

# 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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# Summary of Work

## 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

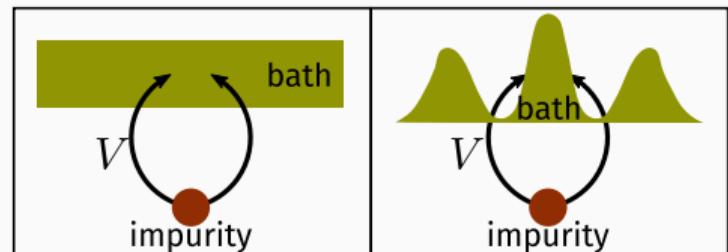
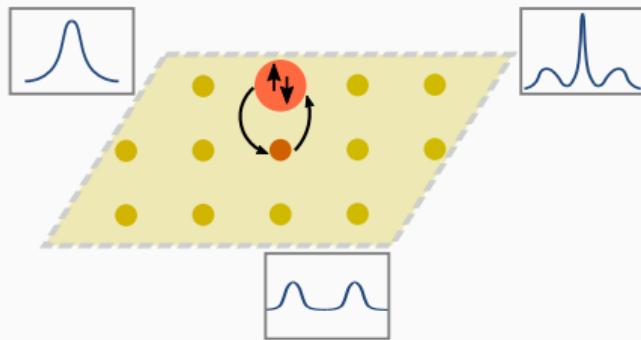
- ✓ Metal-insulator transition in an extended Anderson impurity model (*manuscript in preparation*)
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- ✓ Holography and topology of entanglement scaling in free fermions (*manuscript in preparation*)

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

# Local MIT in an extended Anderson impurity model

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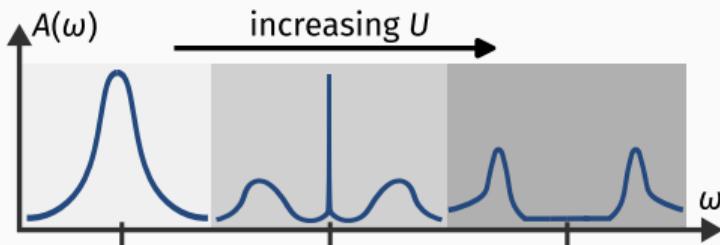


## **Introducing the extended Anderson impurity model**

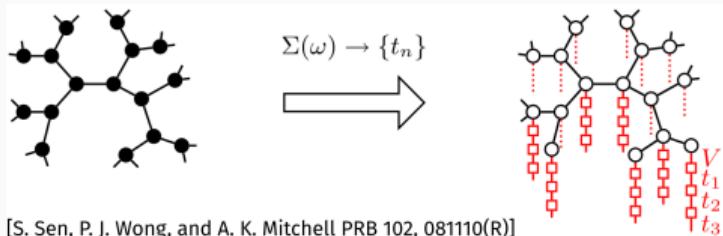
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## DMFT on the Bethe lattice: Exact in $d = \infty$

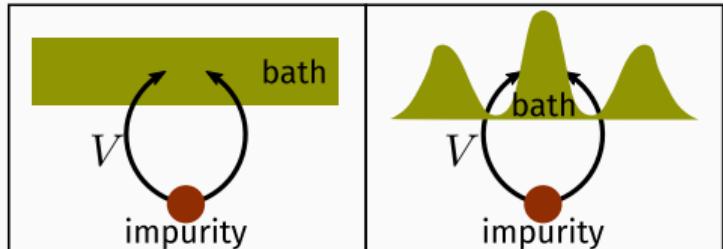
- ✓ shows **metal-insulator transition** on the Bethe lattice with  $\infty$  coordination number



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

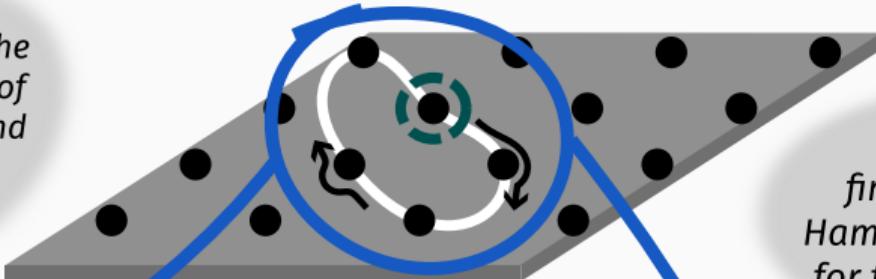


- ✓ Spectral function develops three peaks and then **gaps out**



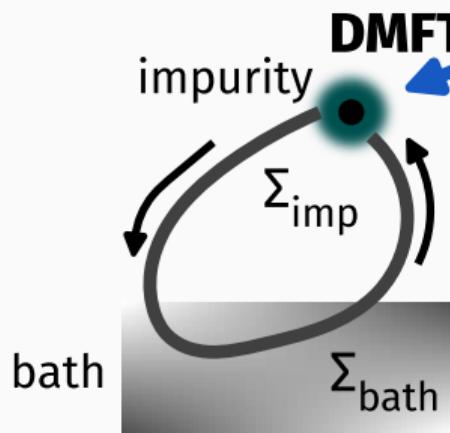
# DMFT on the Bethe lattice: Exact in $d = \infty$

**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.

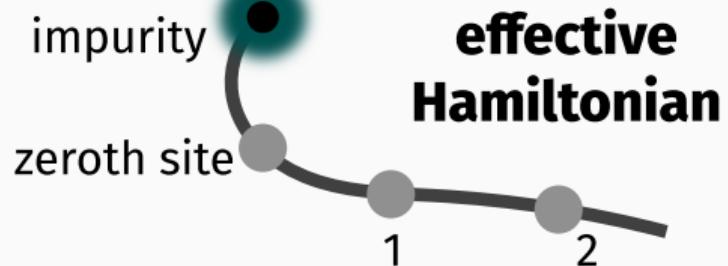


**Our Goal:**

finding an effective Hamiltonian description for the  $\Sigma$  that gives rise to the MIT.



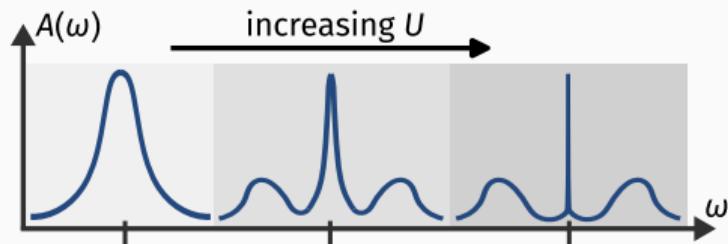
Similar approach adopted by Si & Kotliar for extended Hubbard model



# Introducing the extended Anderson impurity model

## Standard Anderson impurity model

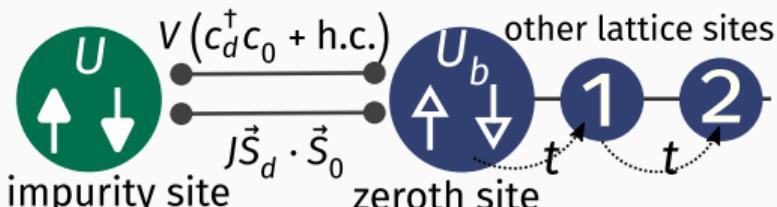
- ✓ no local-moment phase,  $A(\omega)$  gapless
- ✓ cannot explain insulating phase of DMFT



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**

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## Nature of RG flows

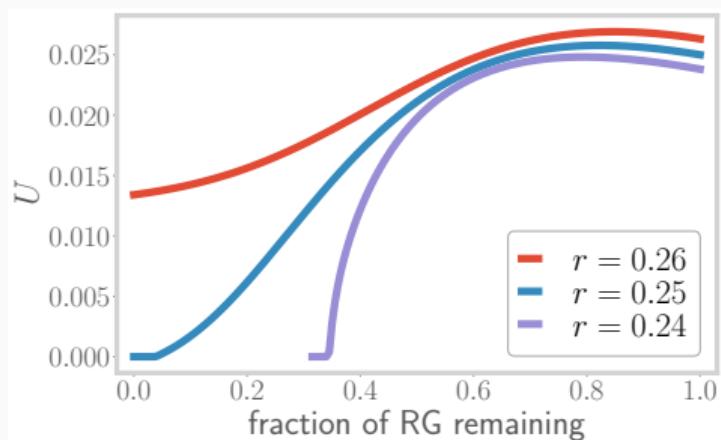
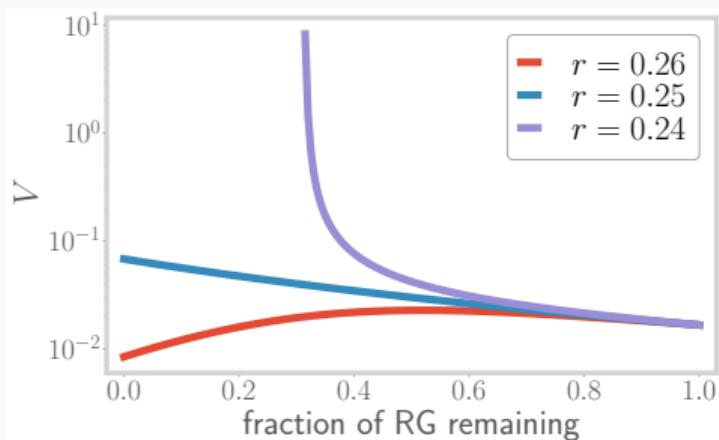
- ✓ URG Equations reveal **critical** point at  $r = -U_b/J = 1/4$
- ✓ RG equation for most dominant coupling  $J$ :

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

- ✓ Numerator structure allows **averting** strong-coupling behaviour

## Nature of RG flows

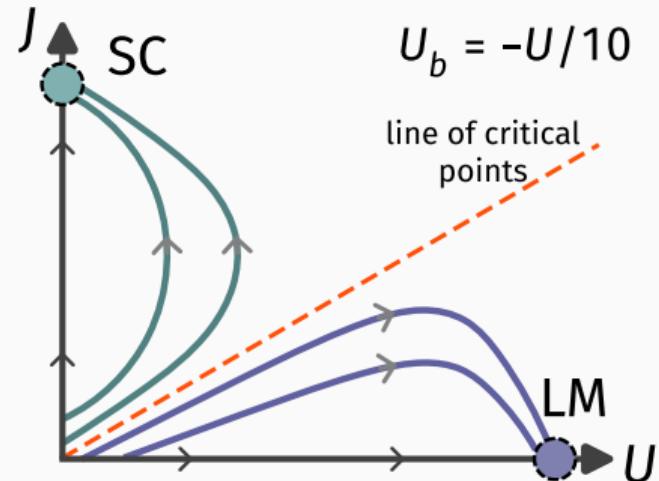
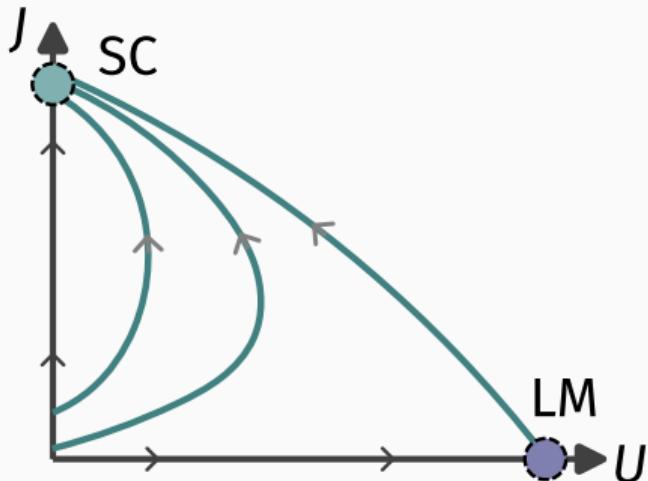
- ✓ Bath correlation  $U_b$  is always **marginal**



## Nature of RG flows

- ✓ RG equation reveals competition between Kondo flow and pairing physics

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



## RG Phase Diagram

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

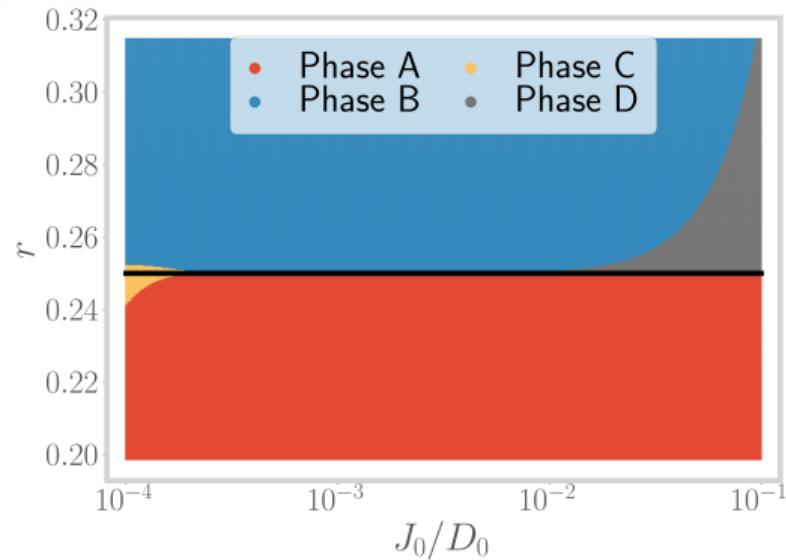
✓ yellow phase:  $J \ll D_0$ : involves  **$V, U, U_b$**

*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

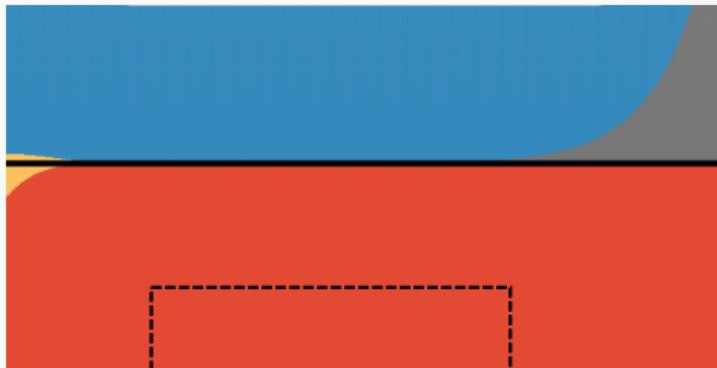
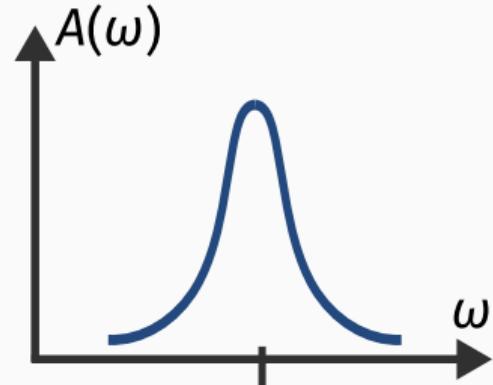


# Low-energy effective Hamiltonians and ground-states

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

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

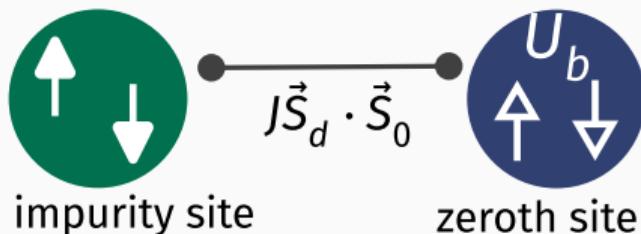
$$H = J\vec{S}_d \cdot \vec{S}_0 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



# Low-energy effective Hamiltonians and ground-states

**Regime 1:**  $|U_h| < J/4$

## 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

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

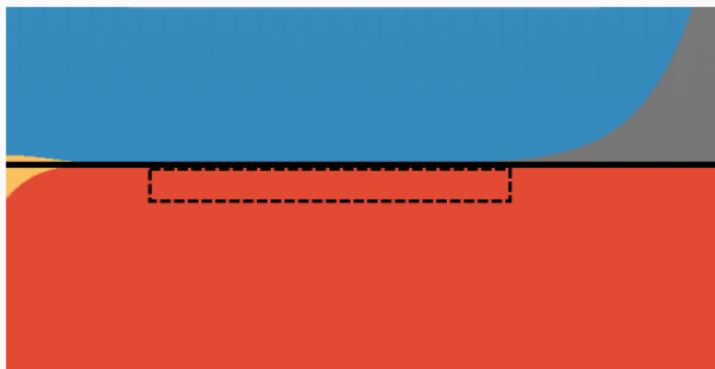
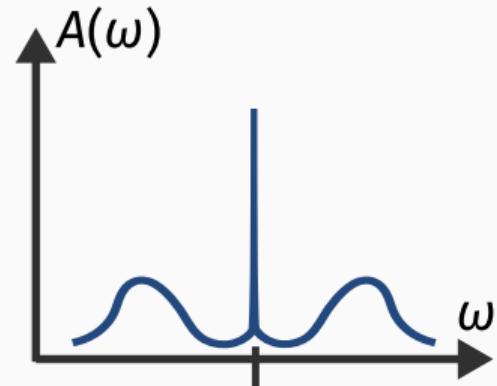


# Low-energy effective Hamiltonians and ground-states

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

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

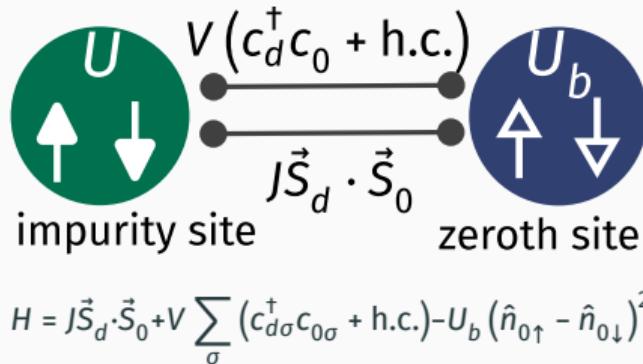
$$H = J\vec{S}_d \cdot \vec{S}_0 + V \sum_{\sigma} (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



# Low-energy effective Hamiltonians and ground-states

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

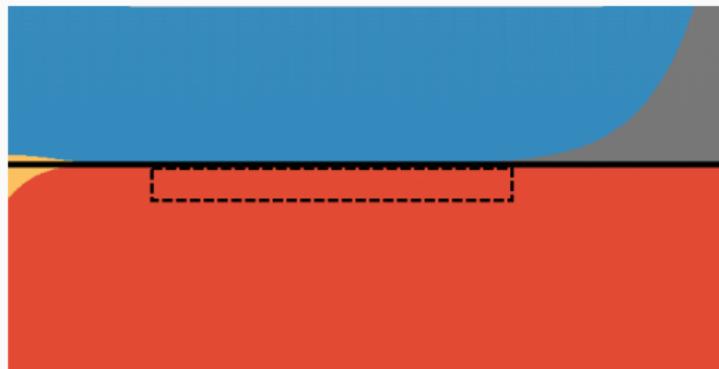
**Zero-bandwidth limit**



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

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

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



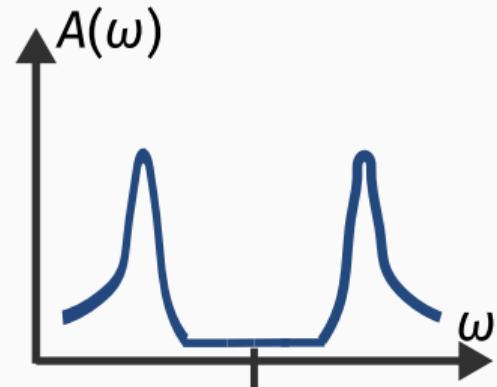
# Low-energy effective Hamiltonians and ground-states

**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

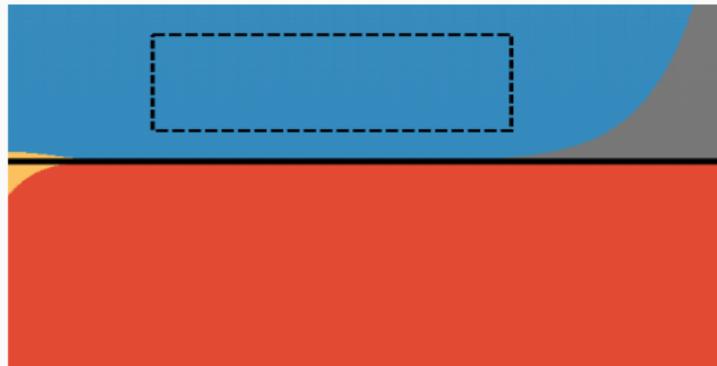


zeroth site

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

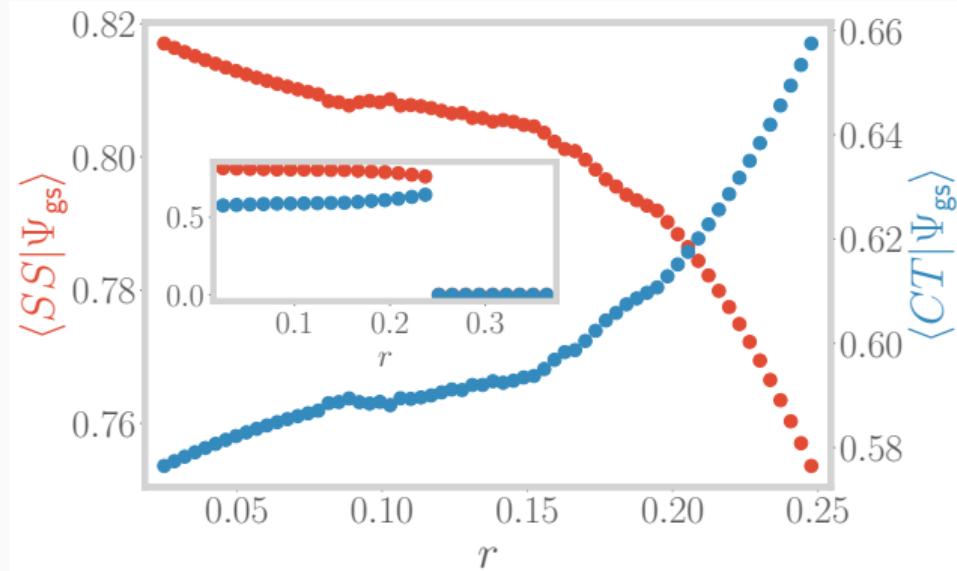
$$|\Psi\rangle_{GS} = |\uparrow, \downarrow\rangle_d \otimes |0, 2\rangle_0$$

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



# Low-energy effective Hamiltonians and ground-states

Ground-state overlaps with spin singlet and charge triplet zero

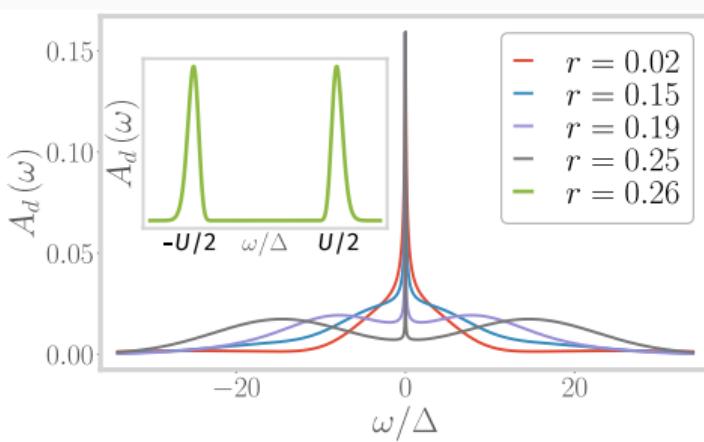


## **Nature of the Transition**

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# Gapping of the impurity spectral function

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



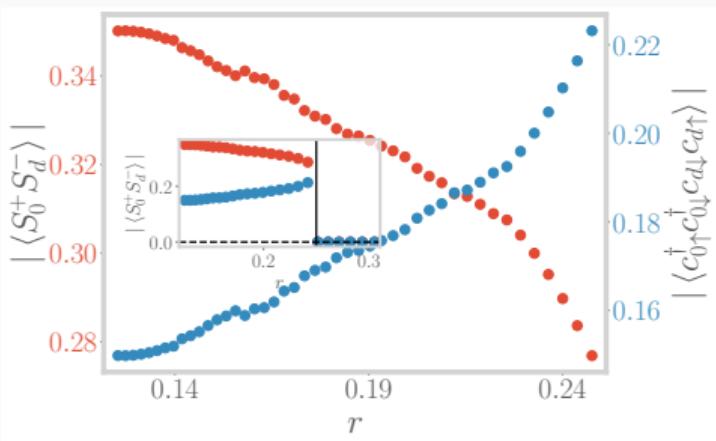
- ✓ hard central gap for  $|U_b| > J/4$

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

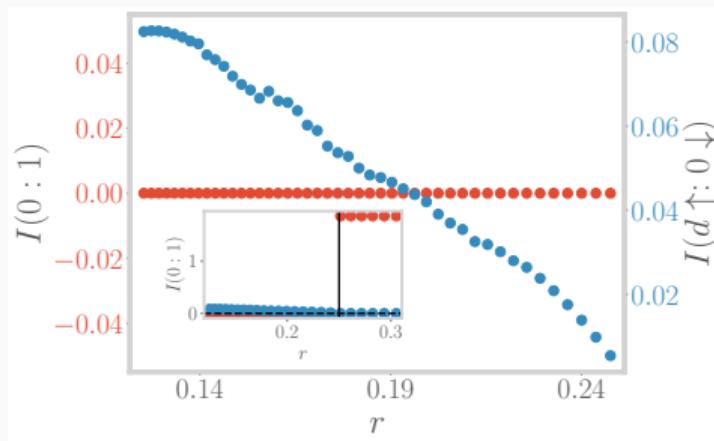
# Destruction of the Kondo cloud

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

- ✓ vanishing of impurity-bath correlations



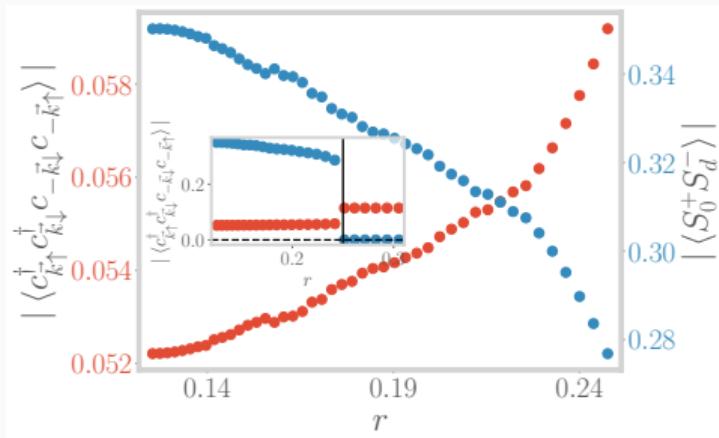
- ✓ transfer of entanglement into the bath



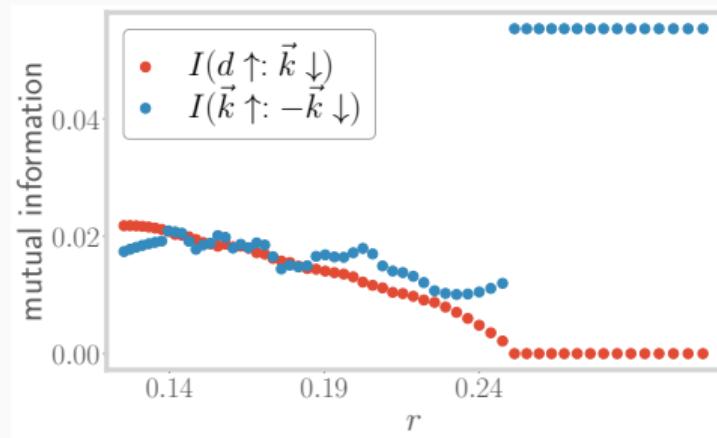
# Growth of pairing fluctuations in the bath

## 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**

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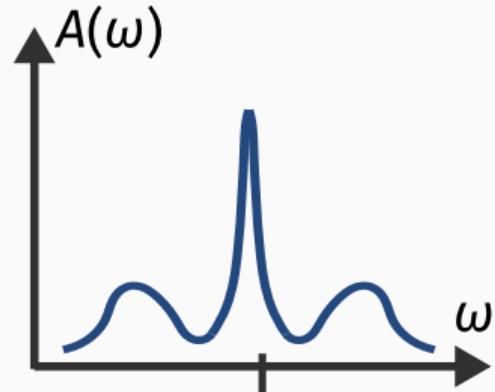
## Minimal effective model for the transition

✓ For  $|U_b| \lesssim J/4$ , central peak and side peaks are **well-separated**

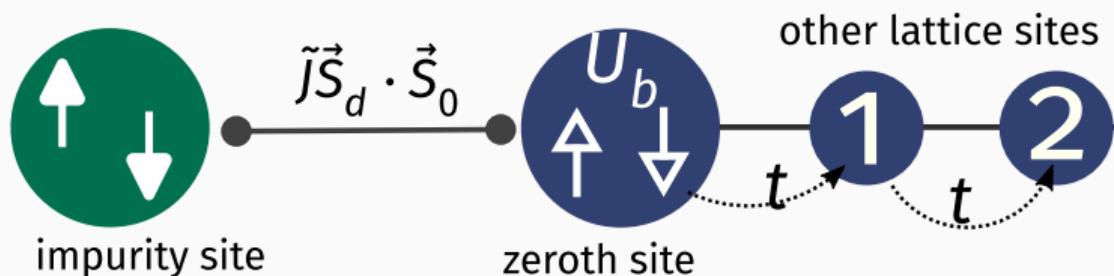
✓ **Integrate out** charge fluctuations through Schrieffer-Wolff transformation

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

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



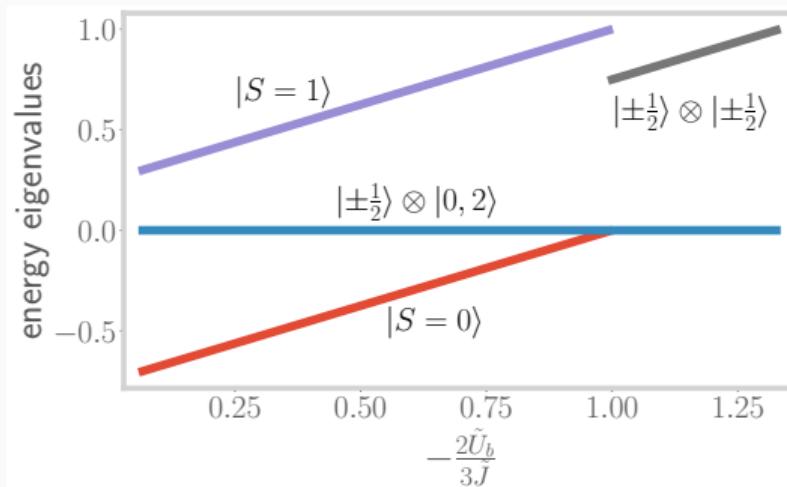
✓ **captures** the criticality, and the strong-coupling and local moment phases



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

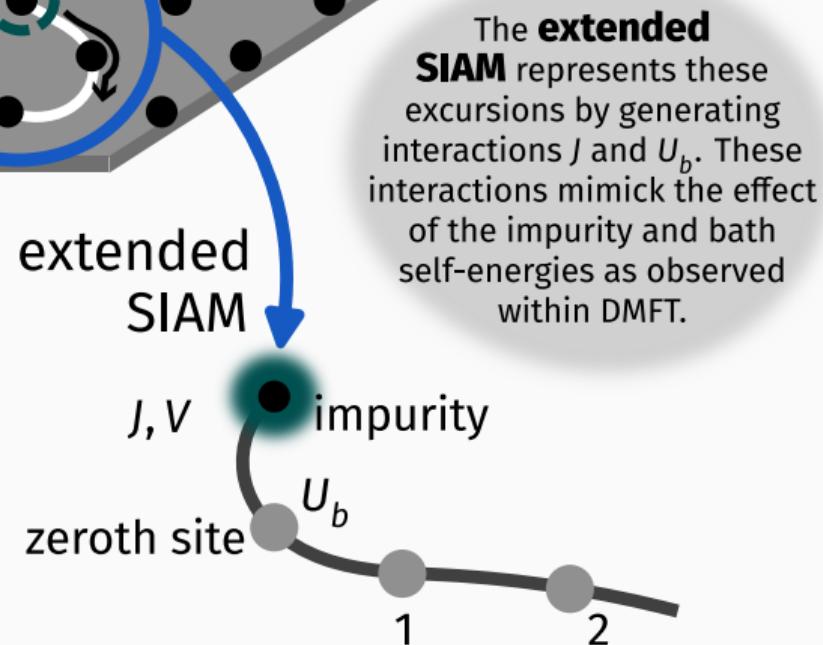
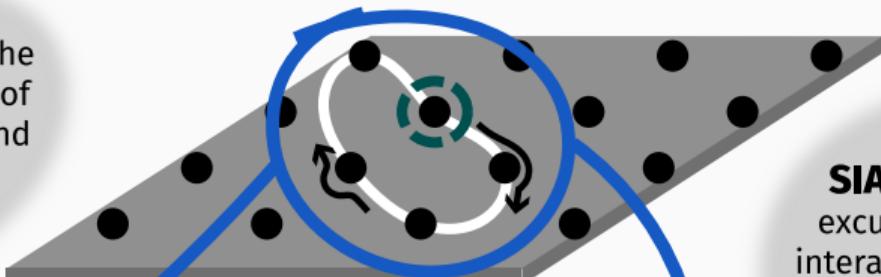
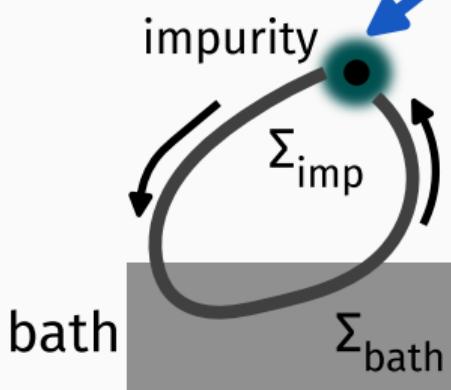


## **Insights into DMFT**

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## Extended SIAM in the context of DMFT

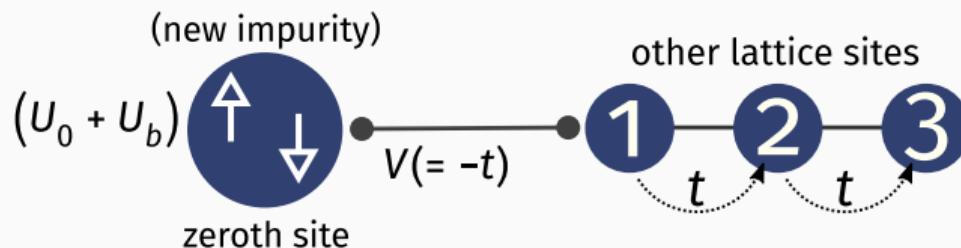
**DMFT** represents excursions from a site into the correlated bath in the form of self-energies for the bath and the impurity. This results in a three-peak DOS of the bath.



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

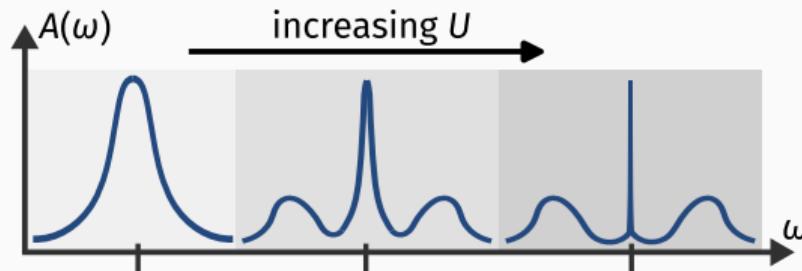


- ✓  $J$  is relevant and the largest scale → **repulsive correlation**:

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

## Equivalence of the impurity site and the bath zeroth site

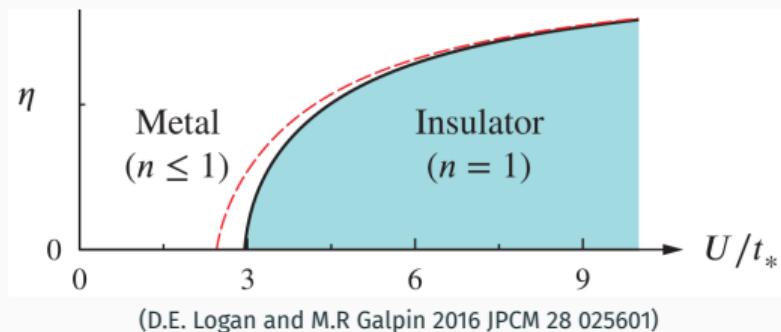
- ✓  $J$  acts a **symmetrisation mechanism** between impurity and zeroth sites
- ✓ **Coherent** spin-flip scatterings ensure similarity of spectral functions



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

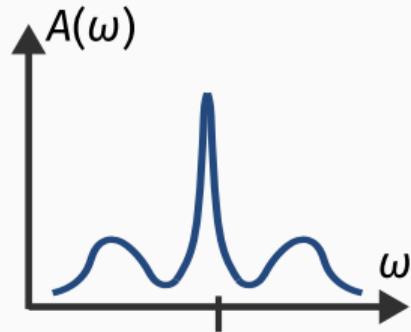
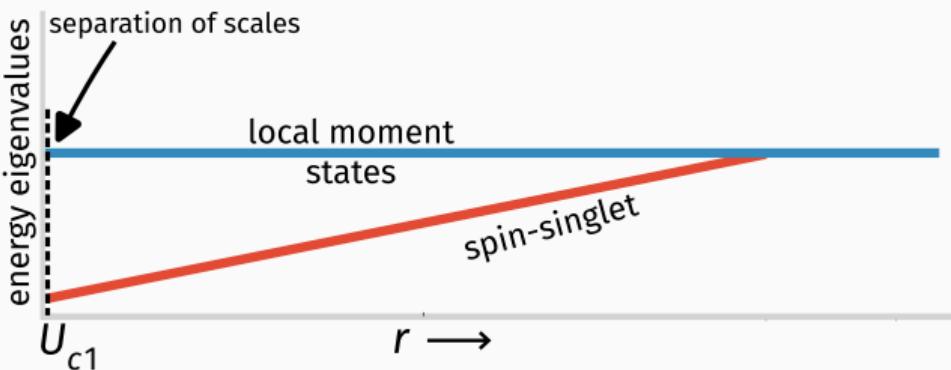


- ✓ Mott gap appears **discontinuously** after the transition, through a **continuous** sharpening of the central peak.
- ✓ **True** transition believed to occur at  $U_{c2}$ .

## Observation of a coexistence region

Can be explained heuristically using the two site spectrum

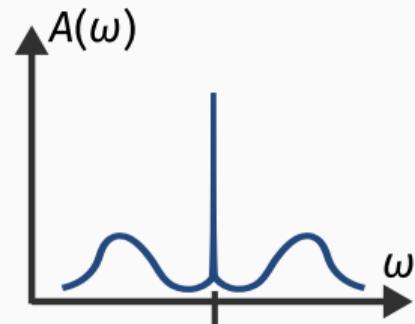
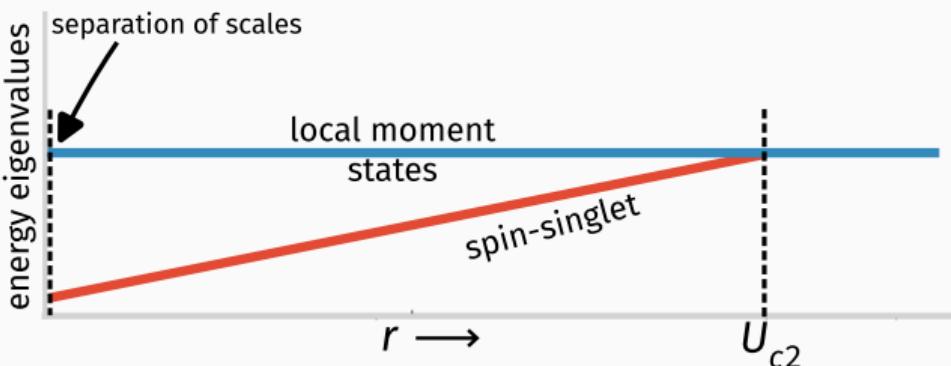
- ✓ Initial point is when the side peaks get separated (near-zeroes in the spectral function)



## Observation of a coexistence region

Can be explained heuristically using the two site spectrum

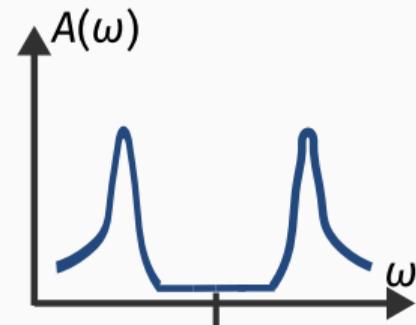
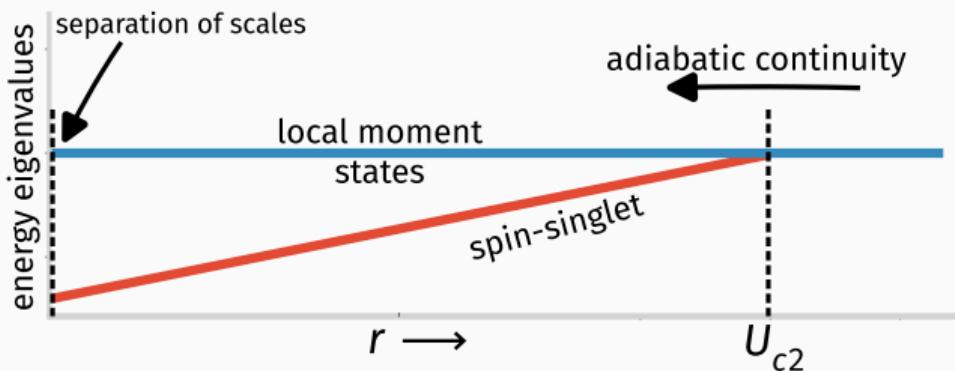
- ✓  $U_{c2}$  is the point where the levels cross



## Observation of a coexistence region

Can be explained heuristically using the two site spectrum

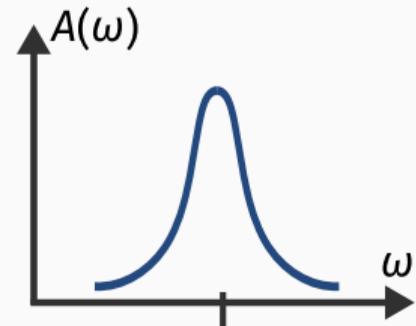
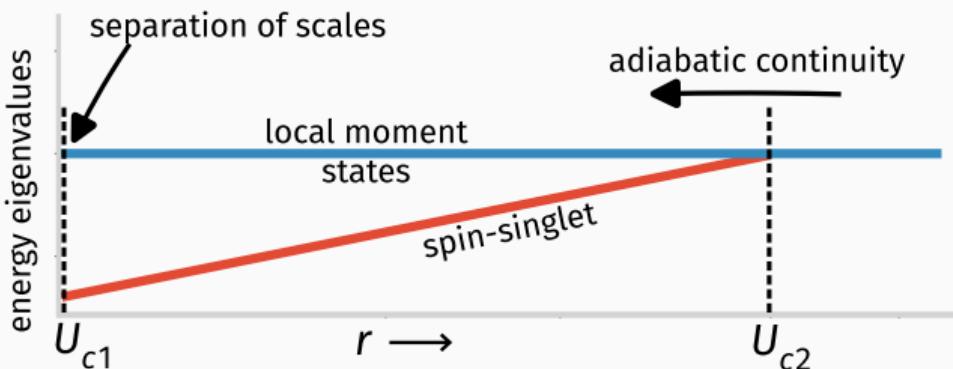
- ✓ Coming from  $U > U_{c2}$ , **adiabatic continuity** allows DMFT to stay on the local moment state...



## Observation of a coexistence region

Can be explained heuristically using the two site spectrum

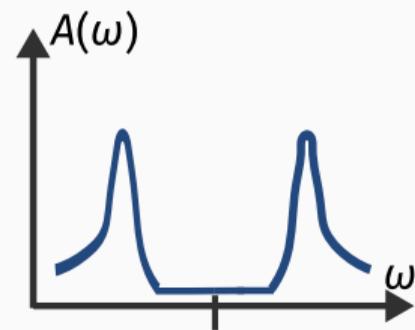
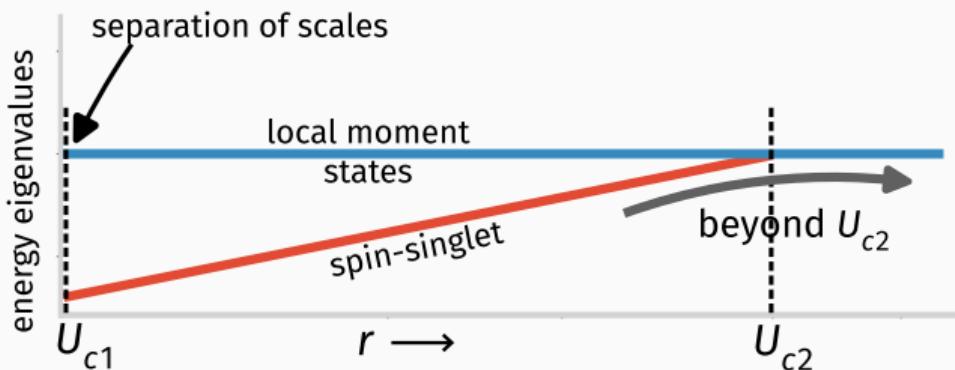
- ✓ For  $U < U_{c1}$ , local moment state is too unstable, relaxes to the true ground state.



## 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



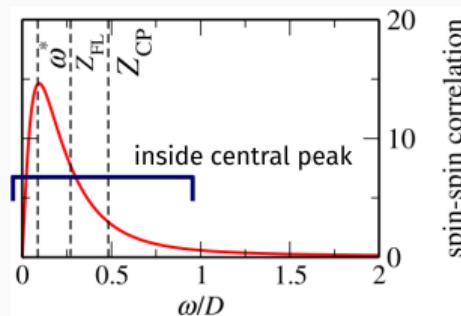
# Comparison against NRG-DMFT correlation functions

## 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

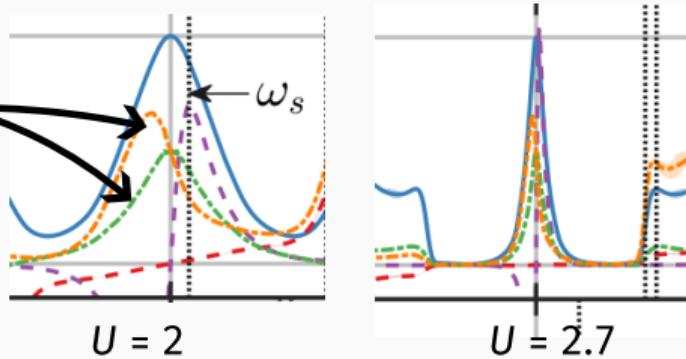
## Doublon-holon correlators of the Hubbard model

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

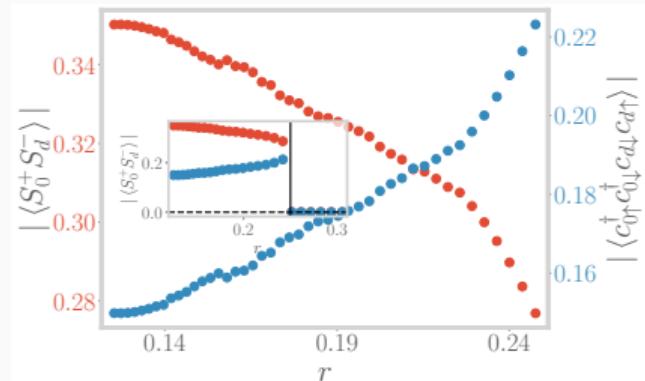
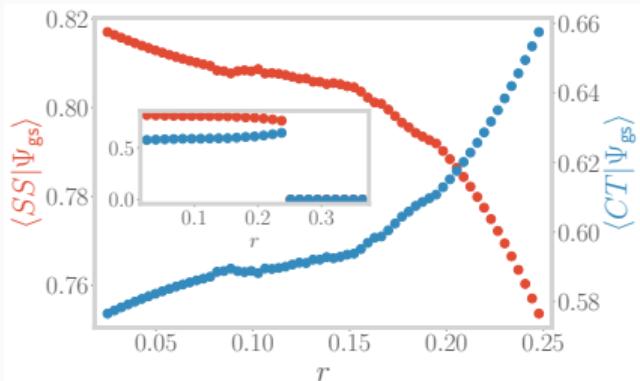
Lee et. al show **peaks** in  
doublon-holon correlators  
near zero energy  
within the central peak.

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**.



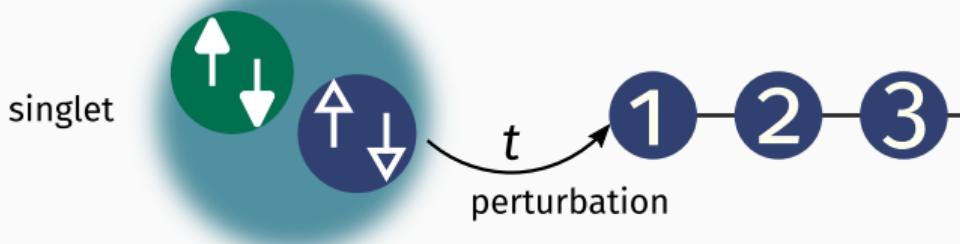
## **Low-energy excitations of the bath**

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## 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...

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

- ✓ 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  $r = -U_b/J_0 \rightarrow \frac{1}{4}$  and  $\Gamma \rightarrow 0$ , 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  $T_K = D^* / k_B$ , 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**  $\Sigma$  and the **quasiparticle residue** behave near the transition?

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- ✓ 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**

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## 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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## **Other Projects**

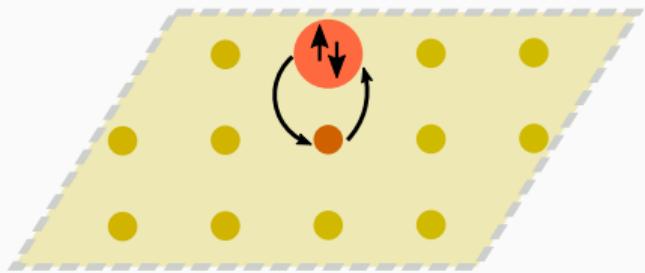
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# Theory for the single-channel Kondo cloud

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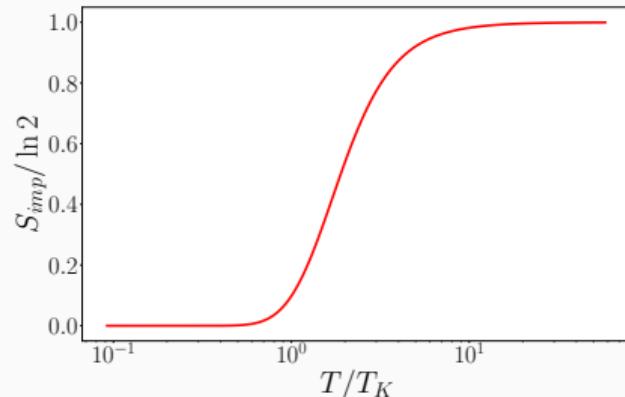
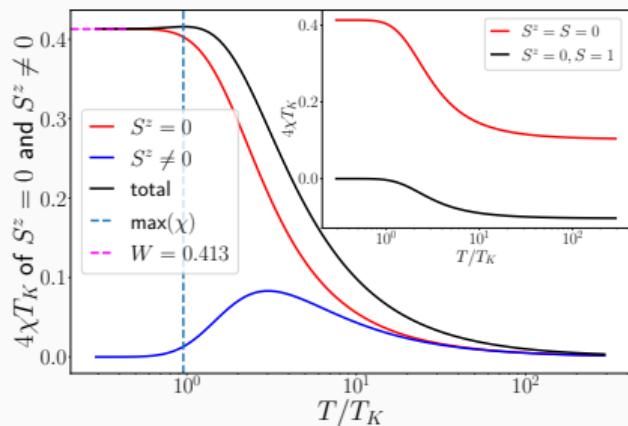
Phys. Rev. B 105, 085119

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



# Theory for the single-channel Kondo cloud

- ✓ spectral function & magnetic susceptibility



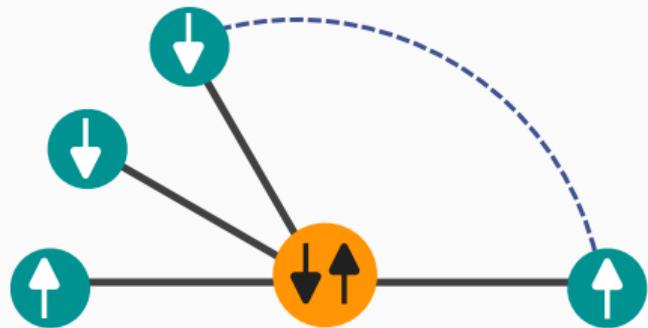
- ✓ local Fermi liq. & orthogonality catastrophe
- ✓ thermal entropy

# Role of degeneracy in the multi-channel Kondo problem

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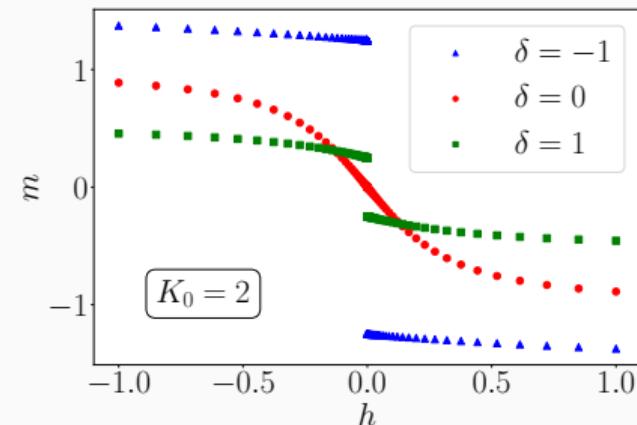
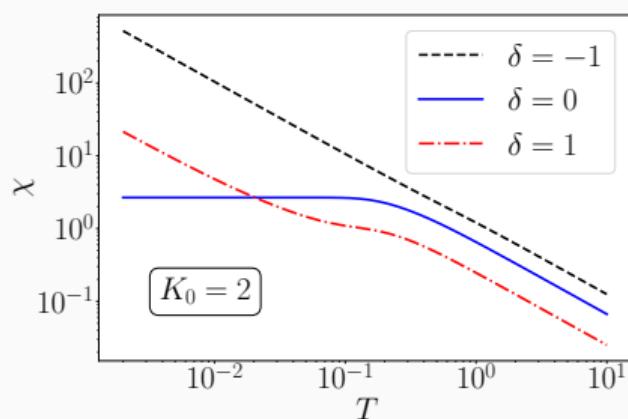
arXiv:2205.00790

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



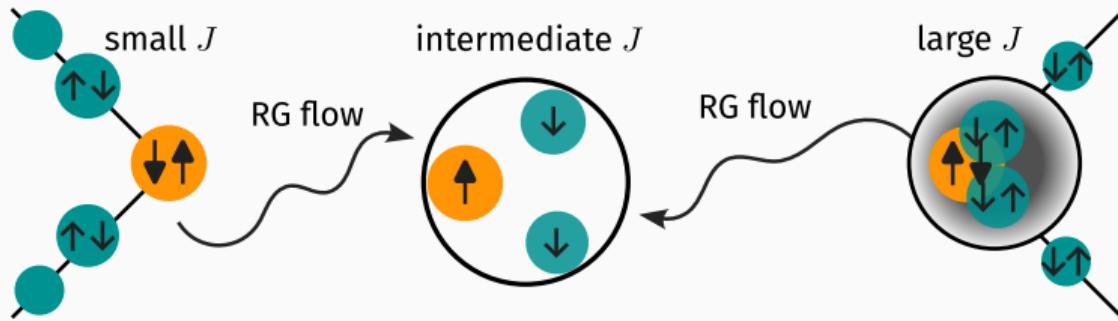
# Role of degeneracy in the multi-channel Kondo problem

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



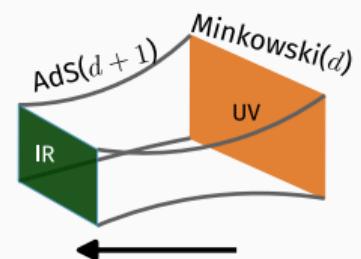
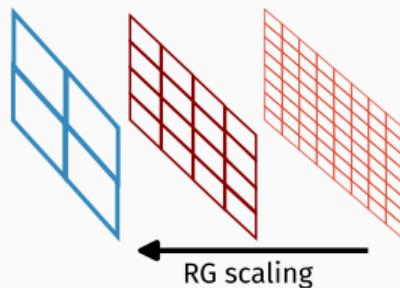
# Role of degeneracy in the multi-channel Kondo problem

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



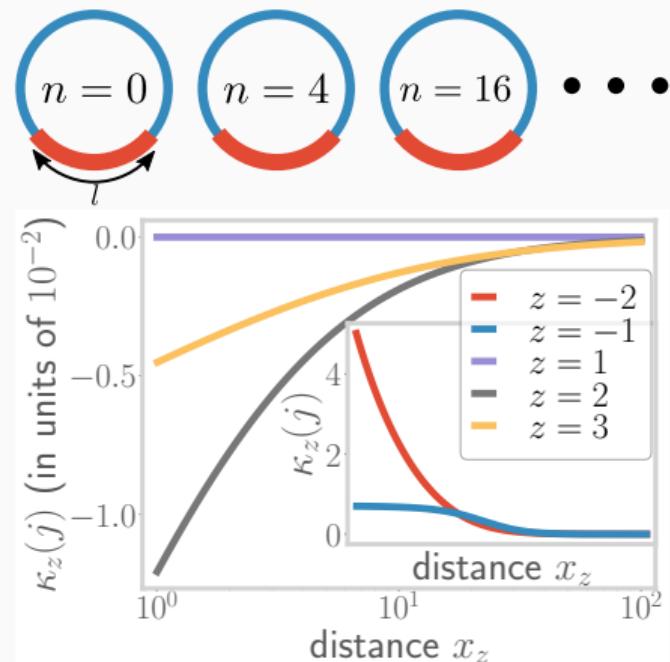
# Entanglement scaling in free fermions: holography & topology

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## 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** =  $\Delta n = 1$

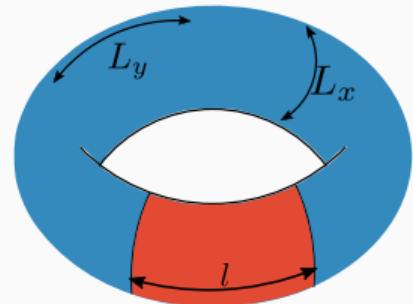
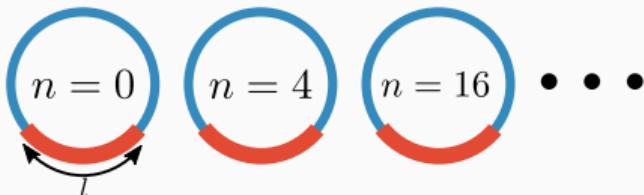
**Simplest** choice: the entire set

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

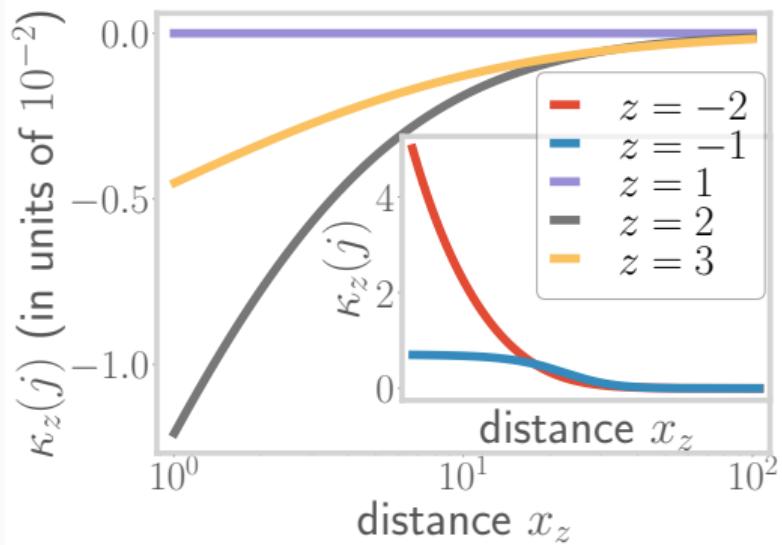
**Mutual information:**  $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$  (non-negative)

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  $\phi$ ,  $\phi = 1$  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