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

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JRF-to-SRF Presentation

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Summary of Work

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Completed Projects

- Single-channel Kondo problem: **Phys. Rev. B 105, 085119** arXiv:2111.10580v3
  A. Mukherjee, *Abhirup Mukherjee*, N. S. Vidhyadhiraja, A. Taraphder, and S. Lal
- Multi-channel Kondo problem: **under review at PRB**, arXiv:2205.00790
  S. Patra, *Abhirup Mukherjee*, A. Mukherjee, N. S. Vidhyadhiraja, A. Taraphder, S. Lal

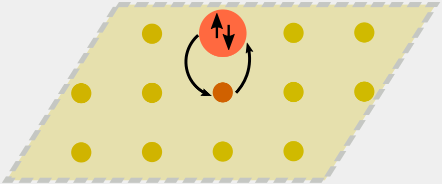
Ongoing Projects

- Metal-insulator transition in an extended Anderson impurity model
- Holography and topology of entanglement scaling in free fermions
- URG-based auxiliary model approach to correlated systems

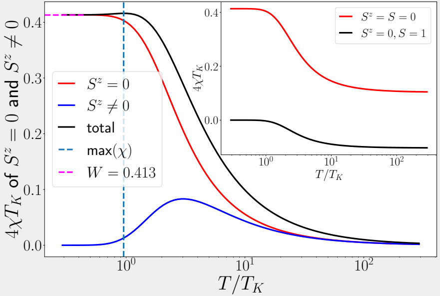
Single-channel Kondo problem

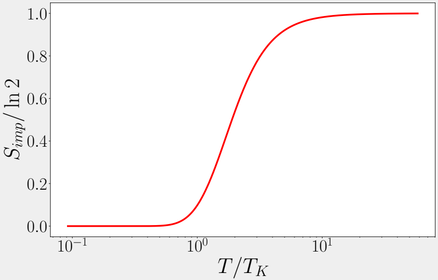
Phys. Rev. B 105, 085119

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



- Comparison of impurity spectral function and magnetic susceptibility with NRG
- Calculation of local Fermi liq., orthogonality catastrophe and thermal entropy



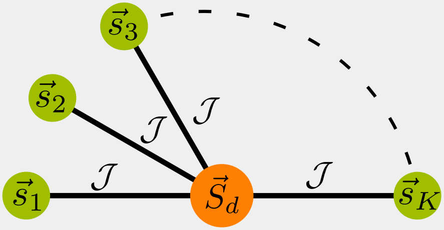


Kondo 1964; Wilson 1975; Andrei et al. 1983; Hewson 1993; Nozieres 1974; Anderson 1970; Tsvelick et al. 1983; Affleck et al. 1993; Goldhaber-Gordon et al. 1998; V. Borzenets et al. 2020; Sakai et al. 1989; Costi et al. 1990; Nozaki et al. 2012; Affleck 1995.

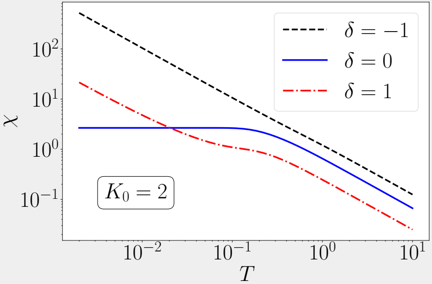
Multi-channel Kondo problem

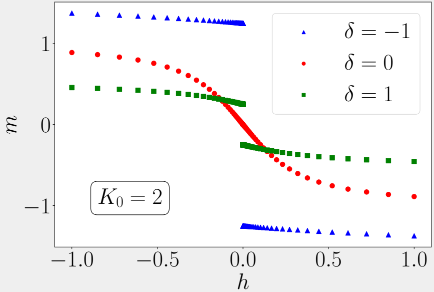
arXiv:2205.00790

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



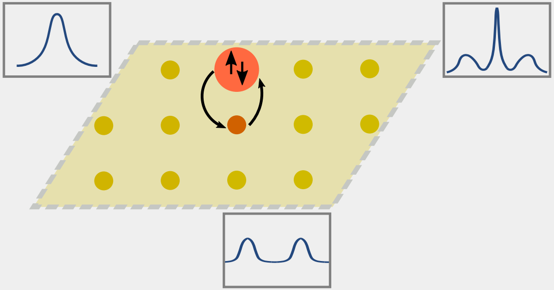
1. Intermediate-coupling RG fixed point Hamiltonian and **degenerate** ground states
2. Degree of compensation, magnetization and susceptibility show **incomplete screening**
3. Local **marginal Fermi liquid** within the low-energy excitations of the bath
4. **Duality** relations constrain the RG flows of the MCK model

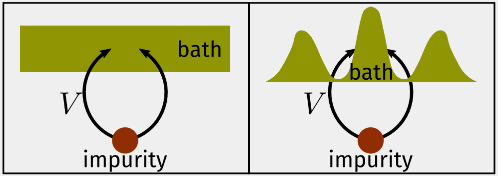




Nozières, Ph. et al. 1980; Tsvelick et al. 1985; Affleck et al. 1993; Gan 1994; Affleck et al. 1991; Emery et al. 1992; Bulla et al. 1998.

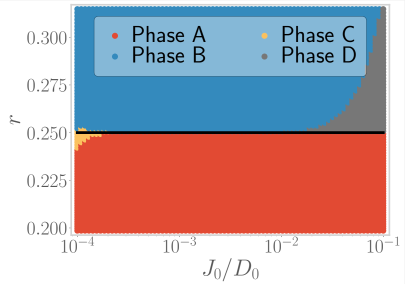
Local metal-insulator transition in an extended Anderson impurity model

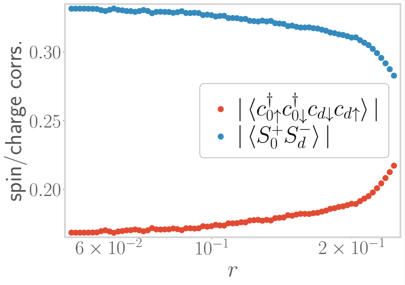




Local metal-insulator transition in an extended Anderson impurity model

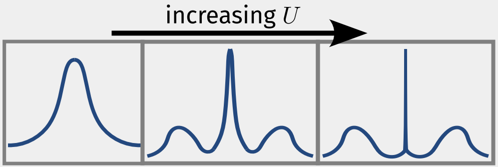
- Competition between J and U_b leads to phase transition from screened singlet phase at $|U_b| \leq 4J$ to unscreened local moment phase at $|U_b| > 4J$.
- Impurity spectral function becomes gapped beyond the critical point.
- Decoupling the impurity model leads to an effective model with the zeroth 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.





Standard Anderson impurity model

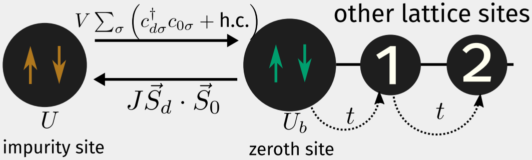
- no local-moment phase, $A(\omega)$ gapless
- cannot explain insulating phase of DMFT



Gap in spectral function requires additional physics!

Extended **Anderson impurity model**

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



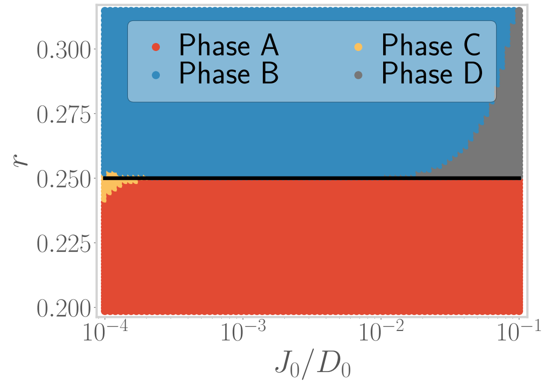
Anderson 1961; Krishna-murthy et al. 1980; Hewson 1993; Costi et al. 1990; Costi 2000; Metzner et al. 1989; Georges et al. 1992.

RG Phase Diagram

RG equations reveal critical point where J, V **become irrelevant**

1. orange phase: J is relevant: strong-coupling
2. blue phase: J is irrelevant: local moment
3. yellow phase: spin+charge liquid
4. gray phase: all couplings irrelevant

$r = -U_b/J$



Presence of a phase transition

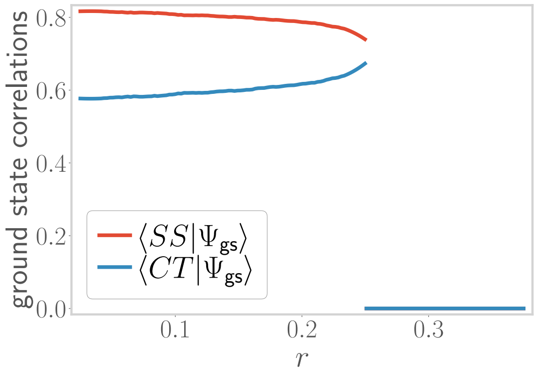
singlet ⟶ spin+charge liquid ⟶ local moment

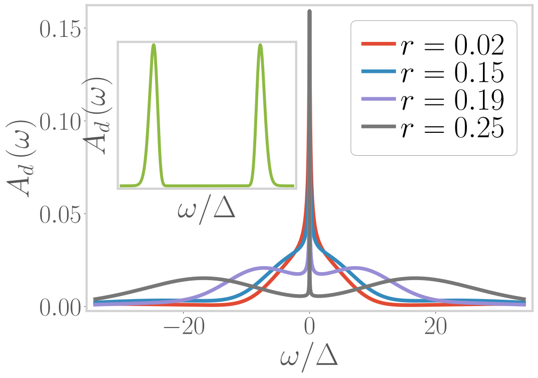
impurity spectral function gaps out

$r = -U_b/J$

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

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





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

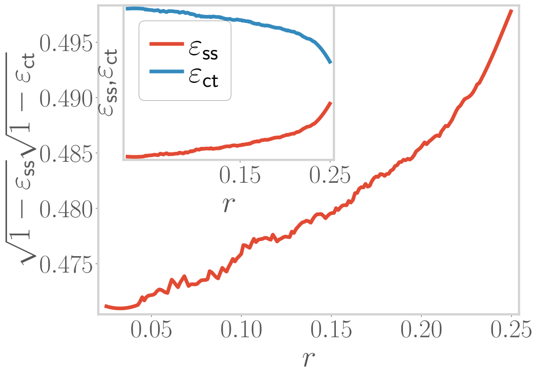
- J symmetrises the two sites, leading to similar spectral functions $\longrightarrow$ essence of self-consistency

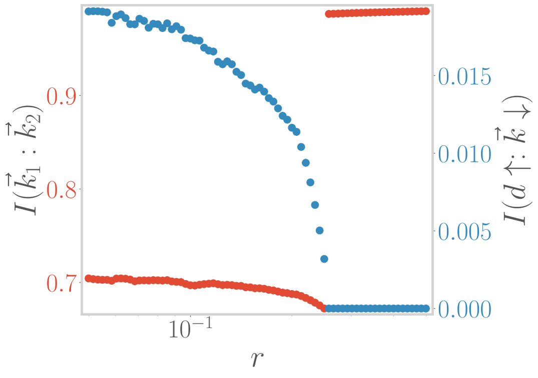
Entanglement as a probe for the transition

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

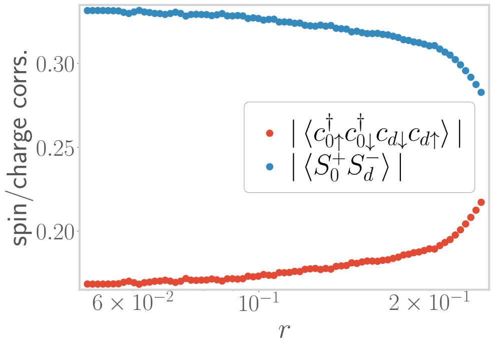
Mutual information between impurity and cloud vanishes

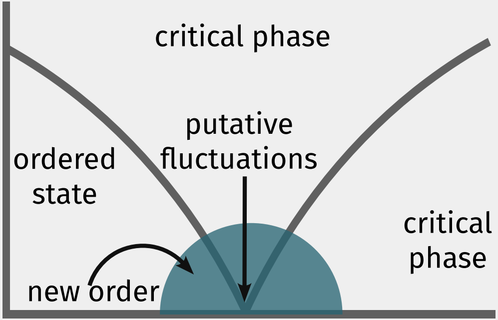




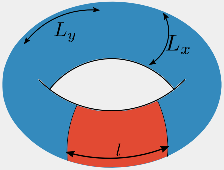
Presence of subdominant pair fluctuations

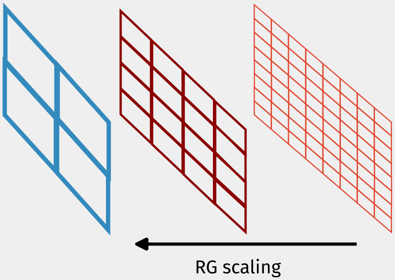
- **pairing tendencies** observed near the quantum critical point
- might lead to **superconductivity** with doping
- seen in cuprates, heavy-fermions materials, pnictides, etc

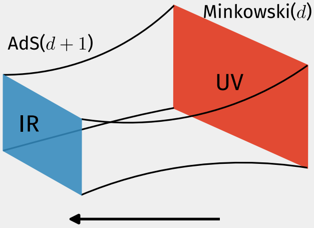




Entanglement scaling in free fermions

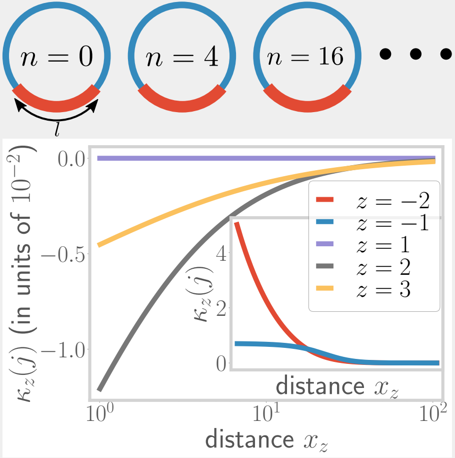






Entanglement scaling in free fermions

- 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 $\longrightarrow$ 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



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)

Acknowledgements

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Further Details

Local metal-insulator transition in extended Anderson impurity model

Entanglement scaling in free fermions

Creating subsystems

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

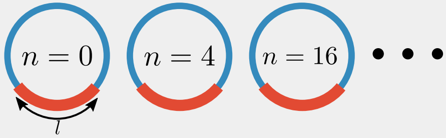
Simplest choice: the entire set

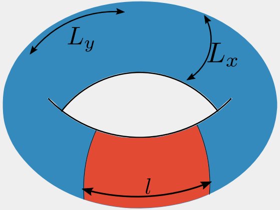
sparsity = 1 $\longrightarrow n \in \{-N, -(N-1), -(N-2), \dots, -1, 0, 1, \dots, N-2, N-1, N\}$

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 $\longrightarrow$ EE distributed across RG steps
  RG transformation $\longrightarrow$ 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.

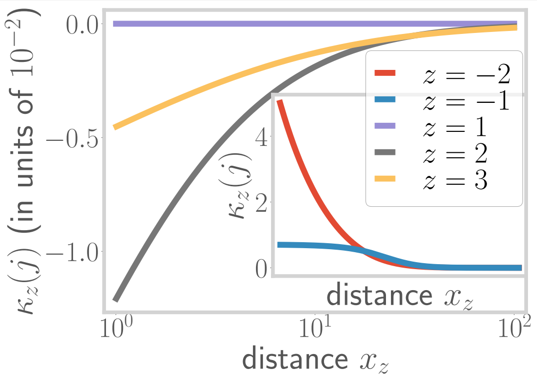
Mutual information: $I^2(A:B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

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

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?

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

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

- 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