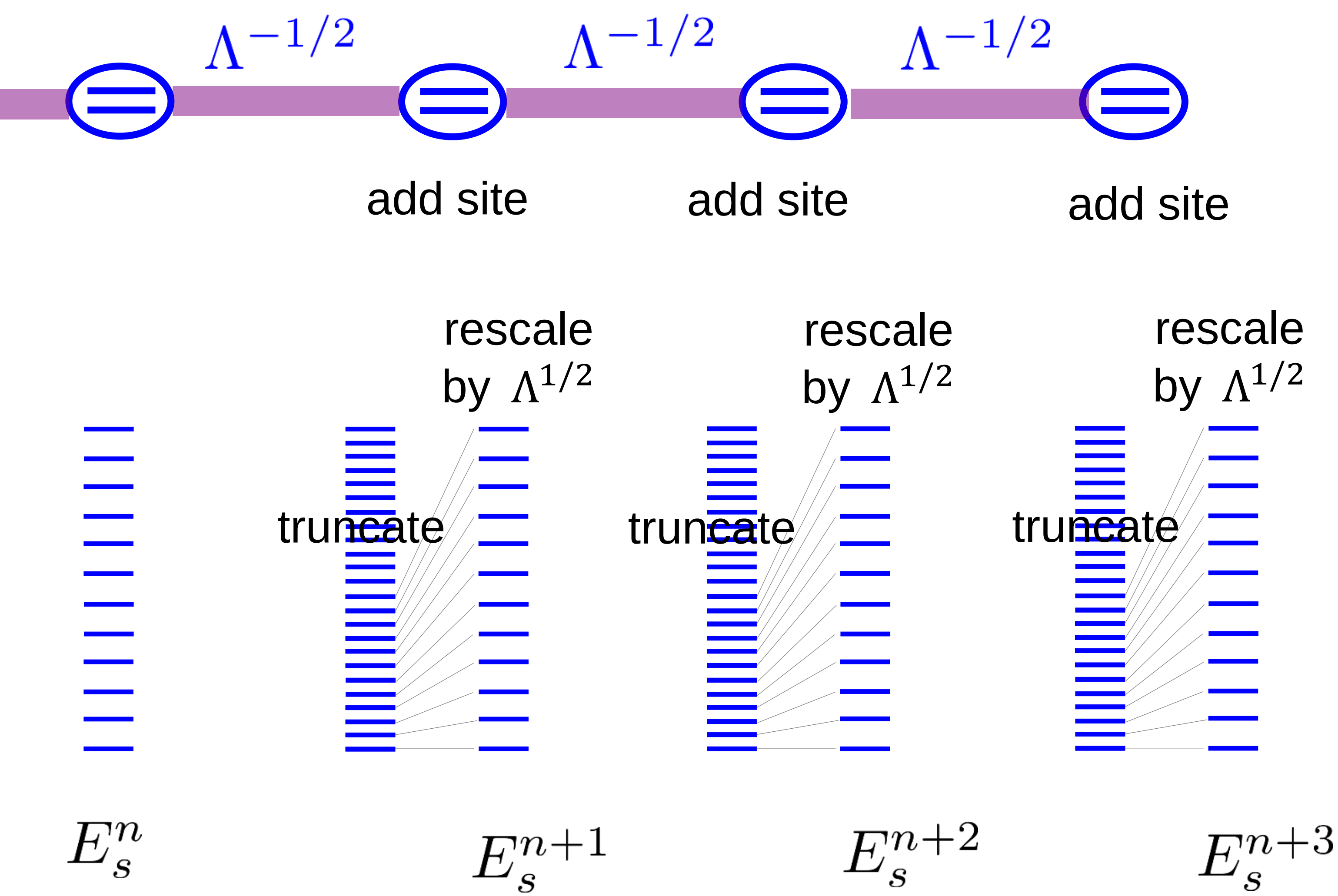
NRG primer: energy level flow diagram

[Wilson, 1975]

level splitting at iteration *n* : $\omega_n \simeq \Lambda^{-n/2} \sim \frac{1}{\text{effective system size}}$

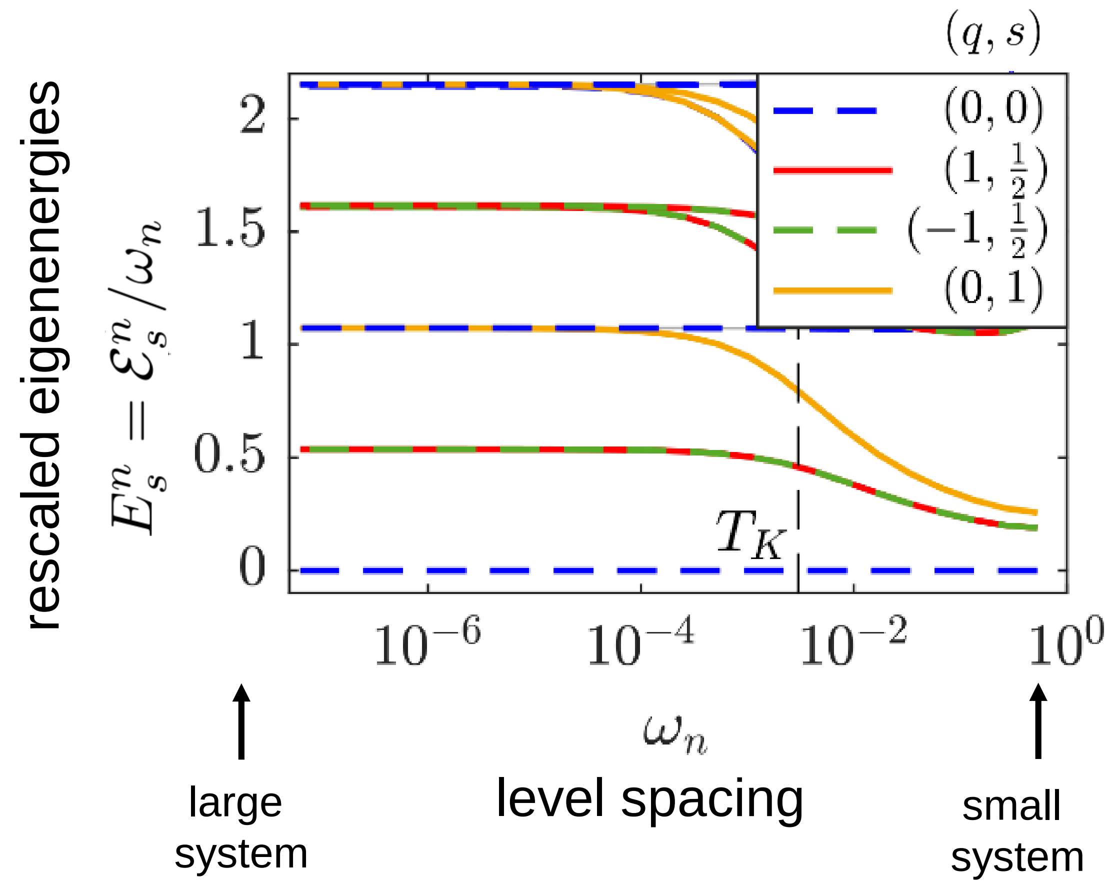
to maintain level splitting $\mathcal{O}(1)$, rescale eigenenergies: $E_s^n \equiv \mathcal{E}_s^n / \omega_n = \Lambda^{n/2} E_s^n$

in rescaled units, each new site perturbs previous spectrum by $\sim \Lambda^{-1/2}$



energy level flow diagram

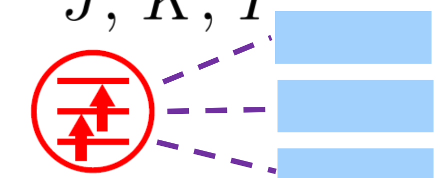
for 1-channel Kondo model



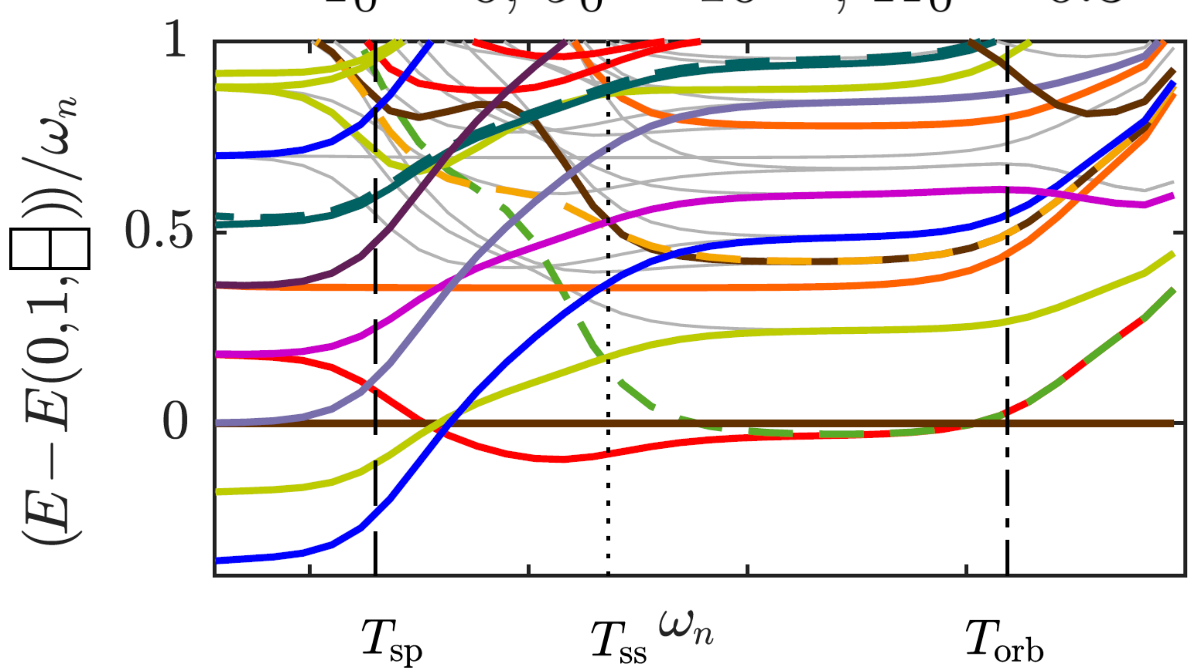
3-channel spin-orbital Kondo model: NRG , CFT

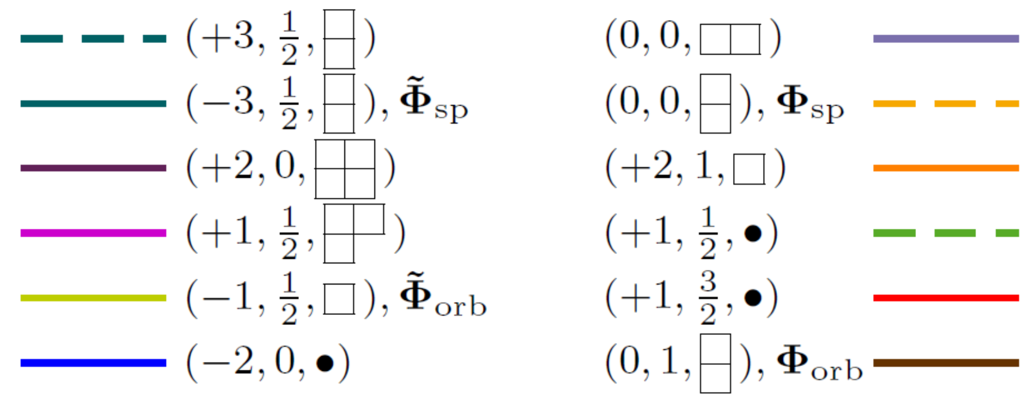
Walter, Stadler, Lee, Wang, Kotliar, Weichselbaum, von Delft, Koliar, arXiv:1908.04362

$$H_{\mathrm{3soK}} = \sum_{k\sigma} \sum_{m=1,2,3} \varepsilon_k c^\dagger_{k\sigma m} c_{k\sigma m} + J_0\, \mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}} + K_0\, \mathbf{T}\cdot\mathbf{J}_{\mathrm{orb}} + I_0\, \mathbf{S}\cdot\mathbf{J}_{\text{sp-orb}}\cdot\mathbf{T}.$$



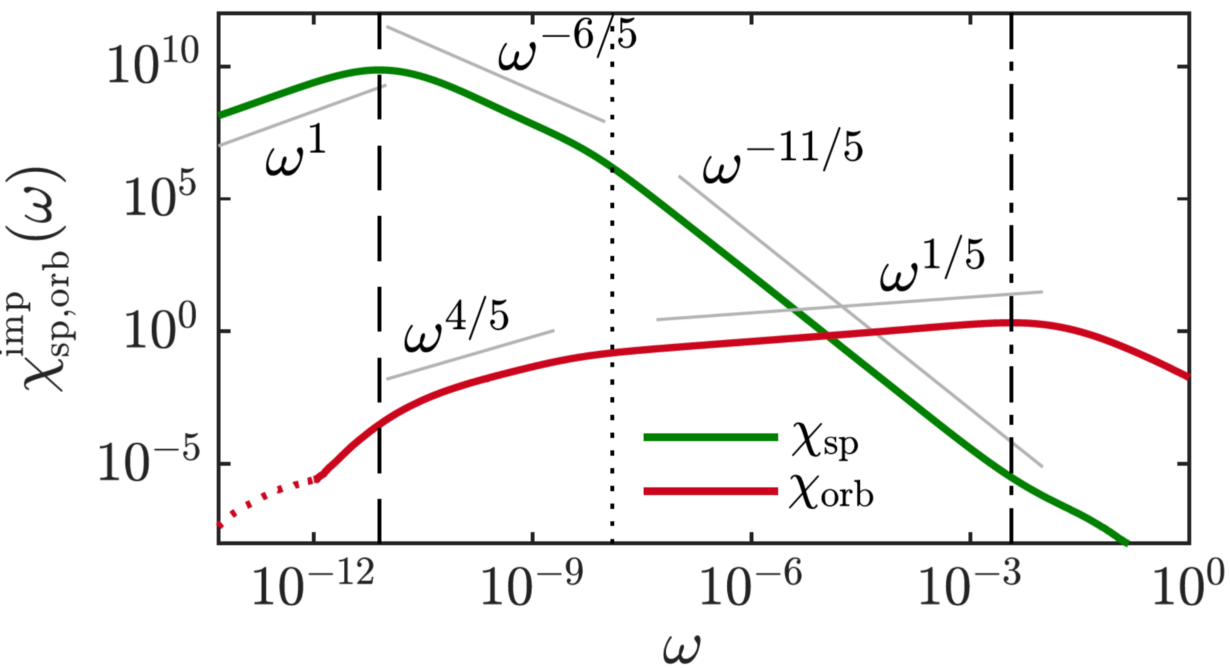
$I_0 = 0,\ J_0 = 10^{-4},\ K_0 = 0.3$





Boundary operator scaling dimensions (from CFT)

$$\Delta_{\mathrm{sp}} = \frac{2}{5},\ \Delta_{\mathrm{orb}} = \frac{3}{5}, \qquad \widetilde{\Delta}_{\mathrm{spin}} = \widetilde{\Delta}_{\mathrm{orb}} = \frac{9}{10}$$



NFL power laws can be explained using CFT [in spirit of Affleck & Ludwig, 1990-1992, using U(1) x $SU(2)_3$ x $SU(3)_2$ Sugawara construction]

For $\omega > T_{\mathrm{ss}}$, effect of J_0 is very small, and we have:

$$\mathbf{J}_{\mathrm{orb}} \mapsto \Phi_{\mathrm{orb}}, \quad \mathbf{T} \mapsto \Phi_{\mathrm{orb}}, \qquad \mathbf{J}_{\mathrm{sp}} \mapsto \Phi_{\mathrm{sp}}, \qquad \mathbf{S} \mapsto \mathbf{S}$$

$$\chi^{\mathrm{imp}}_{\mathrm{orb}} \sim \langle \mathbf{T}\cdot\mathbf{T}\rangle_\omega \mapsto \langle \mathbf{\Phi}_{\mathrm{orb}}\cdot\mathbf{\Phi}_{\mathrm{orb}}\rangle_\omega \sim \omega^{2\Delta_{\mathrm{orb}}-1} \simeq \omega^{1/5}$$

$$\chi^{\mathrm{imp}}_{\mathrm{sp}} \mapsto \langle \mathbf{S}\cdot\mathbf{S}\big(\textstyle\int dt\, \mathbf{S}\cdot\mathbf{\Phi}_{\mathrm{sp}}\big)^2\rangle_\omega \sim \omega^{2\Delta_{\mathrm{sp}}-3} \simeq \omega^{-11/5}$$

For $T_{\mathrm{sp}} < \omega < T_{\mathrm{ss}}$, J_0 reshuffles levels and assignments:

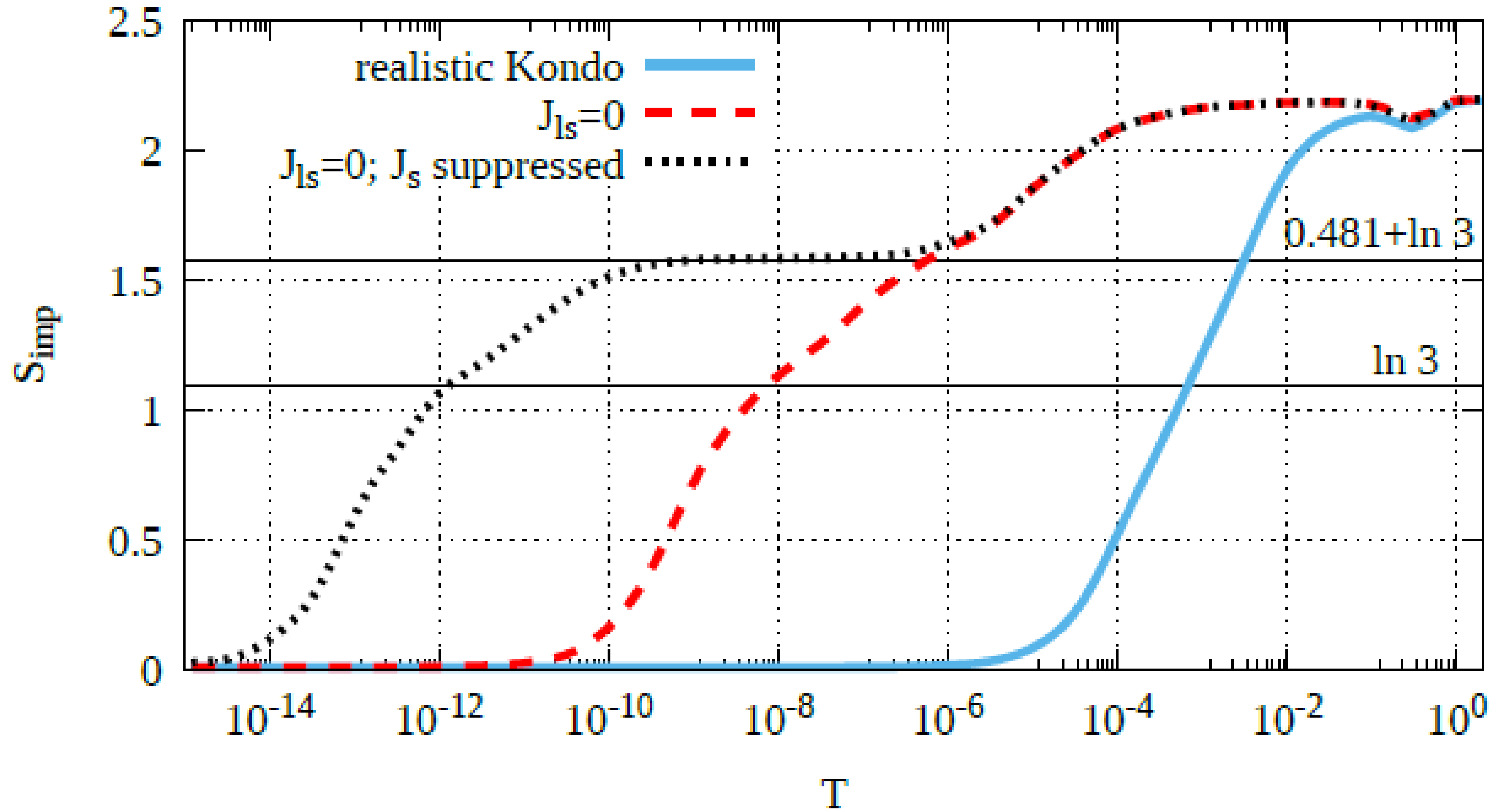
$$\mathbf{J}_{\mathrm{orb}} \mapsto \widetilde{\Phi}_{\mathrm{orb}}, \quad \mathbf{T} \mapsto \widetilde{\Phi}_{\mathrm{orb}}, \quad \mathbf{J}_{\mathrm{sp}} \mapsto \widetilde{\Phi}_{\mathrm{sp}}, \quad \mathbf{S} \mapsto \mathbf{S} + \widetilde{\Phi}_{\mathrm{sp}}$$

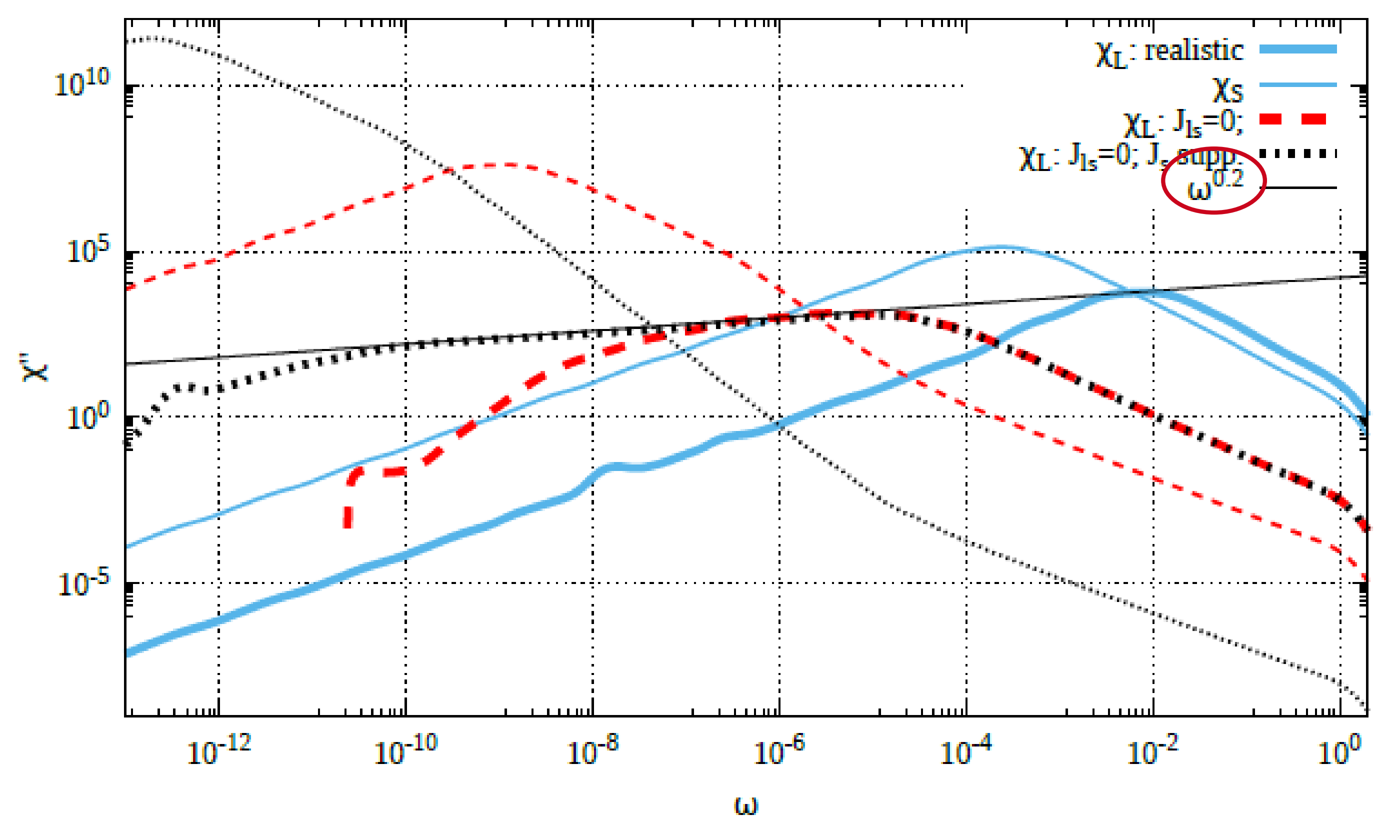
$$\chi^{\mathrm{imp}}_{\mathrm{orb}} \sim \langle \mathbf{T}\cdot\mathbf{T}\rangle_\omega \mapsto \langle \widetilde{\mathbf{\Phi}}_{\mathrm{orb}}\cdot\widetilde{\mathbf{\Phi}}_{\mathrm{orb}}\rangle_\omega \sim \omega^{2\widetilde{\Delta}_{\mathrm{orb}}-1} \simeq \omega^{4/5}$$

$$\chi^{\mathrm{imp}}_{\mathrm{sp}} \mapsto \langle \mathbf{S}\cdot\mathbf{S}\big(\textstyle\int dt\, \mathbf{S}\cdot\widetilde{\mathbf{\Phi}}_{\mathrm{sp}}\big)^2\rangle_\omega \sim \omega^{2\widetilde{\Delta}_{\mathrm{sp}}-3} \simeq \omega^{-6/5}$$

Impurity entropy

Horvat, Zitko, Mravlje, arXiv:1907.07100





Global phase diagram of spin-orbital Kondo model

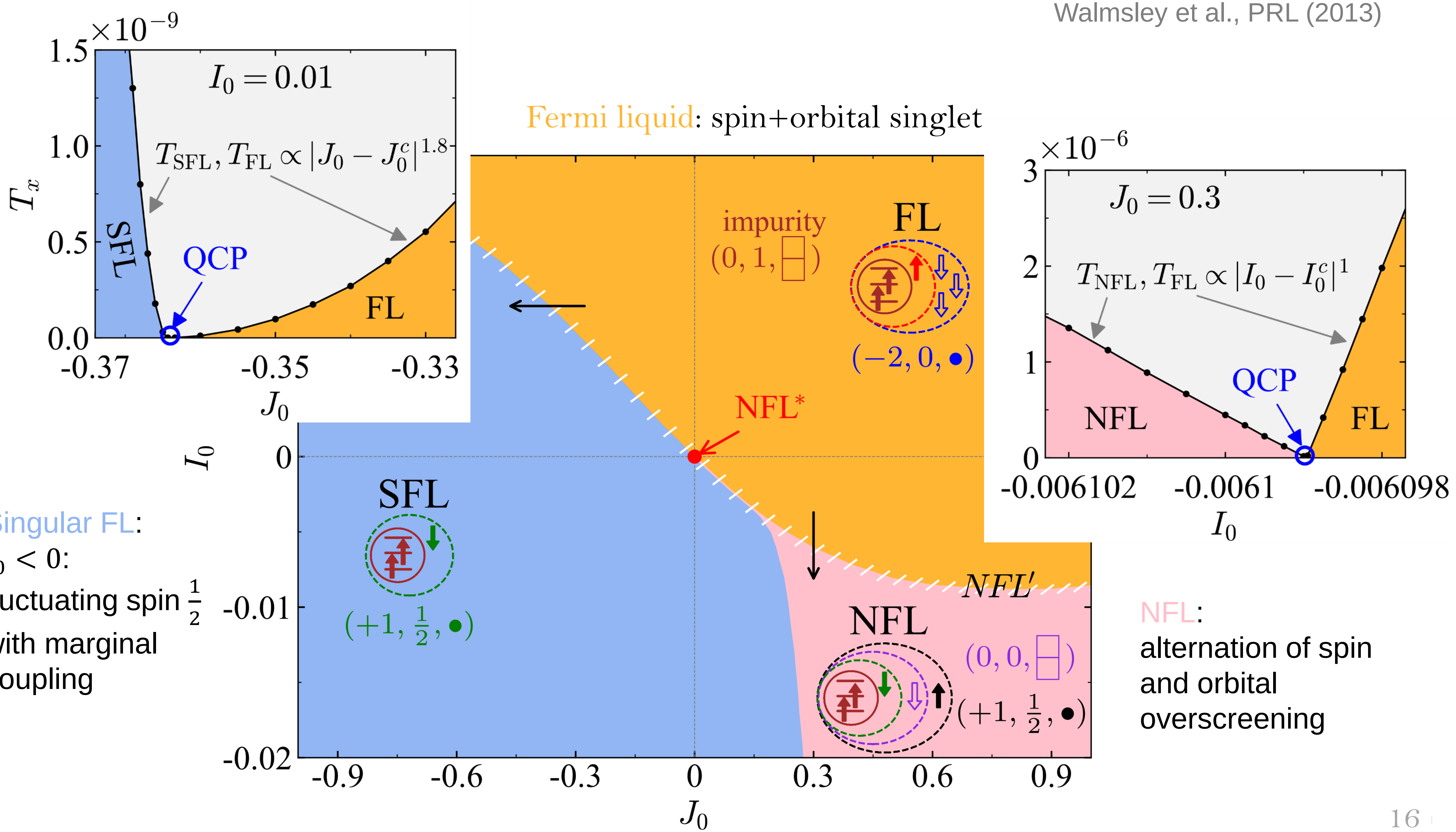
3-channel spin-orbital Kondo model:

$$H_{\mathrm{int}} = J_0\, \mathbf{S}\cdot\mathbf{J}_{\mathrm{sp}} + K_0\, \mathbf{T}\cdot\mathbf{J}_{\mathrm{orb}} + I_0\, \mathbf{S}\cdot\mathbf{J}_{\mathrm{sp-orb}}\cdot\mathbf{T}$$

QCP's: power-law suppression of FL coherence scale

→ large mass enhancement e.g. in $\mathrm{BaFe_2(As_{1-x}P_x)_2}$

Walmsley et al., PRL (2013)



Singular FL:

$J_0 < 0$:

fluctuating spin $\frac{1}{2}$ with marginal coupling

NFL:

alternation of spin and orbital overscreening

Summary

- Minimal 3-band models for Hund metals show spin-orbital separation,
- involving orbital overscreening, leading to non-Fermi-liquid behavior.
- In Anderson-Hund model, the actual NFL fixed point (J=K=0) is not reachable;
- but its properties can be studied using the Kondo-Hund model, where J, K, I can be tuned independently.
- Beautiful NFL power laws were found by NRG and explained by CFT.

Outlook

NRG+DMFT is a highly competitive, powerful, real-frequency, low-energy method !!

- No orbital degeneracy: orbital selective Mott transition Kugler, Lee, Weichselbaum, Kotliar, von Delft, PRB 2019
- Real materials (feasible for three-band models) Kugler, Zingl, Strand, Lee, von Delft, Georges PRL 2019
- Local four-point functions Seung-Sup Lee (poster!)
- Main limitation: currently feasible for at most three spin-full bands