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

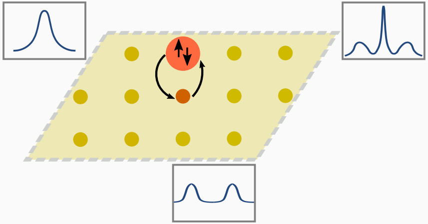
  S. Patra, *Abhirup Mukherjee*, A. Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, S. Lal

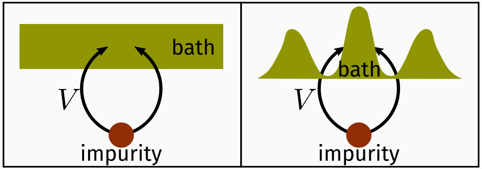
Ongoing Projects

- ✓ 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

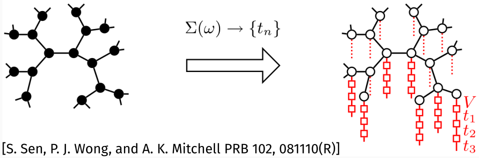




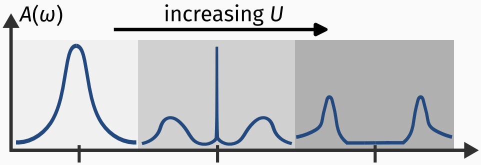
Introducing the extended Anderson impurity model

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

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

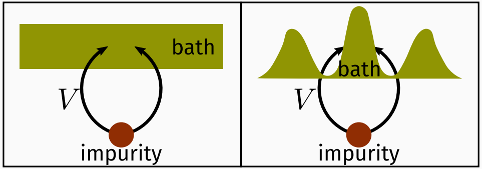


[S. Sen, P. J. Wong, and A. K. Mitchell PRB 102, 081110(R)]



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

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

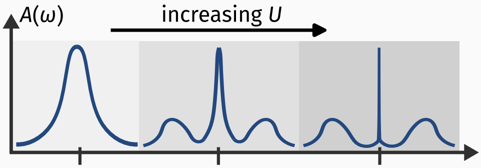


Metzner et al. 1989; Georges et al. 1992; Parcollet et al. 2004; Maier et al. 2005; Kotliar et al. 2006; Ohashi et al. 2008; Held et al. 2013; Sen et al. 2020.

Introducing the extended Anderson impurity model

Standard Anderson impurity model

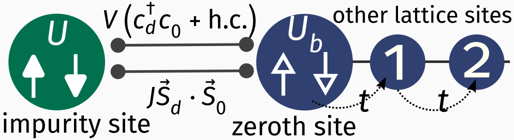
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



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

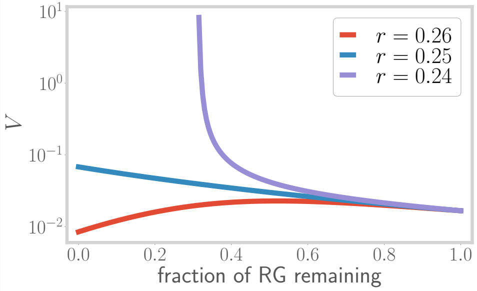
Nature of RG flows

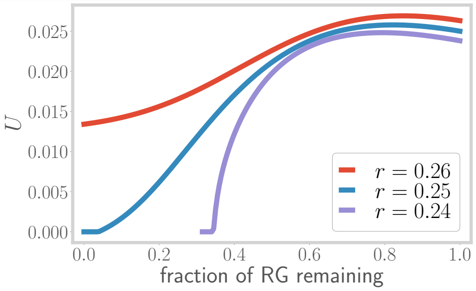
✓ URG Equations reveal **critical** point at $r = -U_b/J = 1/4$

$$\Delta J = J(J + 4U_b)/|d_3|$$

✓ allows averting strong-coupling behaviour

✓ U_b always marginal





RG Phase Diagram

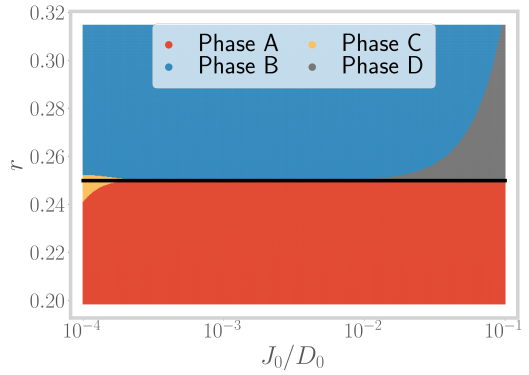
✓ blue phase $\longrightarrow$ $U_b < -J/4$: V, J are **irrelevant** $\longrightarrow$ local moment flows

✓ 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



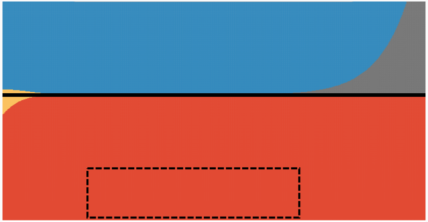
✓ red phase $\longrightarrow$ $U_b > -J/4$: V, J are **relevant** $\longrightarrow$ strong-coupling flows

Low-energy effective Hamiltonians and ground-states

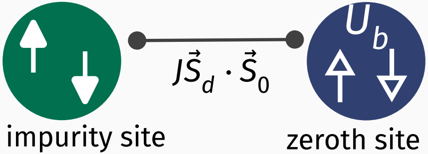
Regime 1: $|U_b| < J/4$

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

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



Zero-bandwidth limit



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

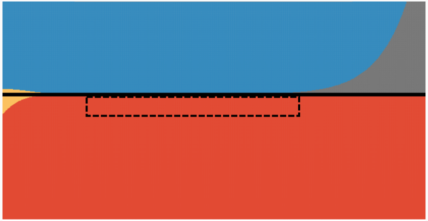
- ✓ two-spin Heisenberg, attractive zeroth site
- ✓ **singlet** ground state

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

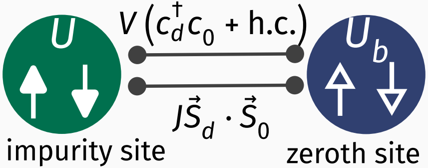
Regime 2: $|U_b| \sim J/4$

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

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



Zero-bandwidth limit



- ✓ **spin+charge** dimer with attractive zeroth site
- ✓ spin-singlet + charge-triplet-zero in gr-state

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

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

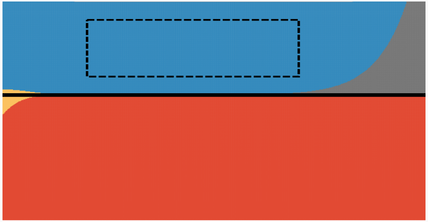
Low-energy effective Hamiltonians and ground-states

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

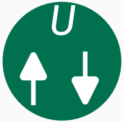
✓ J, V irrelevant,

✓ U relevant,

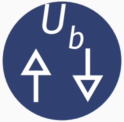
$$H = -U/2\left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 - U_b\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2 + \sum_{k<\Lambda^*} \epsilon_k \hat{n}_{k\sigma}$$



Zero-bandwidth limit



impurity site



zeroth site

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

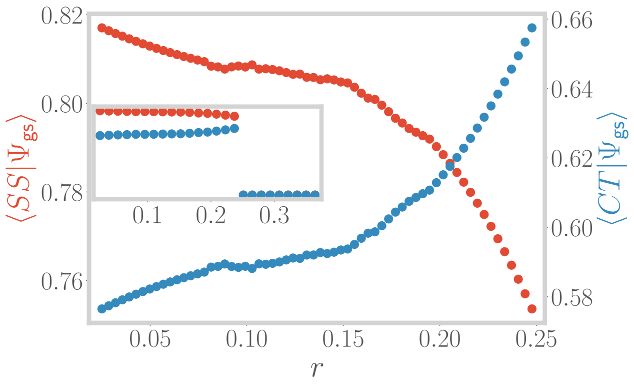
✓ impurity site detaches from bath

✓ **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

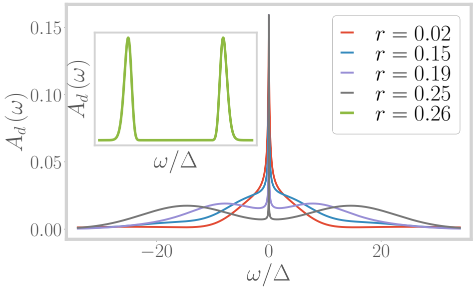


Nature of the Transition

Gapping of the impurity spectral function

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

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

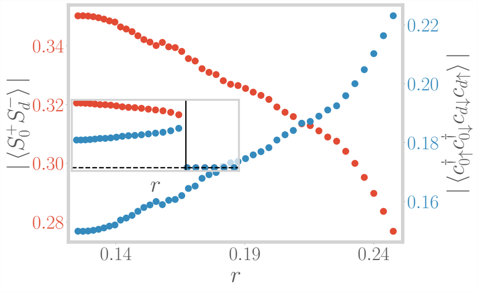


✓ hard central **gap** for $|U_b| > J/4$

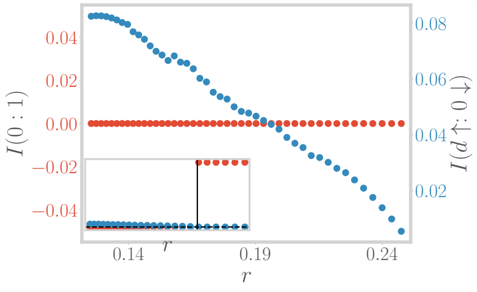
Destruction of the Kondo cloud

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

✓ vanishing of impurity-bath correlations



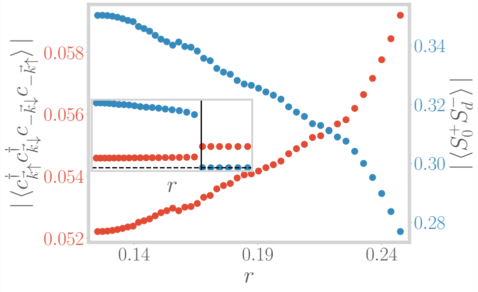
✓ transfer of entanglement into the bath



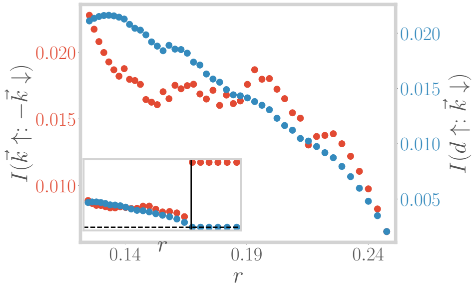
Growth of pairing fluctuations in the bath

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



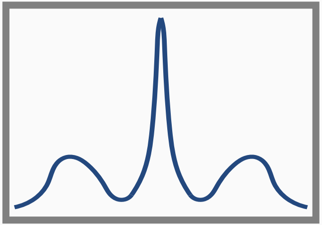
Universal Theory near the Transition

Minimal effective model for the transition

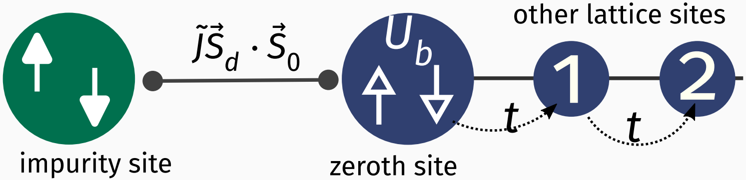
- ✓ For $|U_b| \lesssim J/4$, central peak and side peaks are **well-separated**
- ✓ **Integrate out** charge fluctuations through Schrieffer-Wolff transformation

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

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



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

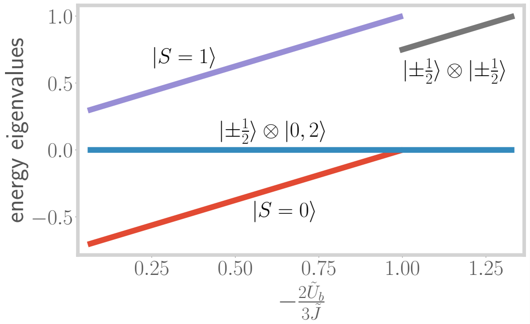


Suggests that ***J* and U_b are the minimal & universal ingredients** for transition!

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

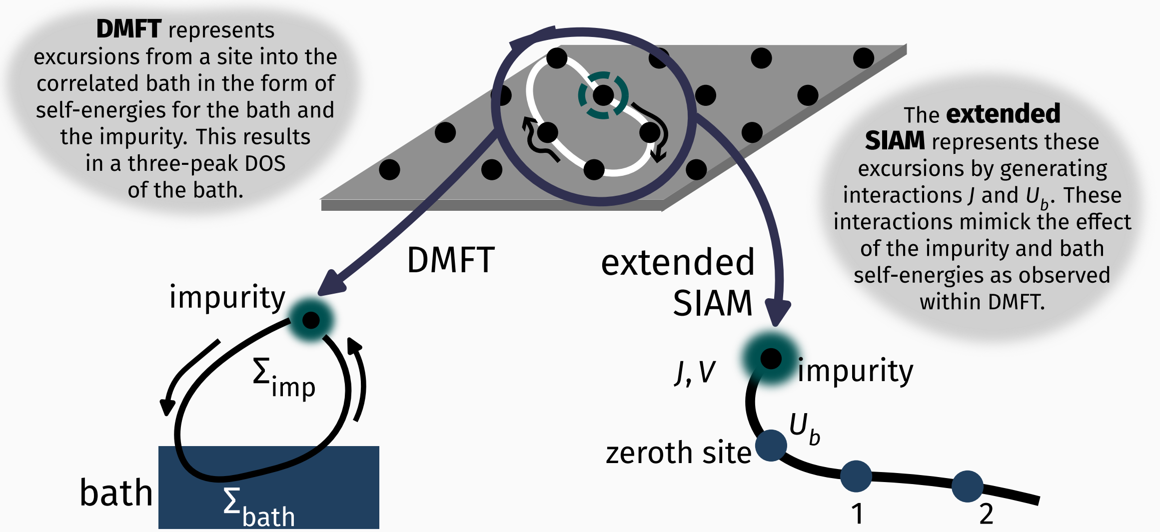
✓ Obtain two-site model by taking **zero bandwidth** limit

✓ spectrum shows **level crossing** between singlet and local moment states



Insights into DMFT

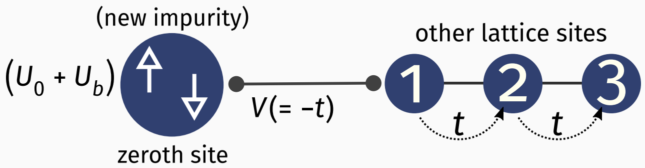
Extended SIAM in the context of DMFT



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



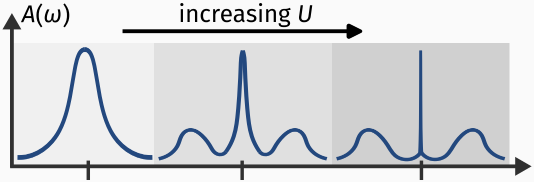
Essence of self-consistency: Equivalence of impurity and zeroth sites!

Equivalence of the impurity site and the bath zeroth site

✓ J is relevant and the largest scale $\longrightarrow$ **repulsive correlation**:

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

✓ J acts a **symmetrisation mechanism** between impurity and zeroth sites

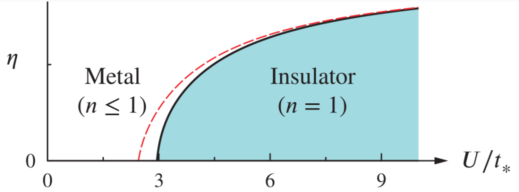


✓ **Coherent** spin-flip scatterings ensure similarity of spectral functions

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

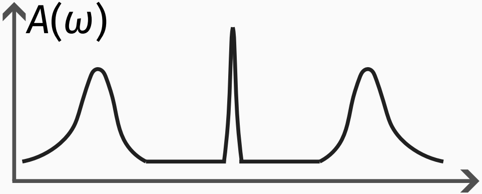
Observation of a coexistence region

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



(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



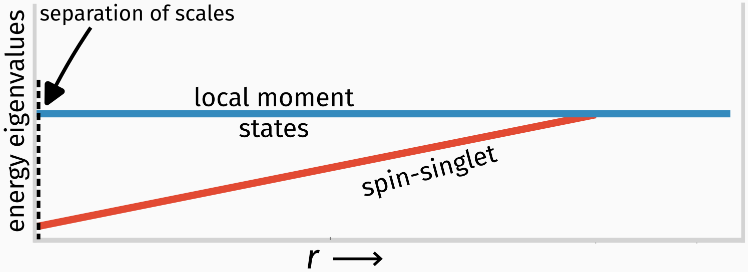
- ✓ spectral function shows preformed gap from metallic side

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

Observation of a coexistence region

Can be explained heuristically using the two site spectrum

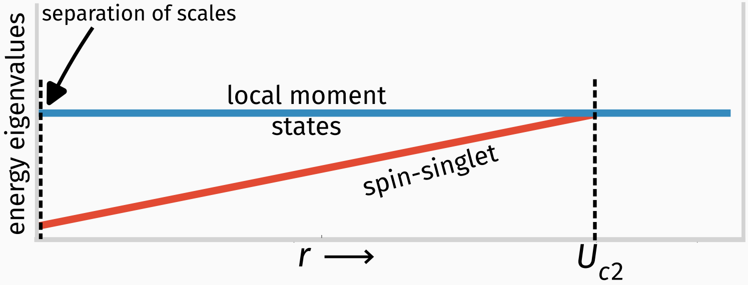
✓ Initial point is when the side peaks get separated (near-zeroes in the spectral function)



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

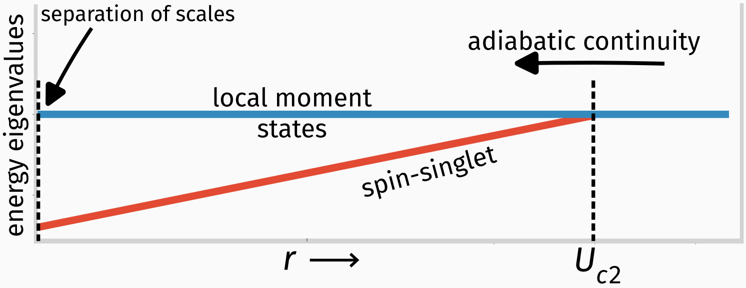
✓ U_{c2} is the point where the levels cross



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

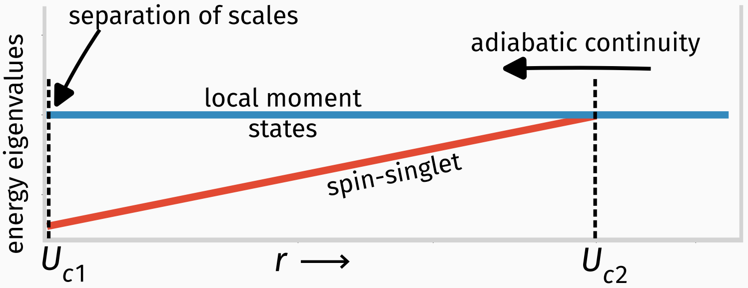
✓ Coming from $U > U_{c2}$, **adiabatic continuity** allows DMFT to stay on the local moment state...



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 of correlation functions

held-toshi and lee-von delft

Low-energy excitations of the bath

effective Hamiltonian for the excitations of the bath near the transition

emergence of NFL terms at the critical point

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. Taraphdar** and **Prof. N. S. Vidhyadhiraja**,
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- ✓ **Prof. H. Casini, Prof. N. Banerjee** and **Shibendu G. Chowdhury** for very fruitful discussions, and
- ✓ IISER Kolkata for funding.

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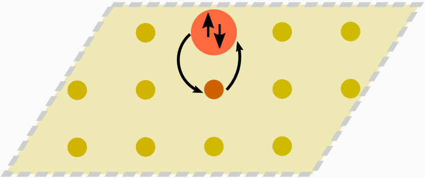
Further Details

Theory for the single-channel Kondo cloud

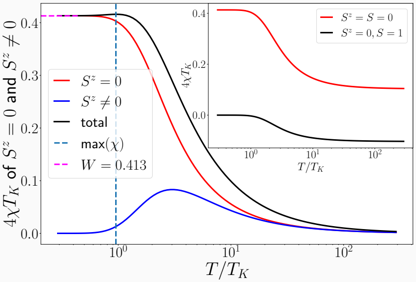
Phys. Rev. B 105, 085119

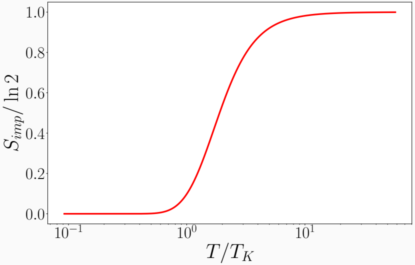
Anirban Mukherjee, **Abhirup Mukherjee**, N. S. Vidhyadhiraja, A. Taraphder, and Siddhartha Lal



Theory for the single-channel Kondo cloud

✓ spectral function & magnetic susceptibility





✓ local Fermi liq. & orthogonality catastrophe

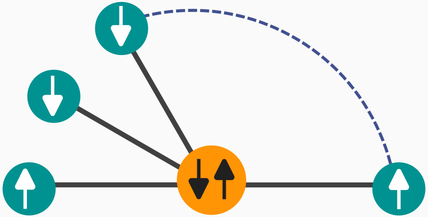
✓ thermal entropy

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

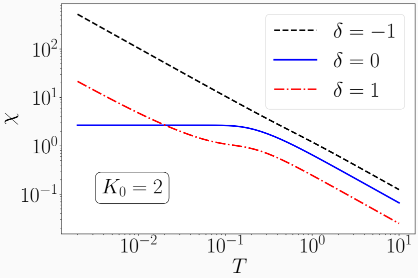
Siddhartha Patra, **Abhirup Mukherjee**, Anirban Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, Siddhartha Lal

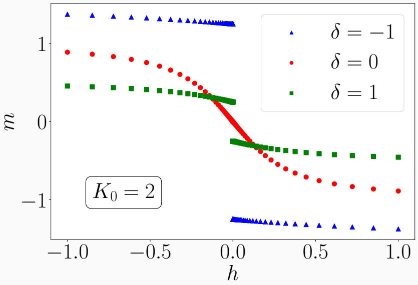


Role of degeneracy in the multi-channel Kondo problem

✓ Intermediate-coupling RG fixed point Hamiltonian and **degenerate** ground states

✓ Degree of compensation, magnetization and susceptibility show **incomplete screening**



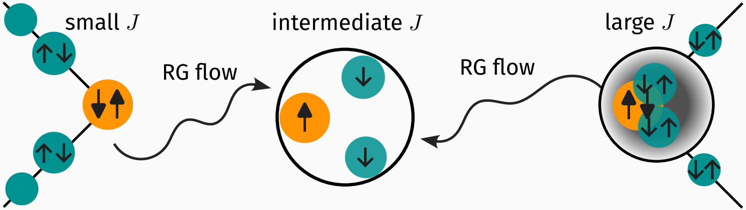


Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

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

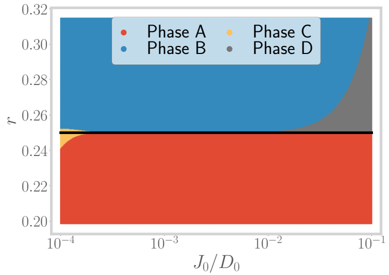


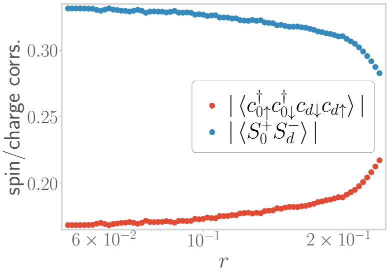
Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

RG Phase diagram:

Local MIT in an extended Anderson impurity model

- ✓ Competition between J and U_b leads to phase transition from screened singlet phase at $|U_b| \leq 4J$ to unscreened local moment phase at $|U_b| > 4J$.
- ✓ Impurity spectral function becomes gapped beyond the critical point.
- ✓ Decoupling the impurity model leads to an effective model with the zeroth site as the correlated impurity, demonstrating the symmetry between the impurity and zeroth site.
- ✓ Geometric entanglement and mutual information track the transition by vanishing beyond the critical point.
- ✓ Subdominant pairing tendencies are observed near the quantum critical point.





Presence of a phase transition

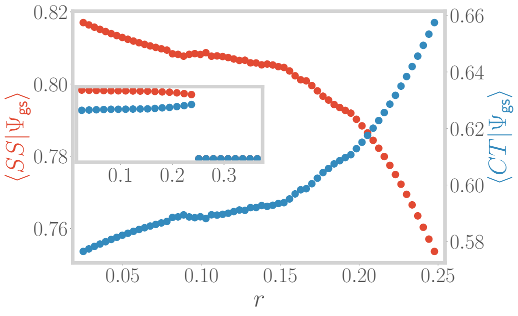
singlet ⟶ spin+charge liquid ⟶ local moment

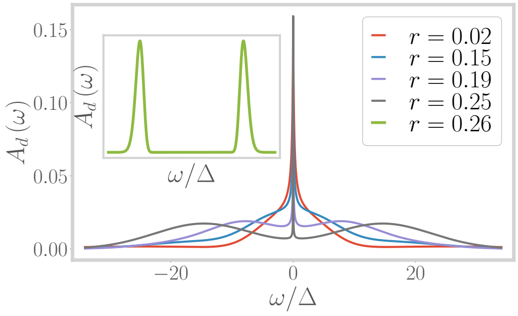
impurity spectral function gaps out

$r = -U_b/J$

$|SS\rangle = |\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle$

$|CT\rangle = |2,0\rangle + |0,2\rangle$





Bath spectral function: towards self-consistency

✓ Decoupling the impurity site leads to an Anderson impurity model

$$H_{0+\text{rest}} = \underbrace{-\left(U_0 + U_b\right)\left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow}\right)^2}_{\text{new correlated impurity}} \underbrace{- t \sum_{\substack{j\in\text{n.n. of } 0,\\ \sigma}} \left(c^\dagger_{0\sigma} c_{j\sigma} + \text{h.c.}\right)}_{\text{hopping between new impurity \& new bath}} \underbrace{- t \sum_{\langle i,j \rangle} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right)}_{\text{K.E. of new bath}}$$

✓ correlated, dominant spin-flip processes lead to repulsive $U_{\text{eff}} = U_0 + U_b \sim J^*/8$

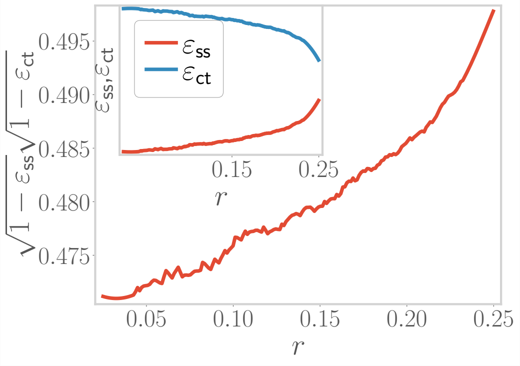
✓ J symmetrises the two sites, leading to similar spectral functions $\longrightarrow$ essence of self-consistency

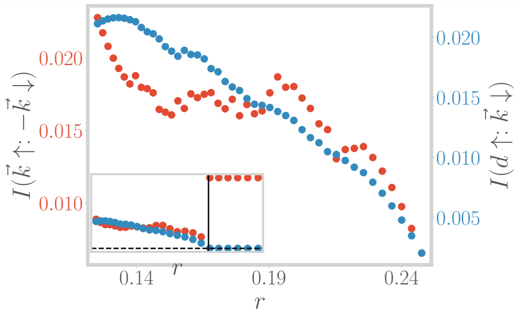
Entanglement as a probe for the transition

Geometric entanglement: $\varepsilon(\psi_1, \psi_2) = 1 - |\langle\psi_1|\psi_2\rangle|^2$

$\longrightarrow \sqrt{1-\varepsilon_{SS}}\sqrt{1-\varepsilon_{CT}}$ is maximised, then vanishes

Mutual information between impurity and cloud vanishes



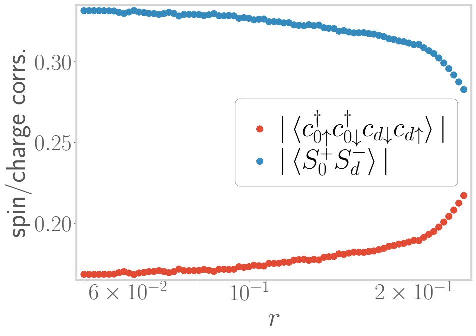


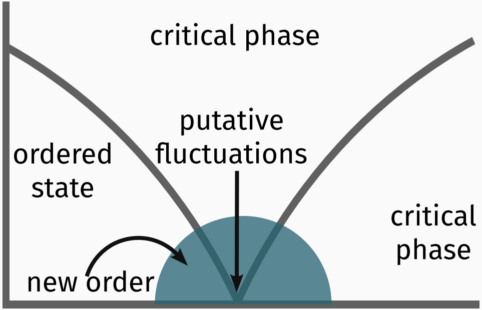
Presence of subdominant pair fluctuations

✓ **pairing tendencies** observed near the quantum critical point

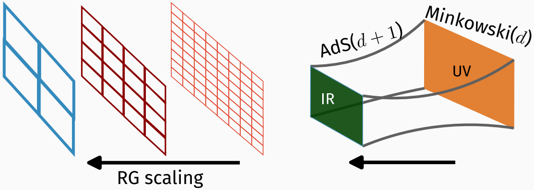
✓ might lead to **superconductivity** with doping

✓ seen in cuprates, heavy-fermions materials, pnictides, etc





Entanglement scaling in free fermions: holography & topology



Creating subsystems

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

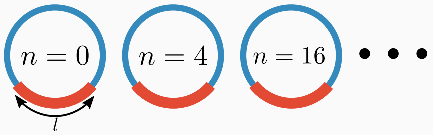
Simplest choice: the entire set

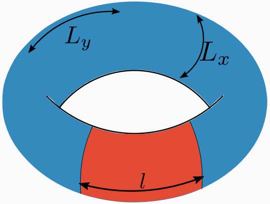
sparsity $= 1 \longrightarrow n \in \{-N, -(N-1), -(N-2), \dots, -1, 0, 1, \dots, N-2, N-1, N\}$

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

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

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

✓ 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

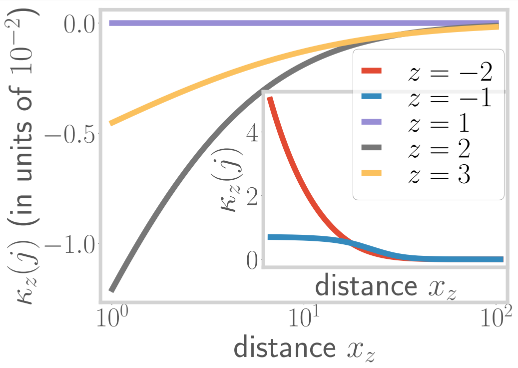
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

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



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

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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.

Holography and topology of entanglement scaling in free fermions

Future Prospects

Improvements to the auxiliary model

- ✓ Better model can be obtained by using multiple impurities
- ✓ Allows entangled liquid-like insulating phases
- ✓ Might also provide k–space resolution
  - ✓ partial gapping of Fermi surface?
  - ✓ pseudogap phases
- ✓ Introducing general impurity filling
  - ✓ new phases?
  - ✓ dominant pair fluctuations?

A novel auxiliary model approach

✓ Using local impurity models to create bulk lattice models (Bloch's theorem)

$$H_{\text{bulk}} = \sum_i H_{\text{local}}(i), \quad \Psi_{\text{bulk}}(\vec{k}) \sim \sum_i e^{i\vec{k}\cdot\vec{r}_i} \Psi_{\text{local}}(i)$$

✓ Relates bulk correlation functions to those of the auxiliary model

✓ phase transition in the extended AIM $\longrightarrow$ phase transition inthe bulk model, **metal-insulator transition** in Hubbard-Heisenberg model

A novel auxiliary model approach

- ✓ Should be useful for studying other models of strong-correlations
  - ✓ periodic Anderson/Kondo models
  - ✓ Heisenberg models
- ✓ Another potential application: topologically active systems:
  - ✓ Fractional quantum hall systems
- ✓ Extend the formalism towards higher order Greens functions
  - ✓ two-particle Greens functions, doublon-holon correlations
  - ✓ can provide more info on the MIT

Heavy-fermion materials

- ✓ Materials with very high quasiparticle masses
- ✓ Outstanding questions exist about the nature of phases and phase transitions
  - ✓ microscopic justification of certain phases
  - ✓ theory for the strange metal excitations
  - ✓ microscopic justification for the origin of unconventional superconductivity
- ✓ the URG, MERG and auxiliary model methods should prove useful