Local metal-insulator transition in an extended Anderson impurity model

JRF-to-SRF Upgradation Presentation

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August 20, 2022

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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

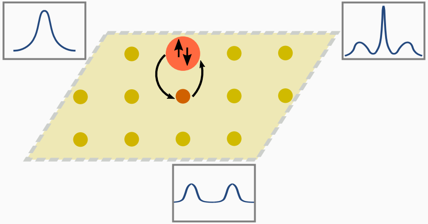
Ongoing Projects

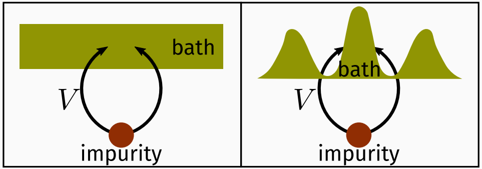
✓ Metal-insulator transition in an extended Anderson impurity model (*manuscript in preparation*)

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

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

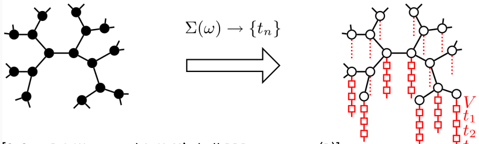
Local MIT in an extended Anderson impurity model





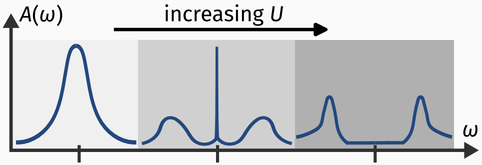
Introducing the extended Anderson impurity model

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



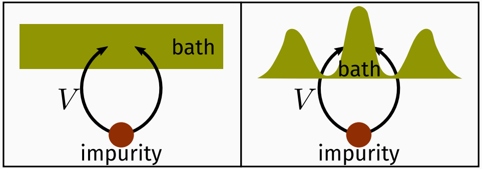
[S. Sen, P. J. Wong, and A. K. Mitchell PRB 102, 081110(R)]

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



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

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



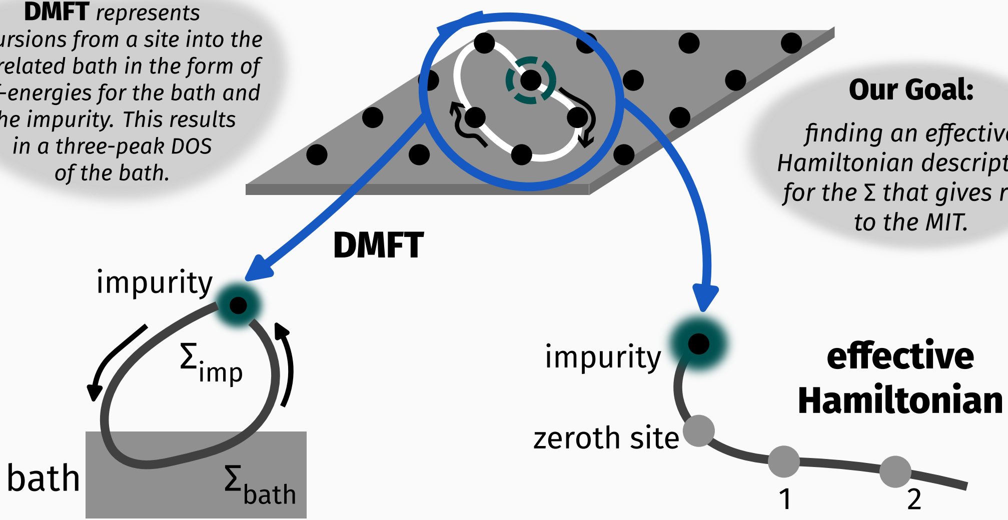
Metzner et al. 1989; Georges et al. 1992; Parcollet et al. 2004; Maier et al. 2005; Kotliar et al. 2006; Ohashi et al. 2008; Held et al. 2013; Sen et al. 2020.

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:

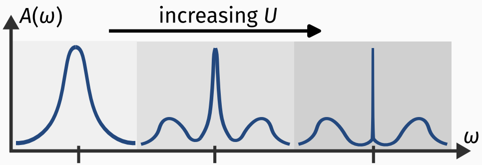
finding an effective Hamiltonian description for the Σ that gives rise to the MIT.



Introducing the extended Anderson impurity model

Standard Anderson impurity model

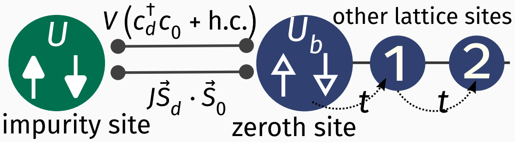
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



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.

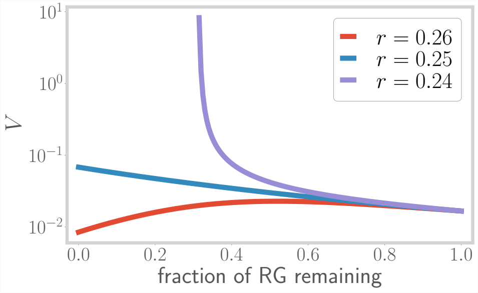
Phase Diagram & Ground-States

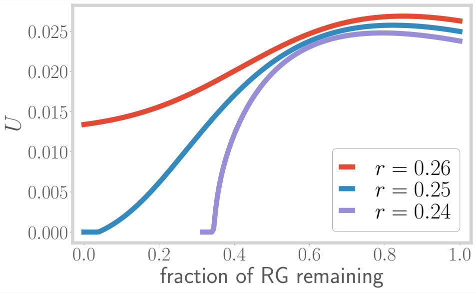
Nature of RG flows

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

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

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





RG Phase Diagram

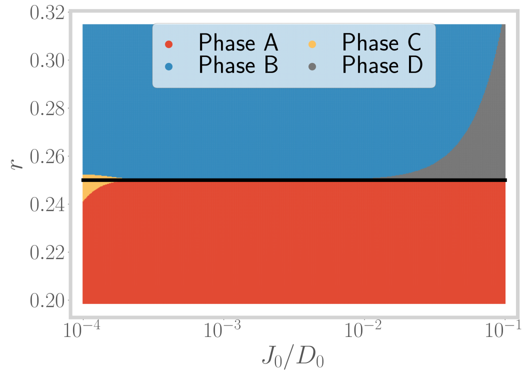
✓ blue phase ⟶ $U_b < -J/4$: V, J are **irrelevant** ⟶ local moment flows

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

vanishes for large systems

✓ gray phase: $J \sim D_0$: **all** couplings irrelevant

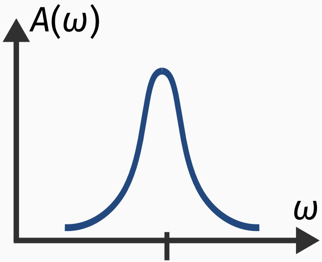
vanishes for large systems



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

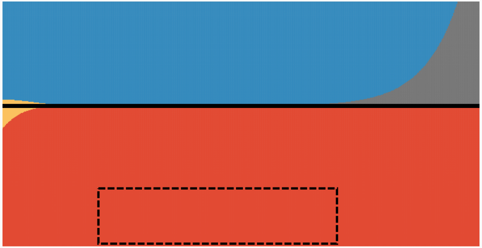
Low-energy effective Hamiltonians and ground-states

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



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

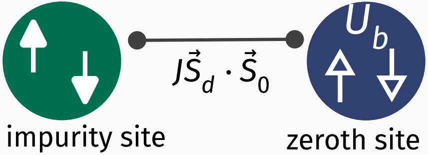
$$H = J\vec{S}_d \cdot \vec{S}_0 - U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2 + \sum_{k<\Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Low-energy effective Hamiltonians and ground-states

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

Zero-bandwidth limit

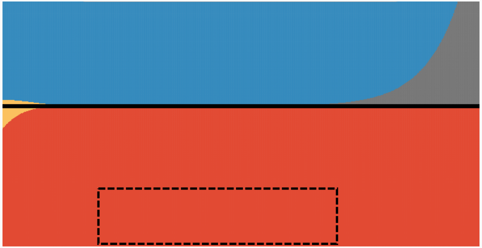


$$H = J\vec{S}_d \cdot \vec{S}_0 - U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2$$

✓ two-spin Heisenberg, attractive zeroth site

✓ **singlet** ground state

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

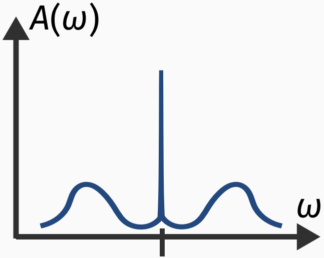


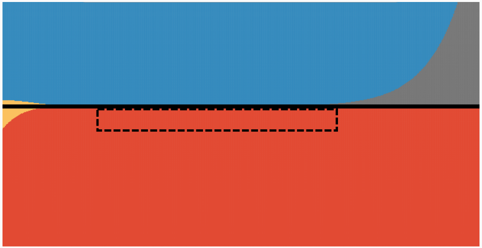
Low-energy effective Hamiltonians and ground-states

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

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

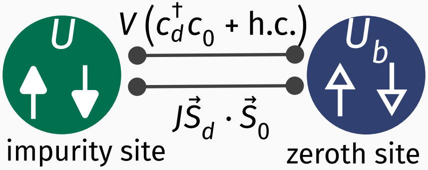
$$H = J\vec{S}_d\cdot\vec{S}_0 + V\sum_\sigma\left(c^\dagger_{d\sigma}c_{0\sigma} + \text{h.c.}\right) - U_b\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2 + \sum_{k<\Lambda^*}\epsilon_k\hat{n}_{k\sigma}$$





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

Zero-bandwidth limit

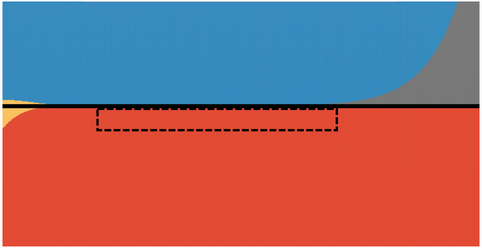


$$H = J\vec{S}_d\cdot\vec{S}_0 + V\sum_\sigma\left(c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}\right) - U_b\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2$$

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

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

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

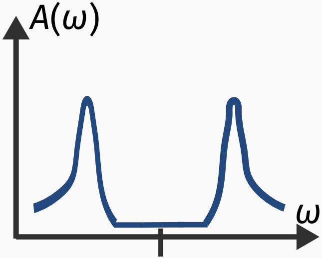


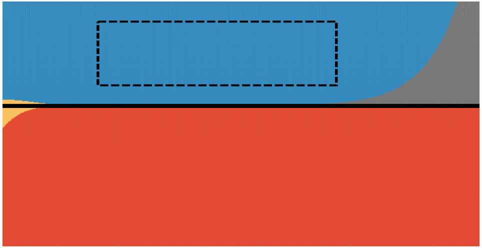
Low-energy effective Hamiltonians and ground-states

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

- ✓ J, V irrelevant,
- ✓ U relevant,

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

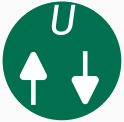




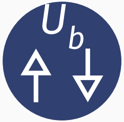
Low-energy effective Hamiltonians and ground-states

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

Zero-bandwidth limit



impurity site

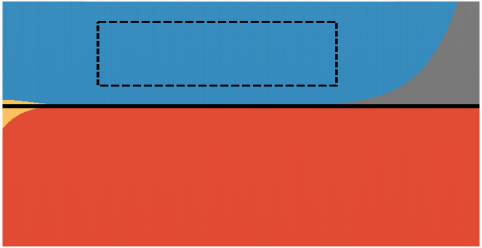


zeroth site

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

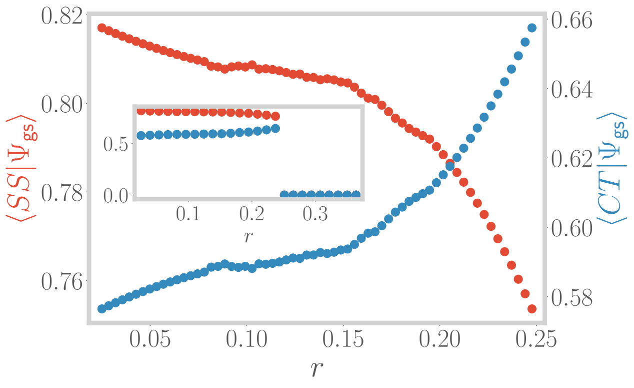
- ✓ impurity site detaches from bath
- ✓ **local moment** ground-state

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



Low-energy effective Hamiltonians and ground-states

Ground-state overlaps with spin singlet and charge triplet zero

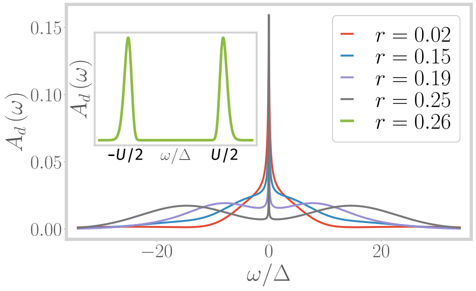


Nature of the Transition

Gapping of the impurity spectral function

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

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

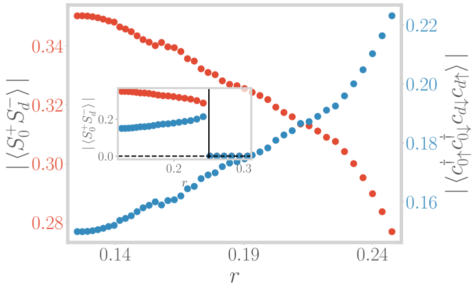


✓ hard central **gap** for $|U_b| > J/4$

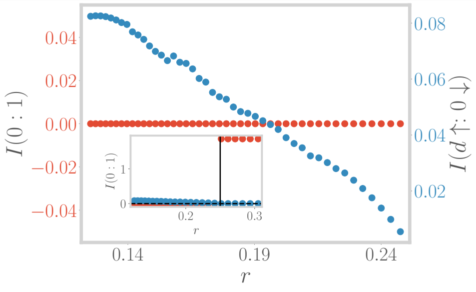
Destruction of the Kondo cloud

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

✓ vanishing of impurity-bath correlations



✓ transfer of entanglement into the bath

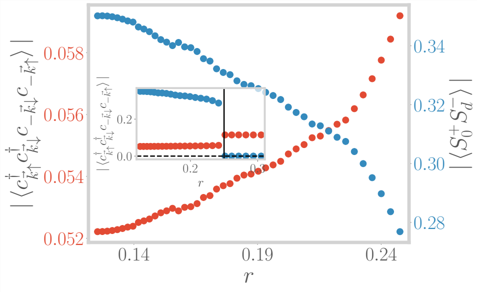


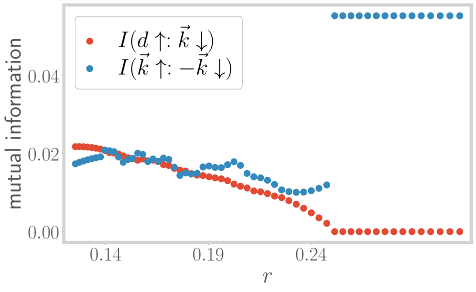
Growth of pairing fluctuations in the bath

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

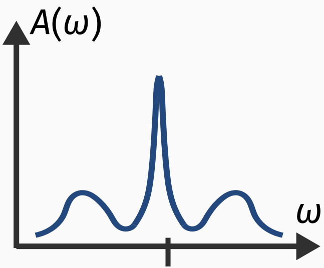
Minimal effective model for the transition

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

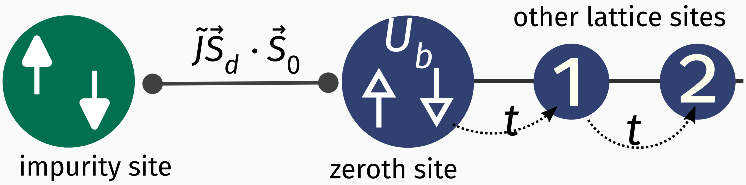
✓ **Integrate out** charge fluctuations through Schrieffer-Wolff transformation

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

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



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

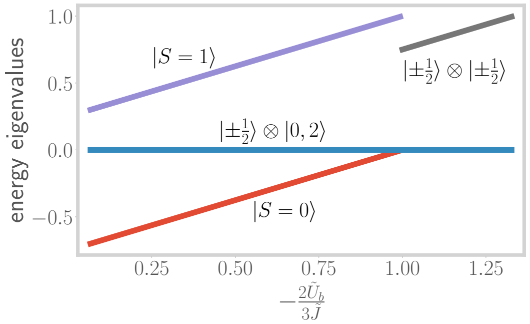


Suggests that ***J* and U_b are the minimal & universal ingredients** for transition!

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

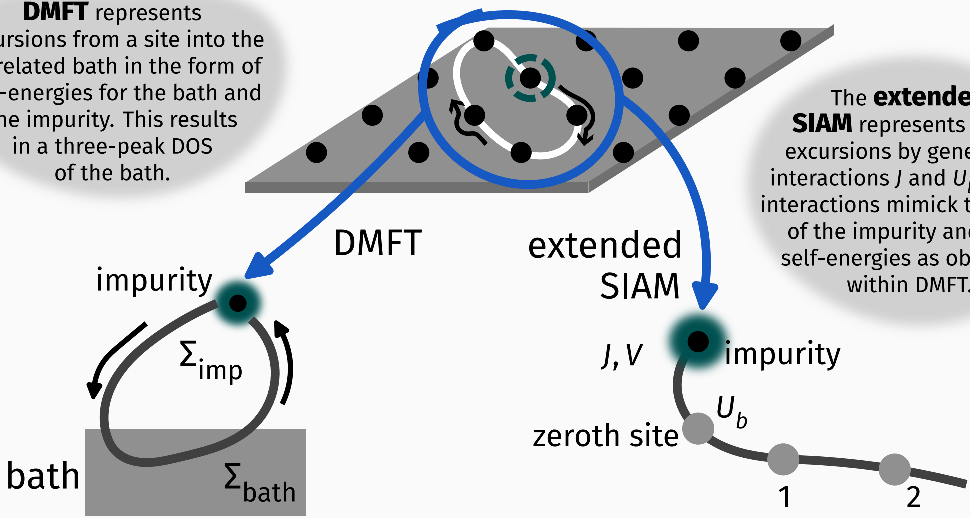


Insights into DMFT

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.

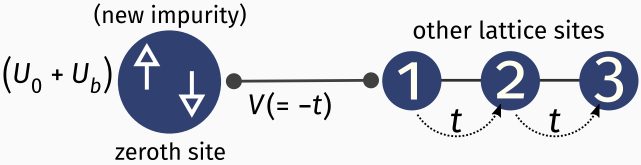
The **extended SIAM** represents these excursions by generating interactions J and U_b. These interactions mimick the effect of the impurity and bath self-energies as observed within DMFT.



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 $\longrightarrow$ **repulsive correlation**:

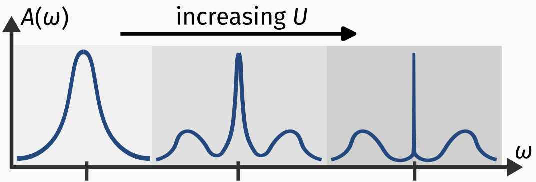
$$U_0 + U_b \simeq J > 0$$

Moeller et al. 1995.

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

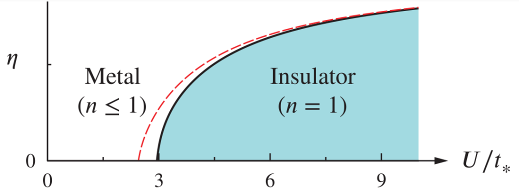


Essence of self-consistency: Equivalence of impurity and zeroth sites!

Moeller et al. 1995.

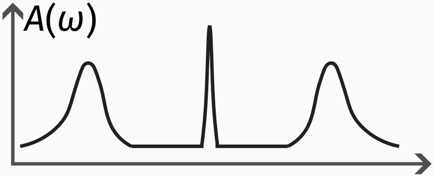
Observation of a coexistence region

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



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

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



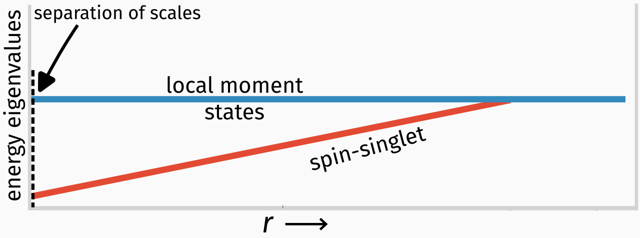
✓ spectral function shows **preformed gap** from metallic side

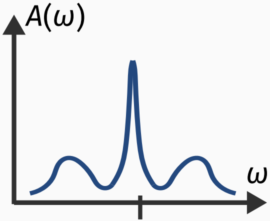
✓ **True** transition believed to occur at U_{c2}

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)

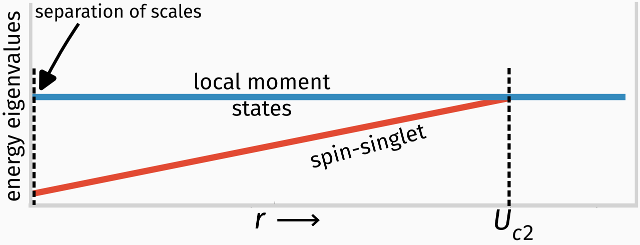


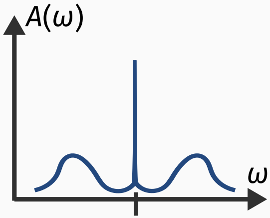


Observation of a coexistence region

Can be explained heuristically using the two site spectrum

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

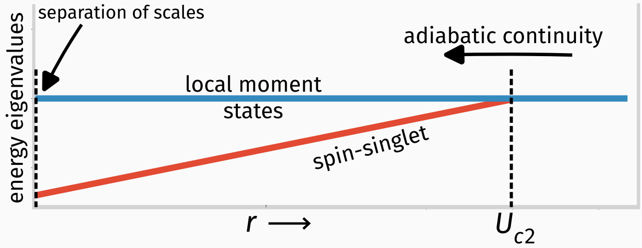


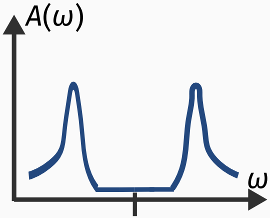


Observation of a coexistence region

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...

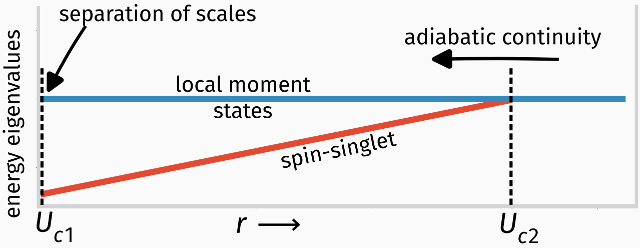


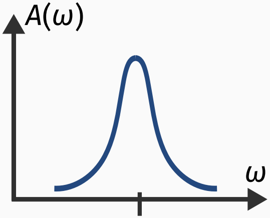


Observation of a coexistence region

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.



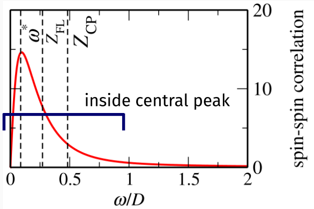


Comparison against NRG-DMFT correlation functions

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)]

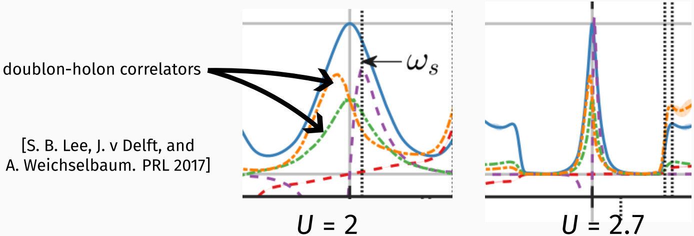


- ✓ Our $J - U_b$ model **goes further** by capturing physics beyond the transition

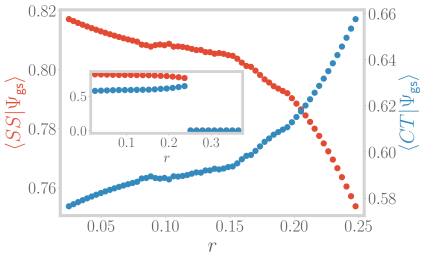
Comparison against NRG-DMFT correlation functions

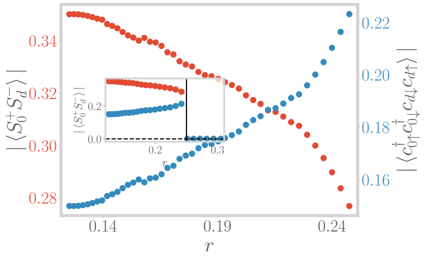
Doublon-holon correlators of the Hubbard model *[S. B. Lee, J. v Delft, and A. Weichselbaum. PRL 2017]*

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



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



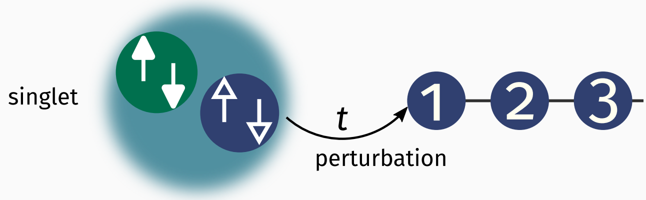


Low-energy excitations of the bath

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...

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

✓ 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

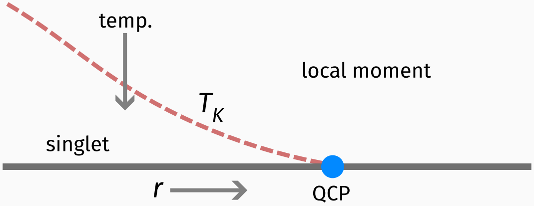
✓ Near the transition $r = -U_b/J_0 \to \frac{1}{4}$, the fixed-point momentum scale Λ^* can be approximated as

$$\Lambda^* \sim \Lambda_0 (1 - 4r)^{\frac{|2\omega + U_b + J_0/2|}{8\rho U_b}}, \quad \Lambda_0 = \text{UV cutoff}, \quad \rho = \text{bath D.O.S}$$

✓ Λ^* vanishes as $r \to 1/4$

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

$$T_K \sim \frac{\hbar}{k_B}\Lambda_0 (1 - 4r)^{\frac{|2\omega + U_b + J_0/2|}{8\rho U_b}}$$



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, $\text{Im}\left[\Sigma(\omega)\right]$ is

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

✓ As $r \to 0$, $u \to \infty$, signalling a vanishing lifetime of the quasiparticles

✓ Quasiparticle residue Z for 1-particle excitations is proportional to T_K:

$$Z \sim T_K$$

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

Hewson 1993; Coleman 2015.

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).

Acknowledgements

Gracious thanks to

- ✓ my collaborators **S. Patra, A. Mukherjee, Prof. A. Taraphder** and **Prof. N. S. Vidhyadhiraja**,
- ✓ my RPC members **Prof. Ritesh Singh** and **Prof. Anandamohan Ghosh** for instructive feedback,
- ✓ **Prof. H. Casini, Prof. N. Banerjee** and **Shibendu G. Chowdhury** for very fruitful discussions, and
- ✓ IISER Kolkata for funding.

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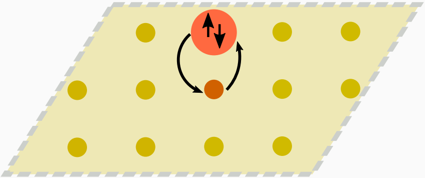
Other Projects

Theory for the single-channel Kondo cloud

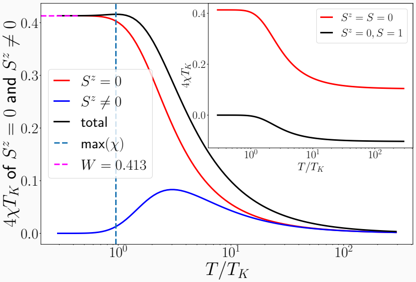
Phys. Rev. B 105, 085119

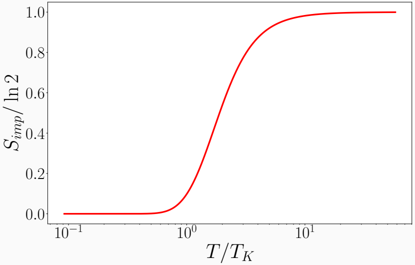
Anirban Mukherjee, **Abhirup Mukherjee**, N. S. Vidhyadhiraja, A. Taraphder, and Siddhartha Lal



Theory for the single-channel Kondo cloud

✓ spectral function & magnetic susceptibility



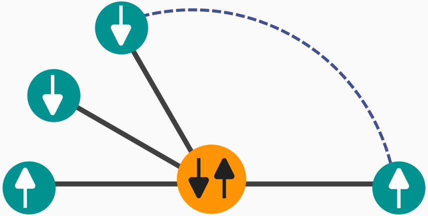


✓ local Fermi liq. & orthogonality catastrophe

✓ 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



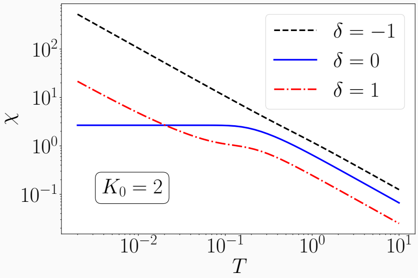
arXiv:2205.00790

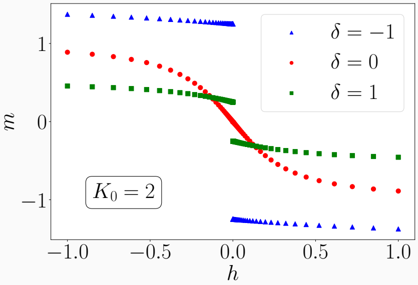
Siddhartha Patra, **Abhirup Mukherjee**, Anirban Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, Siddhartha Lal

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**



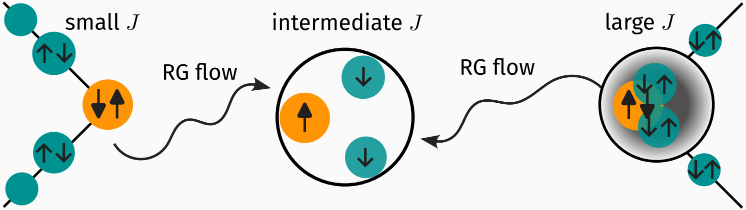


Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

Role of degeneracy in the multi-channel Kondo problem

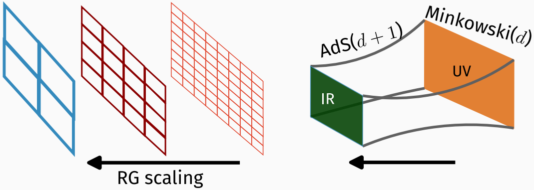
✓ Local **marginal Fermi liquid** within the low-energy excitations of the bath

✓ **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



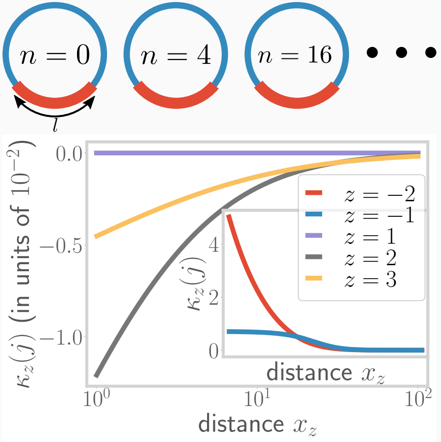
Entanglement scaling in free fermions: holography & topology - Summary

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

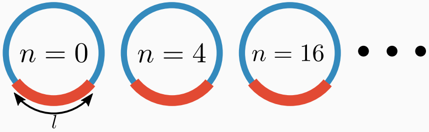
Simplest choice: the entire set

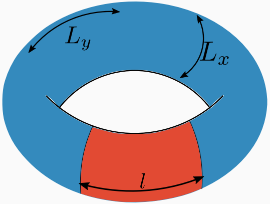
sparsity = 1 $\longrightarrow n \in \{-N, -(N-1), -(N-2), \ldots, -1, 0, 1, \ldots, N-2, N-1, N\}$

Coarser choices: increase sparsity

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

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





Subsystem entanglement entropy: Entanglement hierarchy

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

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

✓ presents a **hierarchy** of entanglement ⟶ EE distributed across RG steps
RG transformation ⟶ reveals entanglement

✓ distribution of entanglement also present in **multipartite** entanglement

---

Calabrese et al. 2004; Casini et al. 2005; Arias et al. 2015; Chen et al. 2017; Murciano et al. 2020.

Mutual information = distance

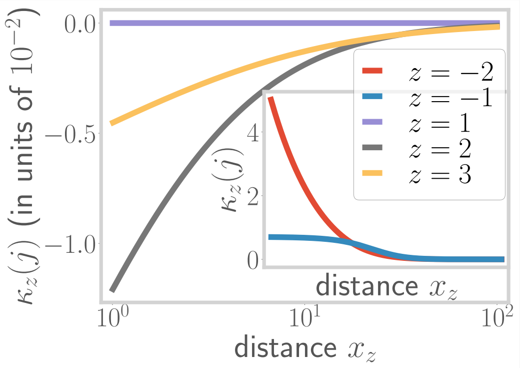
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

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: $\kappa_z(j) = \dfrac{v_z'(j)}{\left[1 + v_z(j)^2\right]^{\frac{3}{2}}}$



Van Raamsdonk 2010; Lee et al. 2016; Mukherjee et al. 2022; Lee 2010; Lee 2014; Qi 2013; Lee et al. 2016; Mukherjee et al. 2020a; Mukherjee et al. 2020b; Ryu et al. 2006b; Ryu et al. 2006a; Nozaki et al. 2012.

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

Maldacena 1999; Ryu et al. 2006a; Holzhey et al. 1994.

Topological nature of geometry-independent term

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

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

Luttinger et al. 1960; Luttinger 1960; Oshikawa 2000; Seki et al. 2017; Mukherjee et al. 2020a; Heath et al. 2020.