Emergence in free and correlated fermions: from impurity models to the bulk

JRF-to-SRF Presentation

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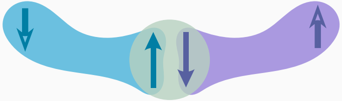
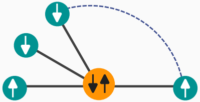
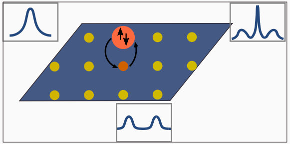
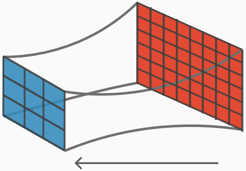




Summary of Work





Summary of Work

Completed Projects

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

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

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

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

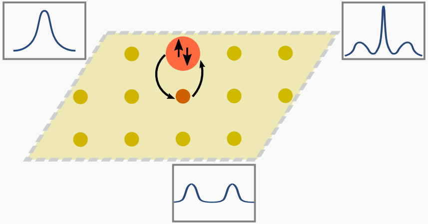
  under review at PRB, arXiv:2205.00790

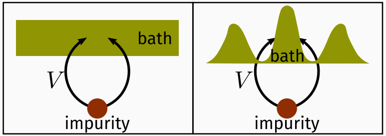
  S. Patra, *Abhirup Mukherjee*, A. Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, S. Lal

Ongoing Projects

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



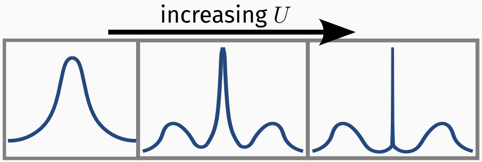


Introducing the extended Anderson impurity model

Introducing the extended Anderson impurity model

Standard Anderson impurity model

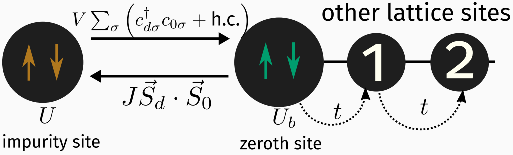
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



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

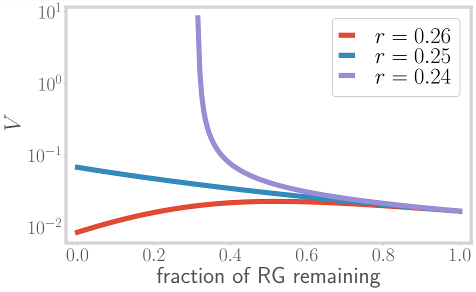
Phase Diagram & Ground-States

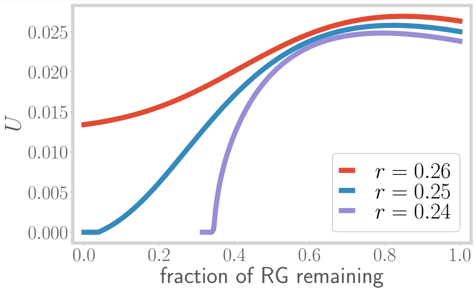
Nature of RG flows

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

✓ allows averting strong-coupling behaviour

✓ U_b always marginal





RG Phase Diagram

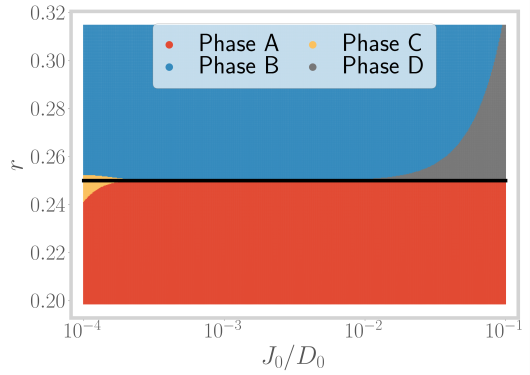
✓ orange phase ⟶ $U_b > -J/4$

V, J are **relevant** ⟶ strong-coupling flows

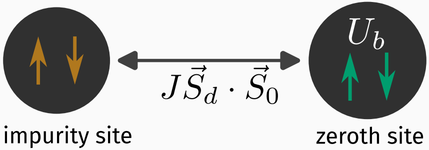
✓ blue phase ⟶ $U_b > -J/4$

V, J are **irrelevant** ⟶ local moment flows

$r = -U_b/J$



Low-energy effective Hamiltonians and ground-states



$U_b > -J/4$

✓ two-spin Heisenberg, attractive zeroth site

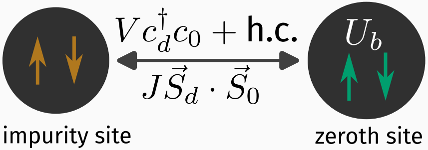
✓ **singlet** ground state

Low-energy effective Hamiltonians and ground-states

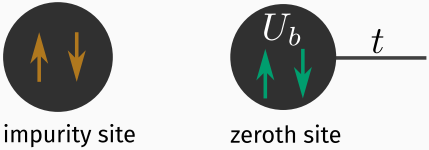
$U_b \sim -J/4$

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

✓ spin-singlet + charge triplet zero in ground state



Low-energy effective Hamiltonians and ground-states



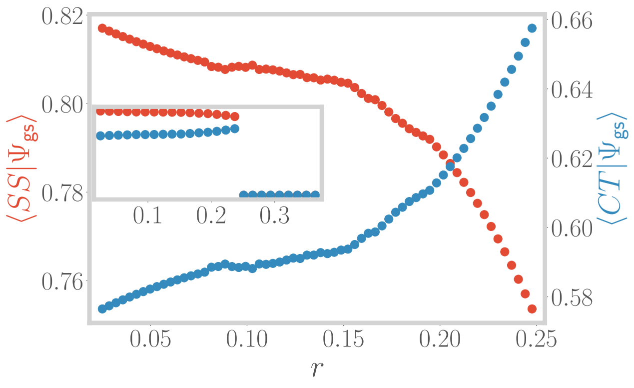
$U_b < -J/4$

✓ impurity site detaches from bath

✓ **local moment** ground-state

Low-energy effective Hamiltonians and ground-states

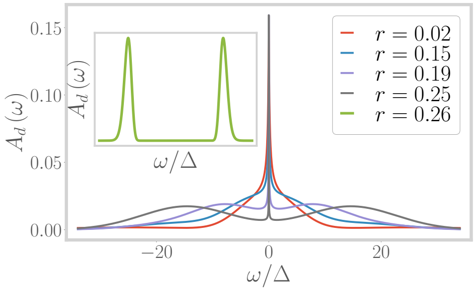
Ground-state overlap with spin singlet and charge triplet zero



Nature of the transition

Gapping of the impurity spectral function

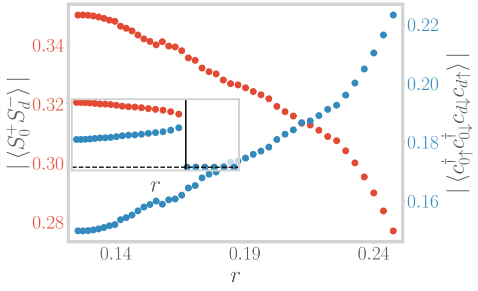
- ✓ Broad central peak at $|U_b| \ll J/4$
- ✓ Correlated **three peak** structure at $|U_b| \lesssim J/4$
- ✓ hard central **gap** for $|U_b| > J/4$

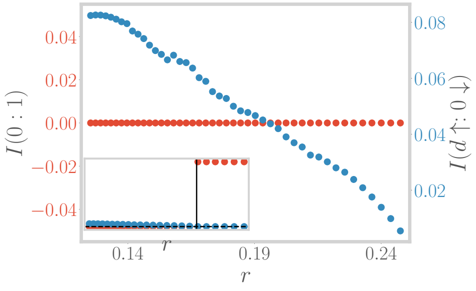


Destruction of the Kondo cloud

The Kondo cloud gets destroyed during the transition.

- ✓ vanishing of impurity-bath correlations
- ✓ transfer of entanglement into the bath



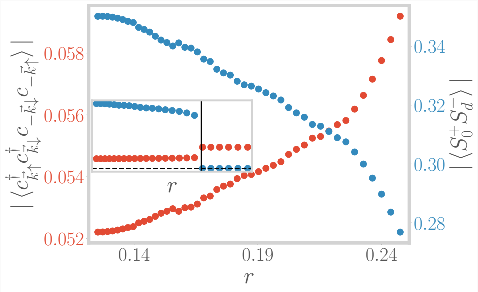


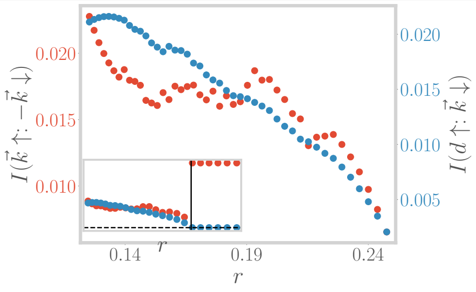
Growth of pairing fluctuations in the bath

Subdominant pairing fluctuations, near the transition

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

✓ mutual information in the same channel 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

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

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

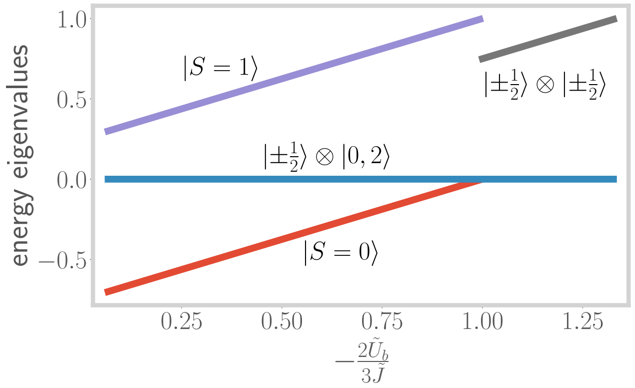
$$\Delta\tilde{J} \sim \tilde{J}\left(\tilde{J} + 4U_b\right)$$

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

equivalence of two sites, as seen through the bath spectral function

explanation of coexistence region from the two site spectrum

comparison of correlation functions from held-toshi and lee-von delft

Low-energy excitations of the bath

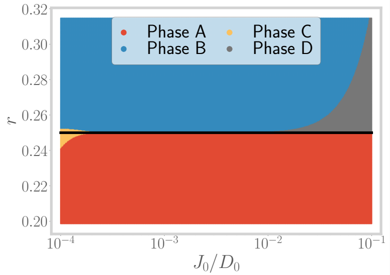
effective Hamiltonian for the excitations of the bath near the transition

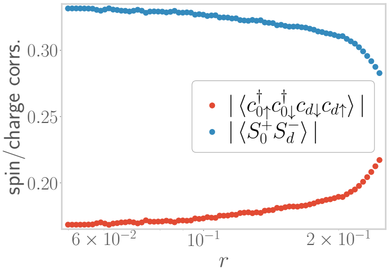
emergence of NFL terms at the critical point

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

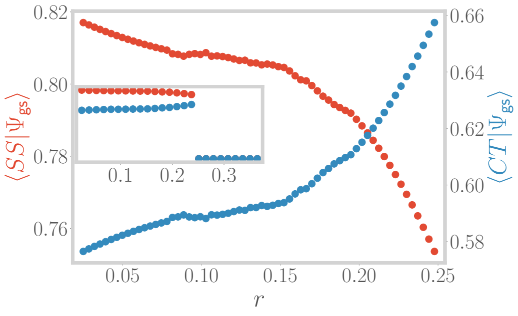
singlet ⟶ spin+charge liquid ⟶ local moment

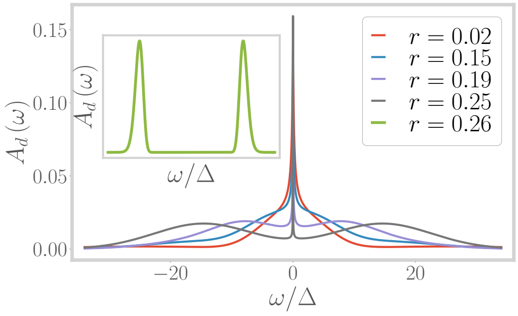
impurity spectral function gaps out

$r = -U_b/J$

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

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





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 $U_{\text{eff}} = U_0 + U_b \sim J^*/8$

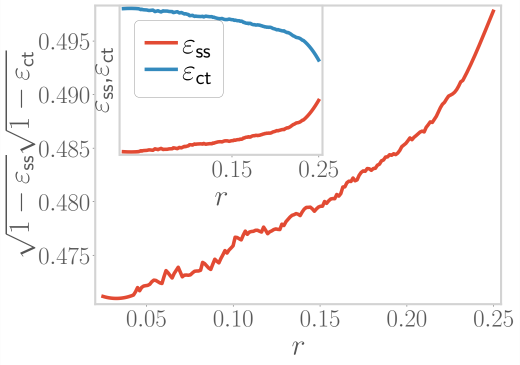
✓ J symmetrises the two sites, leading to similar spectral functions $\longrightarrow$ essence of self-consistency

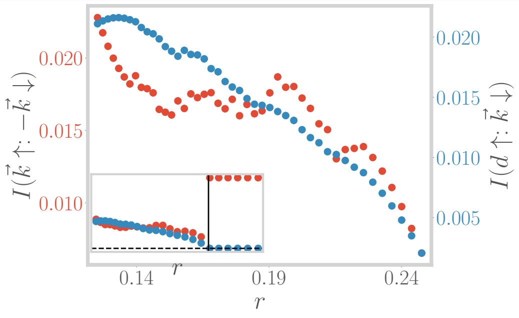
Entanglement as a probe for the transition

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

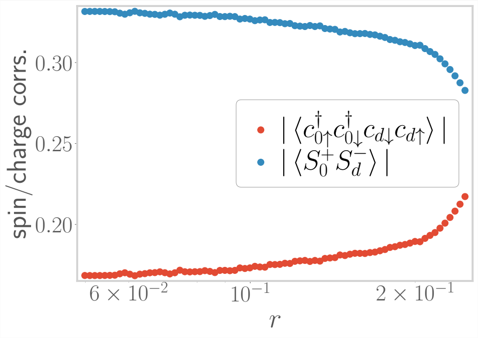
Mutual information between impurity and cloud vanishes

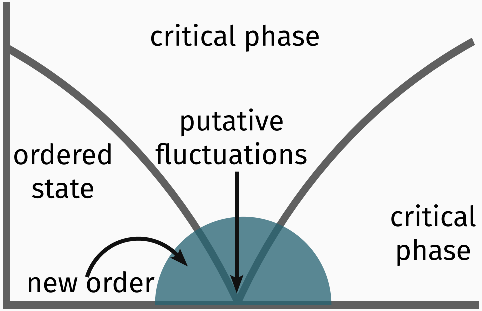




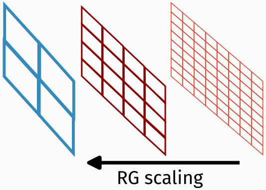
Presence of subdominant pair fluctuations

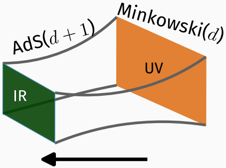
- ✓ **pairing tendencies** observed near the quantum critical point
- ✓ might lead to **superconductivity** with doping
- ✓ seen in cuprates, heavy-fermions materials, pnictides, etc





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** = $\Delta n = 1$

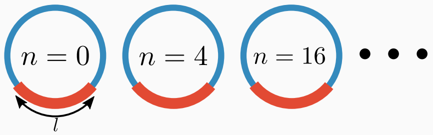
Simplest choice: the entire set

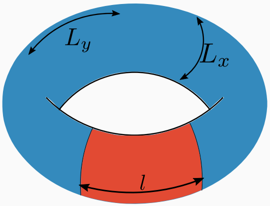
sparsity = 1 $\longrightarrow n \in \{-N, -(N-1), -(N-2), \dots, -1, 0, 1, \dots, N-2, N-1, N\}$

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

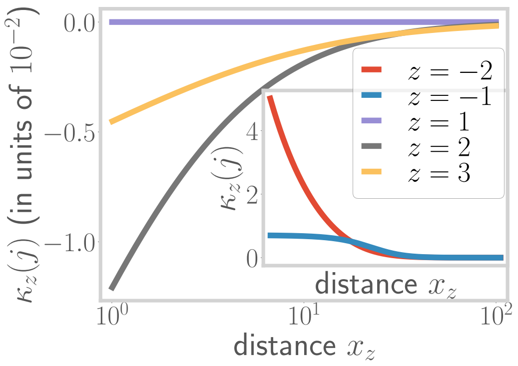
Mutual information: $I^2(A:B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

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



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.

Future Prospects

Future Prospects

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

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Further Details

Theory for the single-channel Kondo cloud

Phys. Rev. B 105, 085119

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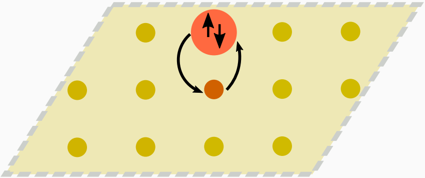
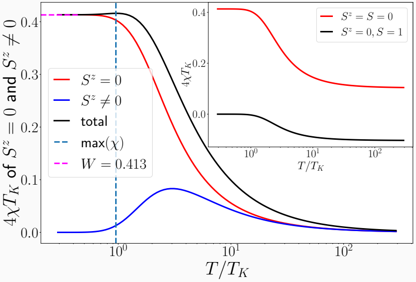
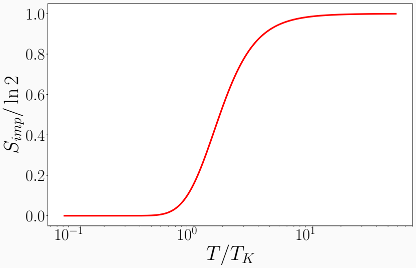


Theory for the single-channel Kondo cloud

✓ spectral function & magnetic susceptibility





✓ local Fermi liq. & orthogonality catastrophe

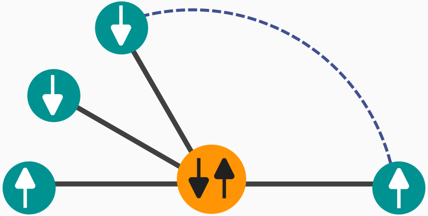
✓ thermal entropy

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

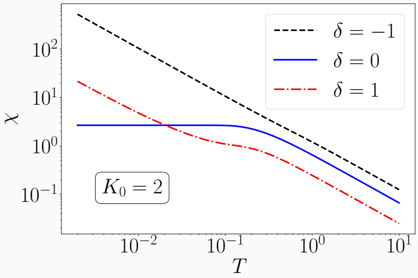
Siddhartha Patra, **Abhirup Mukherjee**, Anirban Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, Siddhartha Lal

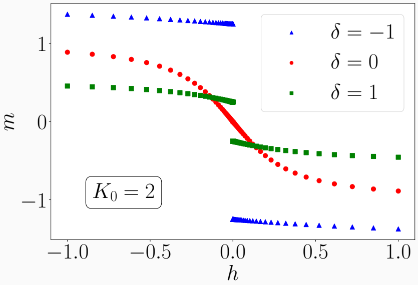


Role of degeneracy in the multi-channel Kondo problem

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

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



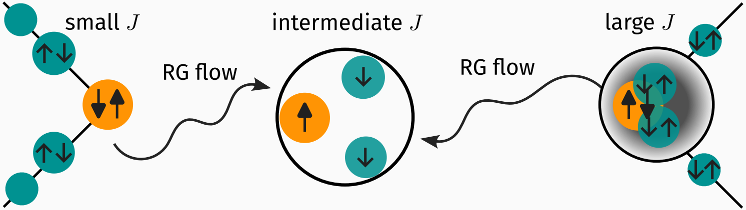


Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

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.

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