

EMERGENCE IN FREE AND CORRELATED FERMIONS: FROM IMPURITY MODELS TO THE BULK

JRF-to-SRF Upgradation Presentation

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Summary of Work

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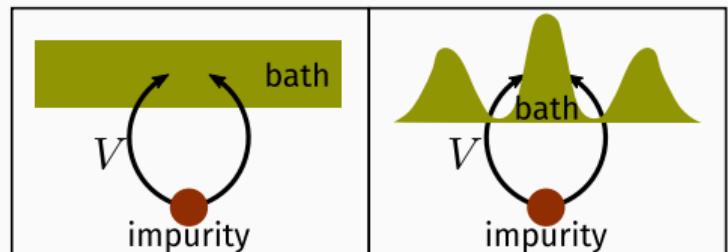
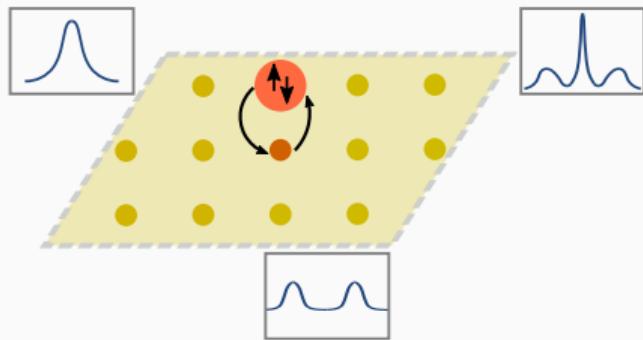
Completed Projects

- ✓ 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

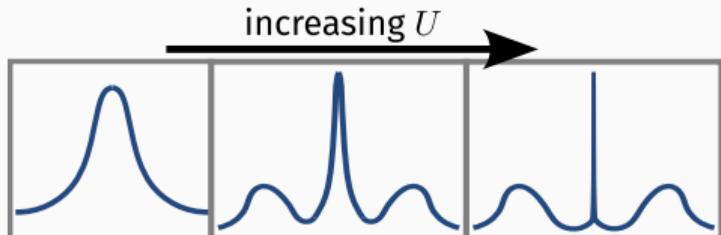


Introducing the extended Anderson impurity model

Introducing the extended Anderson impurity model

Standard Anderson impurity model

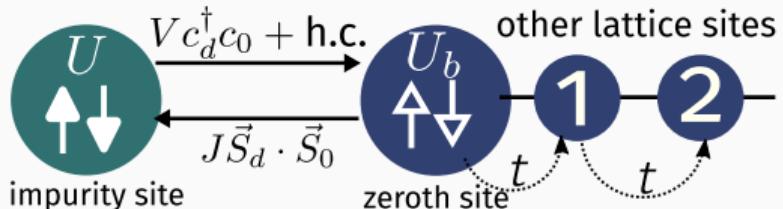
- ✓ no local-moment phase, $A(\omega)$ gapless
- ✓ cannot explain insulating phase of DMFT



Gap in spectral function requires additional physics!

Extended Anderson impurity model

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

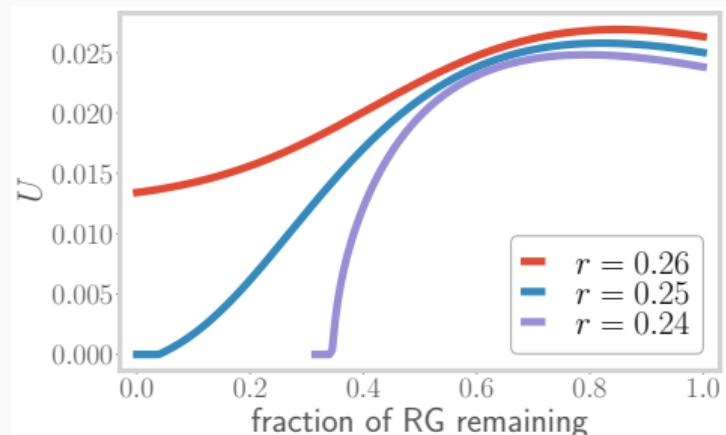
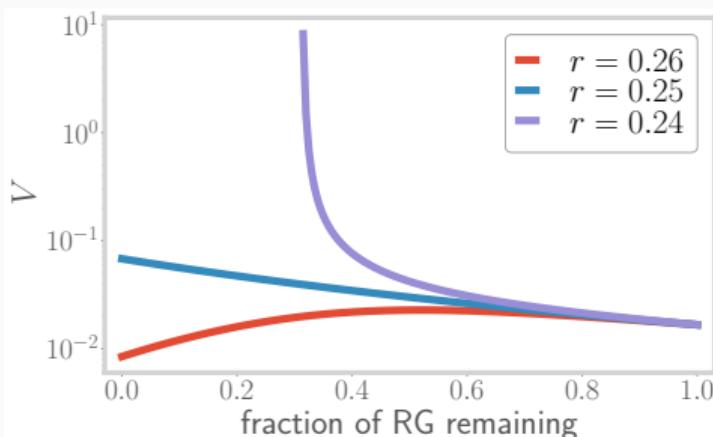


Anderson 1961; Anderson 1978; Wilson et al. 1974; Nozieres 1974; Krishna-murthy et al. 1980; Andrei 1980; Tsvelick et al. 1983; Hewson 1993; Costi et al. 1990; Costi 2000; Kuramoto et al. 1987; Cox et al. 1988; Metzner et al. 1989; Georges et al. 1992; Parcollet et al. 2004; Maier et al. 2005; Kotliar 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

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

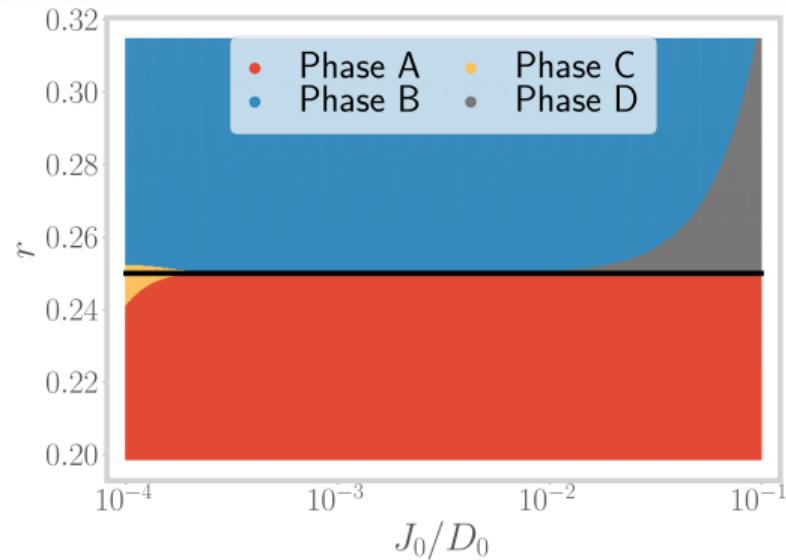
✓ yellow phase: $J \ll D_0$: involves **V, U, U_b**

vanishes for large systems

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

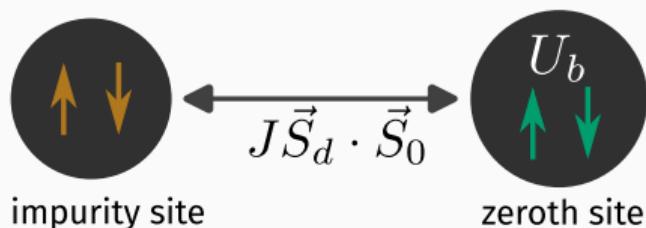
vanishes for large systems

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



Low-energy effective Hamiltonians and ground-states

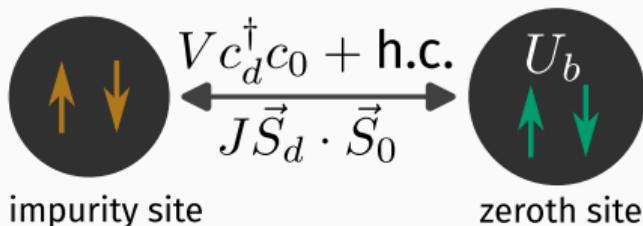
$$\underline{|U_b| < J/4}$$



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

Low-energy effective Hamiltonians and ground-states

$$\underline{|U_b| \sim J/4}$$



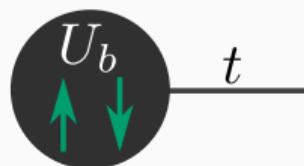
- ✓ **spin+charge** dimer with attractive zeroth site
- ✓ spin-singlet + charge triplet zero in ground state

Low-energy effective Hamiltonians and ground-states

$$\underline{|U_b| > J/4}$$



impurity site

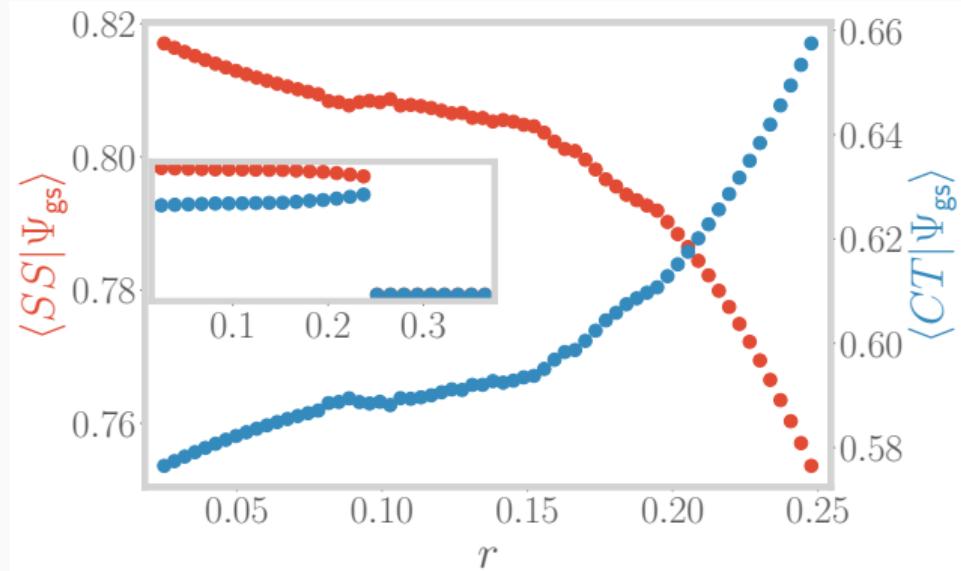


zeroth site

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

Low-energy effective Hamiltonians and ground-states

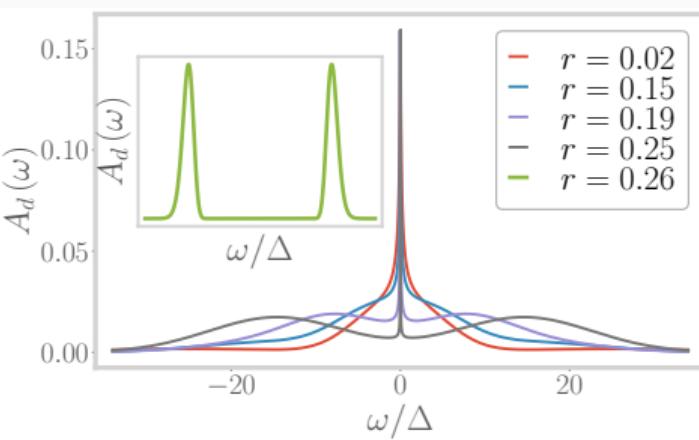
Ground-state overlap with spin singlet and charge triplet zero



Nature of the Transition

Gapping of the impurity spectral function

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



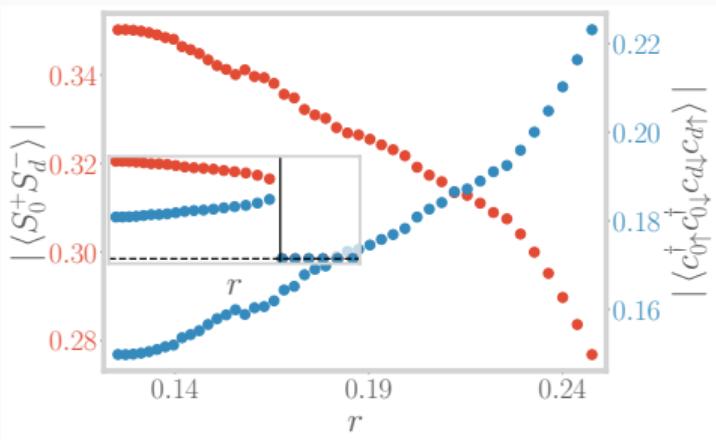
- ✓ Correlated **three peak** structure at $|U_b| \lesssim J/4$

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

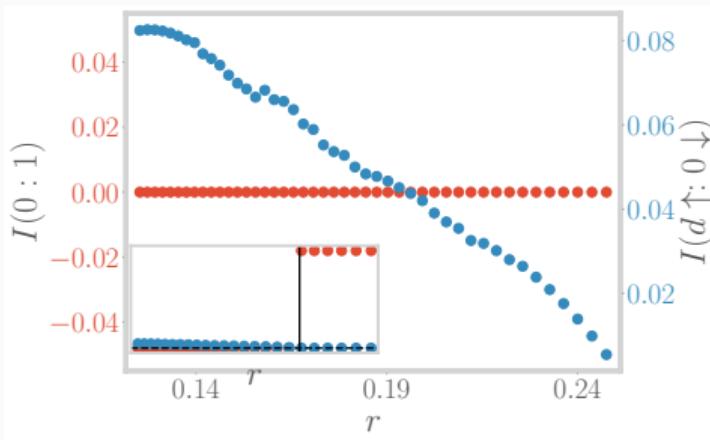
Destruction of the Kondo cloud

The Kondo cloud gets destroyed during the transition.

- ✓ vanishing of impurity-bath correlations



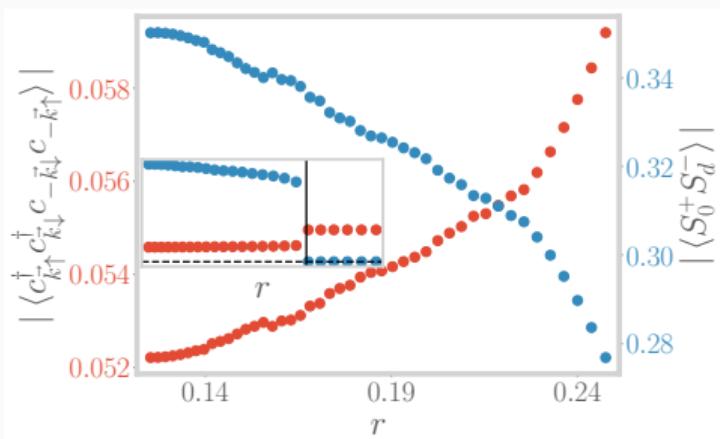
- ✓ transfer of entanglement into the bath



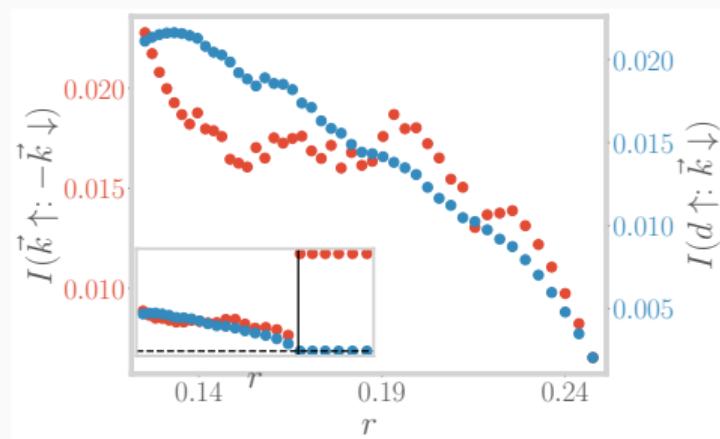
Growth of pairing fluctuations in the bath

Subdominant pairing fluctuations, near the transition...

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



- ✓ mutual information within the bath maximised after transition



Universal Theory near the Transition

Minimal effective model for the transition

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

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

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

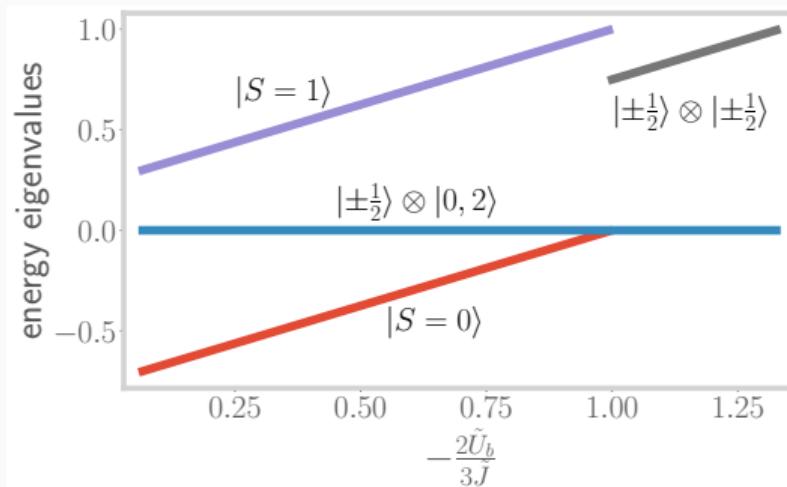
$$\Delta \tilde{J} \sim \tilde{J} (\tilde{J} + 4U_b)$$



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

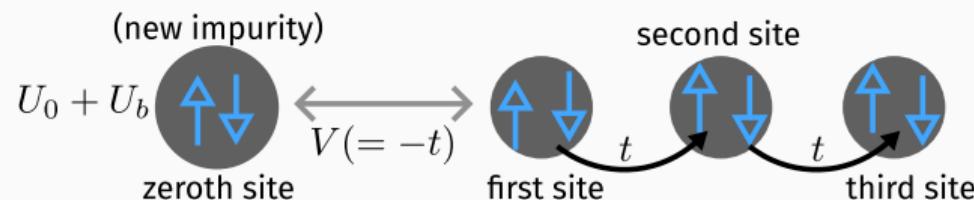
- ✓ Obtain two-site model by taking **zero bandwidth** limit
- ✓ spectrum shows **level crossing** between singlet and local moment states



Insights into DMFT

Equivalence of 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 \rightarrow **repulsive correlation**:

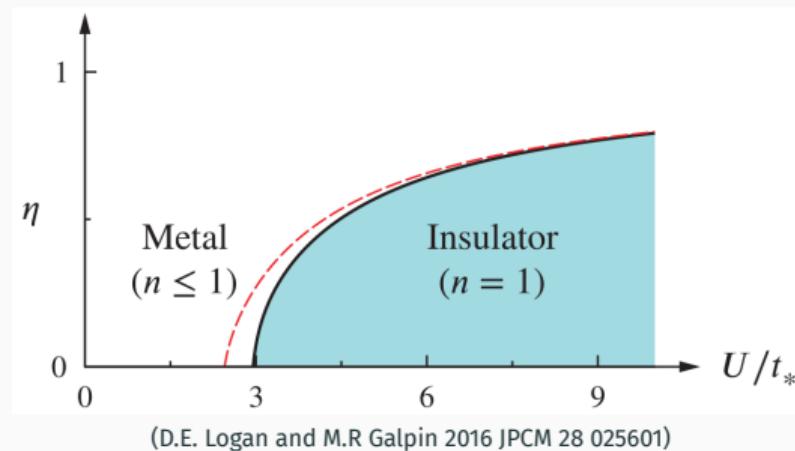
$$U_0 + U_b \approx J > 0$$

- ✓ 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 $U_{c1} < U < U_{c2}$

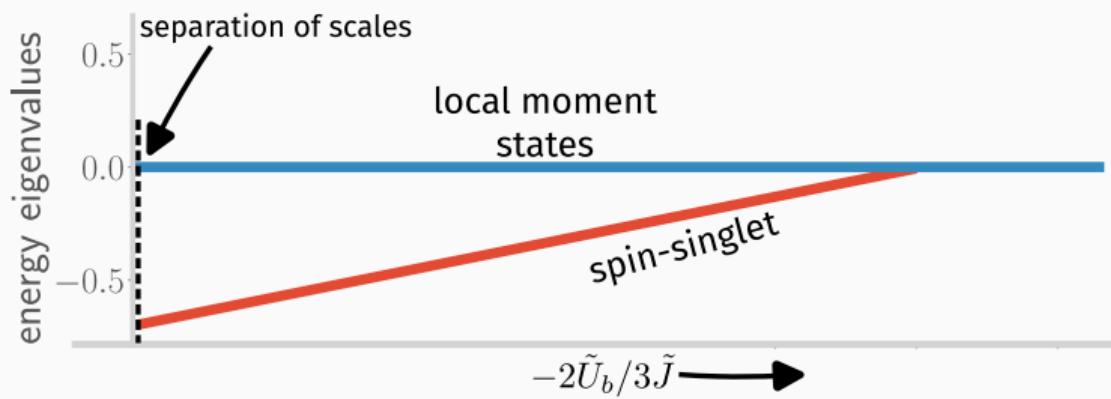


- ✓ Insulating when coming in from the insulator, metallic when coming in from the metal
- ✓ True transition believed to occur at U_{c2}

Observation of a coexistence region

Can be explained heuristically using the two site spectrum

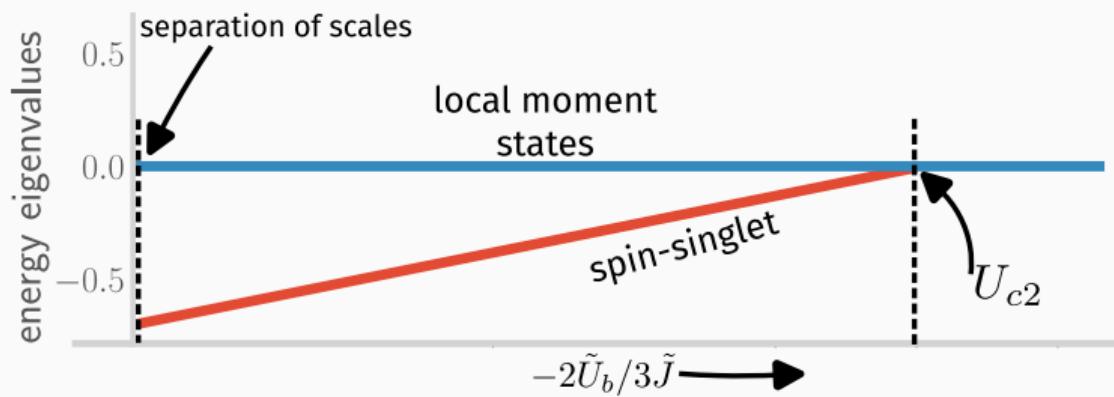
- ✓ Initial point is when the side peaks get separated (near-zeroes in the spectral function)



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

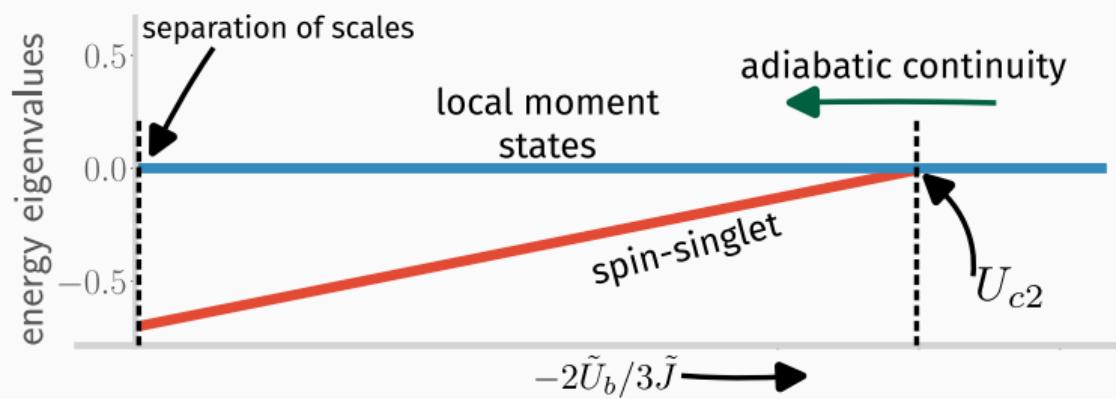
- ✓ U_{c2} is the point where the levels cross



Observation of a coexistence region

Can be explained heuristically using the two site spectrum

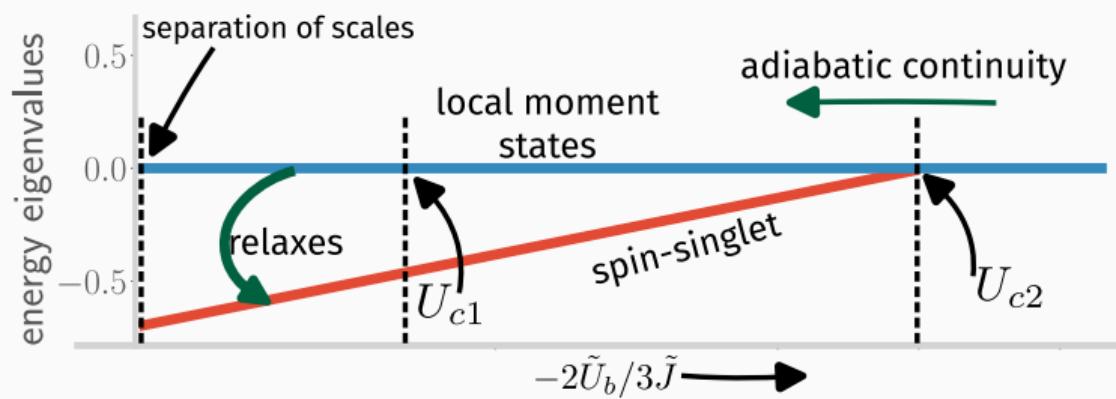
- ✓ Coming from $U > U_{c2}$, **adiabatic continuity** allows DMFT to stay on the local moment state...



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

- ✓ Better model can be obtained by taking multiple impurities and general impurity filling
- ✓ novel auxiliary model method can be 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

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- ✓ **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
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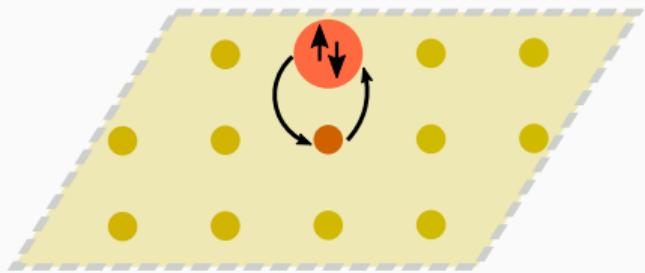
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Further Details

Theory for the single-channel Kondo cloud

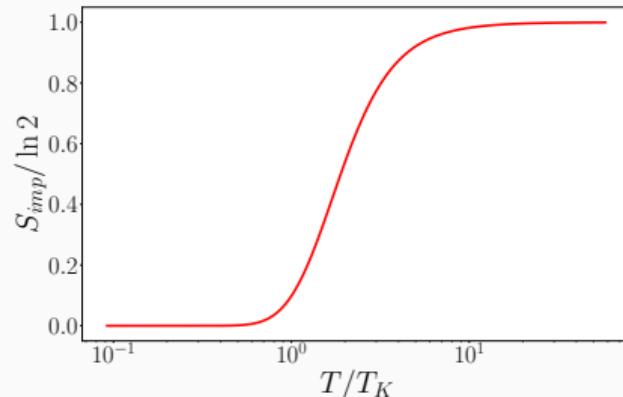
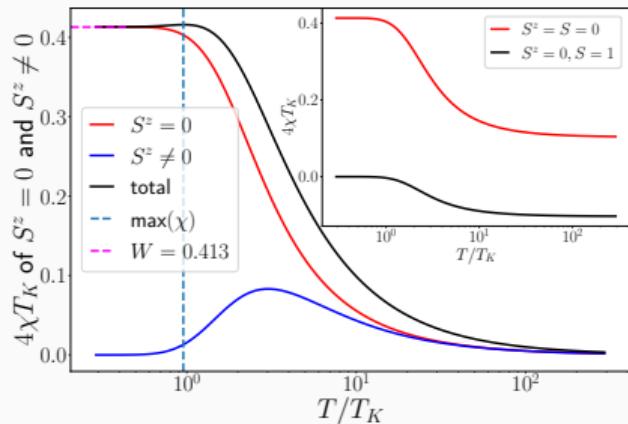
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Theory for the single-channel Kondo cloud

- ✓ spectral function & magnetic susceptibility

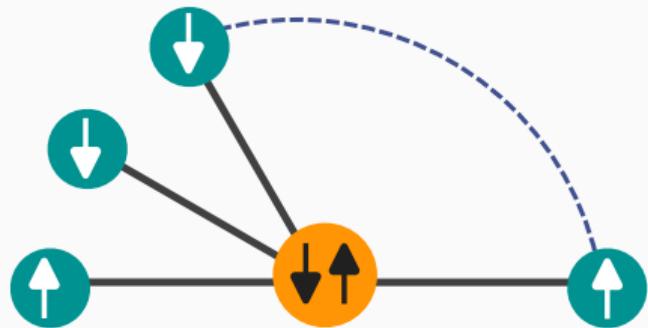


- ✓ local Fermi liq. & orthogonality catastrophe
- ✓ thermal entropy

Role of degeneracy in the multi-channel Kondo problem

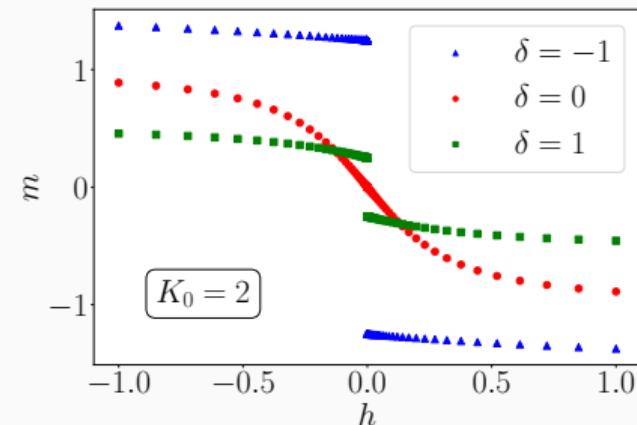
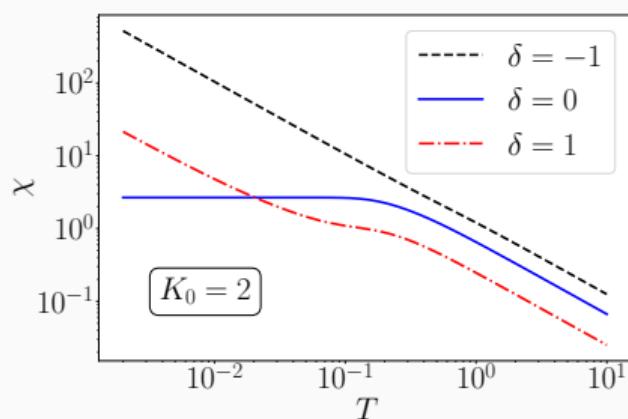
arXiv:2205.00790

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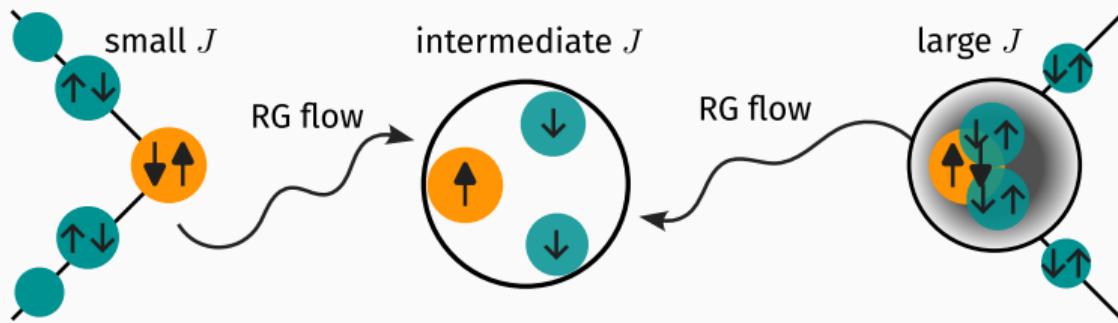
Role of degeneracy in the multi-channel Kondo problem

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



Role of degeneracy in the multi-channel Kondo problem

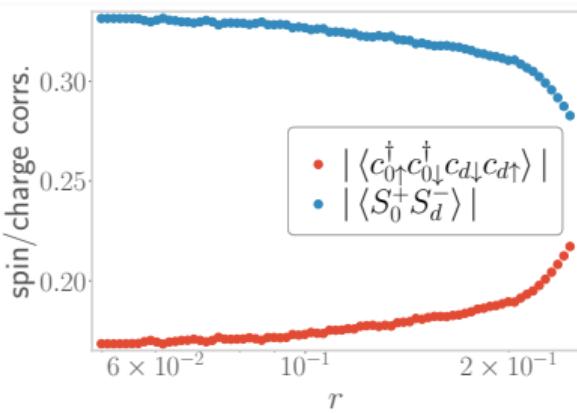
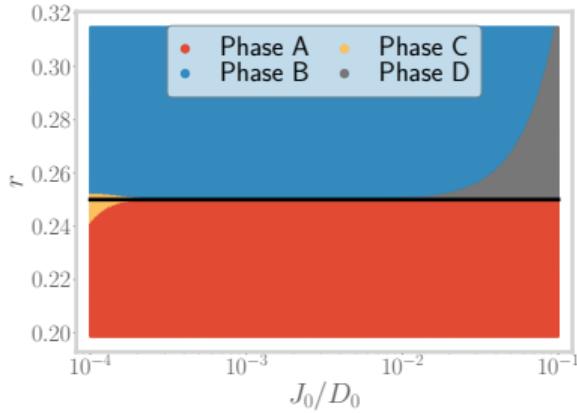
- ✓ Local **marginal Fermi liquid** within the low-energy excitations of the bath
- ✓ **Duality** relations constrain the RG flows of the MCK model



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

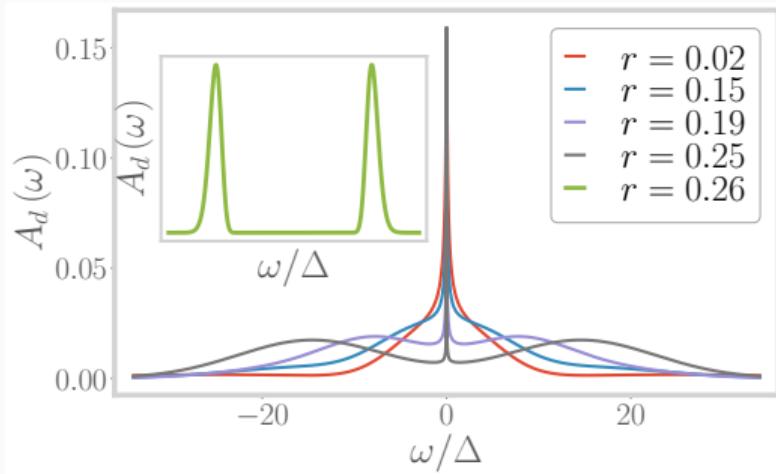
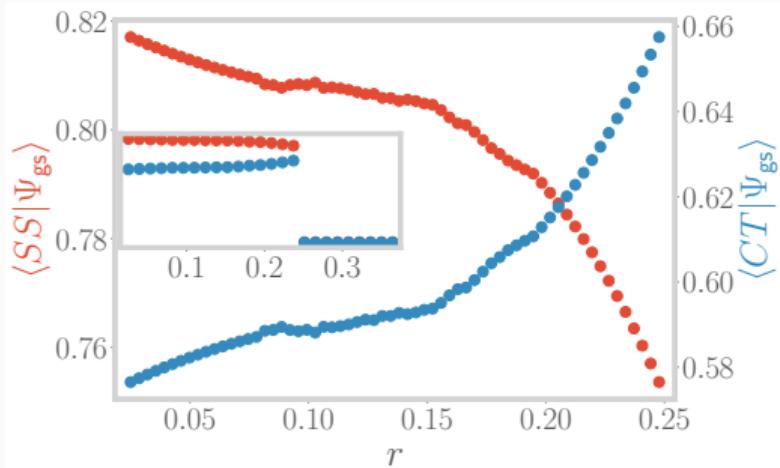
singlet \longrightarrow spin+charge liquid \longrightarrow local moment

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

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

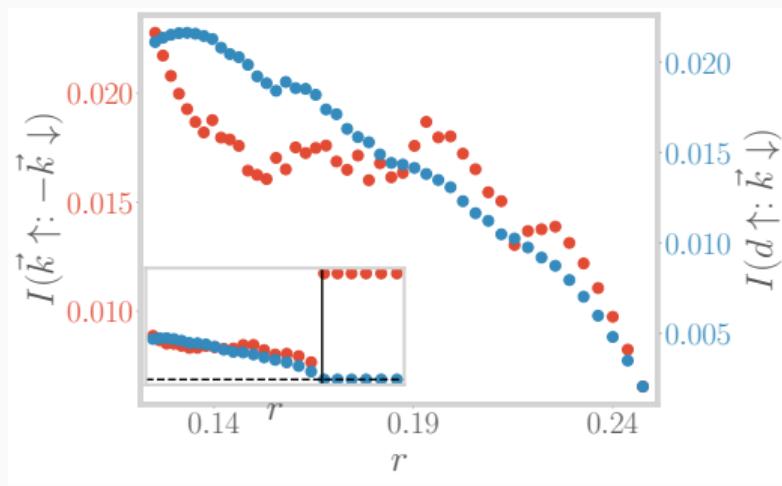
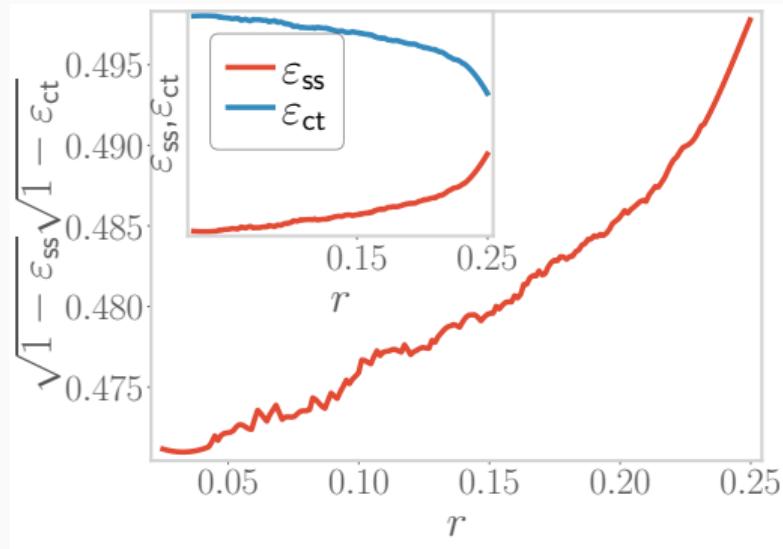
- ✓ correlated, dominant spin-flip processes lead to repulsive $U_{\text{eff}} = U_0 + U_b \sim J^*/8$
- ✓ J symmetrises the two sites, leading to similar spectral functions → essence of self-consistency

Entanglement as a probe for the transition

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

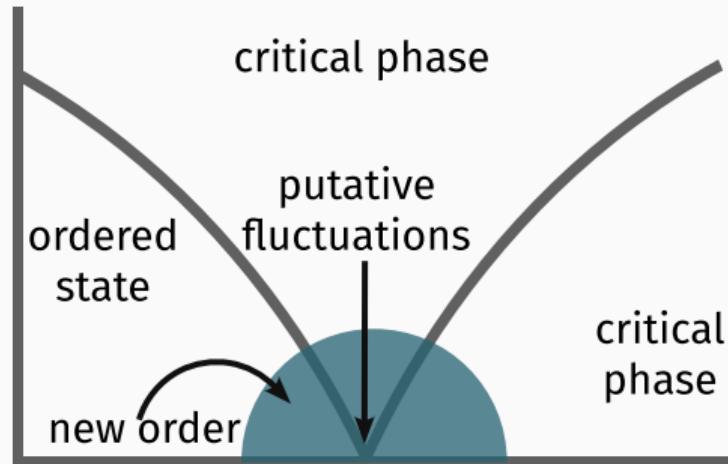
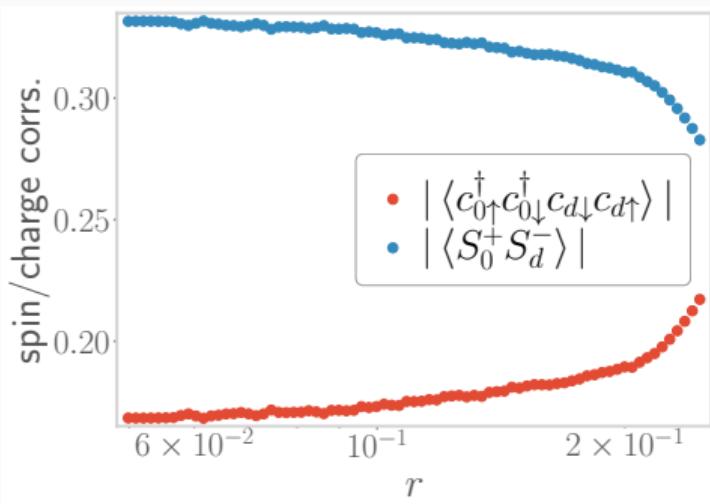
$\rightarrow \sqrt{1 - \varepsilon_{ss}} \sqrt{1 - \varepsilon_{ct}}$ is maximised, then vanishes

Mutual information between impurity and cloud vanishes

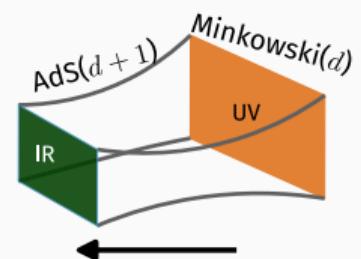
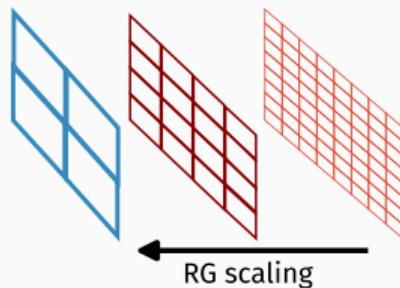


Presence of subdominant pair fluctuations

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

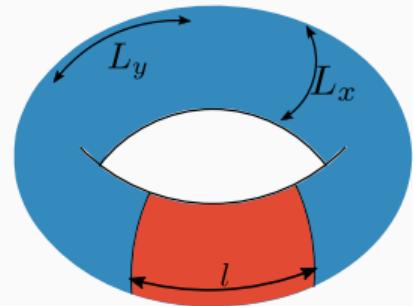
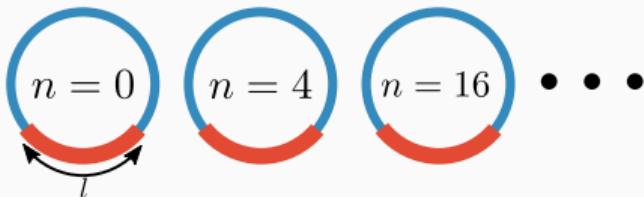
Simplest choice: the entire set

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

$$S_{A_z(j)} = f_z(j)caL_x - c \log |2 \sin(\pi f_z(j)\phi)|$$

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



- ✓ presents a **hierarchy** of entanglement → EE distributed across RG steps
RG transformation → reveals entanglement
- ✓ distribution of entanglement also present in **multipartite** entanglement

Mutual information = distance

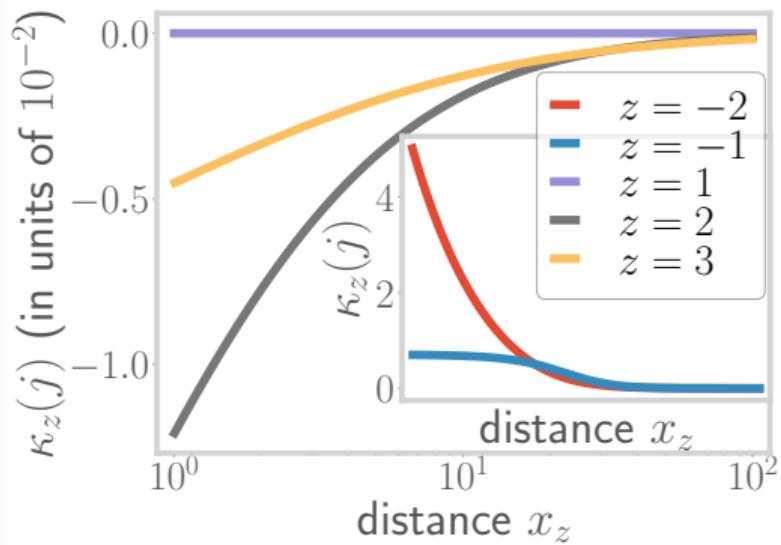
Mutual information: $I^2(A : B) \equiv S(A) + S(B) - S(A \cup B)$ (non-negative)

Define distances using mut. info.

$$x_z(j) = \log t_z(j), \quad y_z(j) = \log t_z(j \pm 1)$$

$$v_z(j) \equiv \Delta y_z(j)/\Delta x_z(j), \quad v' = \Delta v_z(j)/\Delta x_z(j)$$

Curvature as well: $\kappa_z(j) = \frac{v'_z(j)}{\left[1 + v_z(j)^2\right]^{\frac{3}{2}}}$



RG evolution = emergent distance

- ✓ Distances and curvature can be related to an RG **beta function**
- ✓ Amounts to an **explicit demonstration** of the holographic principle
- ✓ Sign of curvature is **topological**, can be written in terms of winding numbers

Topological nature of geometry-independent term

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

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

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 in the 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