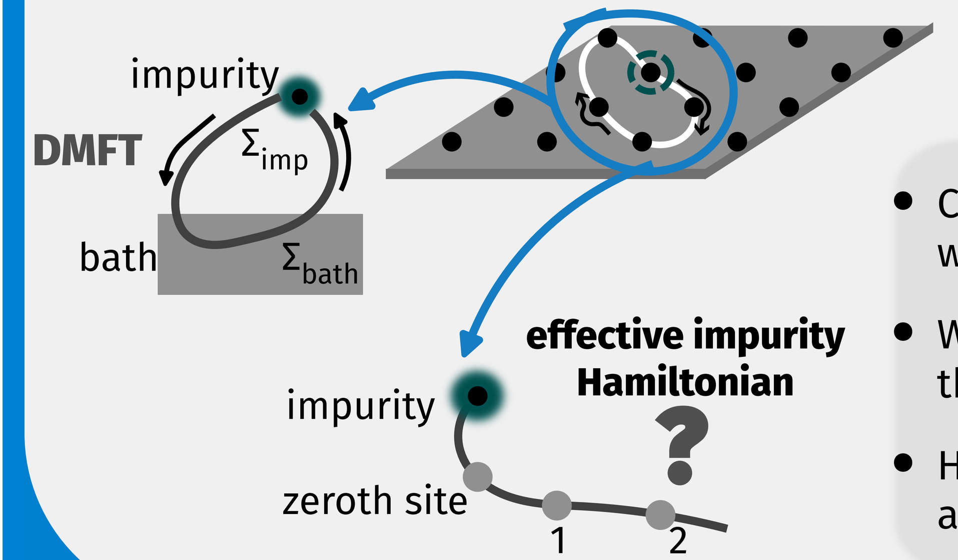
Local metal-insulator transition in an extended Anderson impurity model

Abhirup Mukherjee,[1] N.S. Vidhyadhiraja,[2] A. Taraphder,[3] S. Lal[1]

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

- Dynamical mean-field theory: exact in $d = \infty$
- Solves the bulk model by obtaining a **self-consistent** Anderson impurity model
- Displays Mott MIT on the Bethe lattice
- Standard Anderson model is **always metallic** - the bath must get correlated during self-consistency



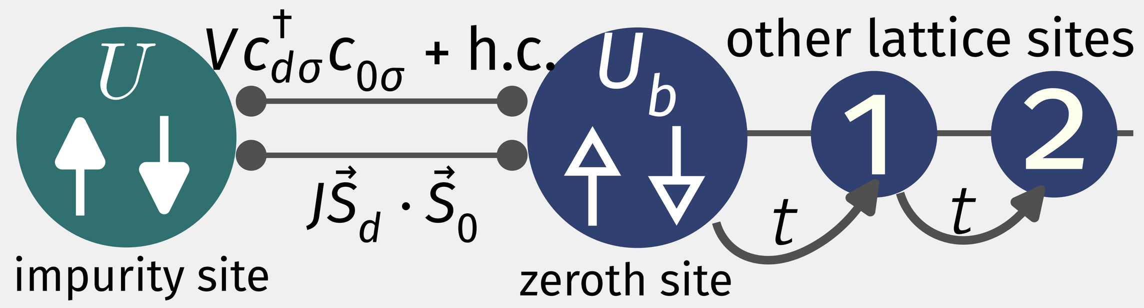
Outstanding Questions

- Can we replace the Σ-based description of correlations with an **effective impurity model** Hamiltonian?
- What fluctuations destabilise the Kondo screening? Is there a **minimal universal theory** near the transition?
- How does the local Fermi liquid die at the critical point, and what low-energy excitations replace it there?

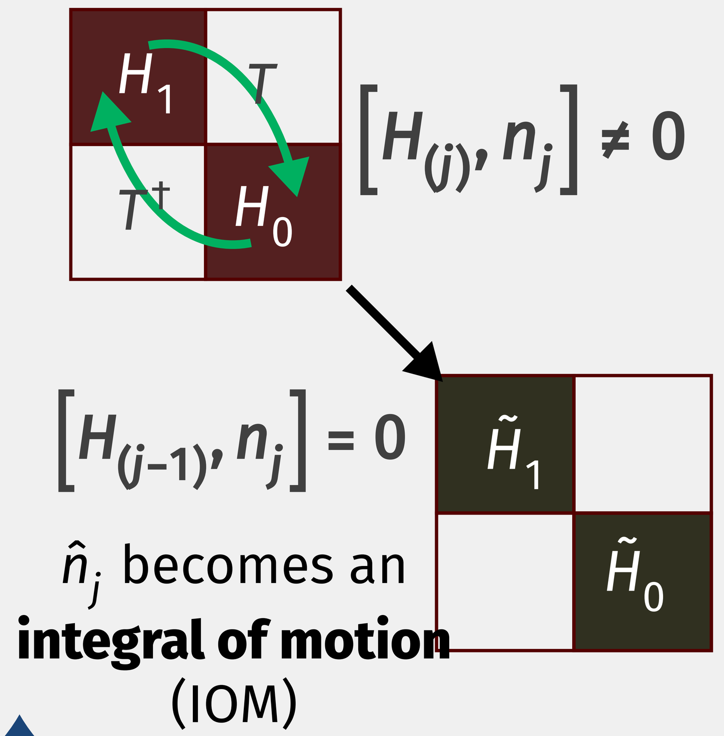
An *extended* Anderson impurity model

Insert two additional interaction terms to the SIAM:

- a **spin-exchange** term $J\vec{S}_d \cdot \vec{S}_0$ between impurity site and bath site that is coupled to the impurity site
- a local particle-hole symmetric **correlation term** $-U_b(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2$ on the same bath site



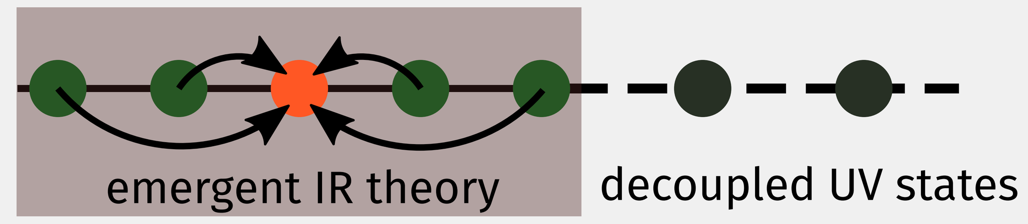
Our impurity solver - the unitary renormalisation group method



- Proceeds by applying **unitary transformations** U_j on the Hamiltonian to generate RG flow H_j

$$H_{j-1} = U_j H_j U_j^\dagger$$

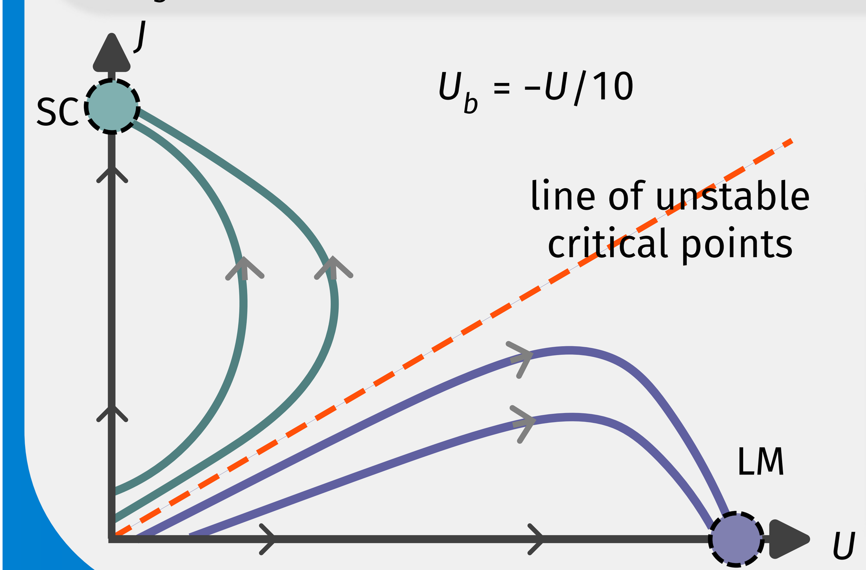
- U_j removes fluctuations in high energy k-states
- Fixed point reached when denominator of RG equation vanishes
- Fixed point Hamiltonian describes **emergent IR theory**



Nature of the RG flows

- RG equations for J, V have critical points at $r = -U_b/J = 1/4$
- Beyond critical point, V and J **turn irrelevant**
- U_b always marginal

$$\frac{dJ}{dD} = \frac{\rho J(J + 4U_b)}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}}$$

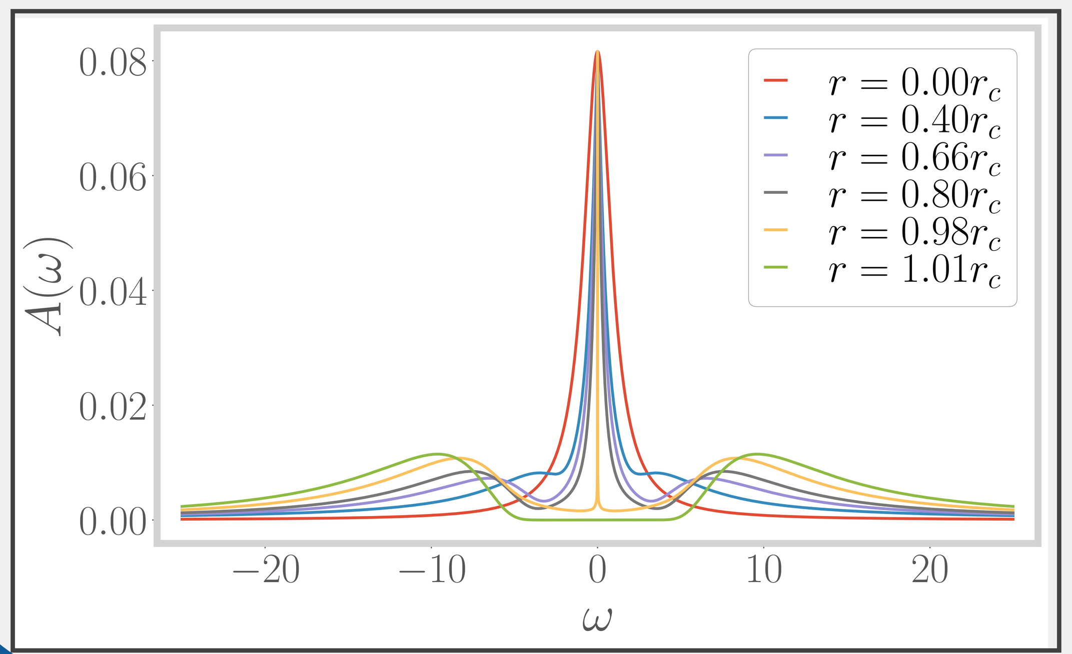


Fixed-point structure

- For $r < 1/4$: strong-coupling Kondo screening **singlet** ground state
- For $r > 1/4$: unscreened impurity spin **local moment** ground state
- At $r = 1/4$: partially screened unstable QCP some **non-Fermi liquid**

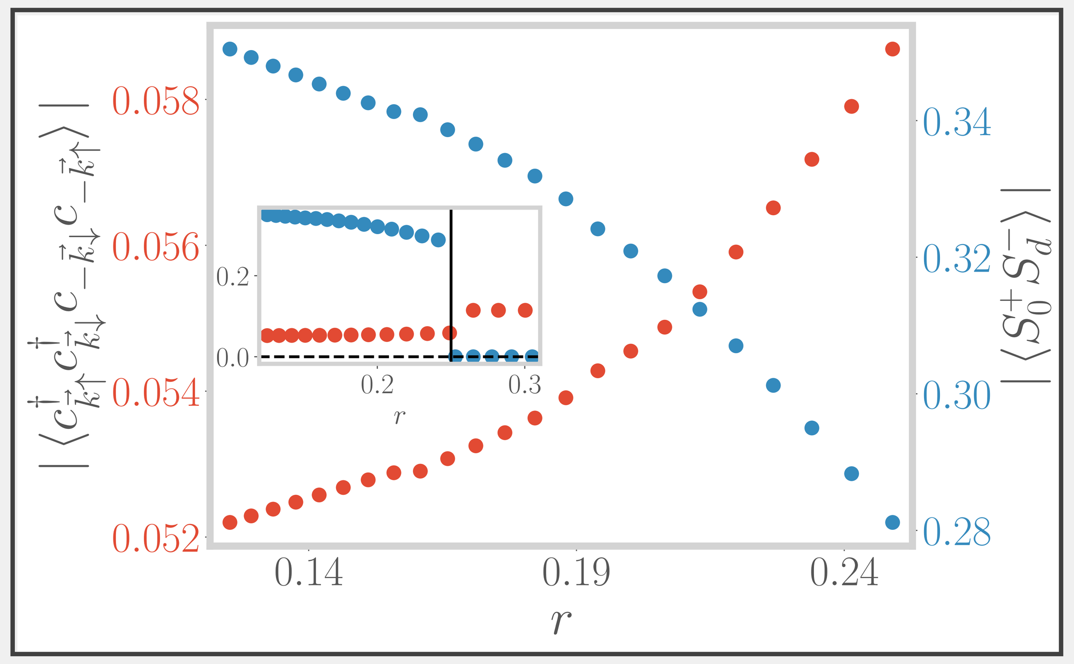
Local metal-insulator transition

Impurity spectral **gaps out** in the insulating phase. Near transition, an approximate **preformed gap** is visible



Growth of charge isospin fluctuations

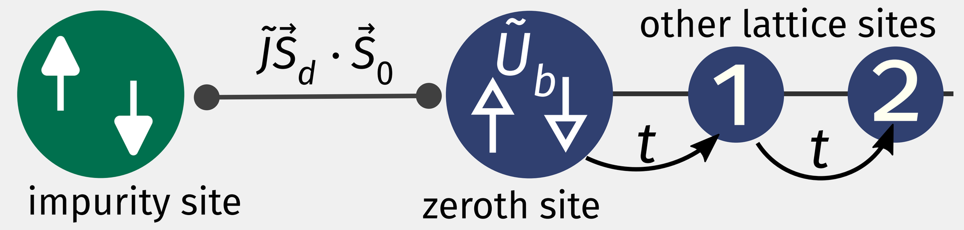
Kondo spin-flip processes get replaced by **pairing fluctuations** in the bath that destroy the Kondo cloud.



Universal theory near the transition

- At large U, eliminate charge states through Schrieffer-Wolffe transformation

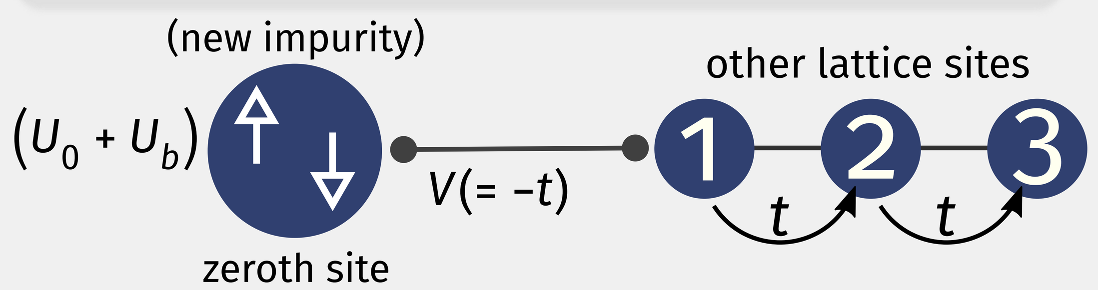
$$\tilde{H} = \tilde{J}\vec{S}_d \cdot \vec{S}_0 - \tilde{U}_b(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + H_{K.E.}$$



- Reduced model has both strong-coupling and local moment phases
- Is able to capture the phase transition!

A parallel to self-consistency in our study

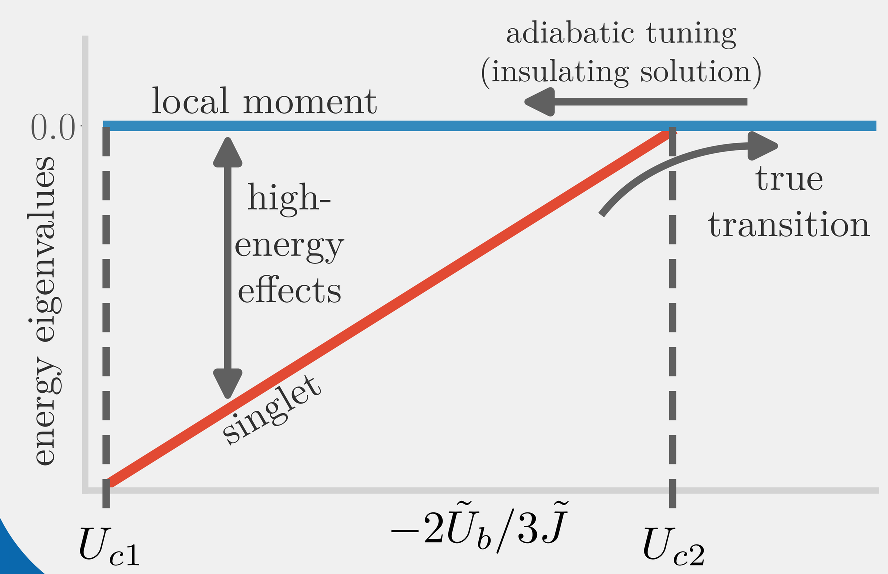
- Self-consistency requires **equality of impurity and zeroth site spectral functions**.
- To study zeroth site, we integrate out the impurity through 1-shot URG transformation.



- Renormalised bath correlation: $U_0 + U_b \simeq J^* + \frac{64}{3}\frac{V^{*2}}{J^*}$; overall positive, increases towards transition
- Implies that the hybridisations V, J **symmetrise the impurity and bath spectral functions**.

Presence of a coexistence region

- DMFT observes the **coexistence** of metallic and insulating solutions between U_{c1} and U_{c2}. The meta is found to have a **lower internal energy** in the coexistence region.
- The coexistence of solutions leads to a **first-order transition** at any finite temperature.
- Can be explained using the **spectrum of the** $J - U_b$ **model** shown in the figure.

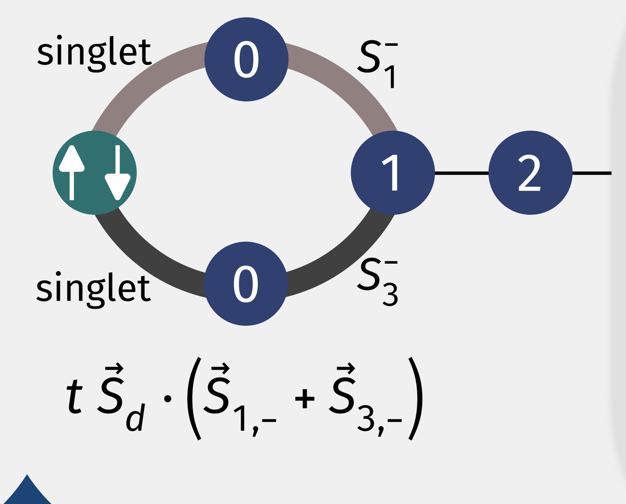


- The **level-crossing** between the singlet and LM states in the figure represents U_{c2} at $T = 0$.
- The point in the spectral function where the central and side peaks **get separated** is U_{c1}.
- The **large degeneracy** of the LM eigenstates stabilises them at finite temperatures.
- This stability allows one to **adiabatically continue** inwards from U_{c2}, hence obtaining an insulator for $U < U_{c2}$.

Fate of the local Fermi liquid

- In the metallic phase, the low-energy excitations involve a **local Fermi liquid** with a coupling that diverges at the transition, indicating the imminent death of the Landau quasiparticles.
- This is also seen in the **vanishing** of the Kondo temperature scale: $\lim_{r\to\frac{1}{4}} T_K = (1 - 4r)^\alpha$.

Nature of the metal exactly at the QCP



- The ground-state has both magnetic and non-magnetic parts, indicating **partial screening** and the NFL nature.
- The SU(2)-symmetric subspace involves the impurity coupled to 2 emergent spins formed by the 0th and 1st sites.
- The new emergent spins spannning two sites show the "**leaking**" of entanglement and the "**stretching**" of the singlet.
- The NFL-like behaviour also manifests in an **"Andreev" scattering** where an incident single electron $c^\dagger_{1\sigma}$ emerges as a hole $c_{1\sigma}$.

Concluding Remarks

- Our extended SIAM appears to be a **minimal** model showing a local MIT on the Bethe lattice. The transition is driven by the **enhanced pairing fluctuations** in the bath.
- The QCP shows **NFL behaviour** with a vanishing Z. It also shows an emergent **correlation of doublon-holon** pairs, as a precursor to their localisation in the insulator.
- The $T = 0$ transition of the $J - U_b$ model provides a description of the **finite temperature QCP** observed from DMFT.

Future directions

Additional insights may be obtained by (i) taking a **general impurity filling**, (ii) expansion of the cluster by taking **multiple impurities**. These can provide finer k-space details and lead to **non-paramagnetic** insulating phases.

Given a suitable analytical framework that **restores translation symmetry**, the model obtained here can be "tiled" throughout the lattice to create a bulk model, and the impurity phase transition observed here will then get promoted to a **bulk MIT**.

References

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