

# Kondo breakdown drives the Mott-Hubbard transition

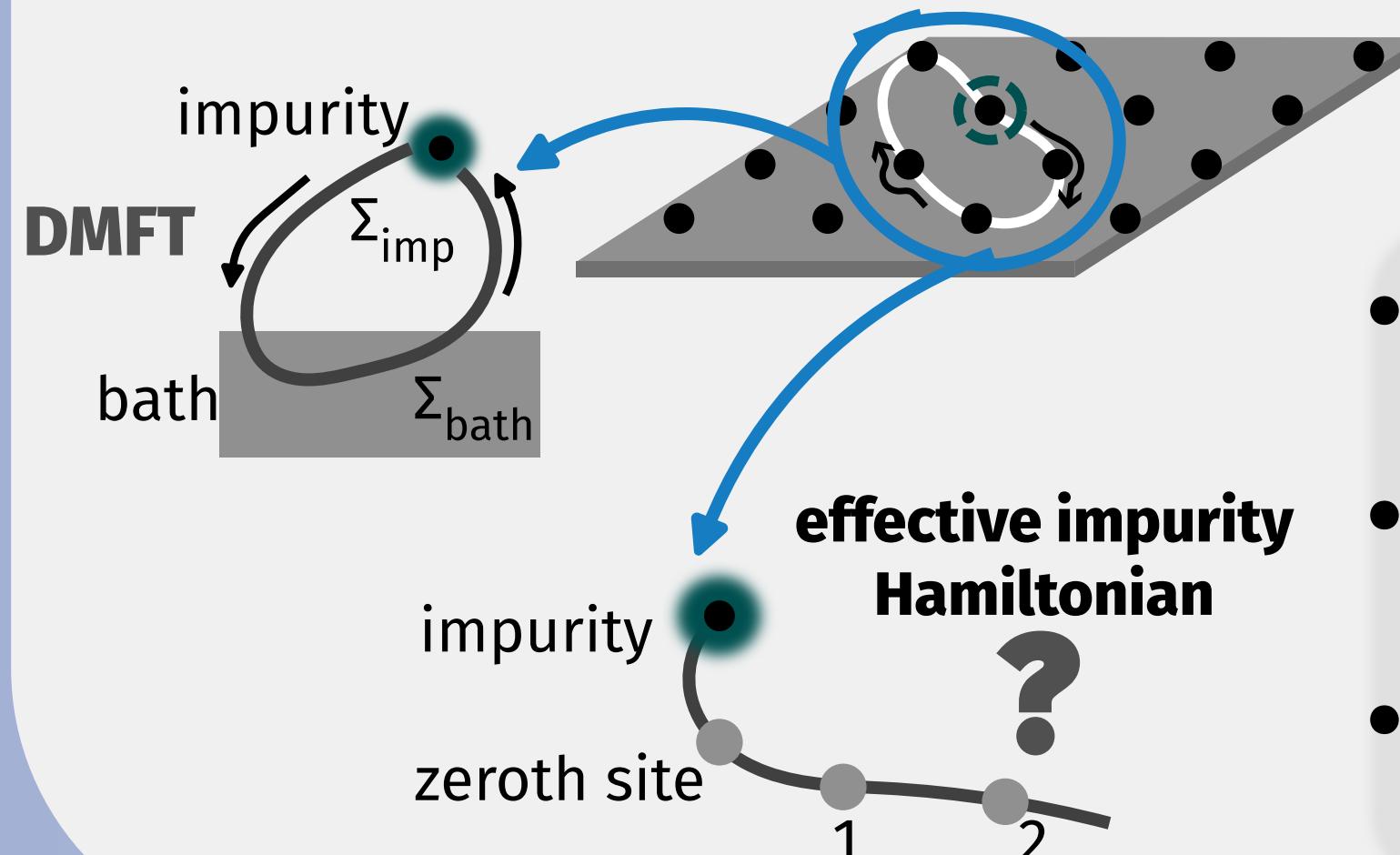
## Charge fluctuations as a route towards the Mott insulator

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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

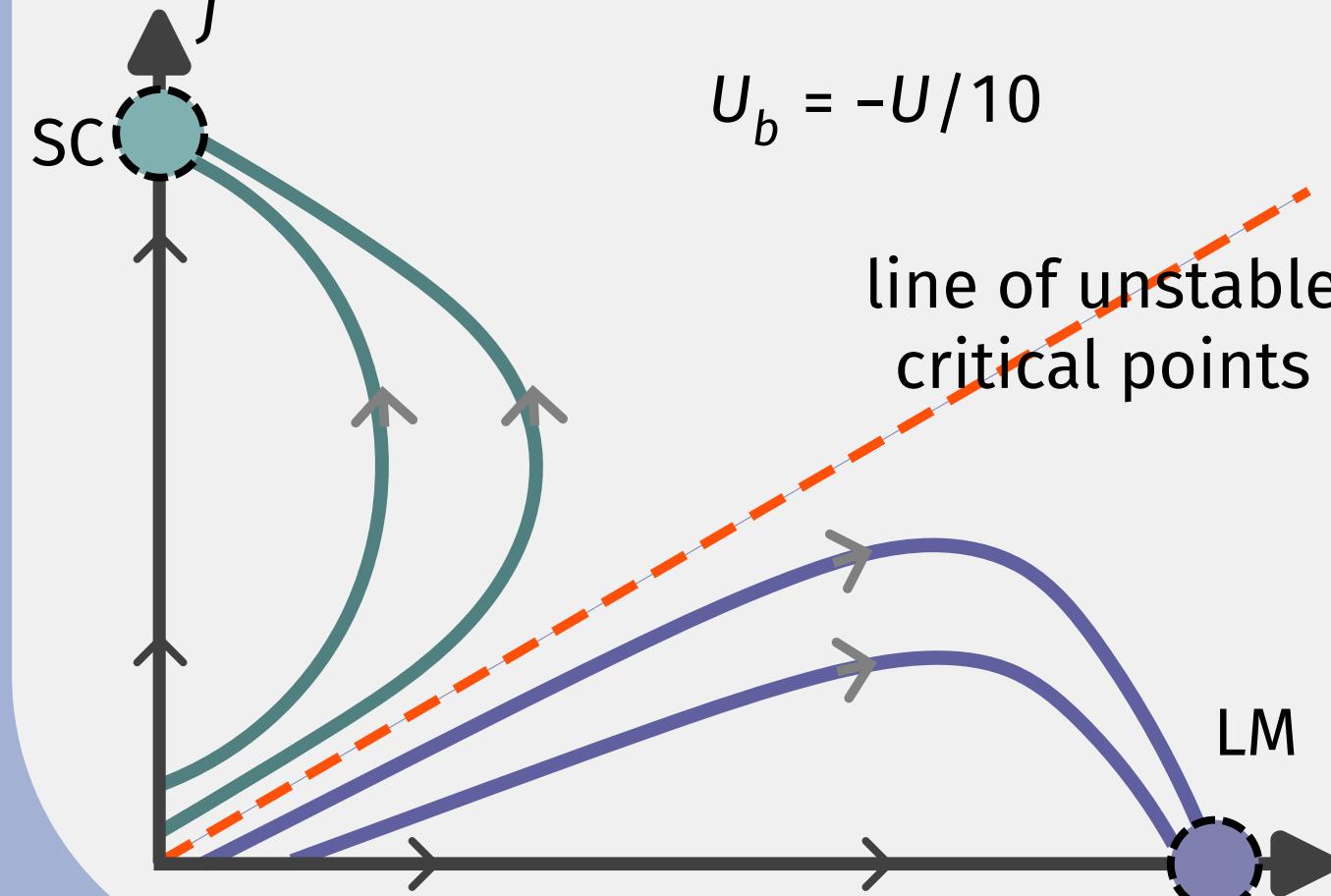


### Outstanding Questions

- Can we replace the  $\Sigma$ -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?

### Nature of the RG flows

- RG equations for  $J, V$  have critical points at finite  $U_b$ .
- Beyond critical point, both  $V$  and  $J$  will have **turned irrelevant**
- $U$  irrelevant before the QCP, relevant after it.  $U_b$  always marginal

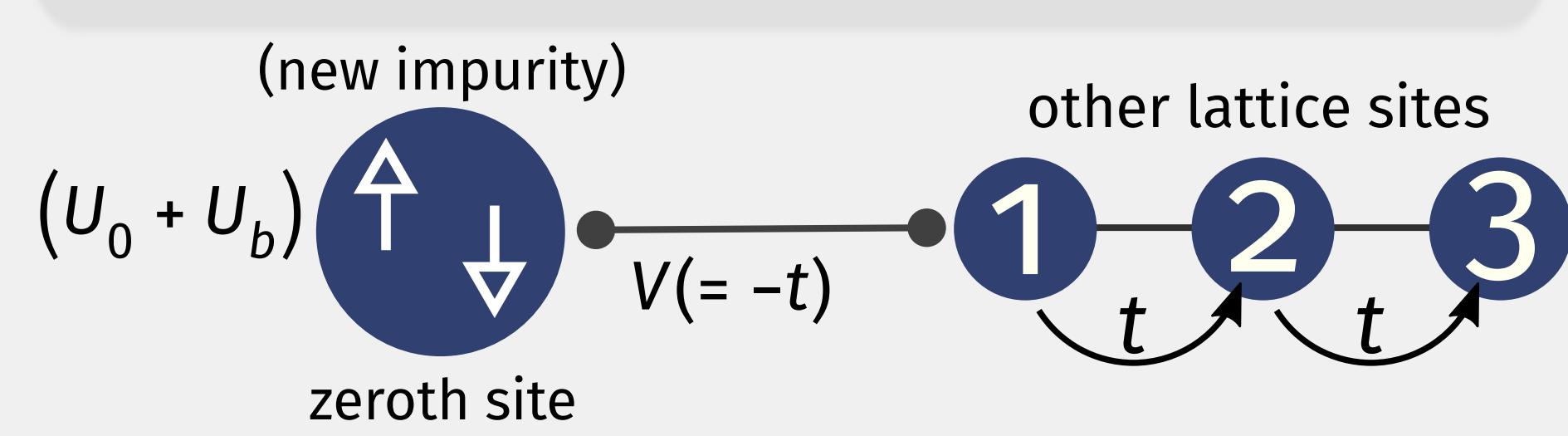


### Fixed-point structure

- For  $r \ll 1/4$ : IR physics described by  $V - J$  model; adiabatically connected to the **small- $U$  SIAM**
- At  $r \leq 1/4$ :  $V$  becomes irrelevant;  $J - U_b$  model is obtained; **singlet** ground state emerges
- For  $r > 1/4$ : unscreened impurity spin **local moment** ground state

### 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.



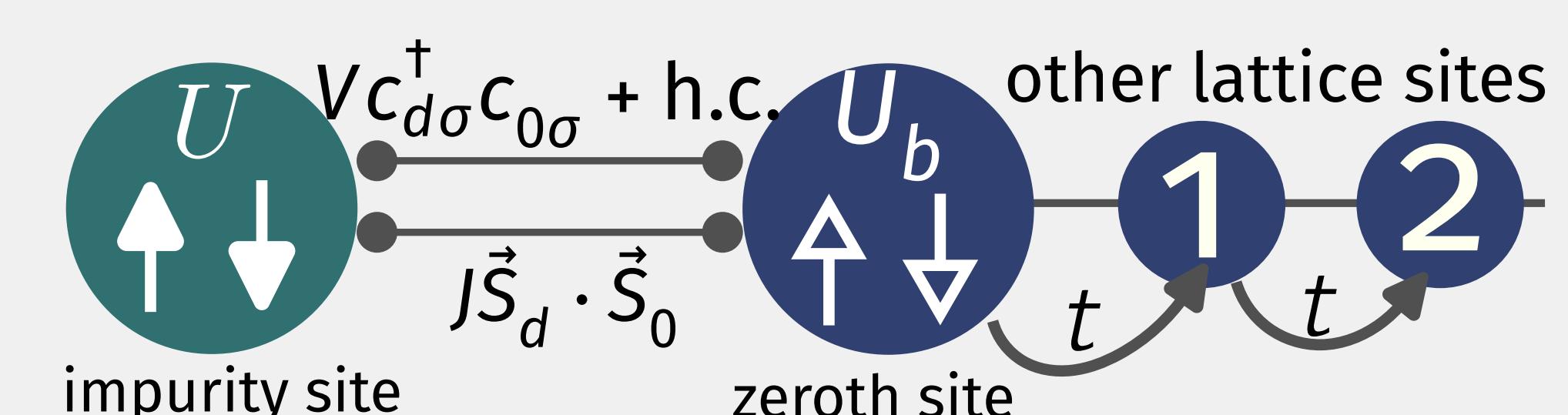
- Renormalised bath correlation:  $U_0 + U_b \approx J^* + \frac{64}{3} \frac{V^2}{J^*}$ ; overall positive, increases towards transition
- Implies that the hybridisations  $V, J$  **symmetrise the impurity and bath spectral functions**.

### 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.

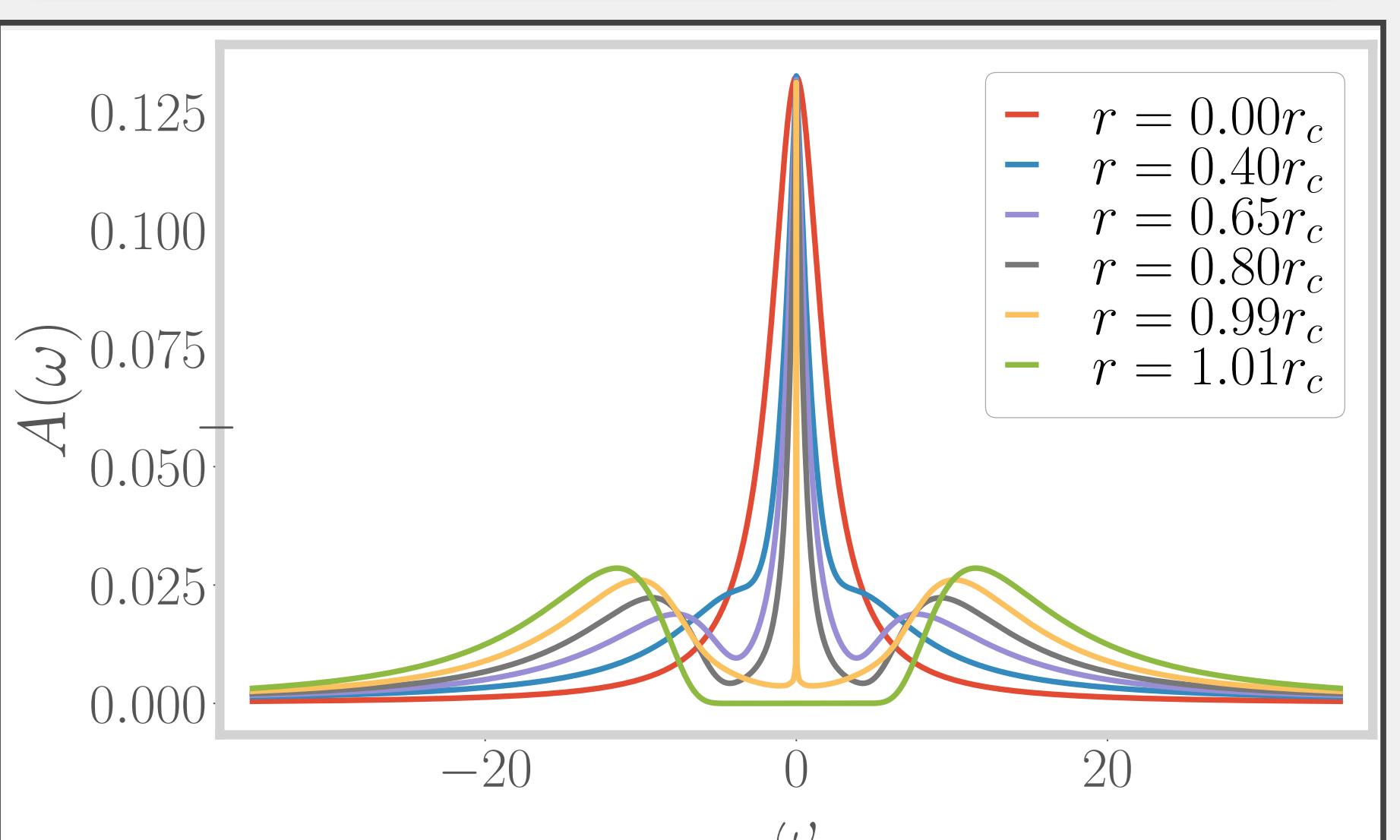
### An extended Anderson impurity model

- 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



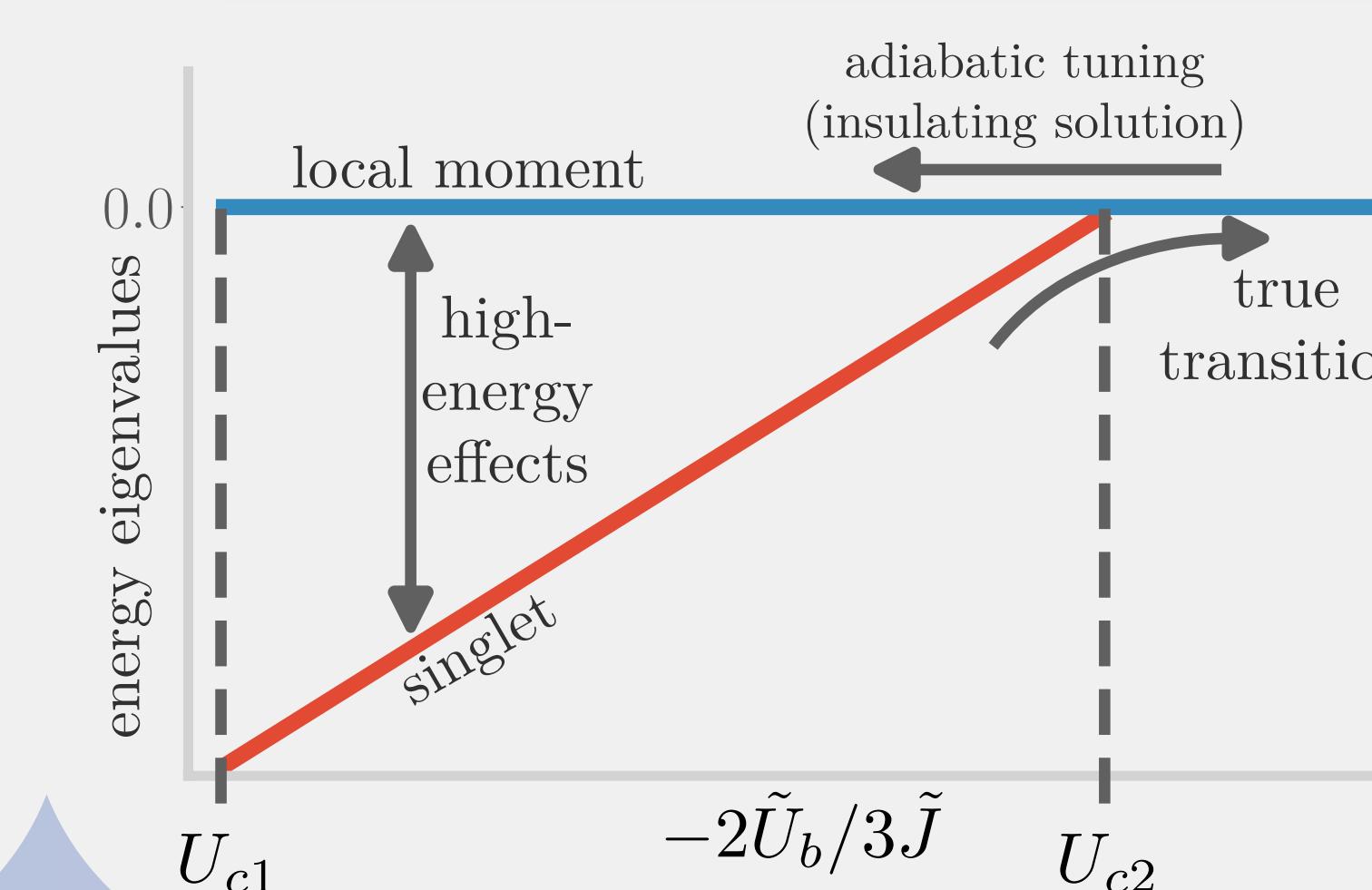
### Local metal-insulator transition

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



### Presence of a coexistence region

- DMFT observes the **coexistence** of metallic and insulating solutions between  $U_{c1}$  and  $U_{c2}$ . The metal 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.

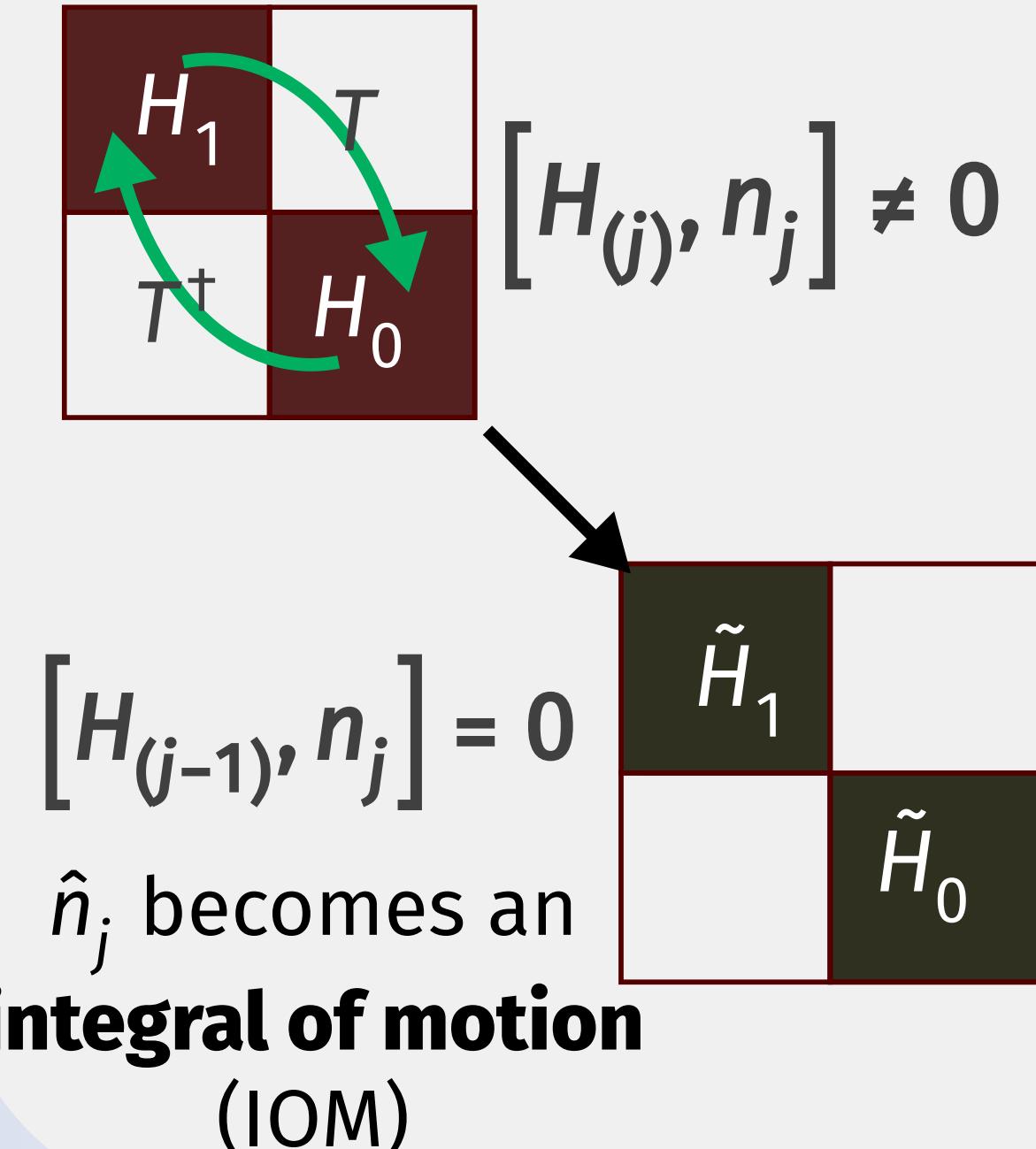


- The **level-crossing** between the singlet and LM states in the figure represents  $U_{c2}$  at  $T = 0$ .
- The point in the spectral function where the central and side peaks **get separated** is  $U_{c1}$ .
- The **large degeneracy** of the LM eigenstates stabilises them at finite temperatures.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

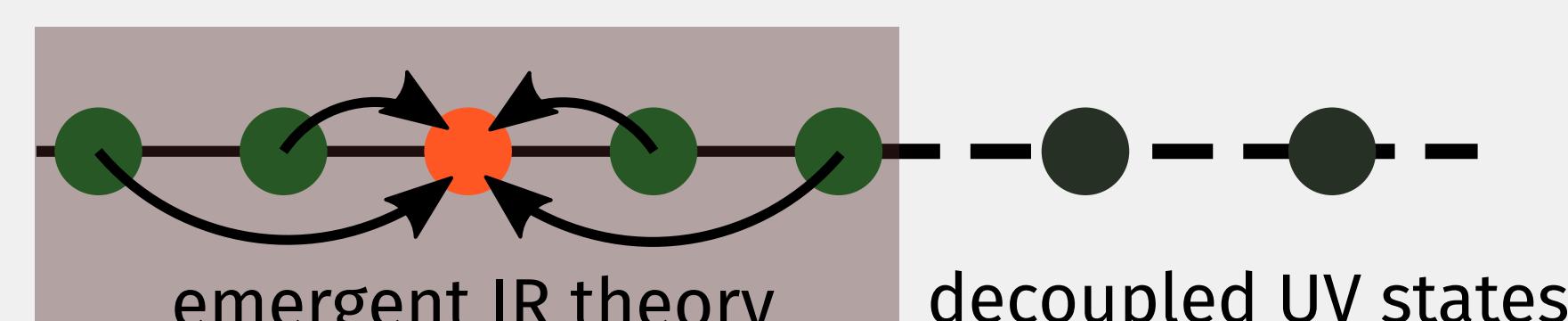
### Future directions

- 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**.

### Our impurity solver - the unitary renormalisation group method

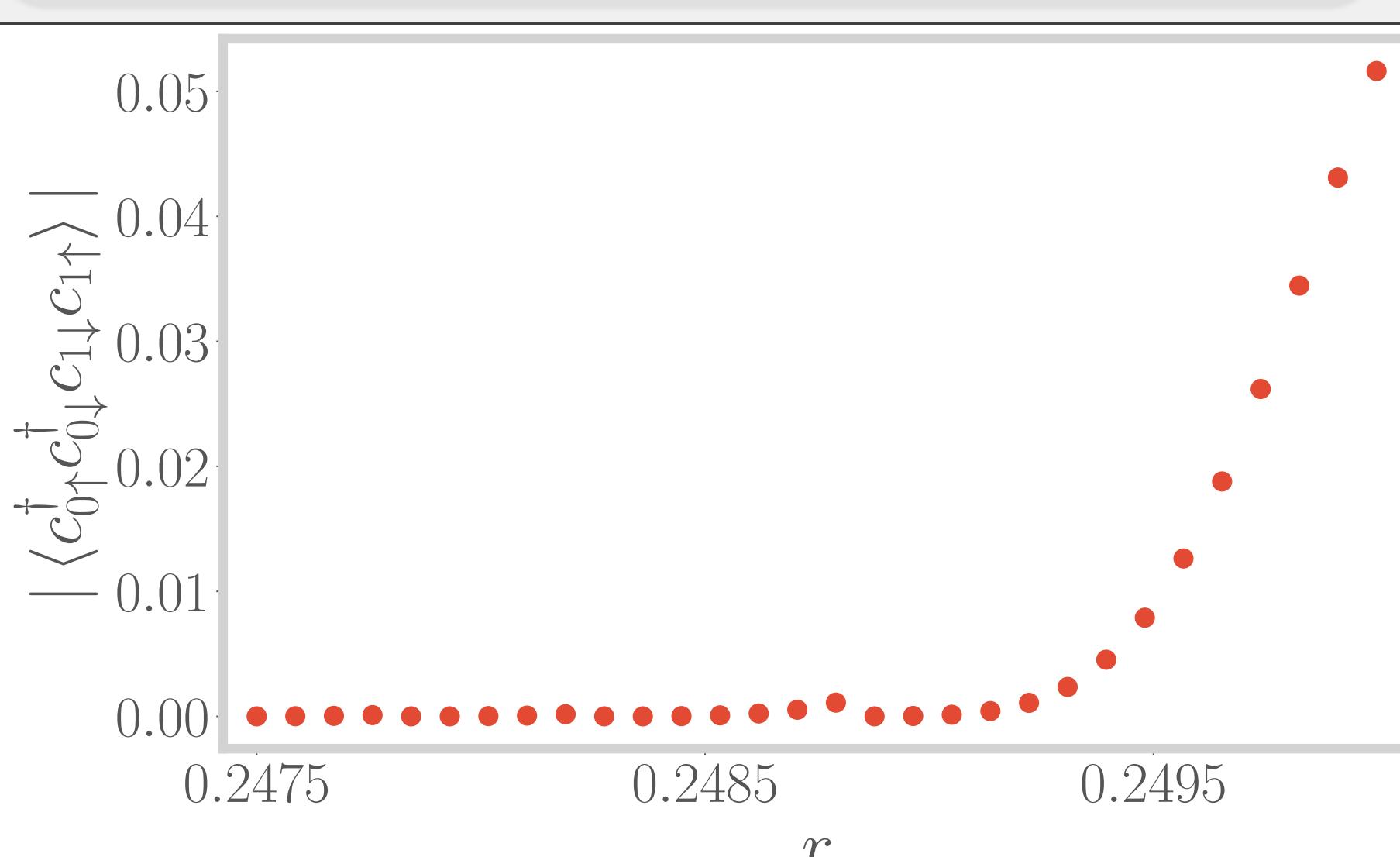


- Proceeds by applying **unitary transformations**  $U_j$  on the Hamiltonian to generate RG flow  $H_j$
- $H_{j-1} = U_j H_j U_j^\dagger$
- $U_j$  removes fluctuations in high energy  $k$ -states
- Fixed point reached when denominator of RG equation vanishes
- Fixed point Hamiltonian describes **emergent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



### Growth of charge isospin fluctuations

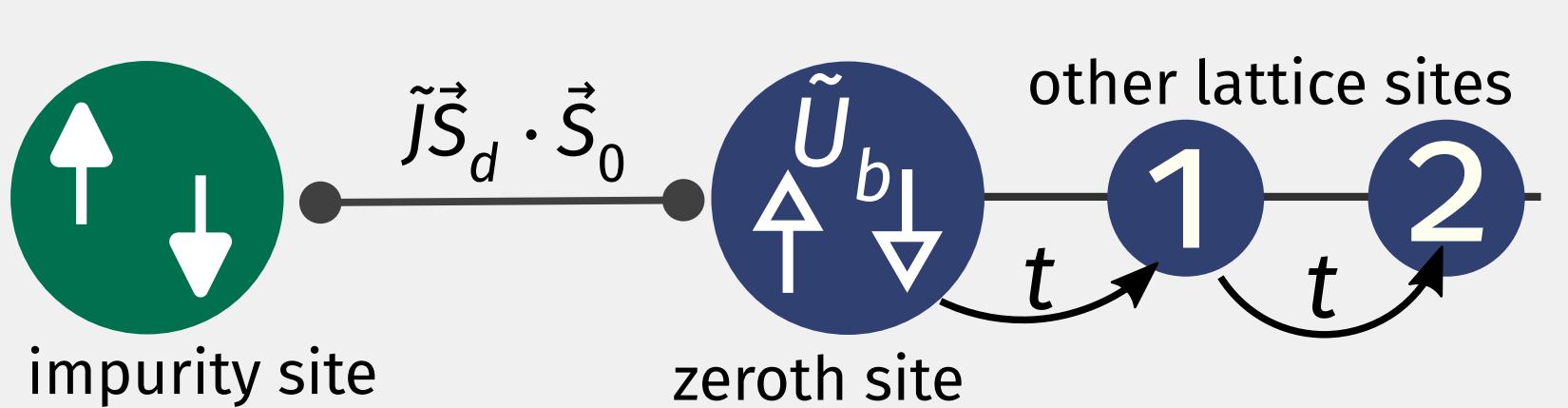
Kondo spin-flip processes get destroyed by real-space **pairing fluctuations** between 0 and 1 sites.



### Universal theory near the transition

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

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



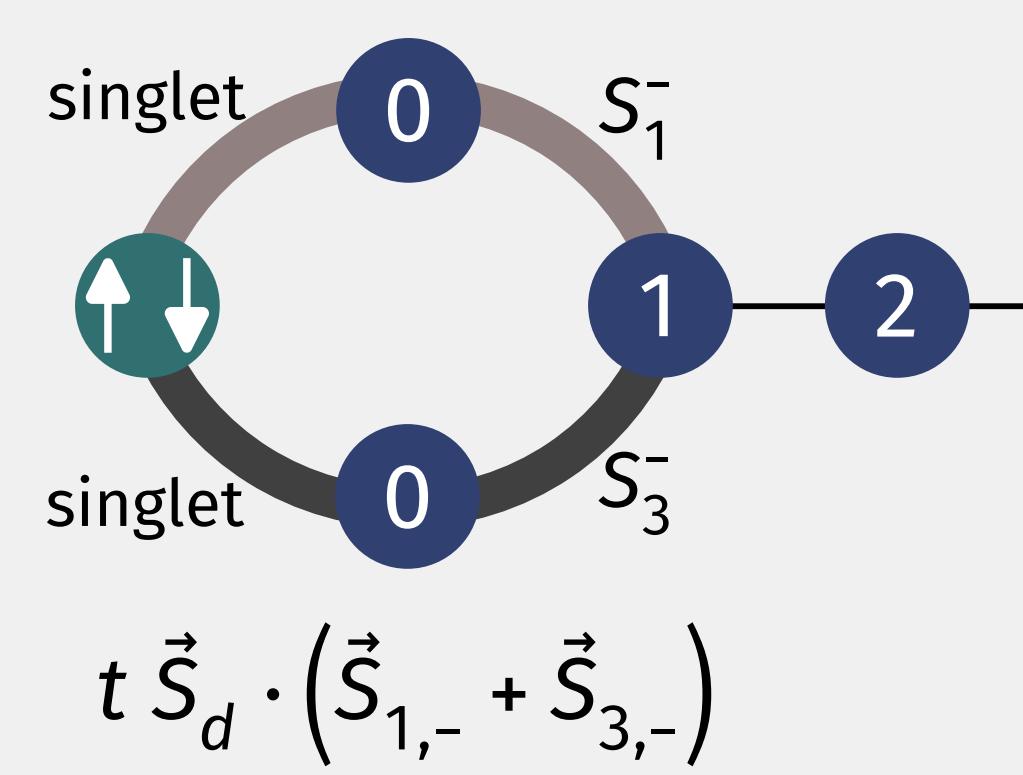
- Reduced model has both strong-coupling and local moment phases
- Is able to capture the phase transition!

### 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:  $\lim_{r \rightarrow \frac{1}{4}} T_K = (1 - 4r)^{\alpha}$ .

### 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 0<sup>th</sup> and 1<sup>st</sup> sites.
- The new emergent spins spanning 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  $c_{1\sigma}^\dagger$  emerges as a hole  $c_{1\sigma}$ .



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