

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

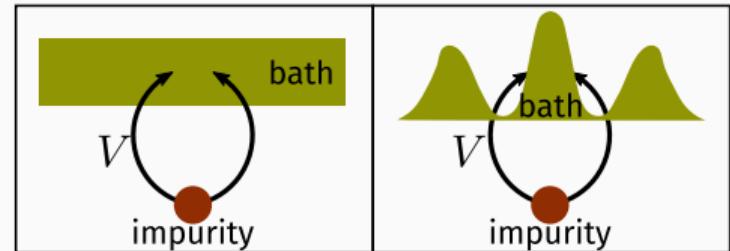
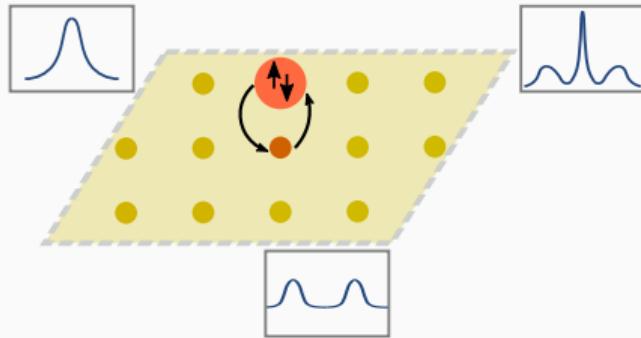
- ✓ Unveiling the Kondo cloud: Unitary renormalization-group study of the Kondo model
Phys. Rev. B 105, 085119, arXiv:2111.10580v3
A. Mukherjee, Abhirup Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, and S. Lal
- ✓ Frustration shapes multi-channel Kondo physics: A star graph perspective
under review at 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*)

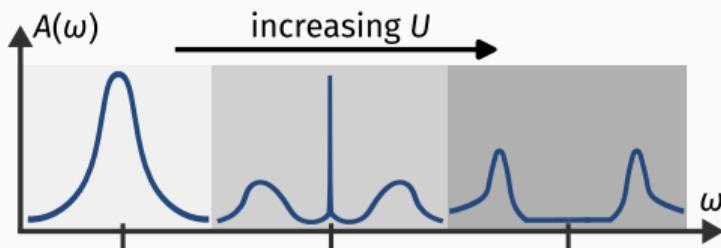
Local MIT in an extended Anderson impurity model



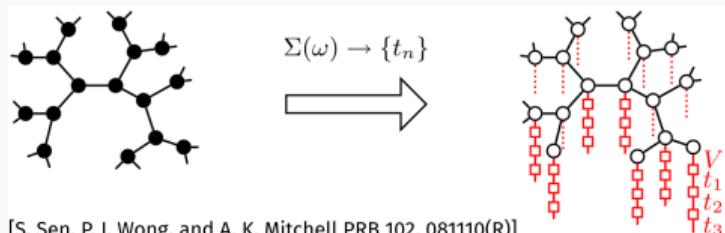
Introducing the extended Anderson impurity model

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

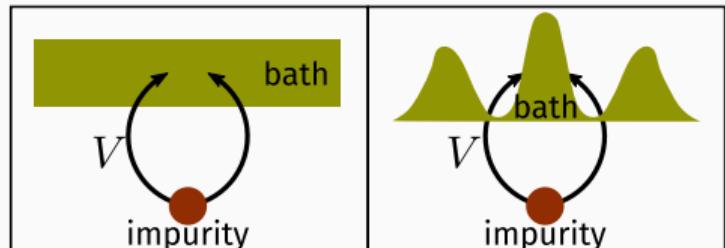
- ✓ shows **metal-insulator transition** on the Bethe lattice with ∞ coordination number



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



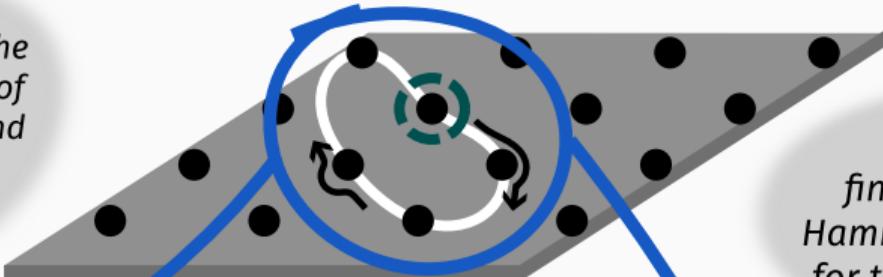
- ✓ Spectral function develops three peaks and then **gaps out**



Metzner et al. 1989; Georges et al. 1992; Parcollet et al. 2004; Maier et al. 2005; Kotliar et al. 2006; Ohashi et al. 2008; Held et al. 2013; Sen et al. 2020.

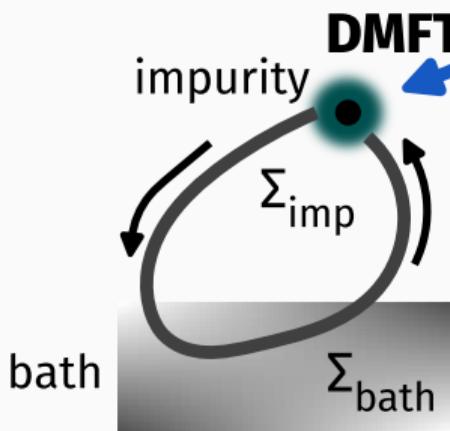
DMFT on the Bethe lattice: Exact in $d = \infty$

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.

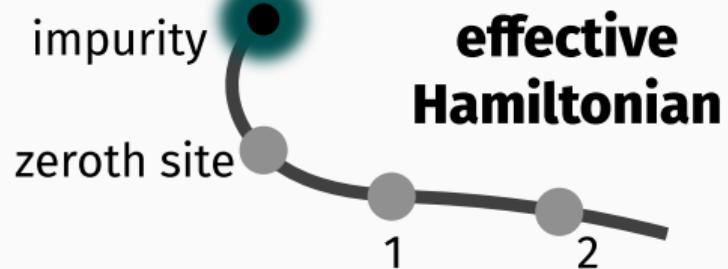


Our Goal:

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



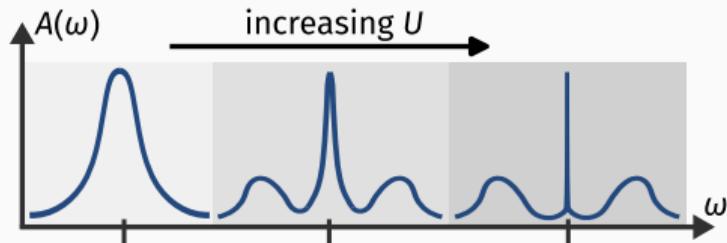
Similar approach adopted by Si & Kotliar for extended Hubbard model



Introducing the extended Anderson impurity model

Standard Anderson impurity model

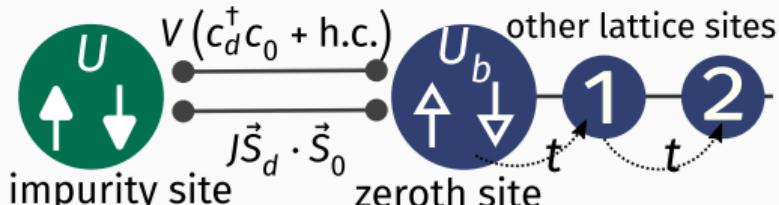
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



Gap in spectral function requires additional physics!

Extended Anderson impurity model

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



Anderson 1961; Anderson 1978; Wilson et al. 1974; Nozieres 1974; Krishna-murthy et al. 1980; Andrei 1980; Tsvelick et al. 1983; Hewson 1993; Costi et al. 1990; Costi 2000; Kuramoto et al. 1987; Cox et al. 1988.

Phase Diagram & Ground-States

Nature of RG flows

- ✓ URG Equations reveal **critical** point at $r = -U_b/J = 1/4$

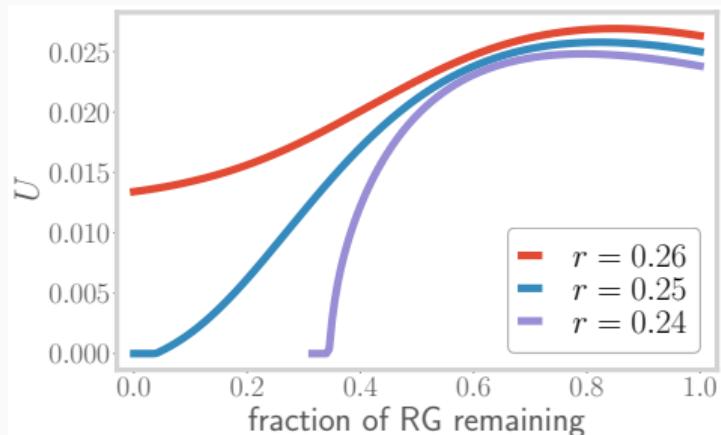
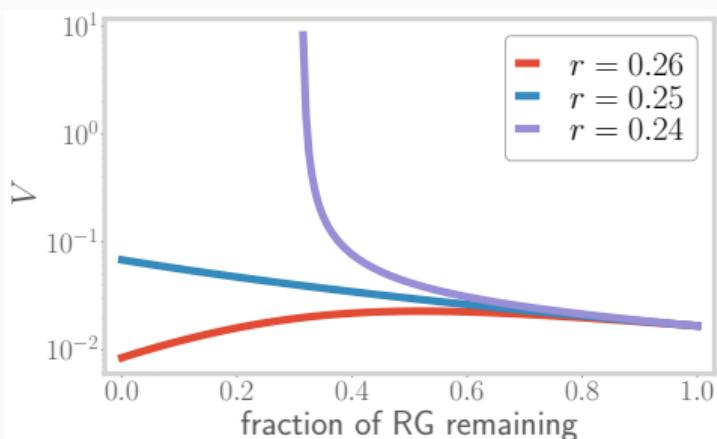
- ✓ RG equation for most dominant coupling J :

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

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

Nature of RG flows

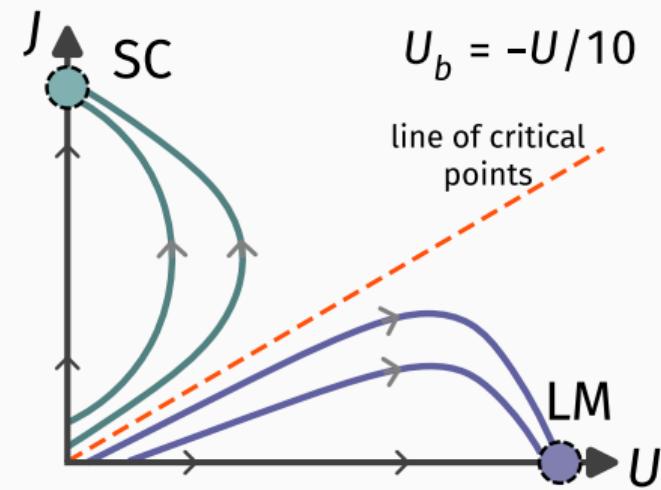
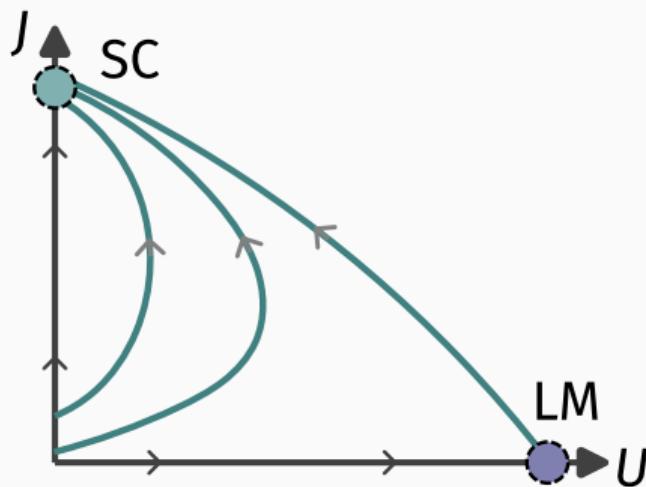
- ✓ Bath correlation U_b is always **marginal**



Nature of RG flows

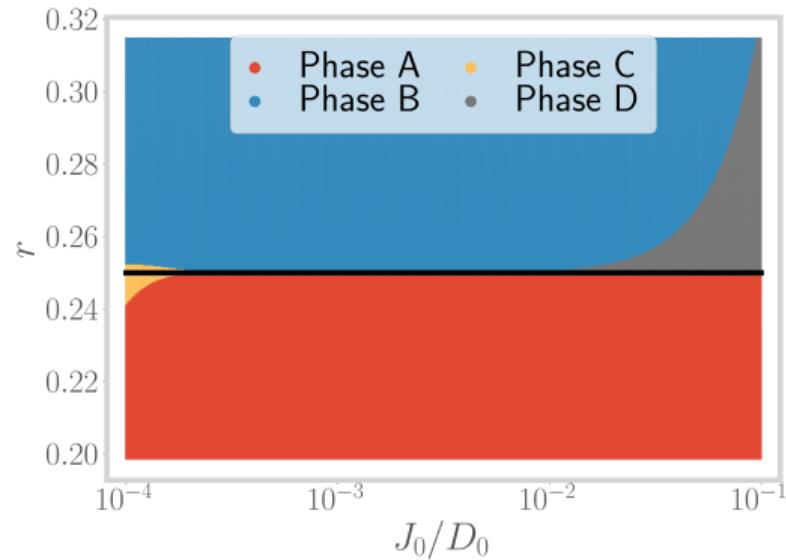
- ✓ RG equation reveals competition between Kondo flow and pairing physics

$$\Delta J = - \underbrace{\frac{(J + 2U_b)^2 n(D)}{\omega - D/2 + U_b/2 + J/4}}_{\text{usual Kondo physics}} + \underbrace{\frac{(2U_b)^2 n(D)}{\omega - D/2 + U_b/2 + J/4}}_{\text{competing pairing physics}}$$



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

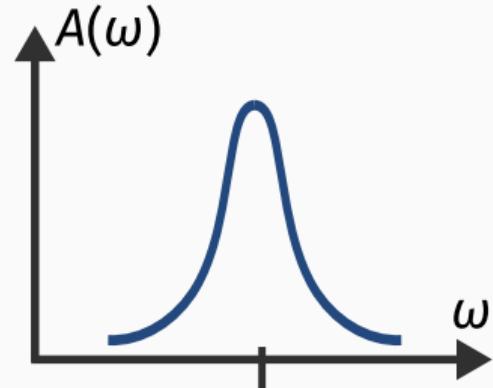


Low-energy effective Hamiltonians and ground-states

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

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

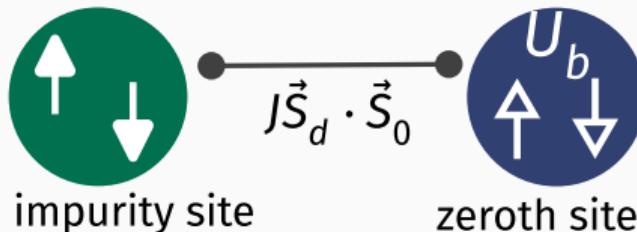
$$H = J \vec{S}_d \cdot \vec{S}_0 - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



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

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

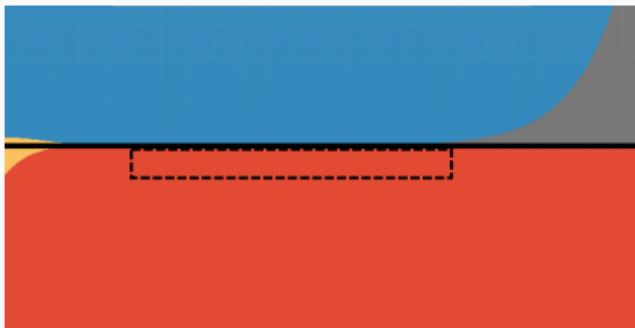
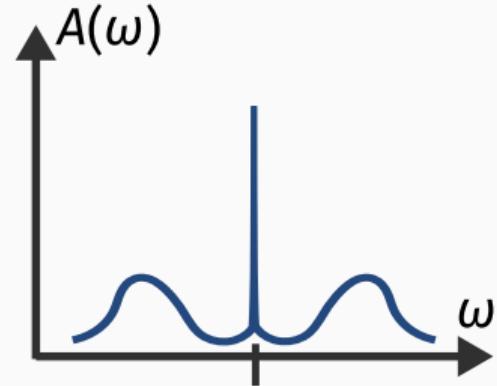


Low-energy effective Hamiltonians and ground-states

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

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

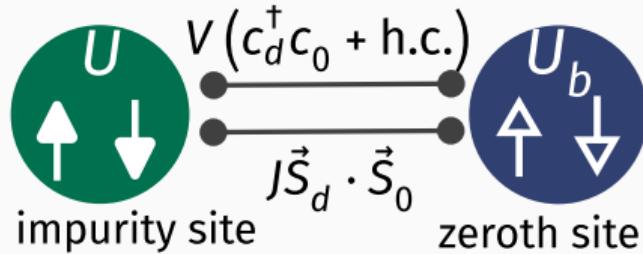
$$H = J\vec{S}_d \cdot \vec{S}_0 + V \sum_{\sigma} (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + \sum_{k < \Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Low-energy effective Hamiltonians and ground-states

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

Zero-bandwidth limit



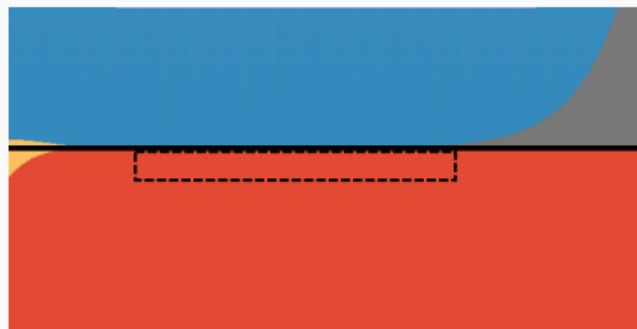
$$H = JS_d \cdot S_0 + V \sum_{\sigma} (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}) - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2$$

✓ **spin+charge** dimer with attractive 0th site

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

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

(1)

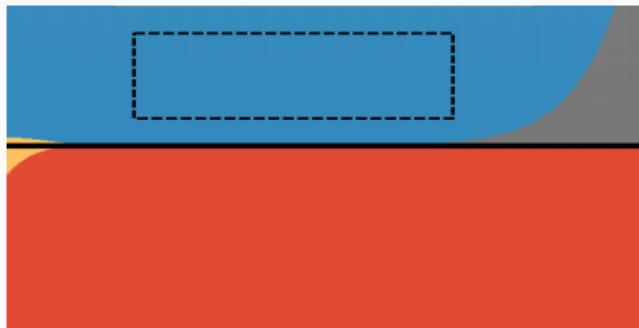
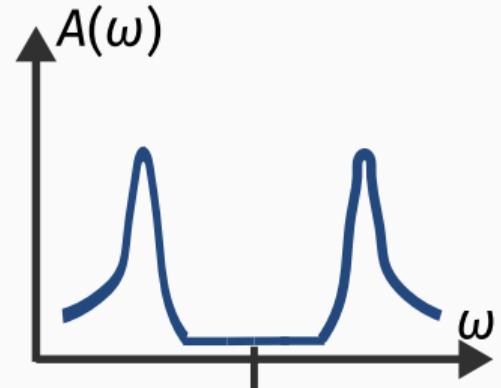


Low-energy effective Hamiltonians and ground-states

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

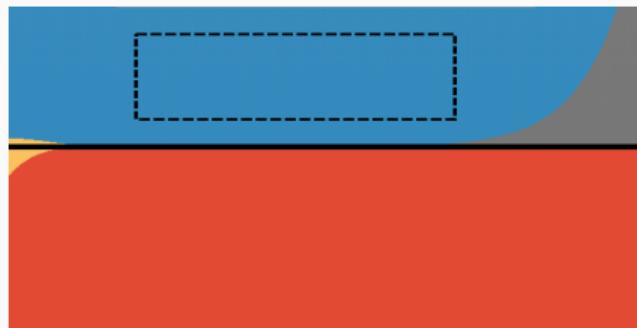


zeroth site

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

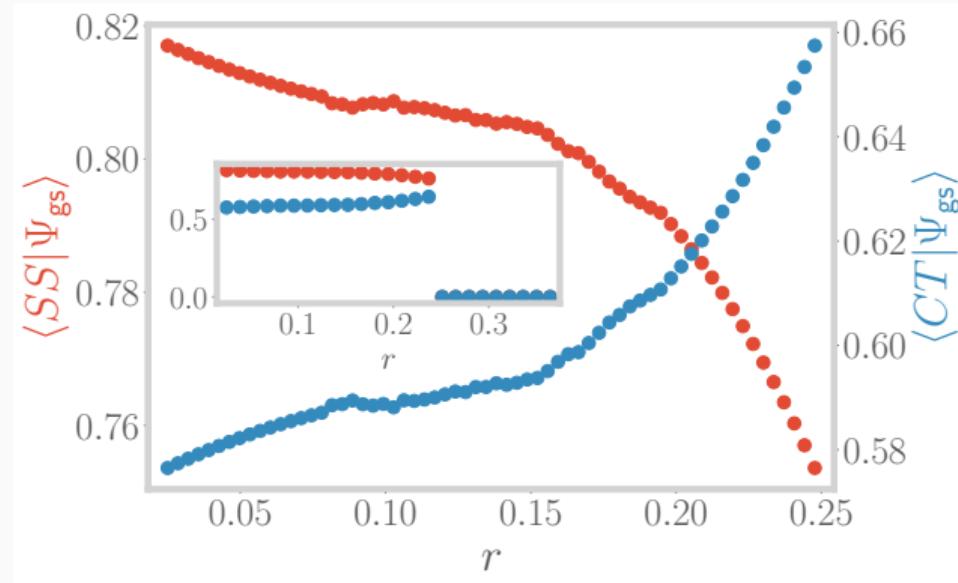
- ✓ impurity site detaches from bath
- ✓ **local moment** ground-state

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



Low-energy effective Hamiltonians and ground-states

Ground-state overlaps with spin singlet and charge triplet zero



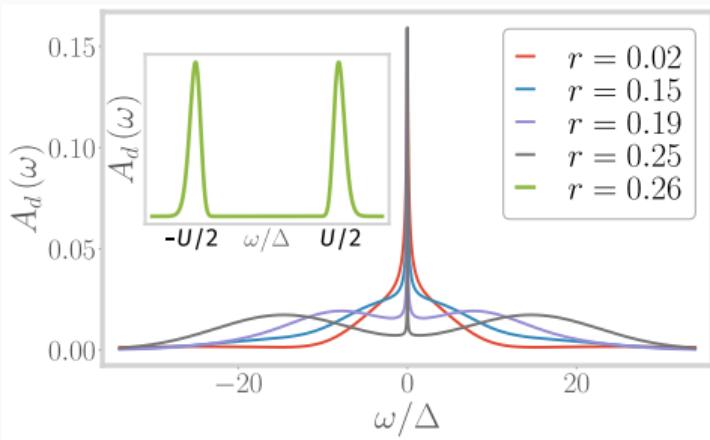
Nature of the Transition

Gapping of the impurity spectral function

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

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

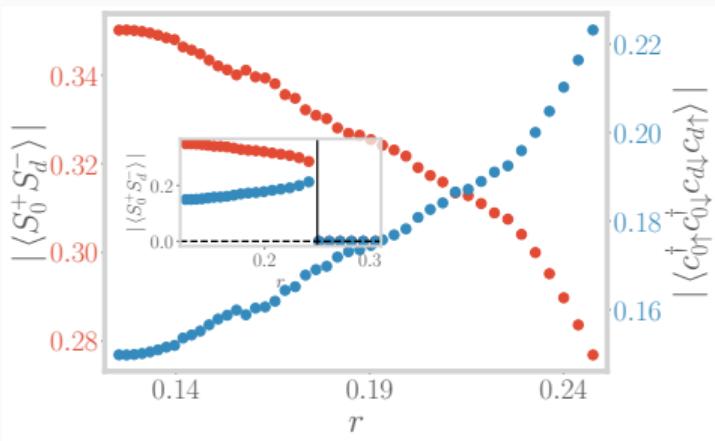
- ✓ hard central **gap** for $|U_b| > J/4$



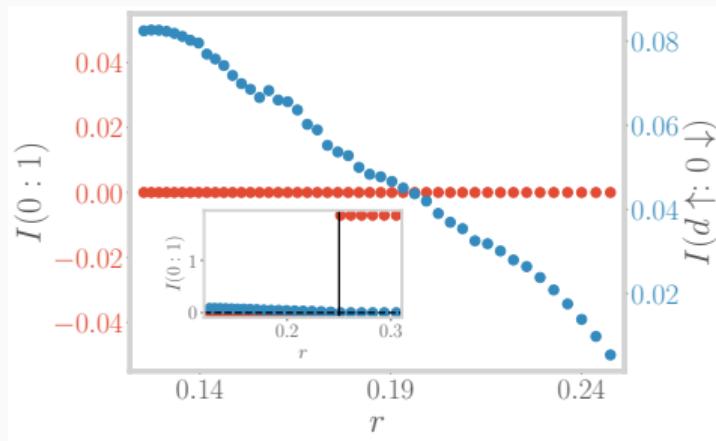
Destruction of the Kondo cloud

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

- ✓ vanishing of impurity-bath correlations



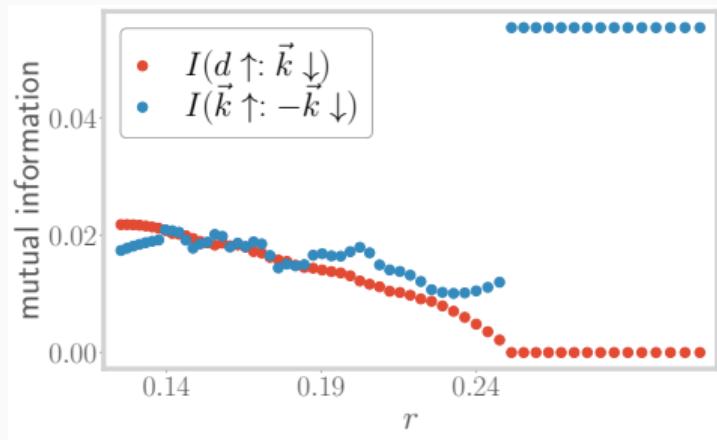
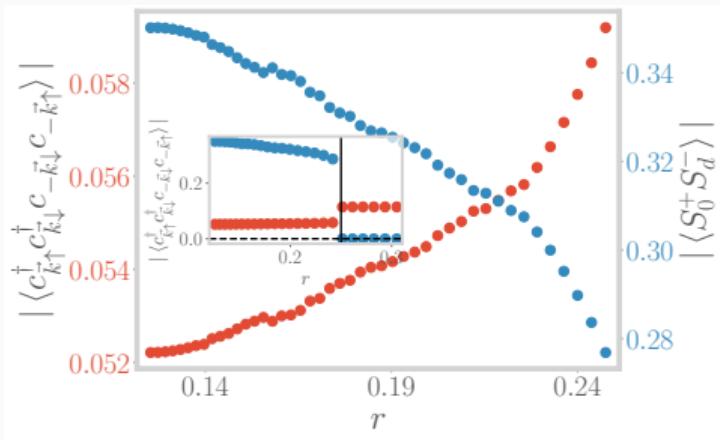
- ✓ transfer of entanglement into the bath



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



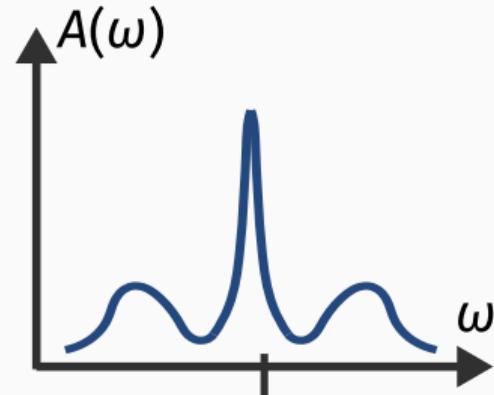
Universal Theory near the Transition

Minimal effective model for the transition

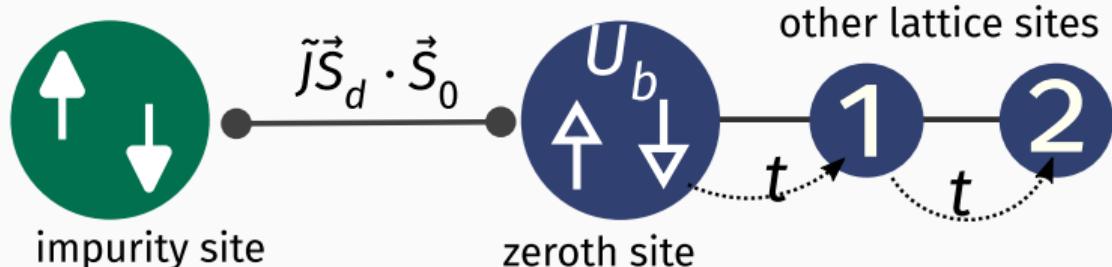
- ✓ For $|U_b| \lesssim J/4$, central peak and side peaks are **well-separated**
- ✓ **Integrate out** charge fluctuations through Schrieffer-Wolff transformation

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

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



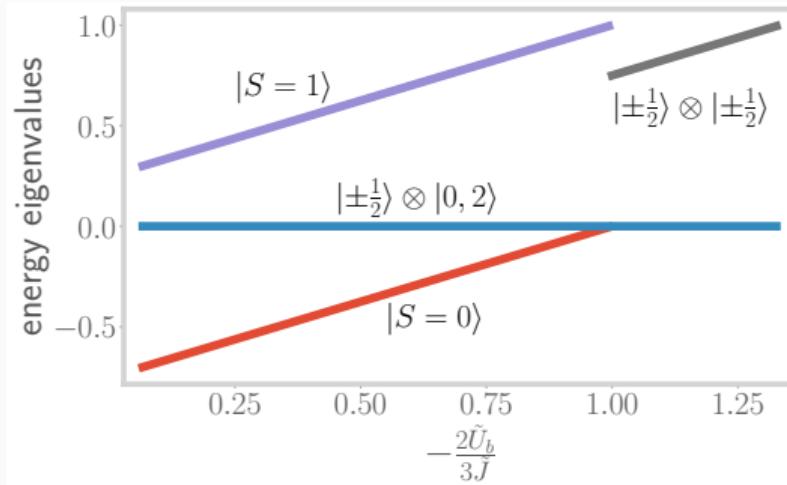
- ✓ **captures** the criticality, and the strong-coupling and local moment phases



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

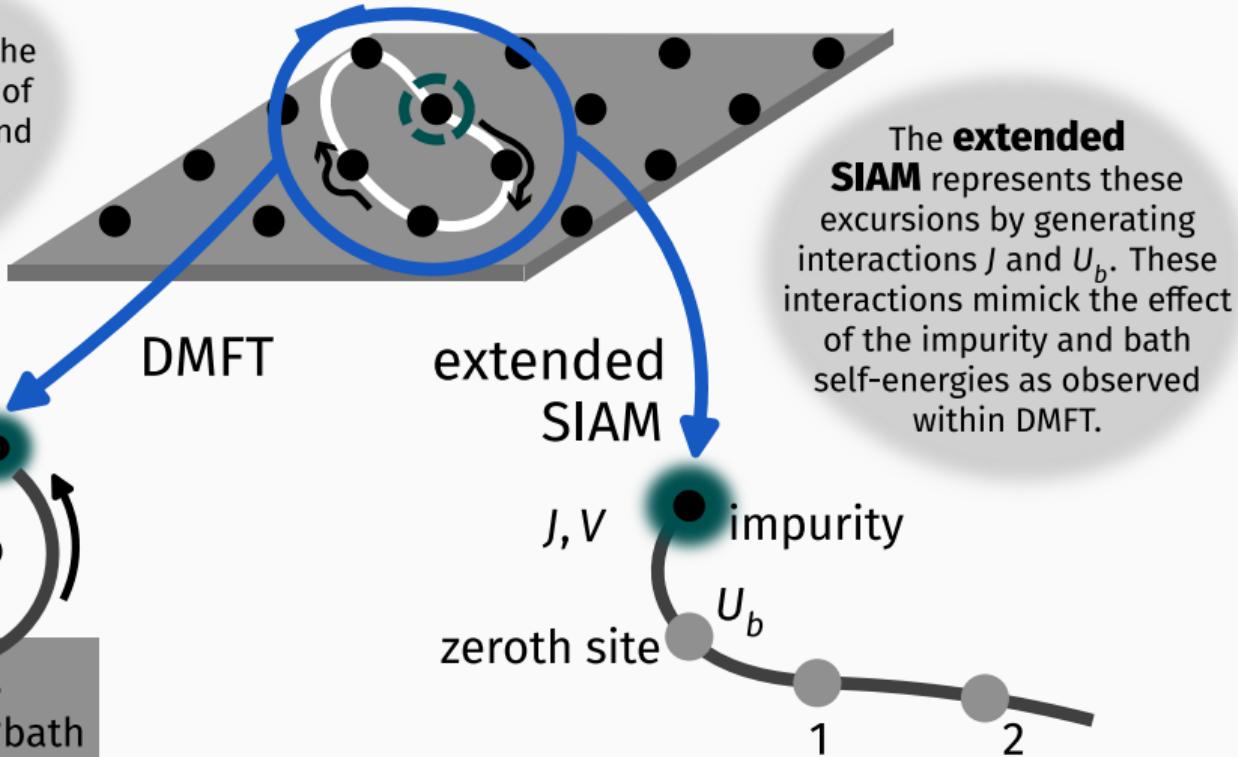
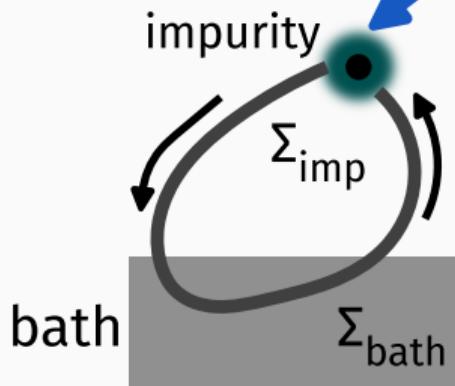
- ✓ Obtain two-site model by taking **zero bandwidth** limit
- ✓ spectrum shows **level crossing** between singlet and local moment states



Insights into DMFT

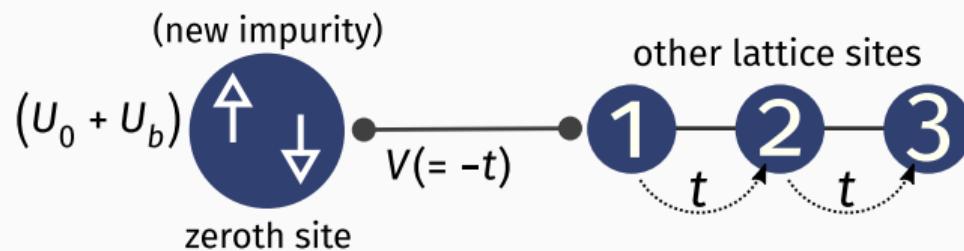
Extended SIAM in the context of DMFT

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.



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

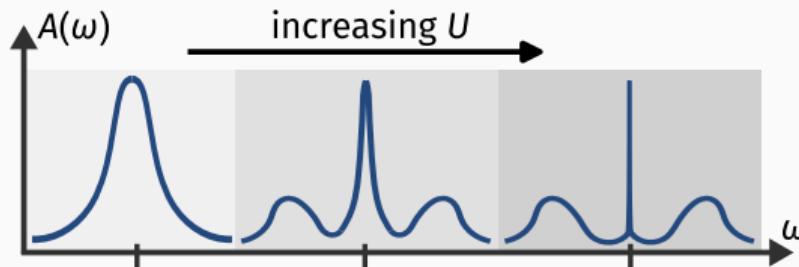


- ✓ J is relevant and the largest scale → **repulsive correlation:**

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

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

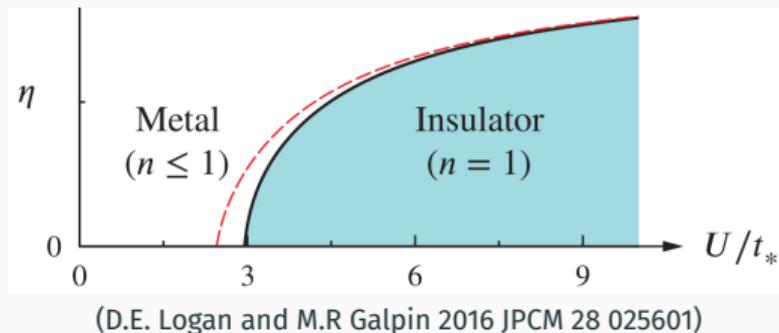


Essence of **self-consistency**: Equivalence of impurity and zeroth sites!

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



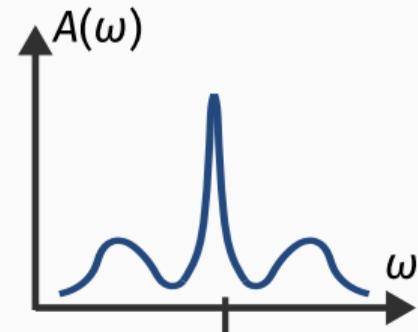
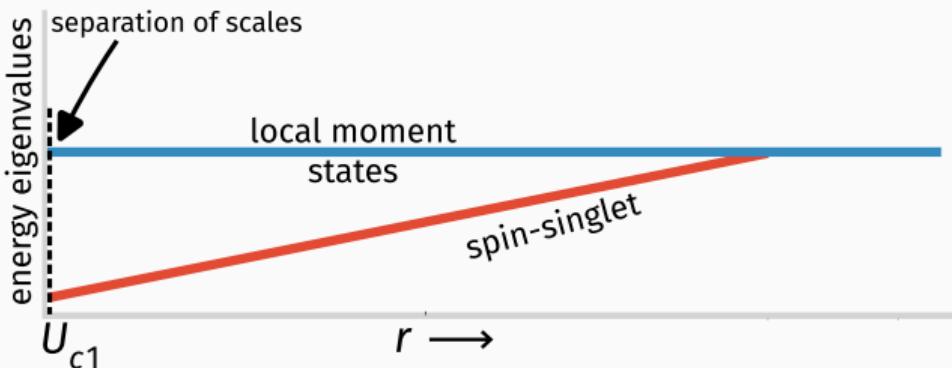
(D.E. Logan and M.R Galpin 2016 JPCM 28 025601)

- ✓ 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

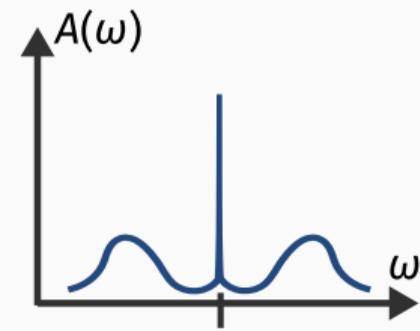
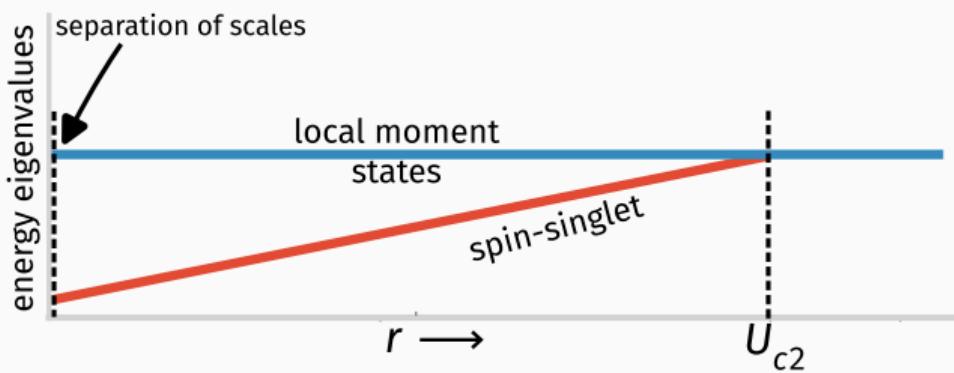
- ✓ Initial point is when the side peaks get separated (near-zeroes in the spectral function)



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

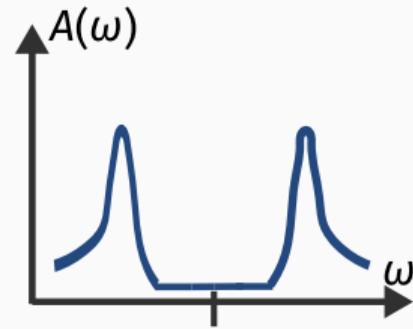
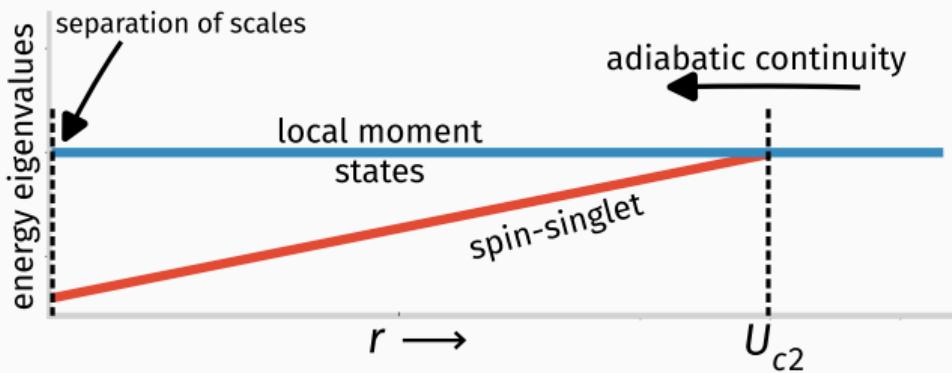
- ✓ U_{c2} is the point where the levels cross



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

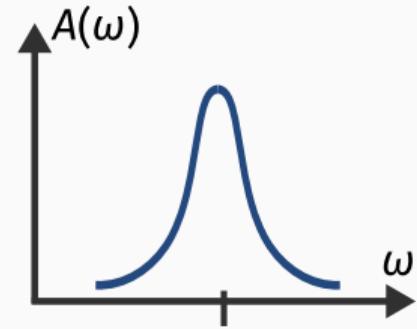
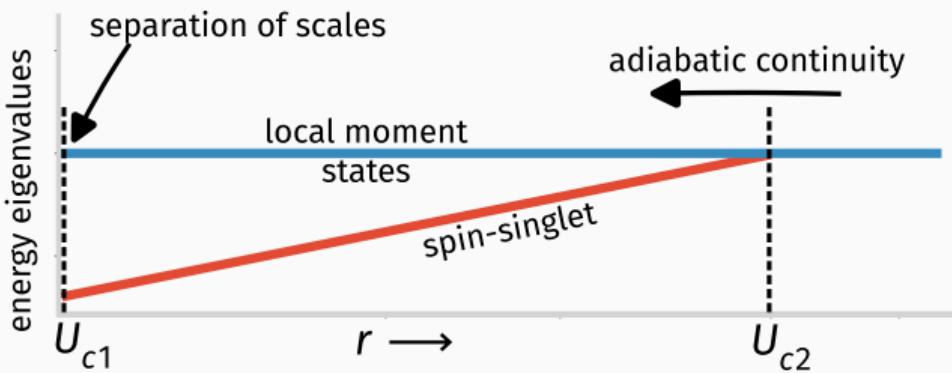
- ✓ Coming from $U > U_{c2}$, **adiabatic continuity** allows DMFT to stay on the local moment state...



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

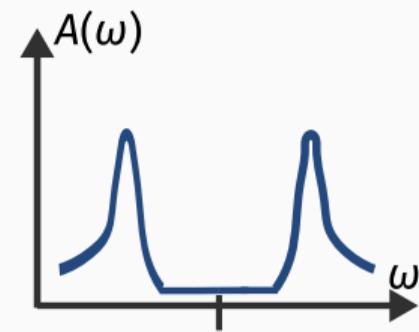
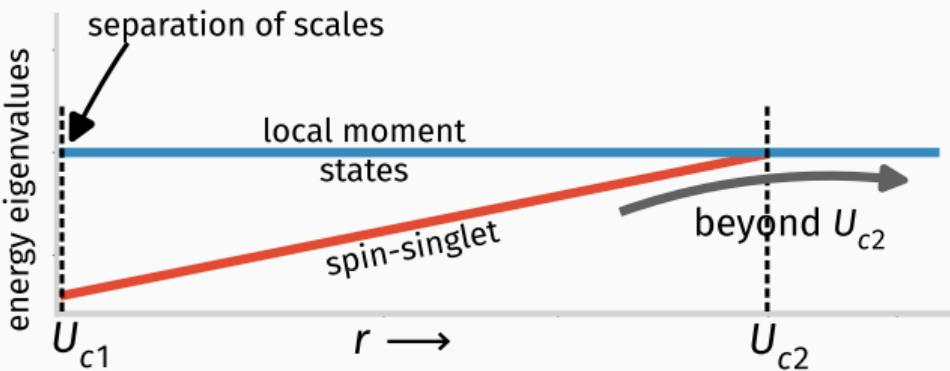
- ✓ For $U < U_{c1}$, local moment state is too unstable, relaxes to the true ground state.



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



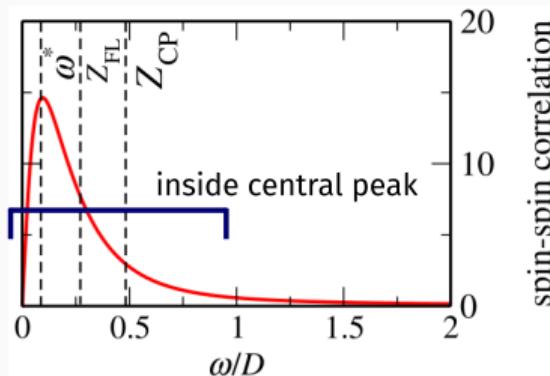
Comparison against NRG-DMFT correlation functions

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

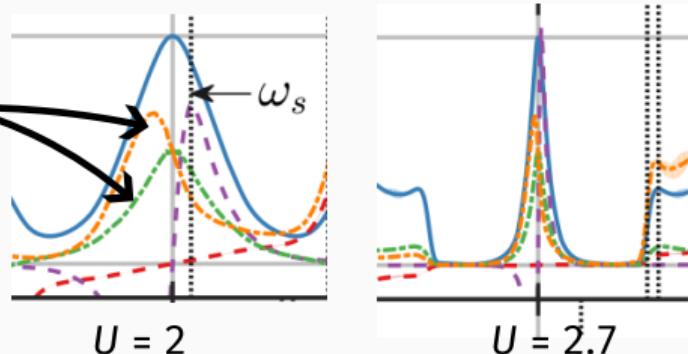
Doublon-holon correlators of the Hubbard model

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

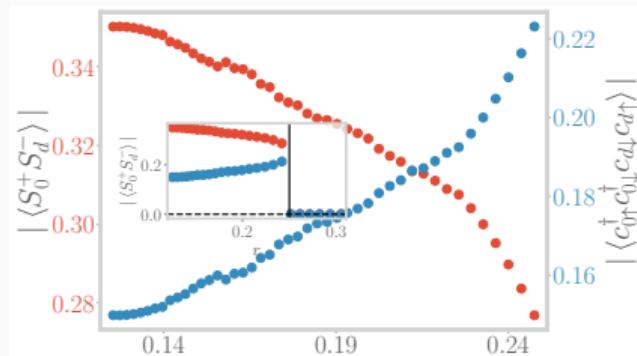
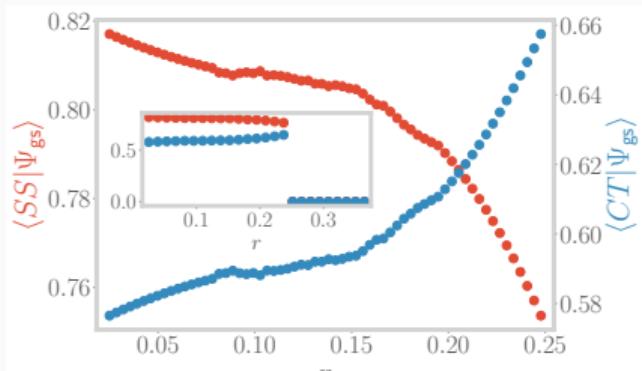
Lee et. al show **peaks** in doublon-holon correlators near zero energy within the central Kondo peak.

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**.

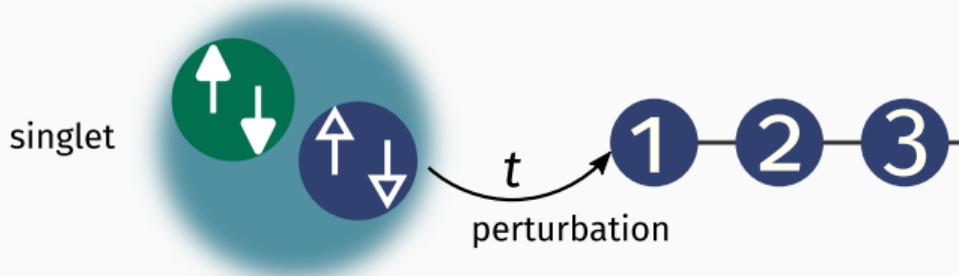


Low-energy excitations of the bath

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 $r = -U_b/J_0 \rightarrow \frac{1}{4}$ 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** 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 :

$$Z \sim T_K$$

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

Effective Hamiltonian at the critical point

What is the nature of the low-energy excitations exactly at the critical point?

- ✓ Singlets become degenerate with local moment states at the critical point - **degenerate perturbation theory**.

- ✓ Hopping perturbation reduces degeneracy to 4-fold:

$$(N_{\text{tot}}, S_{\text{tot}}^z) = (2, 0), (3, 1/2), (3, -1/2), (4, 0)$$

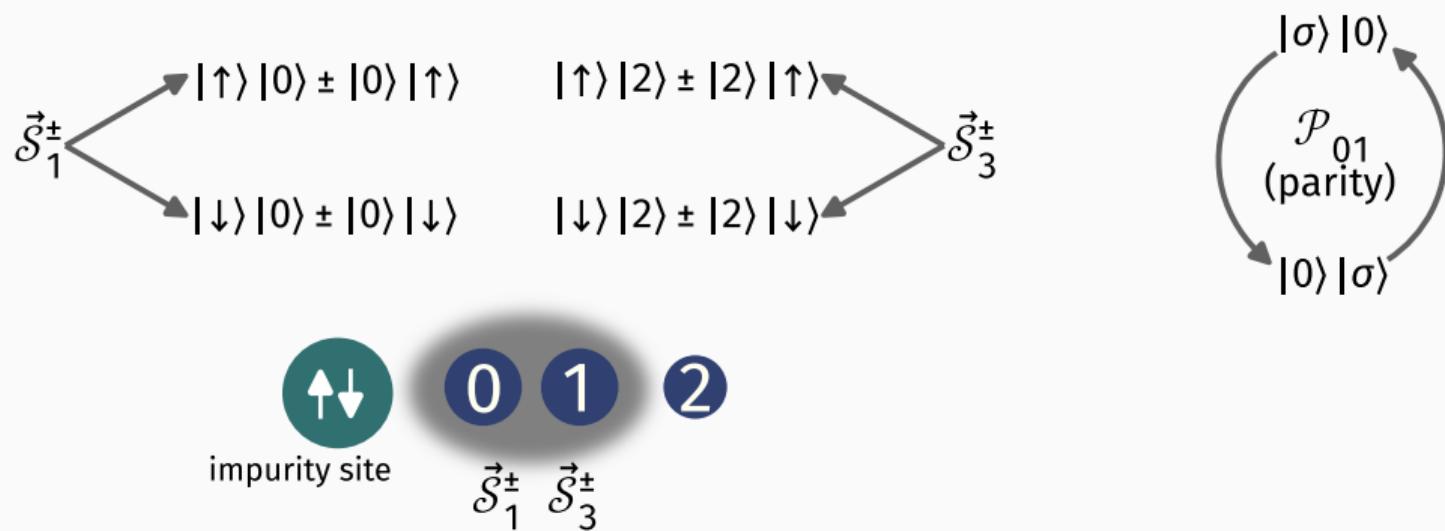
- ✓ Non-vanishing degeneracy will lead to critical correlations and **non-Fermi** liquid physics

Effective Hamiltonian at the critical point

What is the nature of the low-energy excitations exactly at the critical point?

- ✓ $S_{\text{tot}}^z = 0$ first order effective Hamiltonian acquires quasi non-local terms:

$$H_{\text{eff}} = t \vec{S}_d \cdot (\vec{\mathcal{S}}_1^- + \vec{\mathcal{S}}_3^- - \vec{\mathcal{S}}_1^+ - \vec{\mathcal{S}}_3^+) + \frac{t}{4} \mathcal{P}_{01} + H_{\text{K.E.}}$$



Effective Hamiltonian at the critical point

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- ✓ Spreading of bath spin indicates stretching of singlet in real space



- ✓ Shows the dispersion of entanglement across the lattice at critical point. Precursor to decoupling of impurity spin.

Broad conclusions

- ✓ The extended SIAM appears to capture the phenomenology of 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.

Broad conclusions

- ✓ An **emergent self-consistency** is achieved through the qualitative similarity of the spectral functions of the impurity and zeroth sites.
- ✓ Approach towards criticality is marked by **vanishing** metallic energy scale and quasiparticle residue.
- ✓ **Non-Fermi liquid** physics arises at critical point, through the expansion of the singlet into the next lattice site.

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).

Acknowledgements

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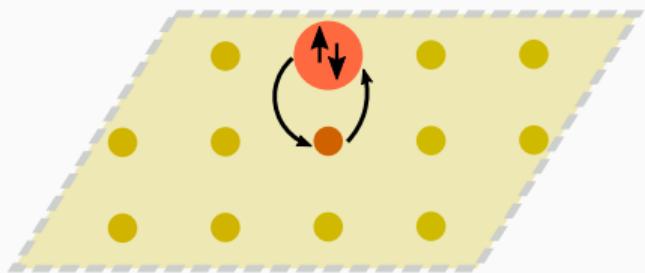
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Other Projects

Theory for the single-channel Kondo cloud

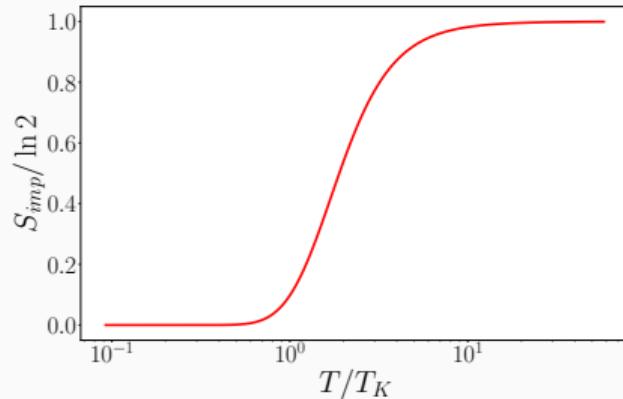
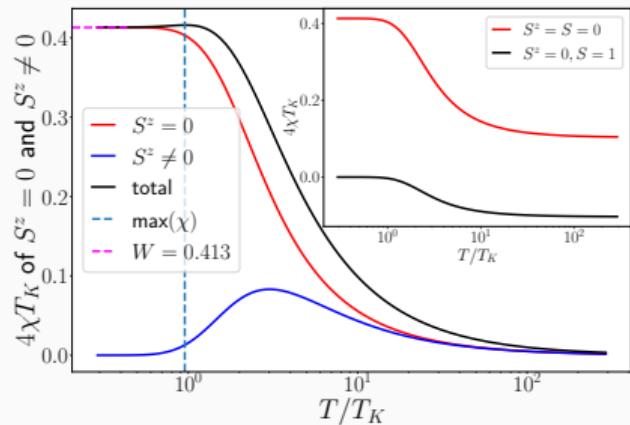
Phys. Rev. B 105, 085119

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



Theory for the single-channel Kondo cloud

- ✓ spectral function & magnetic susceptibility



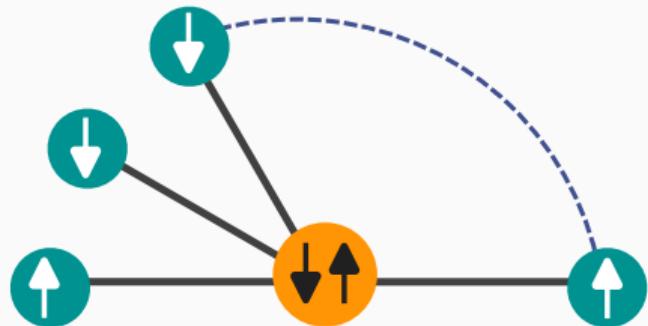
- ✓ local Fermi liq. & orthogonality catastrophe
- ✓ thermal entropy

Kondo 1964; Wilson 1975; Andrei et al. 1983; Hewson 1993; Nozieres 1974; Anderson 1970; Tsvelick et al. 1983; Affleck et al. 1993; Goldhaber-Gordon et al. 1998; V. Borzenets et al. 2020; Sakai et al. 1989; Costi et al. 1990; Nozaki et al. 2012; Affleck 1995.

Role of degeneracy in the multi-channel Kondo problem

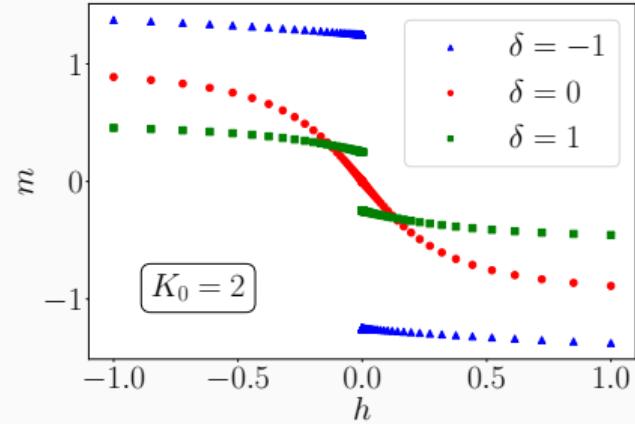
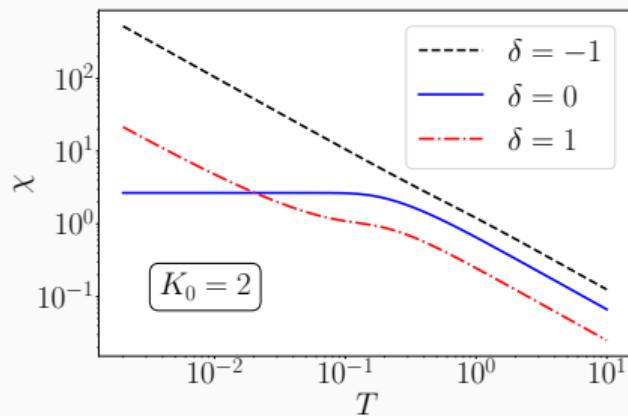
arXiv:2205.00790

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



Role of degeneracy in the multi-channel Kondo problem

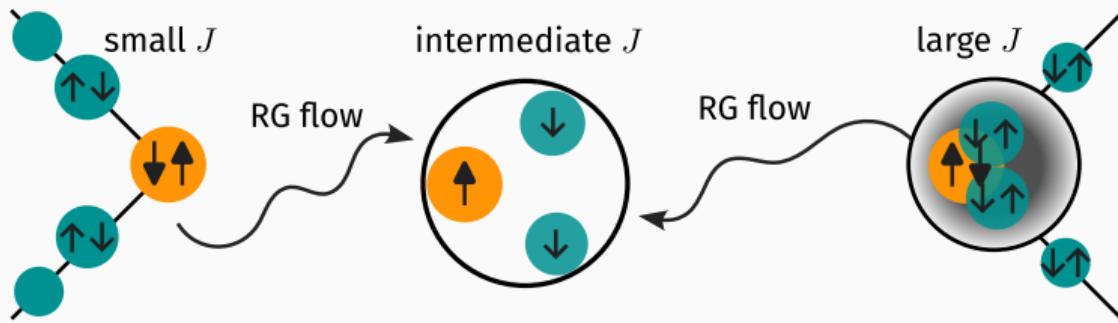
- ✓ Intermediate-coupling RG fixed point Hamiltonian and **degenerate** ground states
- ✓ Degree of compensation, magnetization and susceptibility show **incomplete screening**



Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

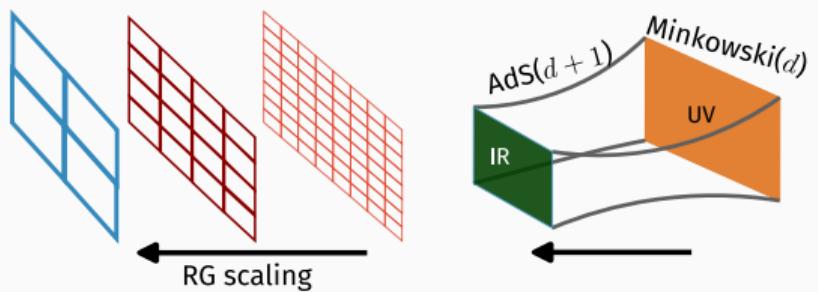
Role of degeneracy in the multi-channel Kondo problem

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



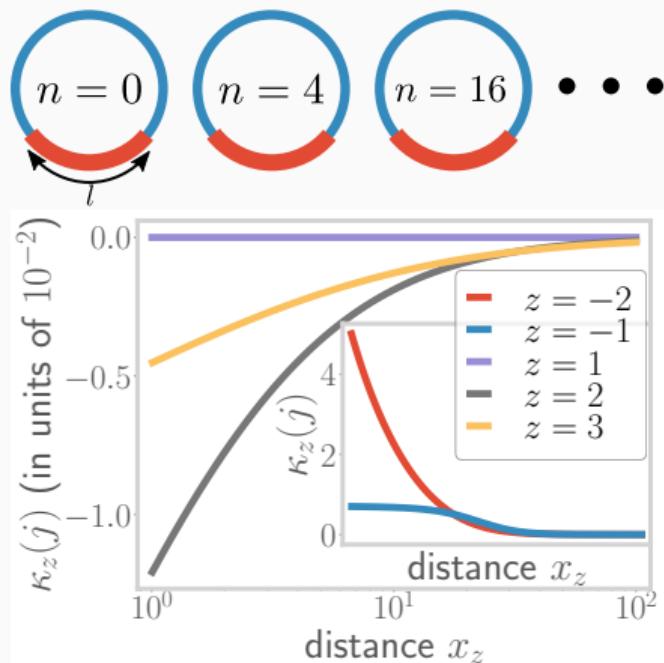
Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

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: $k_x^n = \frac{2\pi}{L_x} n, \quad n \in \mathbb{Z}; \quad \text{define sparsity} = \Delta n = 1$

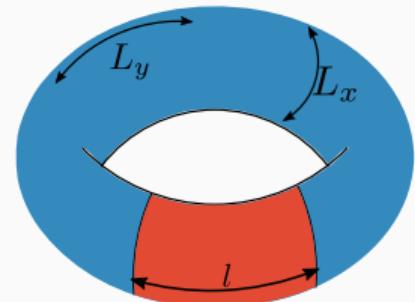
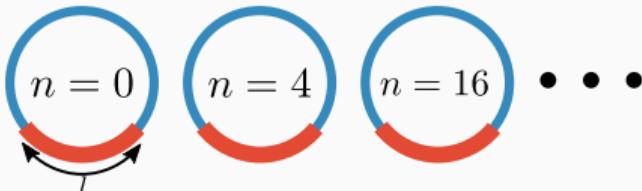
Simplest choice: the entire set

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

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

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



- ✓ 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

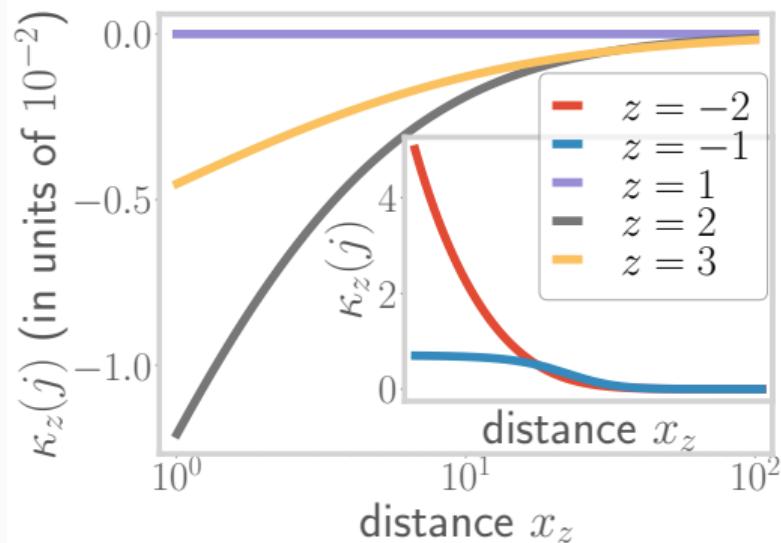
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

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

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

- ✓ $Q(\phi)$ 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