



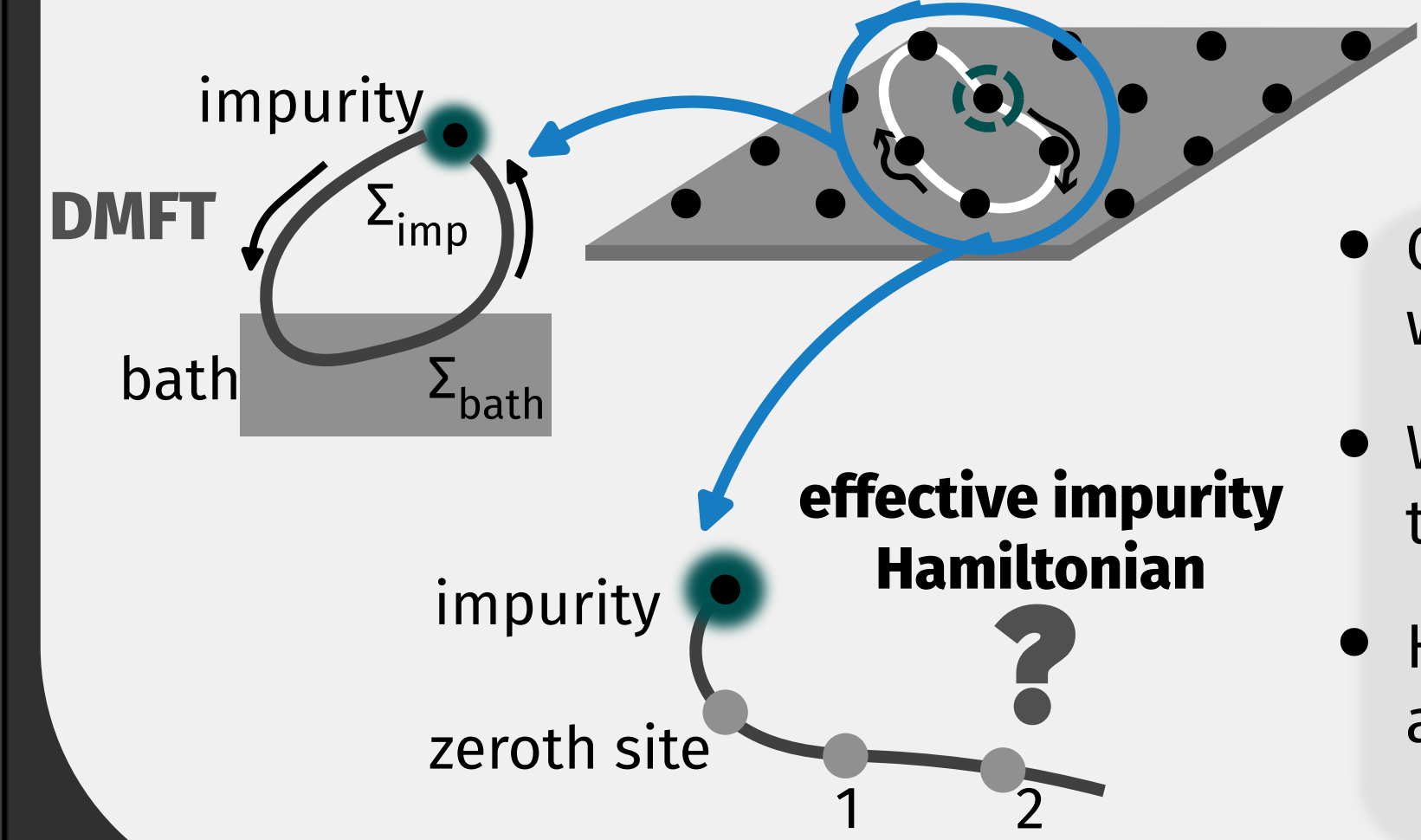
Local metal-insulator transition in an extended Anderson impurity model

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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



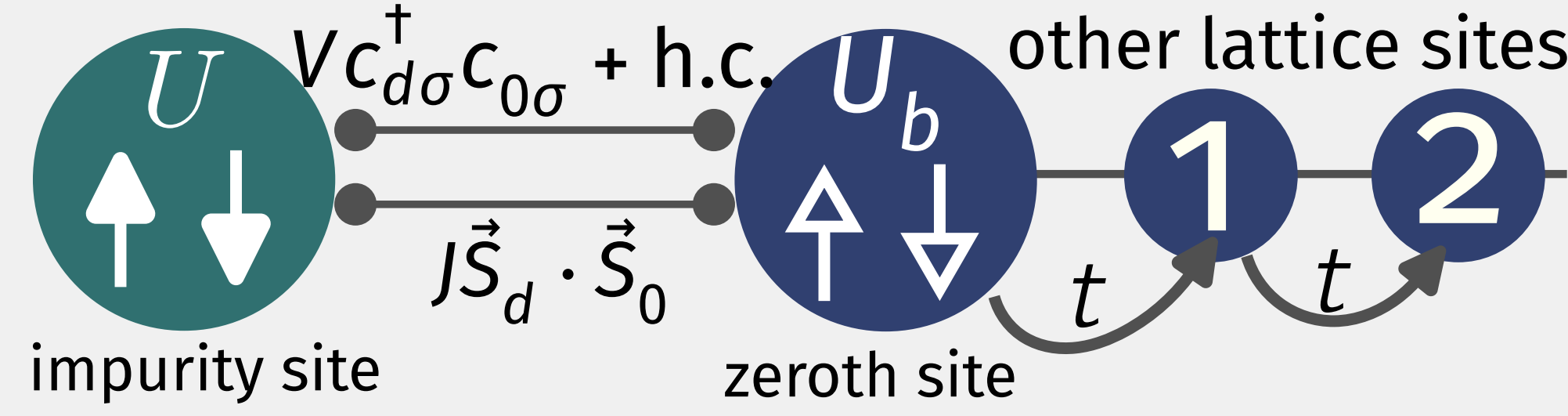
Outstanding Questions

- 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?

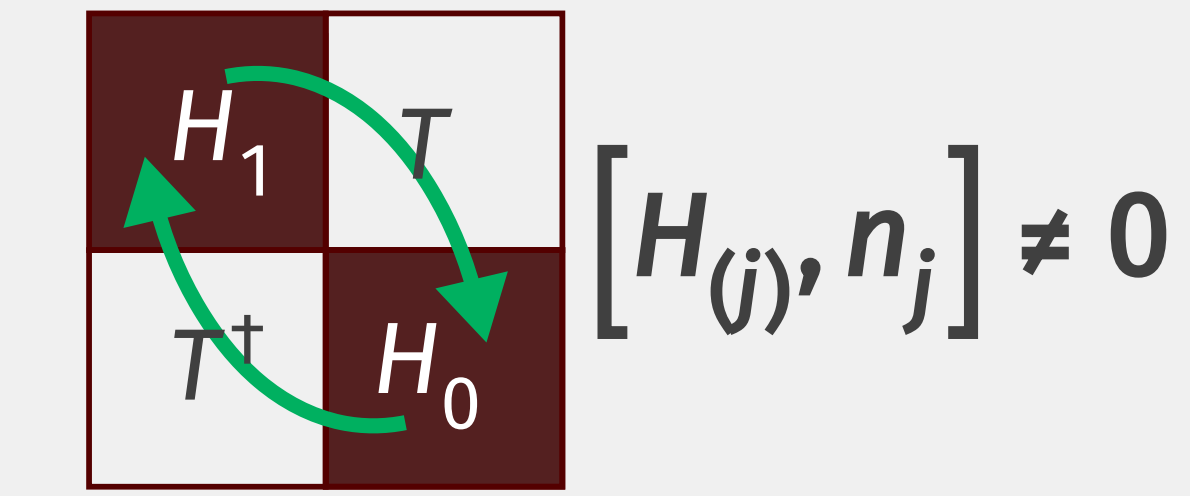
An Extended Anderson Impurity Model

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

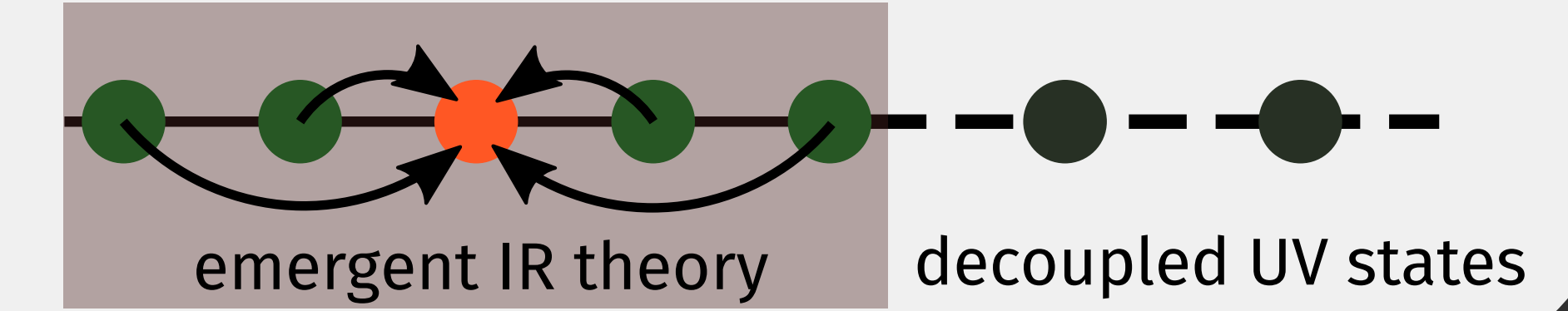


Our Impurity Solver - Unitary Renormalisation Group



$[H_{(j)}, n_j] \neq 0$
 $[H_{(j-1)}, n_j] = 0$
 \hat{n}_j becomes an **integral of motion (IOM)**

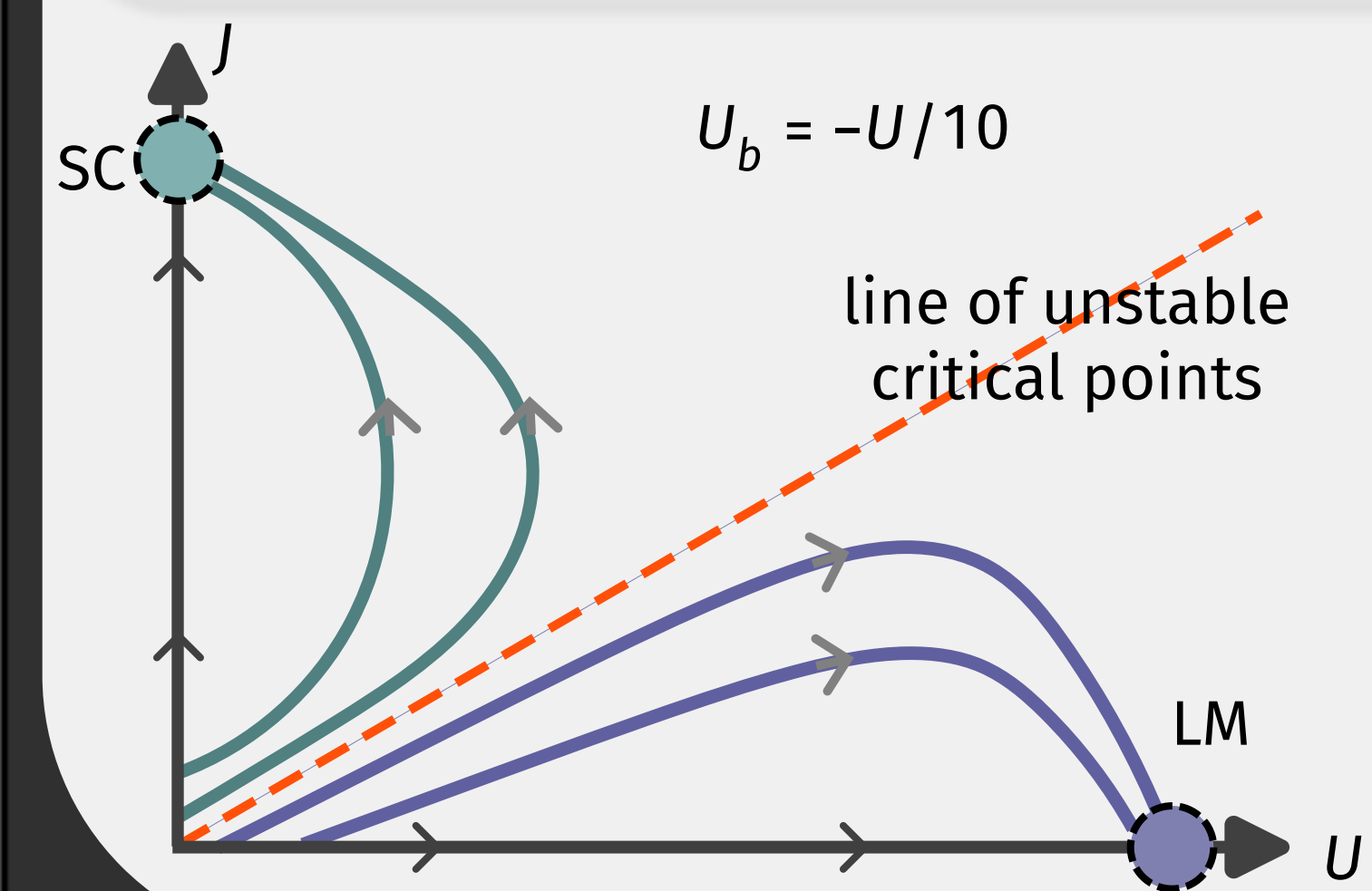
- Proceeds by applying unitary transformations U_j on the Hamiltonian to generate RG flow H_j
 $H_{j-1} = U_j H_j U_j^\dagger$
- U_j removes fluctuations in high energy k -states
- Fixed point reached when denominator of RG equation vanishes
- Fixed point Hamiltonian describes emergent IR theory



Nature of RG Flows

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

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

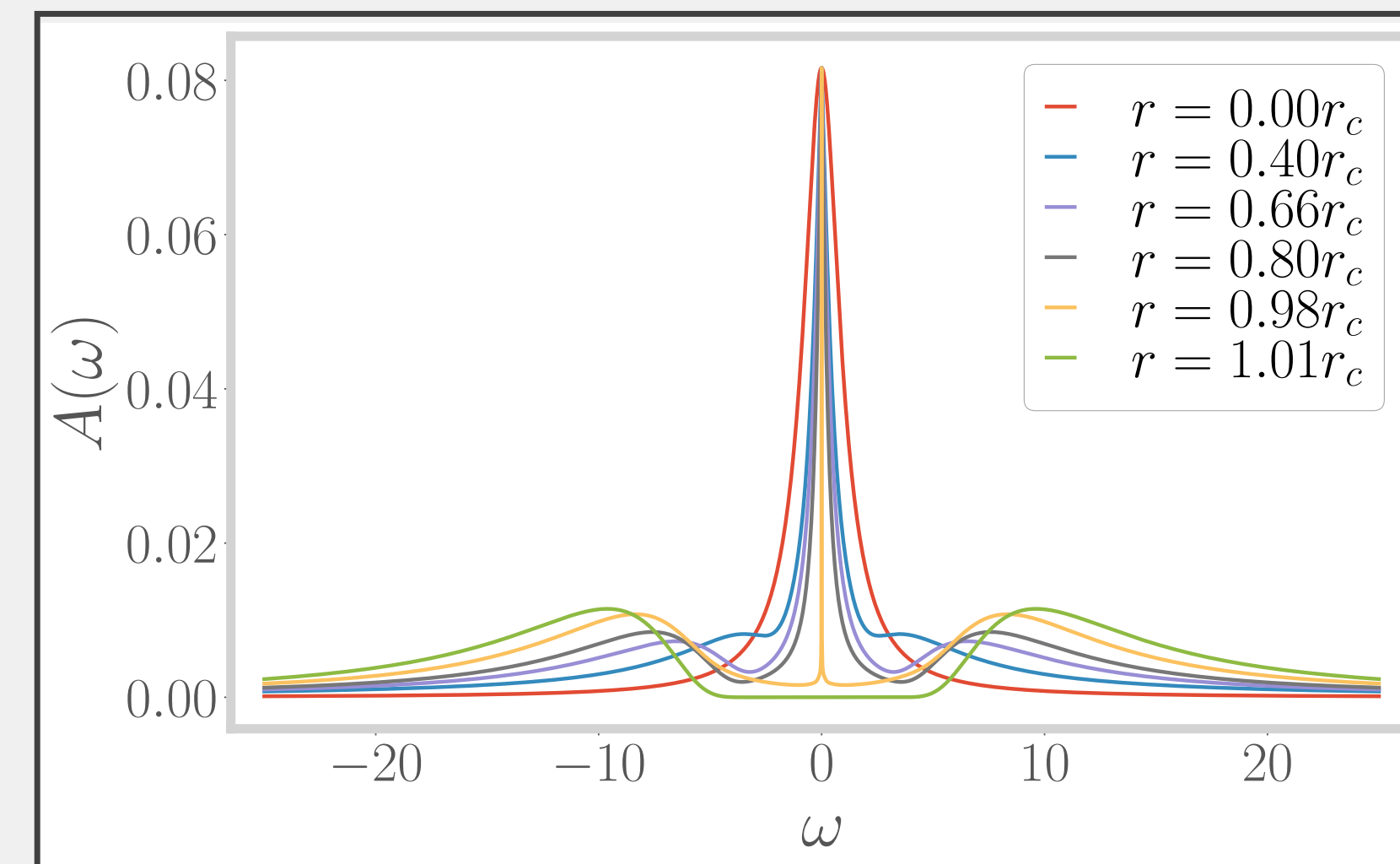


Fixed-Point Structure

- 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

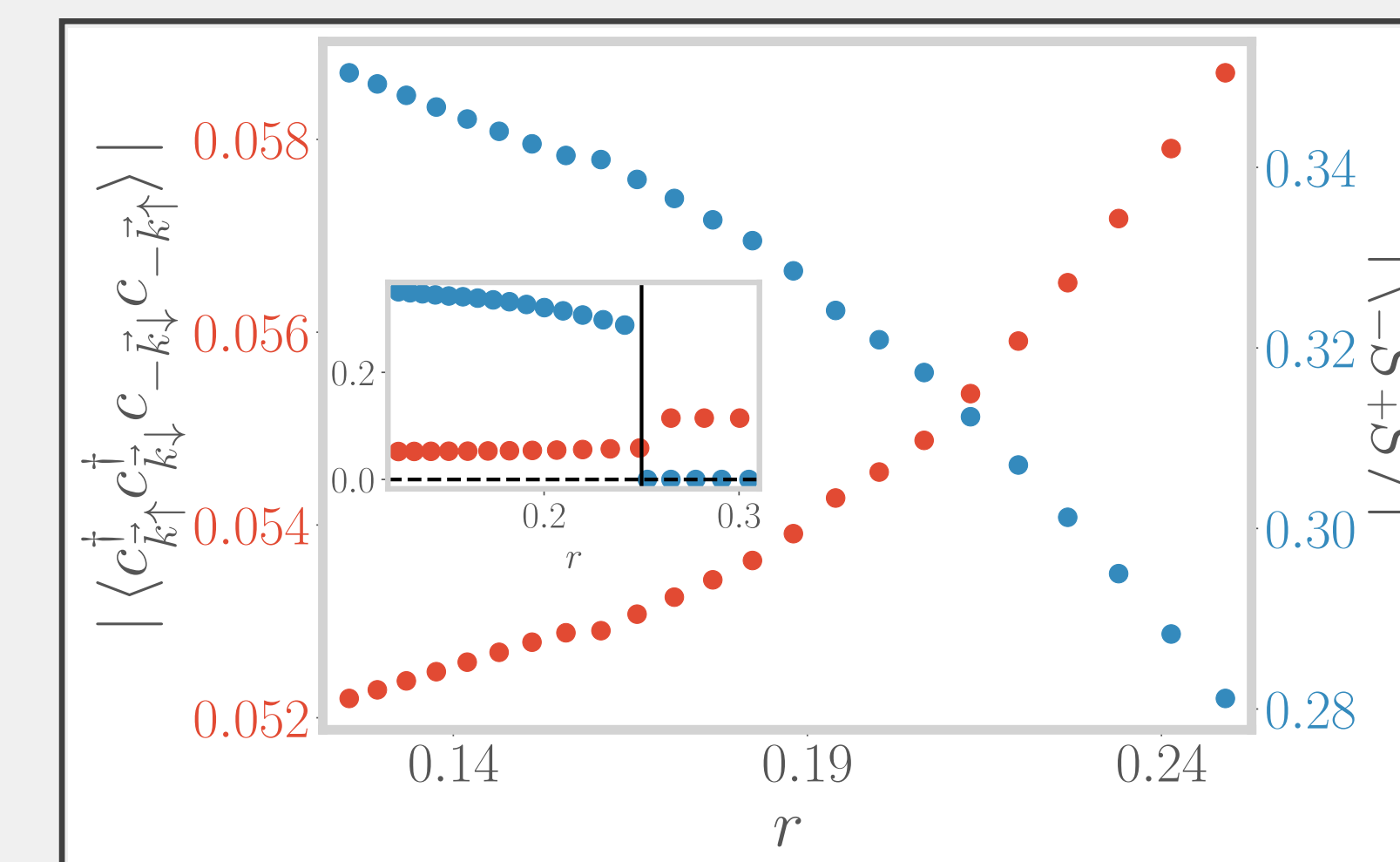
Local metal-insulator transition

Tuning the bath correlation U_b gaps out the impurity spectral function



Growth of charge isospin fluctuations

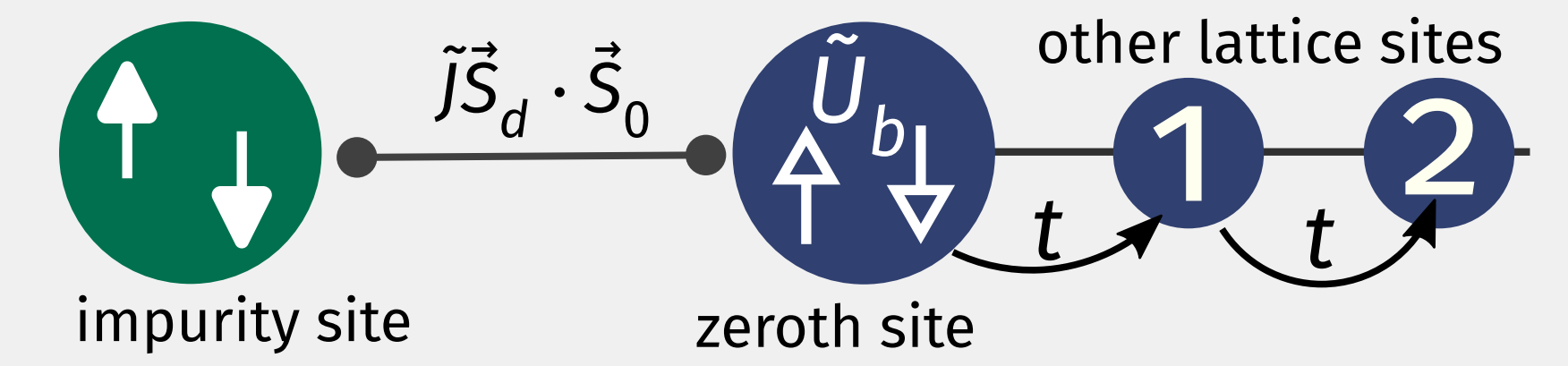
Kondo spin-flip processes get replaced by pairing fluctuations in the bath that destroy the Kondo cloud.



Universal theory near the transition

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

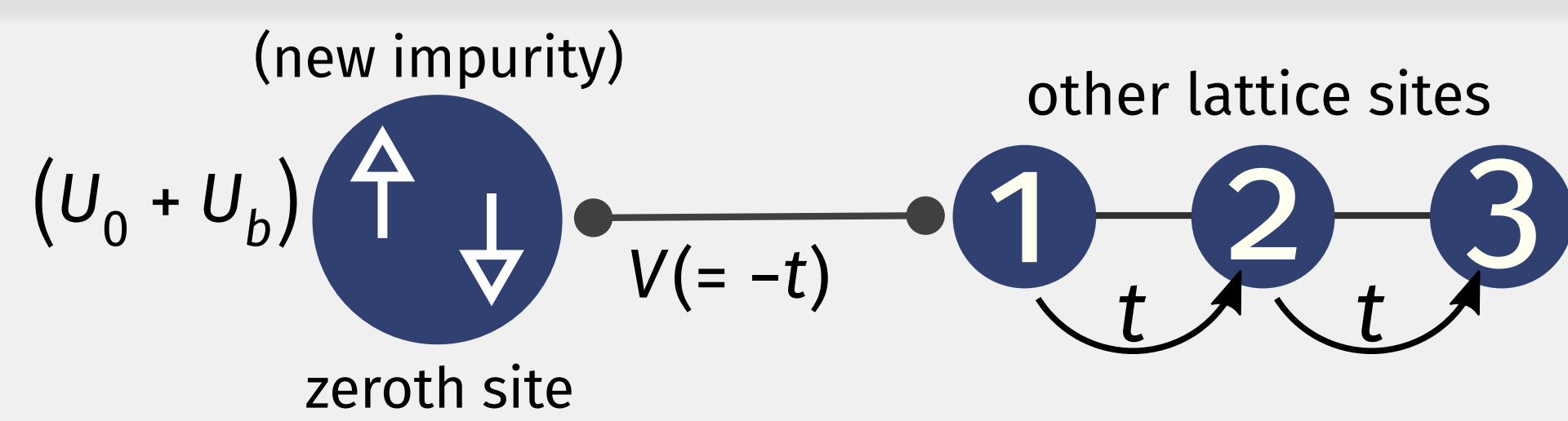
$$\tilde{H} = \tilde{J}\vec{S}_d \cdot \vec{S}_0 - \tilde{U}_b(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 + H_{KE}.$$



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

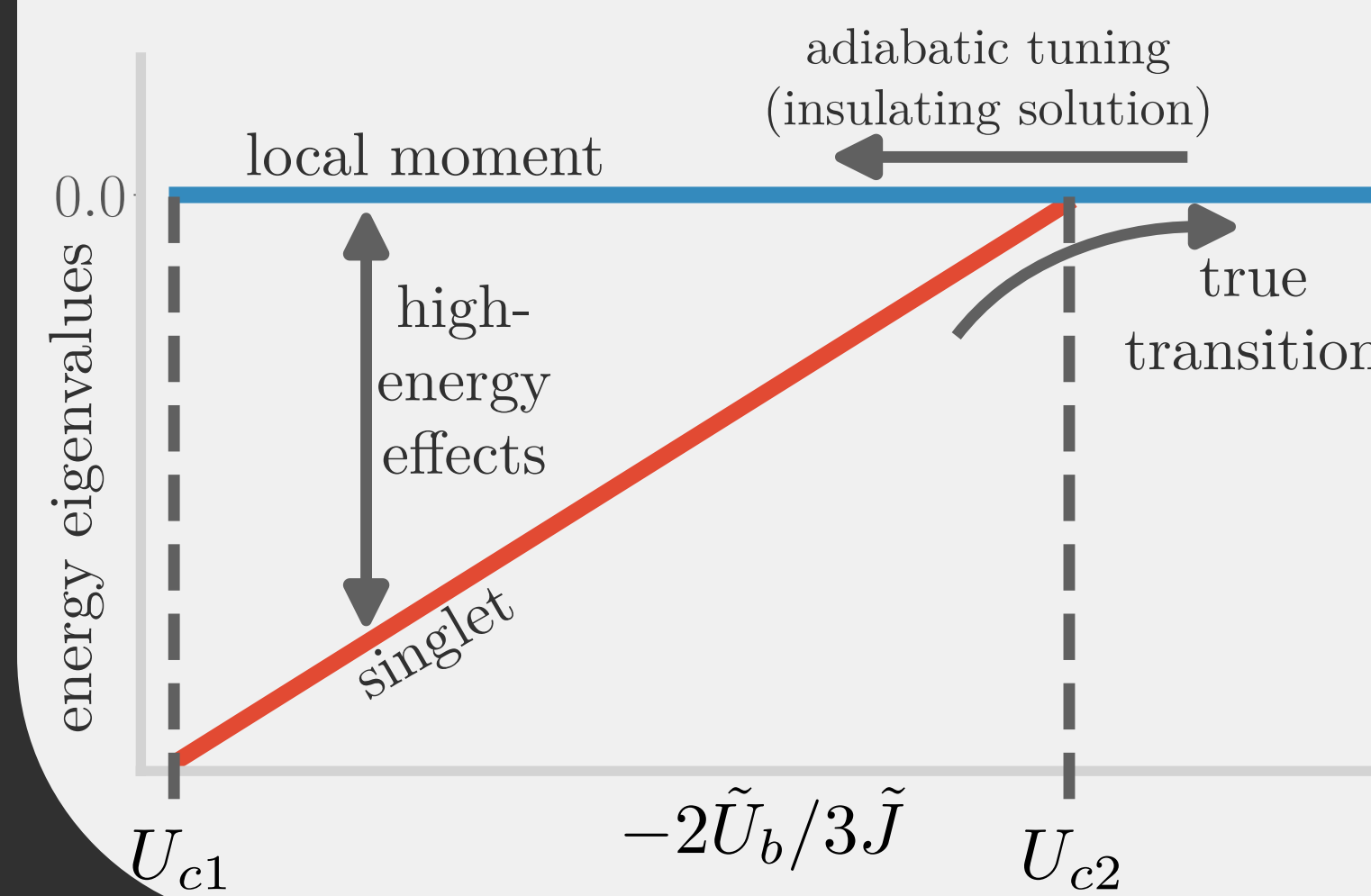
A parallel to self-consistency in our study

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

Presence of a coexistence region



Nature of the low-energy metallic excitations

References

- A. Georges et al., RMP 68, 13 (1996)
- G. Kotliar and Q. Si, Phys. Rev. B 53, 12373 (1996)
- G. Moeller et al., Phys. Rev. Lett. 74, 2082 (1995)
- R. Bulla, Phys. Rev. Lett. 83, 136 (1999)
- H. R. Krishna-murthy et al., Phys. Rev. B 21, 1003 (1980)
- A. Mukherjee and S. Lal, Nuclear Physics B 960, 115170 & 115163 (2020)
- K. Held et al., Phys. Rev. Lett. 110, 246402 (2013)

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**.

Acknowledgements

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