

LOCAL METAL-INSULATOR TRANSITION IN AN EXTENDED ANDERSON IMPURITY MODEL

JRF-to-SRF Upgradation Presentation

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Summary of Work

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Completed Projects

- ✓ Unveiling the Kondo cloud: Unitary renormalization-group study of the Kondo model

Phys. Rev. B 105, 085119, arXiv:2111.10580v3

A. Mukherjee, Abhirup Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, and S. Lal

- ✓ Frustration shapes multi-channel Kondo physics: A star graph perspective

under review at PRB, arXiv:2205.00790

S. Patra, Abhirup Mukherjee, A. Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, S. Lal

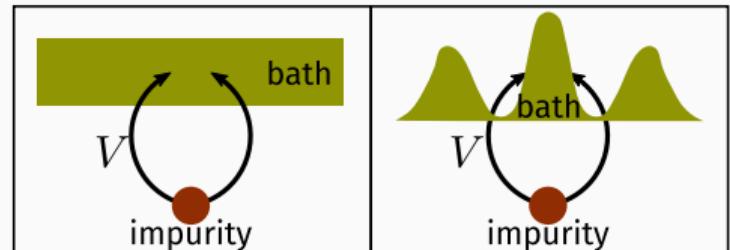
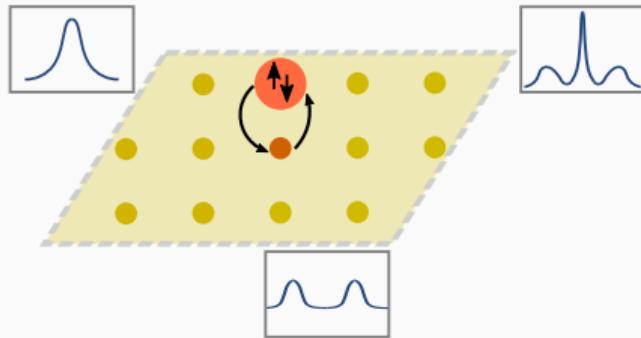
Ongoing Projects

- ✓ Metal-insulator transition in an extended Anderson impurity model (*manuscript in preparation*)
-

- ✓ Holography and topology of entanglement scaling in free fermions (*manuscript in preparation*)

- ✓ URG-based auxiliary model approach to correlated systems (*ongoing*)

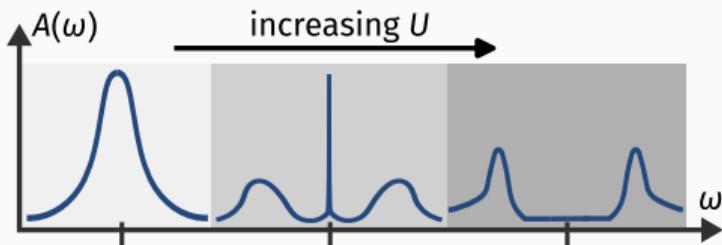
Local MIT in an extended Anderson impurity model



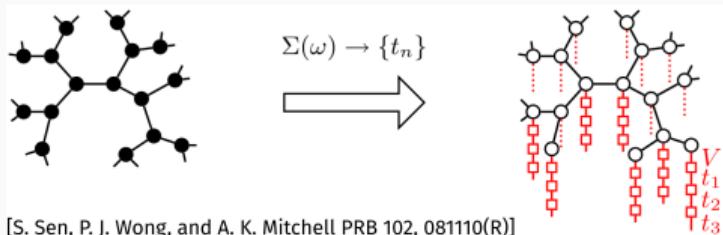
Introducing the extended Anderson impurity model

DMFT on the Bethe lattice: Exact in $d = \infty$

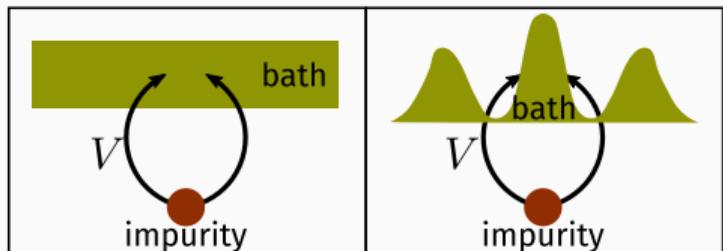
- ✓ shows **metal-insulator transition** on the Bethe lattice with ∞ coordination number



- ✓ Conduction bath obtained by imposing self-consistency shows **non-trivial correlations**

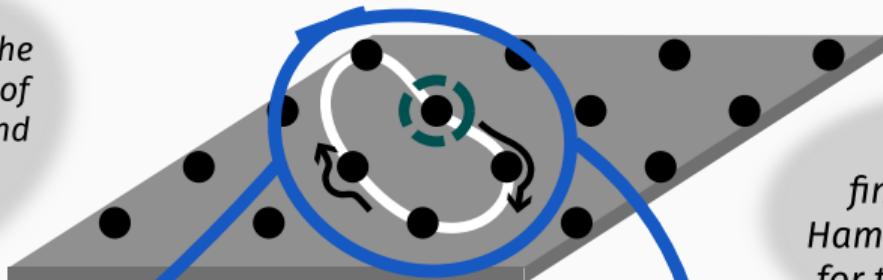
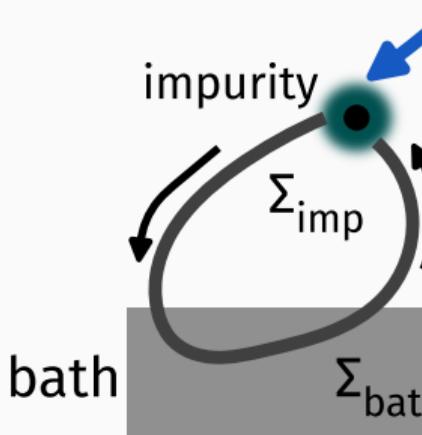


- ✓ Spectral function develops three peaks and then **gaps out**

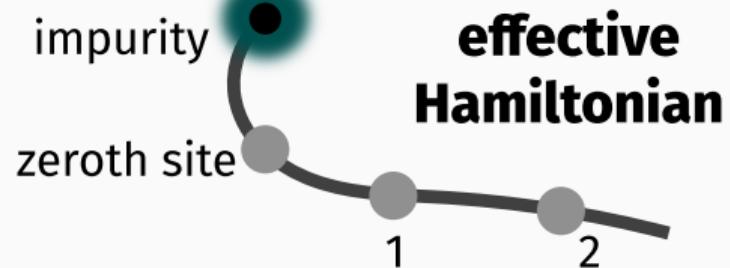


DMFT on the Bethe lattice: Exact in $d = \infty$

DMFT represents excursions from a site into the correlated bath in the form of self-energies for the bath and the impurity. This results in a three-peak DOS of the bath.



DMFT



Our Goal:

finding an effective Hamiltonian description for the Σ that gives rise to the MIT.

DMFT on the Bethe lattice: Exact in $d = \infty$

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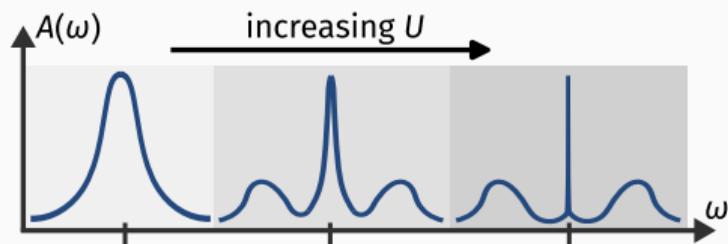
Our Goal:
finding an effective
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Similar approach was adopted by Si & Kotliar for an extended Hubbard model.

Introducing the extended Anderson impurity model

Standard Anderson impurity model

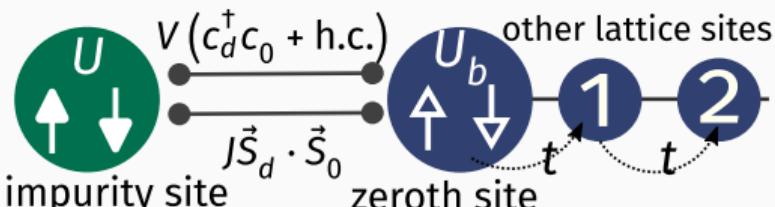
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



Gap in spectral function requires additional physics!

Extended Anderson impurity model

- ✓ impurity-bath spin correlation: J
- ✓ bath zeroth site local correlation: U_b



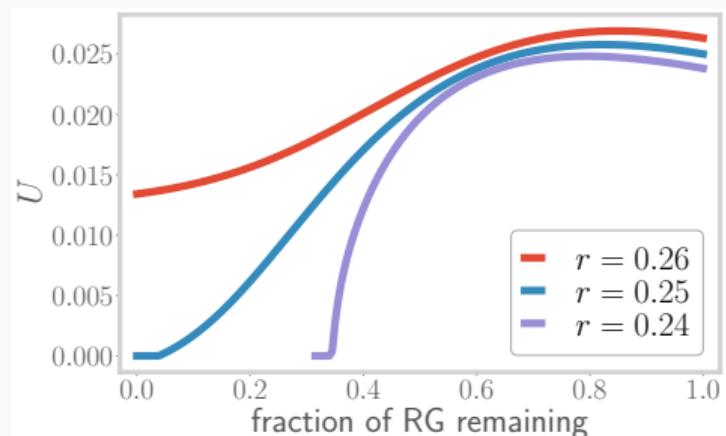
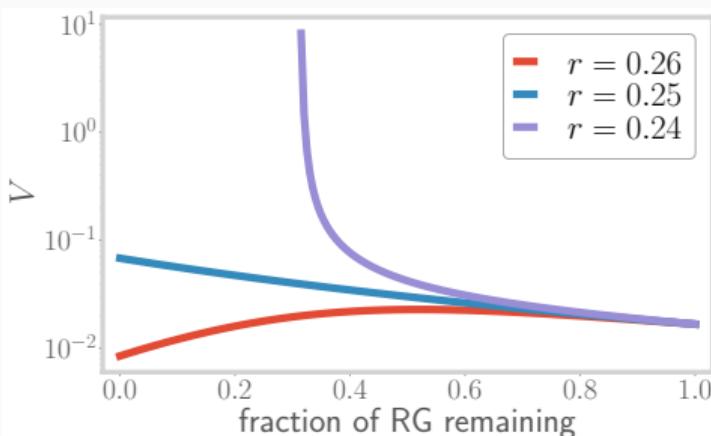
Phase Diagram & Ground-States

Nature of RG flows

- ✓ URG Equations reveal **critical** point at $r = -U_b/J = 1/4$:
- ✓ RG equation for most dominant coupling J :

$$\Delta J = J(J + 4U_b)n(D) \frac{1}{\omega - D/2 + U_b/2 + J/4}$$

- ✓ allows averting strong-coupling behaviour
- ✓ U_b always marginal

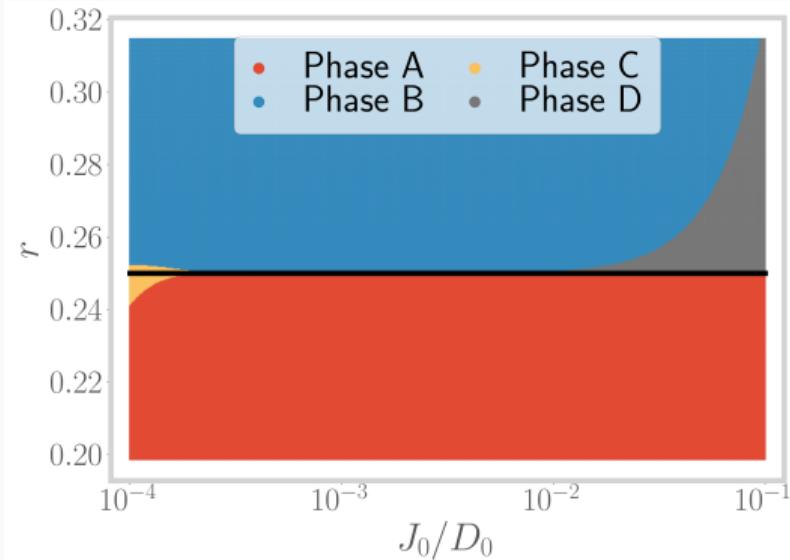


RG Phase Diagram

✓ blue phase $\rightarrow U_b < -J/4$: V, J are **irrelevant** \rightarrow local moment flows

✓ yellow phase: $J \ll D_0$: involves **V, U, U_b**
vanishes for large systems

✓ gray phase: $J \sim D_0$: **all** couplings irrelevant
vanishes for large systems



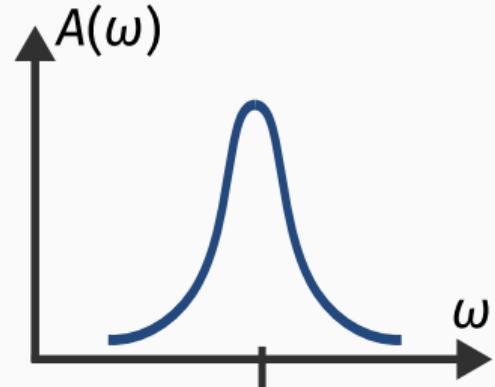
✓ red phase $\rightarrow U_b > -J/4$: V, J are **relevant** \rightarrow strong-coupling flows

Low-energy effective Hamiltonians and ground-states

Regime 1: $|U_b| < J/4$

- ✓ J relevant,
- ✓ V subdominant,
- ✓ U irrelevant

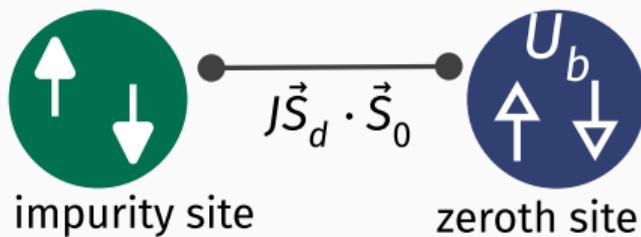
$$H = J\vec{S}_d \cdot \vec{S}_0 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Low-energy effective Hamiltonians and ground-states

Regime 1: $|U_b| < J/4$

Zero-bandwidth limit



$$H = J\vec{S}_d \cdot \vec{S}_0 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2$$

- ✓ two-spin Heisenberg, attractive zeroth site
- ✓ **singlet** ground state

$$|\Psi\rangle_{GS} = \frac{1}{\sqrt{2}} [|\uparrow_d \downarrow_0\rangle - |\downarrow_d \uparrow_0\rangle]$$

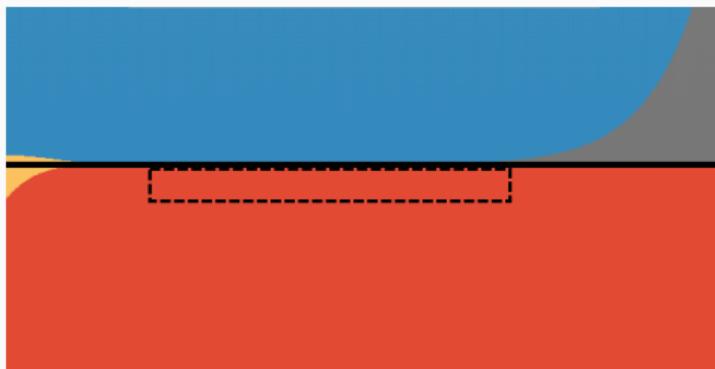
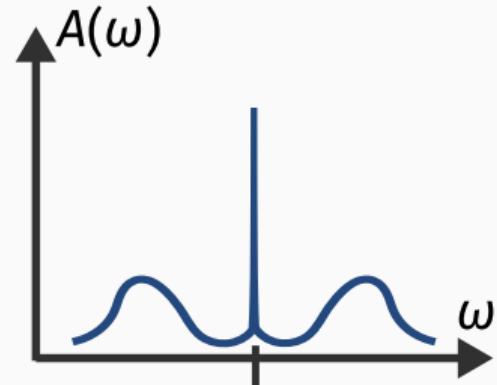


Low-energy effective Hamiltonians and ground-states

Regime 2: $|U_b| \sim J/4$

- ✓ J relevant,
- ✓ V relevant,
- ✓ U irrelevant

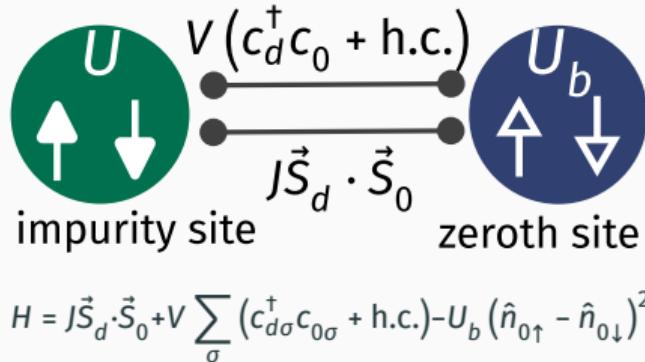
$$H = J\vec{S}_d \cdot \vec{S}_0 + V \sum_{\sigma} (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Low-energy effective Hamiltonians and ground-states

Regime 2: $|U_b| \sim J/4$

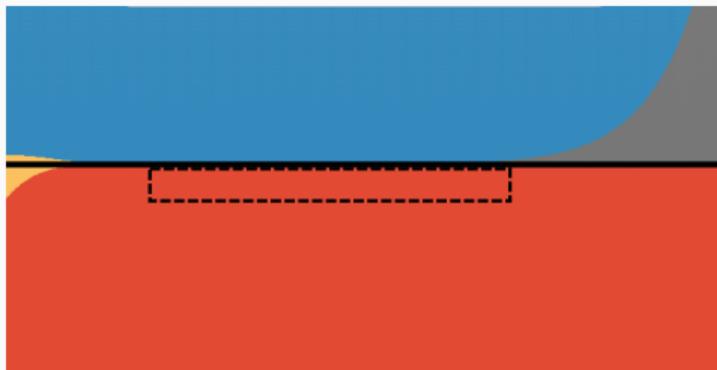
Zero-bandwidth limit



✓ **spin+charge** dimer with attractive zeroth site

✓ spin-singlet + charge-triplet-zero in gr-state

$$|\Psi\rangle_{GS} = \frac{1}{2\sqrt{2}} [|\uparrow_d \downarrow_0\rangle - |\downarrow_d \uparrow_0\rangle] + \frac{1}{2\sqrt{2}} [|\downarrow_d, 0_0\rangle - |0_d, 2_0\rangle]$$

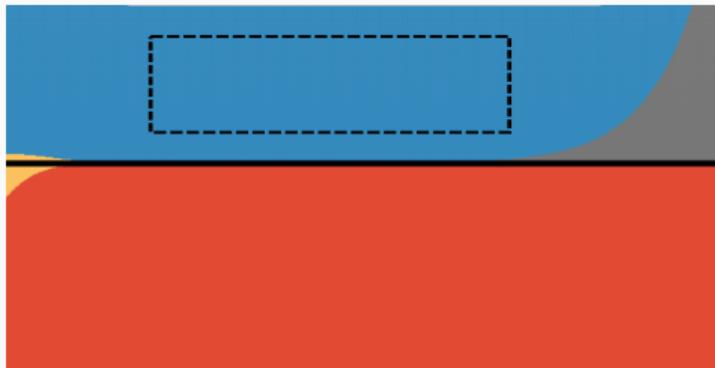
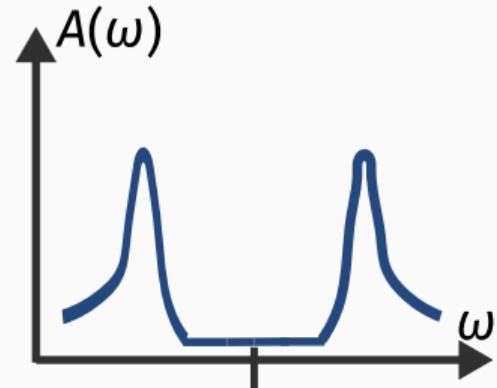


Low-energy effective Hamiltonians and ground-states

Regime 3: $|U_b| > J/4$

- ✓ J, V irrelevant,
- ✓ U relevant,

$$H = -U/2 (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Low-energy effective Hamiltonians and ground-states

Regime 3: $|U_b| > J/4$

Zero-bandwidth limit



impurity site



zeroth site

$$H = -U/2 (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2$$

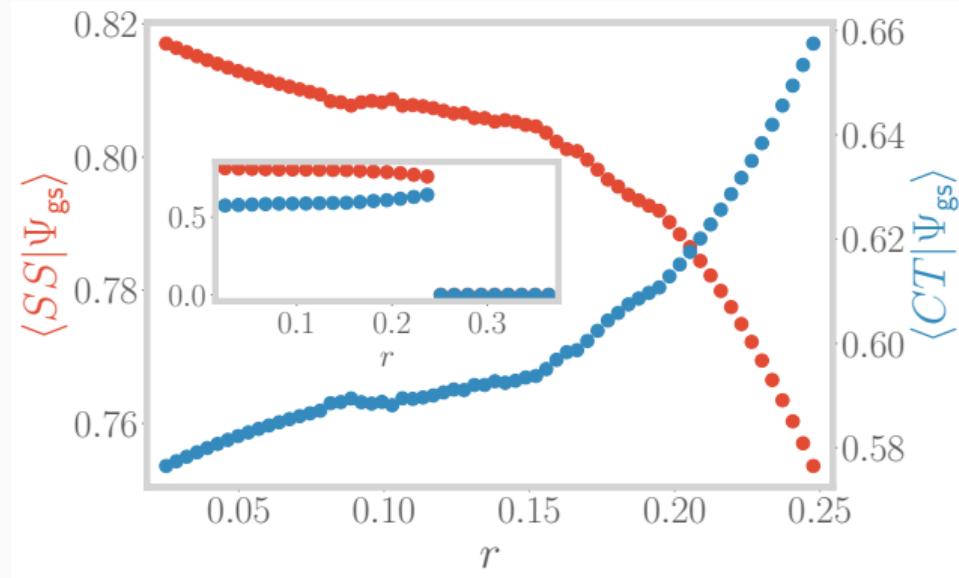
- ✓ impurity site detaches from bath
- ✓ **local moment** ground-state

$$|\Psi\rangle_{GS} = |\uparrow, \downarrow\rangle_d \otimes |0, 2\rangle_0$$



Low-energy effective Hamiltonians and ground-states

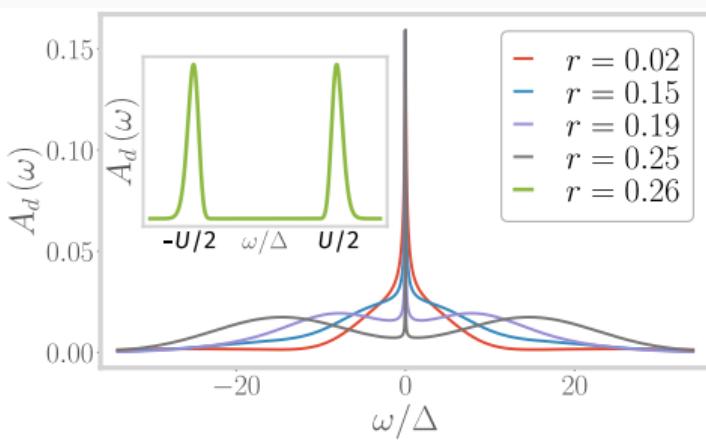
Ground-state overlaps with spin singlet and charge triplet zero



Nature of the Transition

Gapping of the impurity spectral function

- ✓ Broad central peak at $|U_b| \ll J/4$



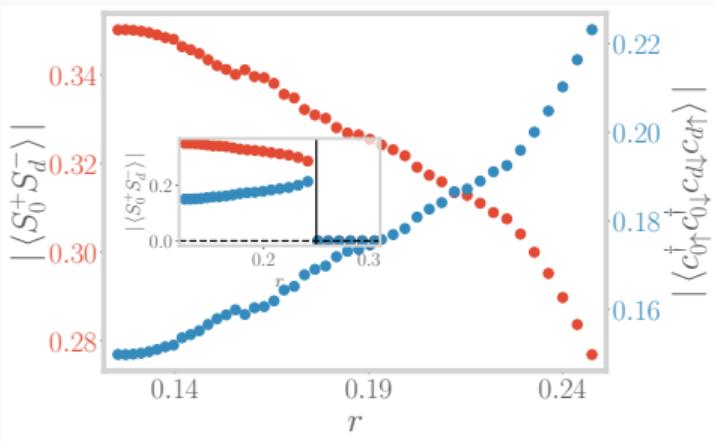
- ✓ hard central gap for $|U_b| > J/4$

- ✓ Correlated **three peak** structure at $|U_b| \lesssim J/4$

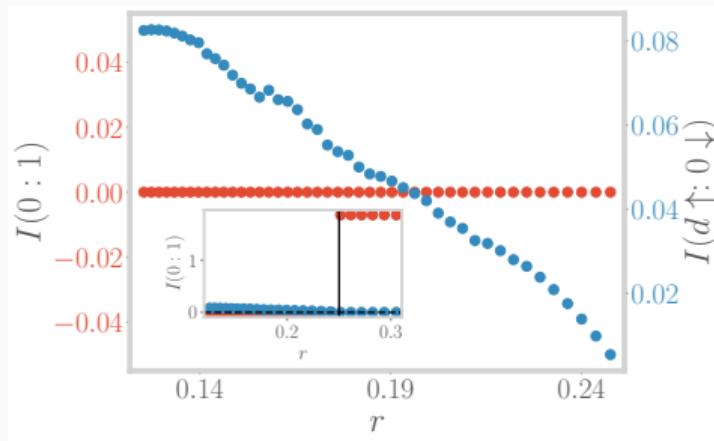
Destruction of the Kondo cloud

The Kondo cloud **weakens, and is destroyed** at the transition.

✓ vanishing of impurity-bath correlations



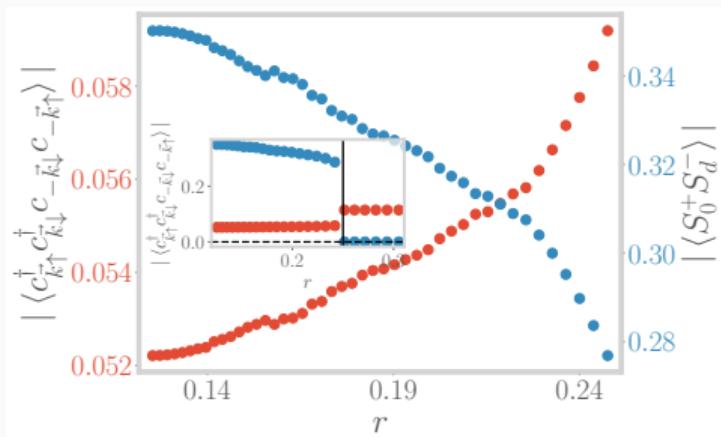
✓ transfer of entanglement into the bath



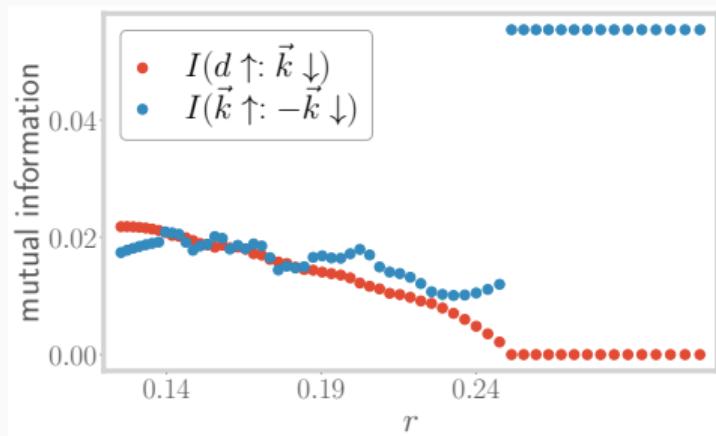
Growth of pairing fluctuations in the bath

Subdominant pairing fluctuations, near the transition...

- ✓ growth of fluctuations in Cooper channel, at the cost of spin-flip fluctuations



- ✓ mutual information within the bath maximised after transition



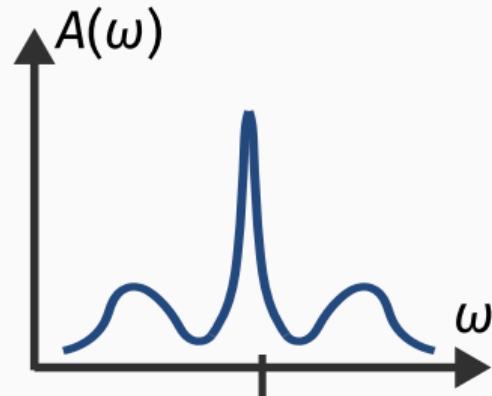
Universal Theory near the Transition

Minimal effective model for the transition

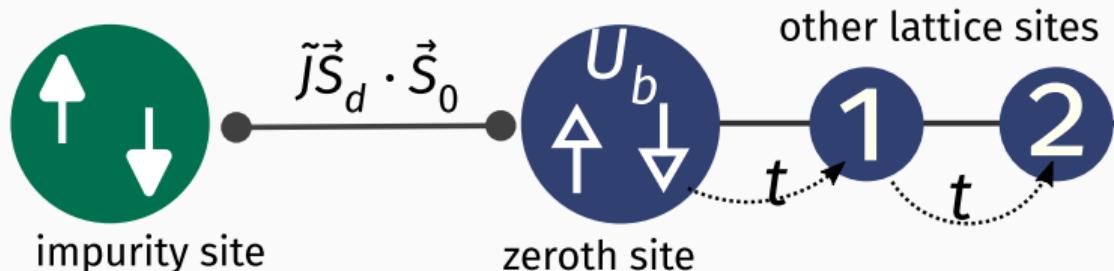
- ✓ For $|U_b| \leq J/4$, central peak and side peaks are **well-separated**
- ✓ **Integrate out** charge fluctuations through Schrieffer-Wolff transformation

$$H_{\text{eff}} = \tilde{J} \vec{S}_d \cdot \vec{S}_0 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + H_{\text{K.E.}}$$

$$\text{RG equation for } \tilde{J} : \Delta \tilde{J} \sim \tilde{J} (\tilde{J} + 4U_b)$$



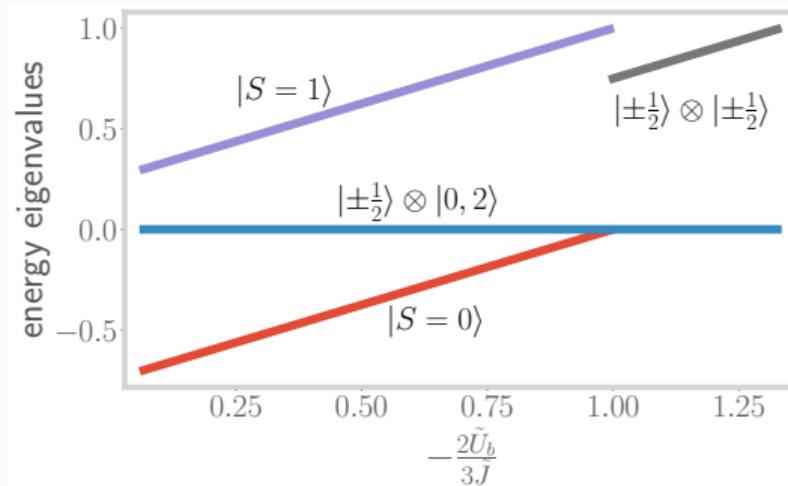
- ✓ **captures** the criticality, and the strong-coupling and local moment phases



Suggests that **J and U_b are the minimal & universal ingredients** for transition!

Capturing the level crossing at the transition from a two-site model

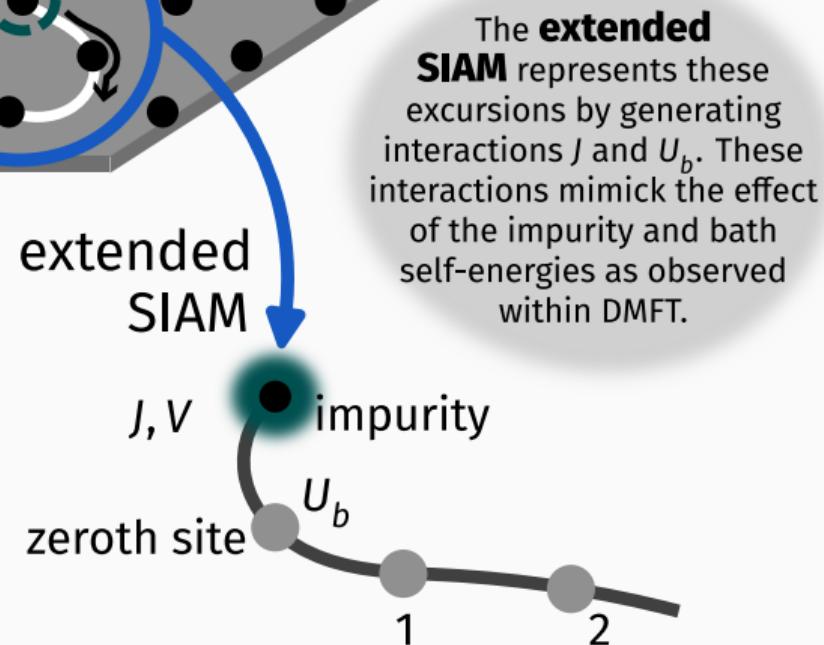
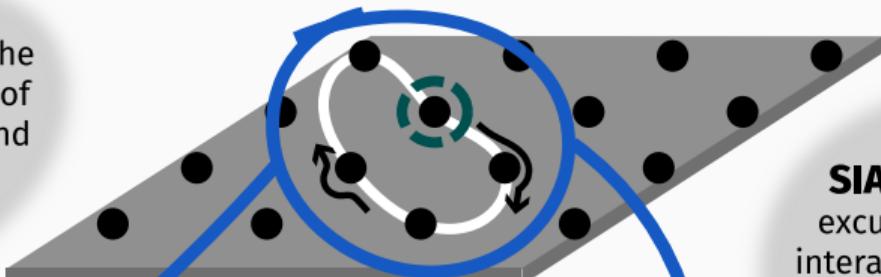
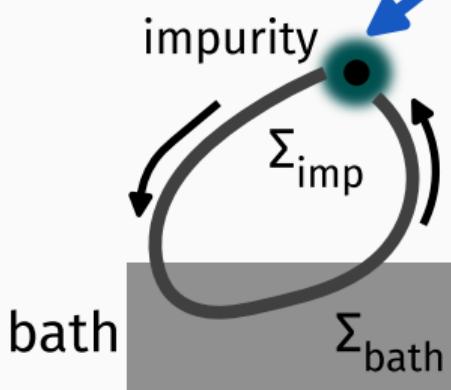
- ✓ Obtain two-site model by taking **zero bandwidth** limit
- ✓ spectrum shows **level crossing** between singlet and local moment states



Insights into DMFT

Extended SIAM in the context of DMFT

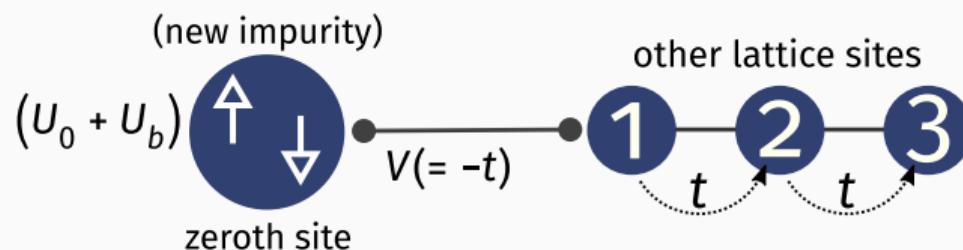
DMFT represents excursions from a site into the correlated bath in the form of self-energies for the bath and the impurity. This results in a three-peak DOS of the bath.



The **extended SIAM** represents these excursions by generating interactions J and U_b . These interactions mimick the effect of the impurity and bath self-energies as observed within DMFT.

Equivalence of the impurity site and the bath zeroth site

- ✓ Integrate out impurity site from fixed point Hamiltonian via a single URG transformation
- ✓ Generates additional correlation U_0 on zeroth site

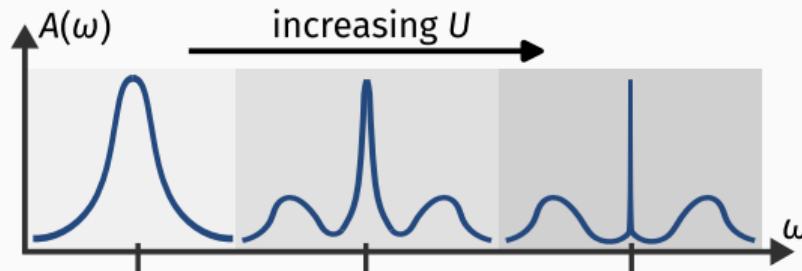


- ✓ J is relevant and the largest scale → **repulsive correlation**:

$$U_0 + U_b \approx J > 0$$

Equivalence of the impurity site and the bath zeroth site

- ✓ J acts a **symmetrisation mechanism** between impurity and zeroth sites
- ✓ **Coherent** spin-flip scatterings ensure similarity of spectral functions



Essence of self-consistency: Equivalence of impurity and zeroth sites!

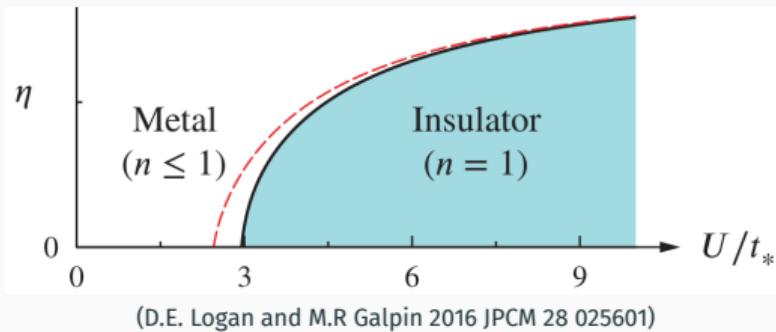
Observation of a coexistence region

- ✓ DMFT observes a **coexistence region** near the critical point, for $U_{c1} < U < U_{c2}$

- ✓ Insulating when coming in from the insulator, metallic when coming in from the metal

- ✓ **True** transition believed to occur at U_{c2}

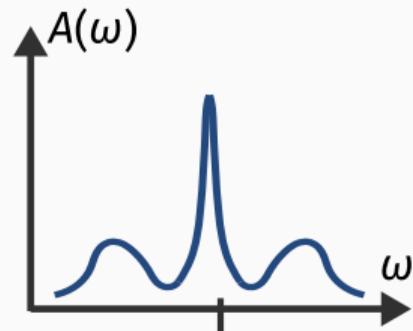
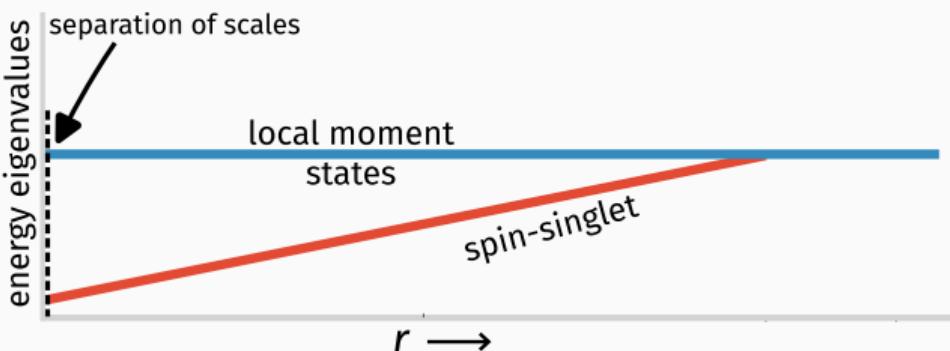
- ✓ Mott gap appears discontinuously after the transition



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

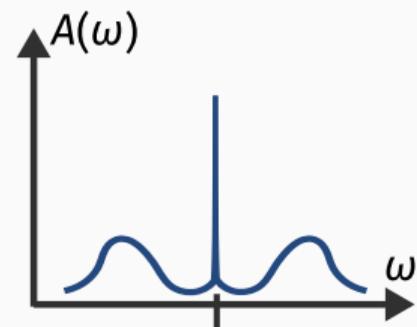
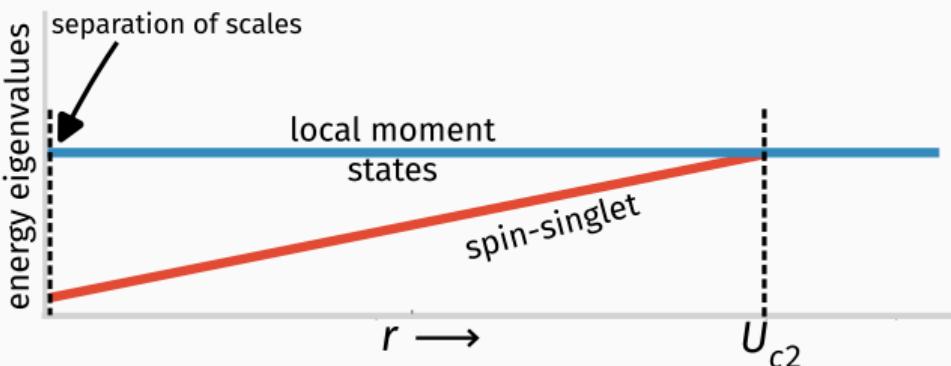
- ✓ Initial point is when the side peaks get separated (near-zeroes in the spectral function)



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

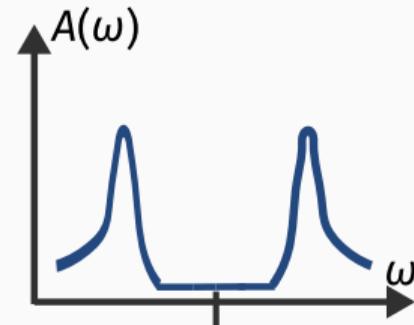
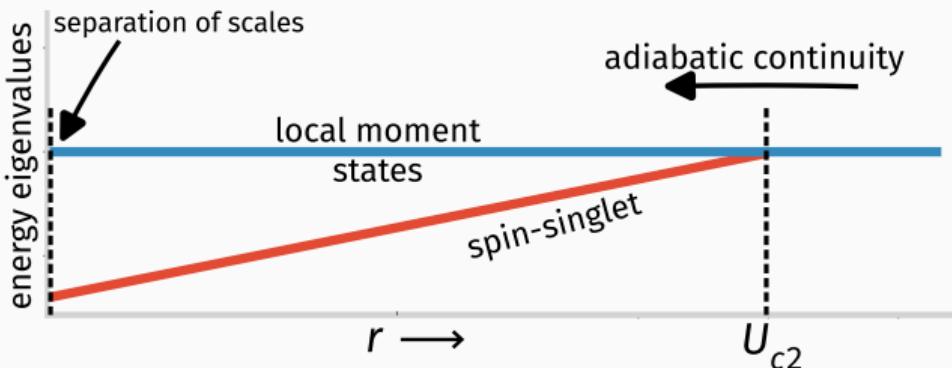
- ✓ U_{c2} is the point where the levels cross



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

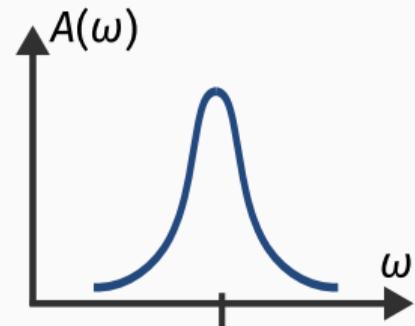
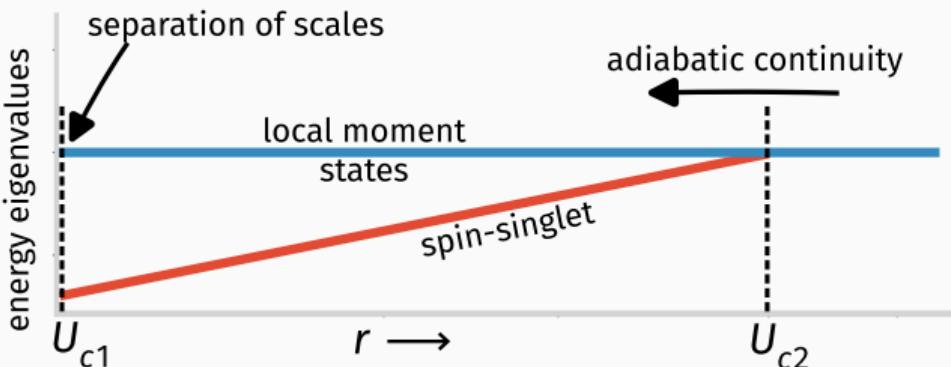
- ✓ Coming from $U > U_{c2}$, **adiabatic continuity** allows DMFT to stay on the local moment state...



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

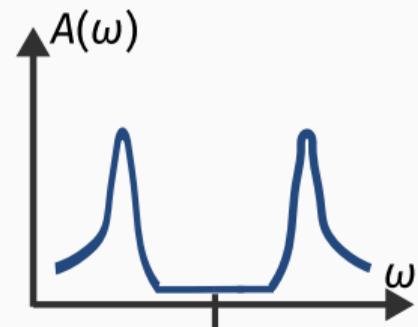
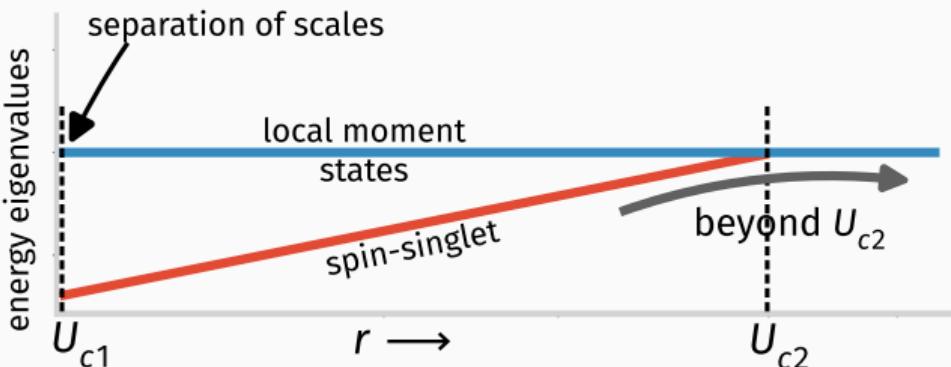
- ✓ For $U < U_{c1}$, local moment state is too unstable, relaxes to the true ground state.



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

- ✓ For $U > U_{c1}$, charge sector separated by large U , leads to the **discontinuous** appearance of finite gap



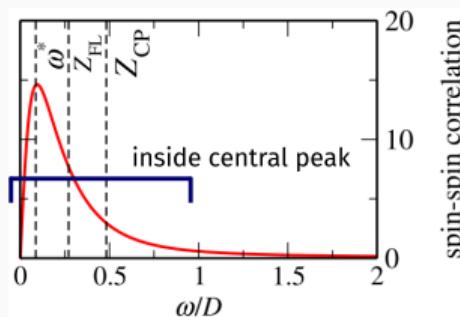
Comparison against NRG-DMFT correlation functions

Poor Man's scaling of the effective Kondo model

[K. Held, R. Peters, and A. Toschi. PRL 2013]

- ✓ shows **quantitative** agreement with NRG-DMFT (crossover scale and kinks in self-energy)
- ✓ Suggests that the minimal model can capture **spin susc.**

[K. Held, R. Peters, and A. Toschi.
PRL 110, 246402 (2013)]



- ✓ Our $J - U_b$ model **goes further** by capturing physics beyond the transition

Comparison against NRG-DMFT correlation functions

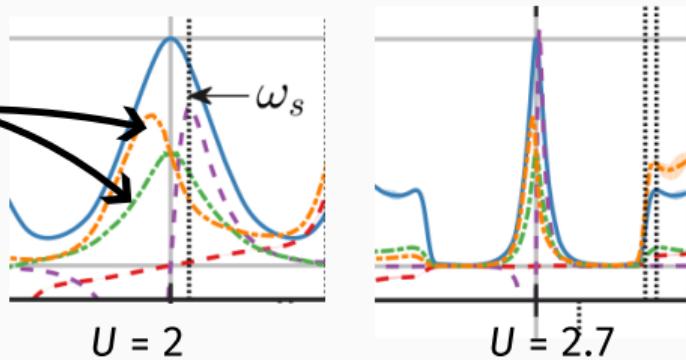
Doublon-holon correlators of the Hubbard model

[S. B. Lee, J. v Delft, and A. Weichselbaum. PRL 2017]

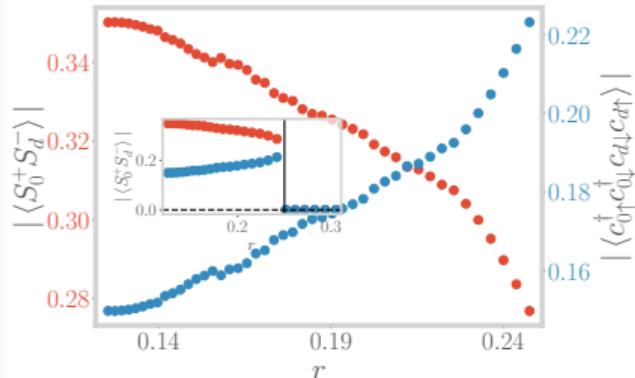
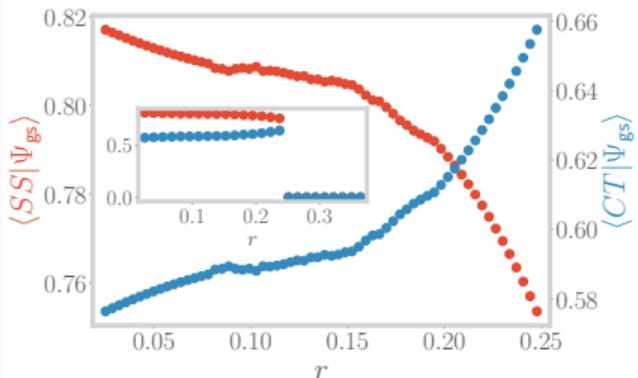
Lee et. al show **peaks** in
doublon-holon correlators
near zero energy
within the central peak.

doublon-holon correlators

[S. B. Lee, J. v Delft, and
A. Weichselbaum. PRL 2017]



We find support for this in the form of **increasing ground-state charge correlations and overlap**.

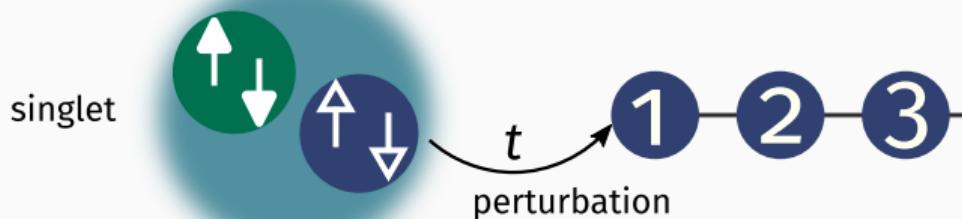


Low-energy excitations of the bath

Effect on the local Fermi liquid

What about the **low-energy excitations** of the bath, that lie above the singlet ground state?

- ✓ treat hopping between singlet and bath as perturbation



- ✓ Up to fourth order, charge sector becomes repulsive...

$$H_{\text{eff}} = \frac{2t^4}{\tilde{J}(3\tilde{J}/4 + \tilde{U}_b)^2} [\hat{n}_{1\uparrow}\hat{n}_{1\downarrow} + p-h] + H_{\text{K.E.}}$$

- ✓ FL term blows up towards transition, signaling **breakdown** of Fermi liquid theory and loss of adiabaticity.

Effect on the local Fermi liquid

Vanishing of the **Kondo scale** T_K towards the transition

- ✓ Kondo temperature scale T_K can be obtained from the $J - U_b$ model, but with a Lorentzian DOS in the bath,
 $\rho = \rho_0 \Gamma^2 / (D^2 + \Gamma^2)$.
- ✓ Near the transition $r = -U_b/J_0 \rightarrow \frac{1}{4}$, the fixed-point momentum energy scale D^* can be approximated as

$$D^* = D_0 \exp \left[\frac{(2\omega + U_b + J_0/2)^2}{8U_b \rho_0 \Gamma^2} \ln |1 - 4r| \right], \quad D_0 = \text{UV cutoff}.$$

- ✓ Kondo temperature can be defined as $T_K = \hbar \Lambda^* / k_B$, vanishes towards the critical point

$$T_K = \frac{D_0}{k_B} \exp \left[\frac{(2\omega + U_b + J_0/2)^2}{8U_b \rho_0 \Gamma^2} \ln |1 - 4r| \right]$$

Effect on the local Fermi liquid

How do the imaginary part of **self-energy** Σ and the **quasiparticle residue** behave near the transition?

- ✓ Following the renormalised perturbation theory approach of Hewson, $\text{Im}[\Sigma(\omega)]$ is

$$\text{Im}[\Sigma(\omega)] \sim u^2 \omega^2, \quad u = \frac{2t^4}{\tilde{J}(3\tilde{J}/4 + \tilde{U}_b)^2}$$

- ✓ As $r \rightarrow 0$, $u \rightarrow \infty$, signalling a vanishing lifetime of the quasiparticles
- ✓ Quasiparticle residue Z for 1-particle excitations is proportional to T_K :

$$Z \sim T_K$$

$$Z \rightarrow 0 \text{ as } r \rightarrow 0$$

Broad conclusions

- ✓ The extended SIAM appears to capture the DMFT transition and **self-consistency**.
- ✓ The key ingredient is a **competition** between Kondo screening physics and a local attractive correlation in the bath.
- ✓ Crucial feature of the journey is the enhancement of **pairing fluctuations** in the bath - leads to destruction of Kondo cloud.
- ✓ An emergent self-consistency is achieved through the qualitative similarity of the spectral functions of the impurity and zeroth sites.
- ✓ SOMETHING ABOUT THE FINAL CALCULATIONS (MAYBE NON-FERMI LIQUID PHYSICS)

Future Prospects

Future Prospects

- ✓ The extended SIAM can be improved by considering **multiple impurities** and general impurity **filling**.
- ✓ We are developing a new **tiling-based auxiliary model method** can used for studying other models of strong-correlations as well as topologically active or flat band systems.
- ✓ The URG can be applied to **heavy-fermion materials** towards a study of phase diagram and unconventional superconductivity, as well as Kondo insulators.
- ✓ Interacting systems in a magnetic field is also a potential area of study, specifically **fractional Chern insulators** (e.g. the fractional quantum hall effects).

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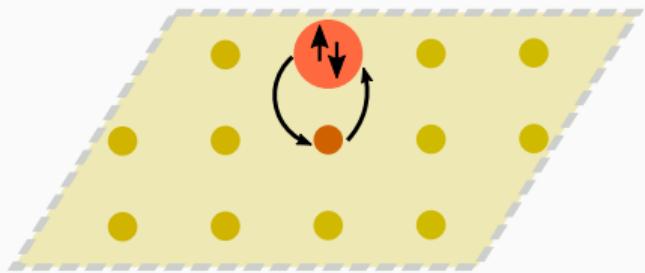
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Other Projects

Theory for the single-channel Kondo cloud

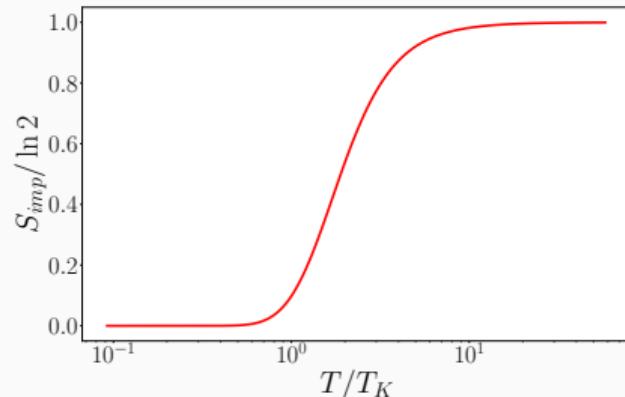
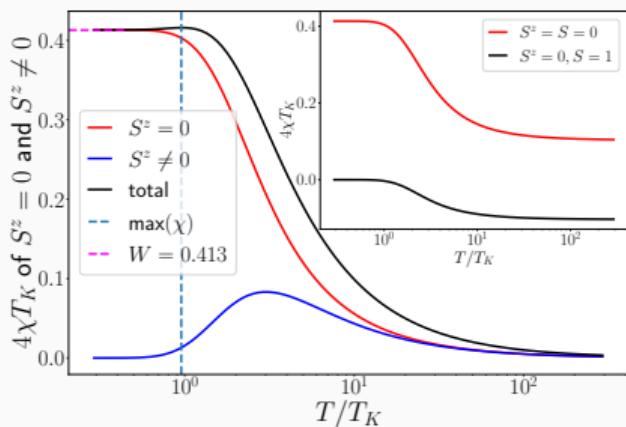
Phys. Rev. B 105, 085119

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Theory for the single-channel Kondo cloud

- ✓ spectral function & magnetic susceptibility

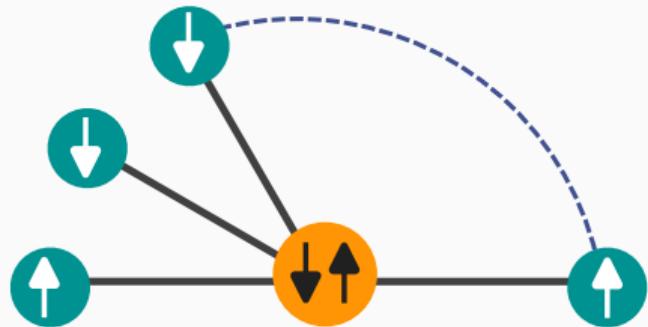


- ✓ local Fermi liq. & orthogonality catastrophe
- ✓ thermal entropy

Role of degeneracy in the multi-channel Kondo problem

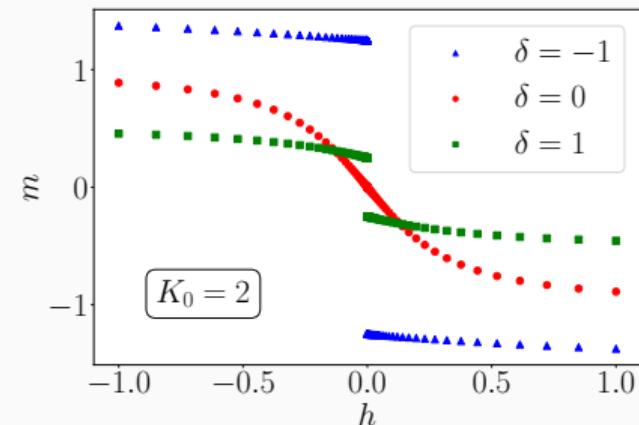
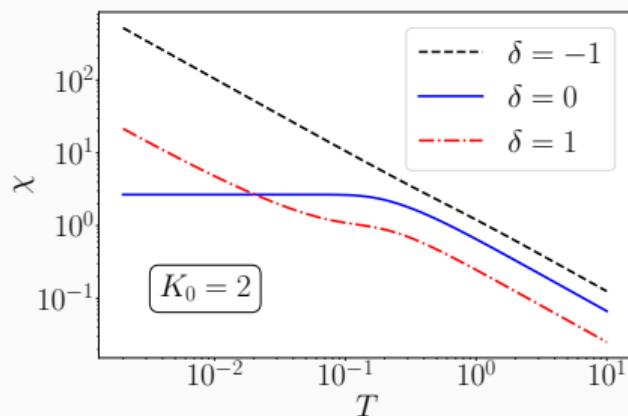
arXiv:2205.00790

Siddhartha Patra, **Abhirup Mukherjee**, Anirban Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, Siddhartha Lal



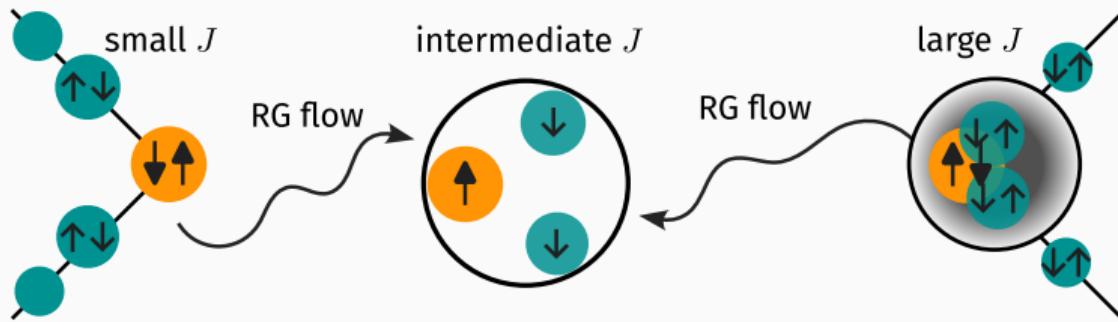
Role of degeneracy in the multi-channel Kondo problem

- ✓ Intermediate-coupling RG fixed point Hamiltonian and **degenerate** ground states
- ✓ Degree of compensation, magnetization and susceptibility show **incomplete screening**

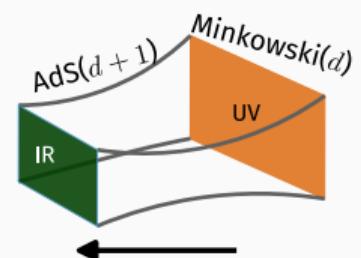
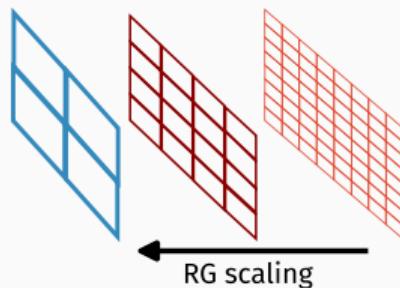


Role of degeneracy in the multi-channel Kondo problem

- ✓ Local **marginal Fermi liquid** within the low-energy excitations of the bath
- ✓ **Duality** relations constrain the RG flows of the MCK model

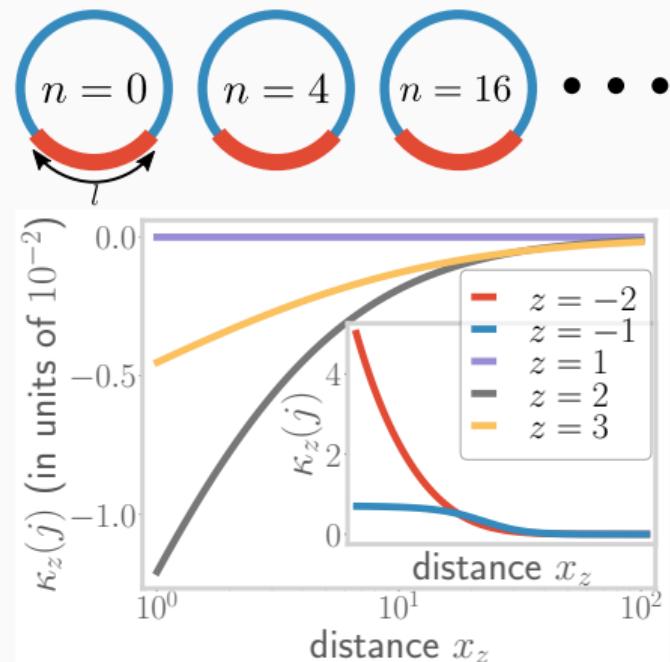


Entanglement scaling in free fermions: holography & topology



Entanglement scaling in free fermions: holography & topology - Summary

- ✓ Under coarse-graining or fine-graining in k -space, entanglement of free Dirac fermions shows hierarchical onion-like structure.
- ✓ Entanglement scaling can be used to define distances, leads to additional spatial dimension \rightarrow holography.
- ✓ Emergent distances and curvature can be related to RG beta function; the sign of the curvature is topological.
- ✓ Pole structure of the entanglement tracks the Luttinger volume - invariant under the scaling transformations.



Creating subsystems

Free Dirac fermions on torus: $k_x^n = \frac{2\pi}{L_x} n, \quad n \in \mathbb{Z}; \quad$ define **sparsity** = $\Delta n = 1$

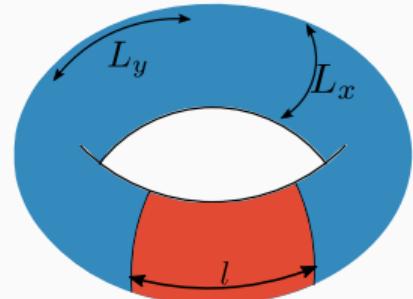
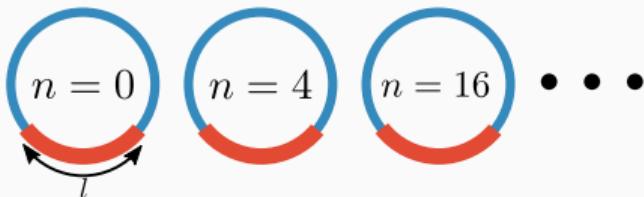
Simplest choice: the entire set

sparsity = 1 $\longrightarrow n \in \{-N, -(N - 1), -(N - 2), \dots, -1, 0, 1, \dots, N - 2, N - 1, N\}$

Coarser choices: increase sparsity

sparsity = 2 $\longrightarrow n \in \{-N, -(N - 2), -(N - 4), \dots, -2, 0, 2, \dots, N - 4, N - 2, N\}$

sparsity = 4 $\longrightarrow n \in \{-N, -(N - 4), -(N - 8), \dots, -4, 0, 4, \dots, N - 8, N - 4, N\}$



Subsystem entanglement entropy: Entanglement hierarchy

$$S_{A_z(j)} = f_z(j) c \alpha L_x - c \log |2 \sin(\pi f_z(j)\phi)|$$

$$i < j, \quad S_{i \cup j} = \begin{cases} S_i, & z > 0 \\ S_j, & z < 0 \end{cases}$$



- ✓ presents a **hierarchy** of entanglement → EE distributed across RG steps
RG transformation → reveals entanglement
- ✓ distribution of entanglement also present in **multipartite** entanglement

Mutual information = distance

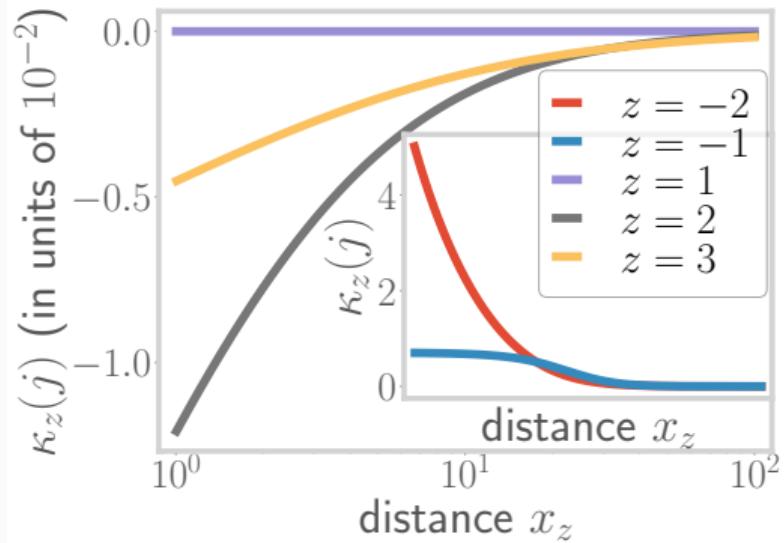
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

Define distances using mut. info.

$$x_z(j) = \log t_z(j), \quad y_z(j) = \log t_z(j \pm 1)$$

$$v_z(j) \equiv \Delta y_z(j)/\Delta x_z(j), \quad v' = \Delta v_z(j)/\Delta x_z(j)$$

Curvature as well: $\kappa_z(j) = \frac{v'_z(j)}{\left[1 + v_z(j)^2\right]^{\frac{3}{2}}}$



RG evolution = emergent distance

- ✓ Distances and curvature can be related to an RG **beta function**
- ✓ Amounts to an **explicit demonstration** of the holographic principle
- ✓ Sign of curvature is **topological**, can be written in terms of winding numbers

Topological nature of geometry-independent term

$$S_{A_z(j)} = f_z(j)caL_x - \underbrace{c \log |2 \sin(\pi f_z(j)\phi)|}_{=Q(\phi), \text{geometry-independent term}}$$

- ✓ $Q(\phi)$ is periodic in the flux ϕ , $\phi = 1$ transports a charge across Fermi surface
- ✓ pole structure of $(\sin \frac{\pi}{4} - |\sin(\pi f_z(j)\phi)|)^{-1}$ counts number of states → tracks Luttinger volume
- ✓ Luttinger volume is topological, so is $Q(\phi)$; $Q(\phi)$ can be expressed in terms of winding numbers