



A New Auxiliary-Model Method for Strongly-Correlated Systems

A fresh look at the Mott transition in d=2

Abhirup Mukherjee¹, N.S. Vidhyadhiraja², A. Taraphder³, Siddhartha Lal¹

IISER Kolkata

Mohanpur

West Bengal

¹IISER Kolkata

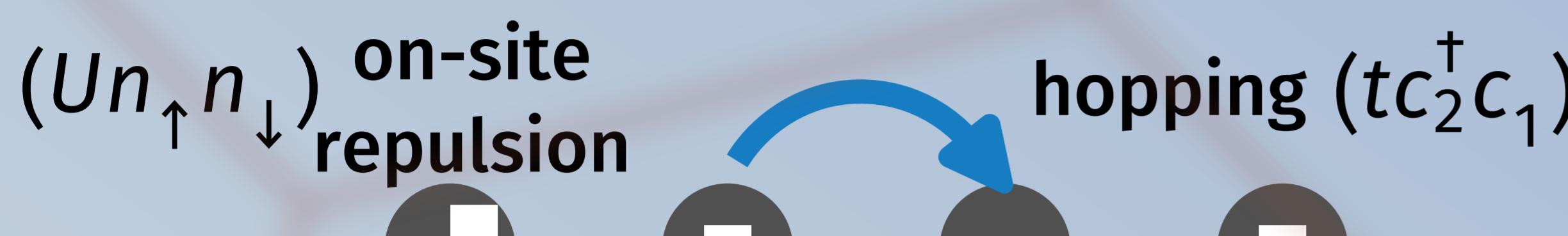
²JNCASR

³IIT Kharagpur

The Mott-Hubbard Transition

Simplest lattice model for correlated electrons

Combines effects of kinetic energy and repulsion.



Metallic for $t \gg U$
Mott insulator for $U \gg t$

DMFT shows MIT at finite U in infinite dimensions, maps Hubbard model to self-consistent impurity model

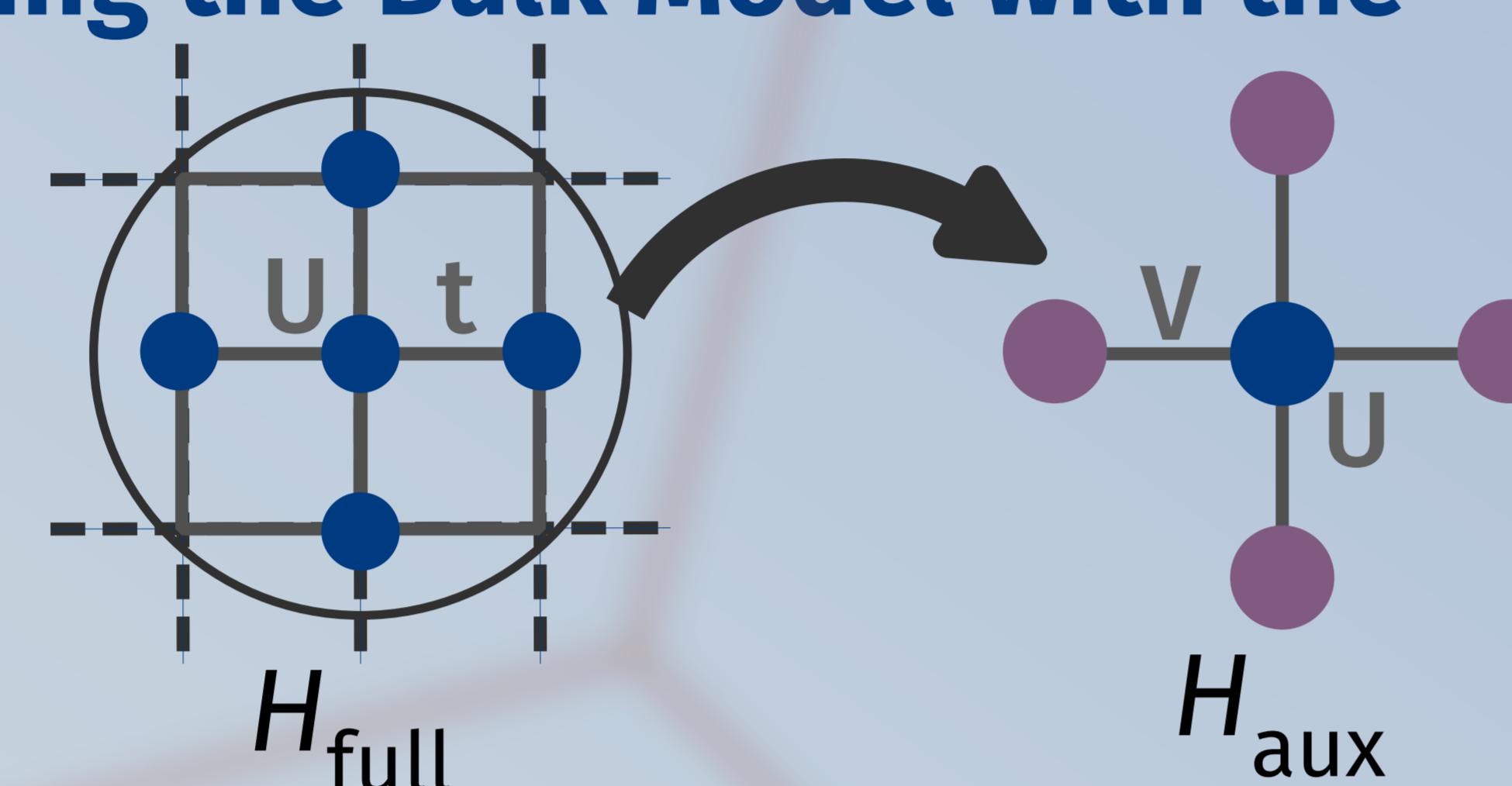
Metal-insulator transition separates the two phases

Metallic

From D=∞ to D=2: Linking the Bulk Model with the Auxiliary Model

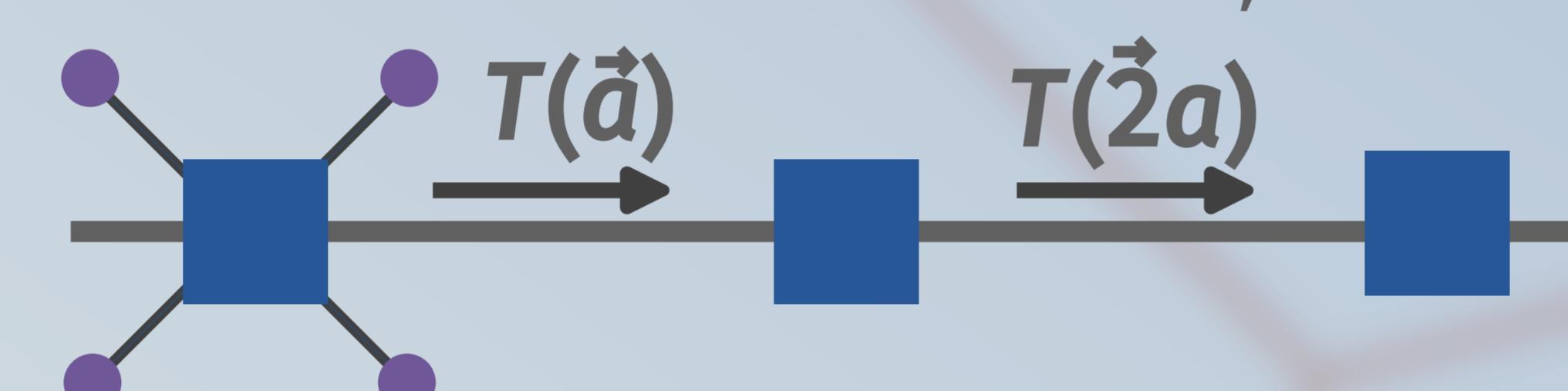
Consider each site of the lattice model as a quantum impurity, and surrounding lattice sites as the bath.

$$H_{\text{aux}} = H_{\text{SIAM}} + J \vec{S}_d \cdot \vec{S}_0 - \frac{1}{2} U_b (n_{0\uparrow} - n_{0\downarrow})^2$$



We translate the auxiliary model Hamiltonian over all lattice sites, to create the full Hamiltonian.

$$H_{\text{full}} = \sum_{\vec{r}} T^\dagger(\vec{r}) H_{\text{aux}} T(\vec{r})$$

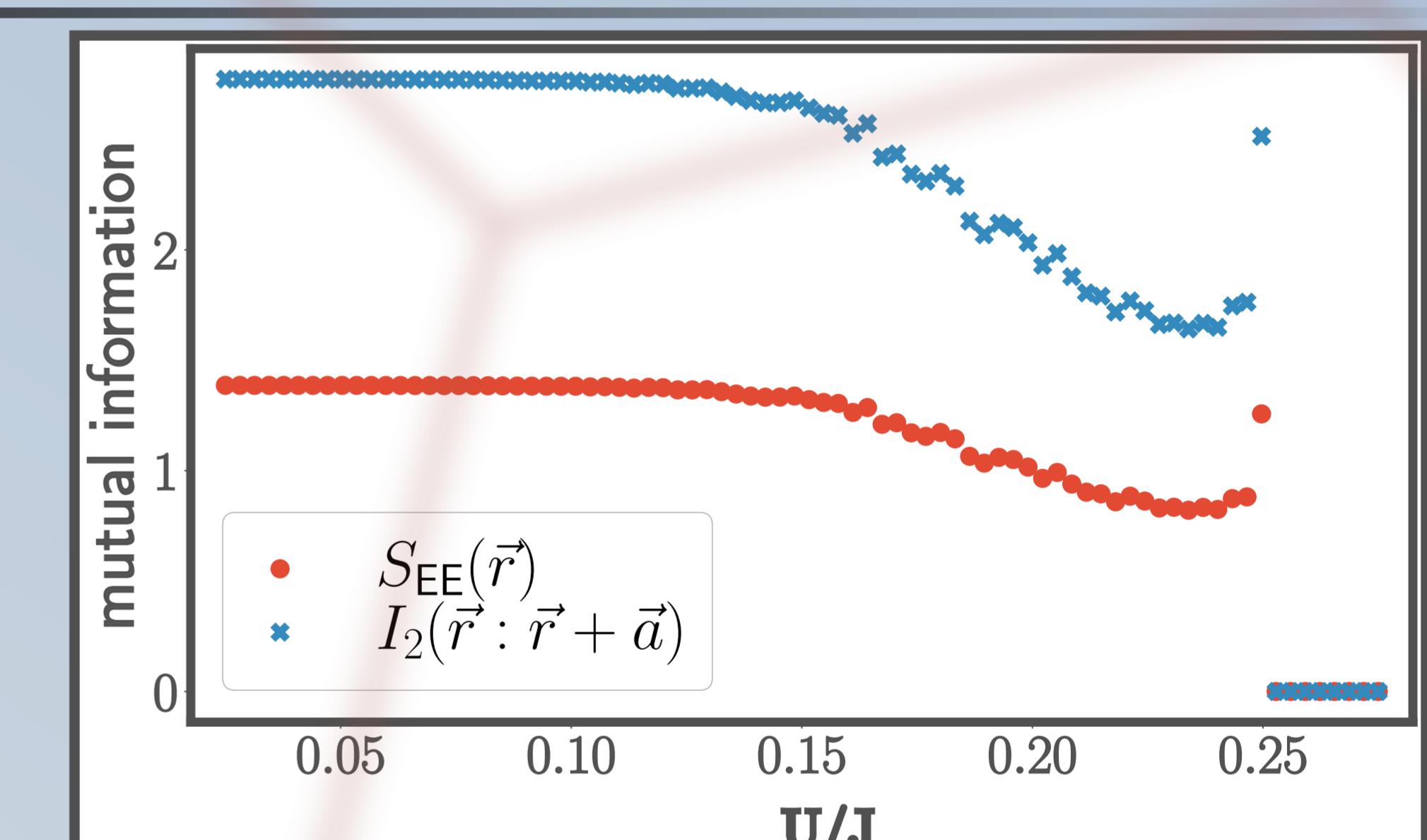
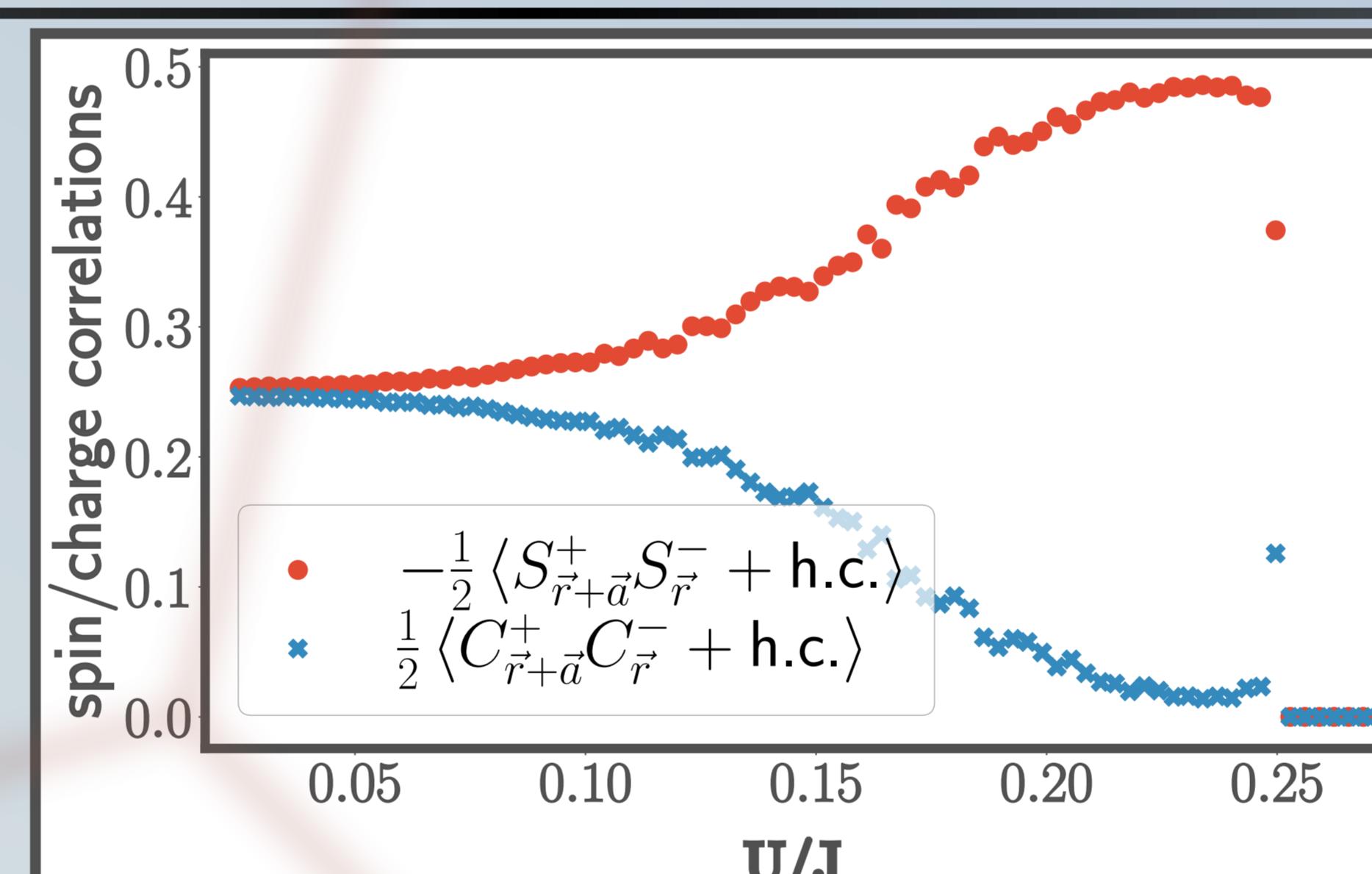


Translating over all sites leads to a Hubbard-Heisenberg model.

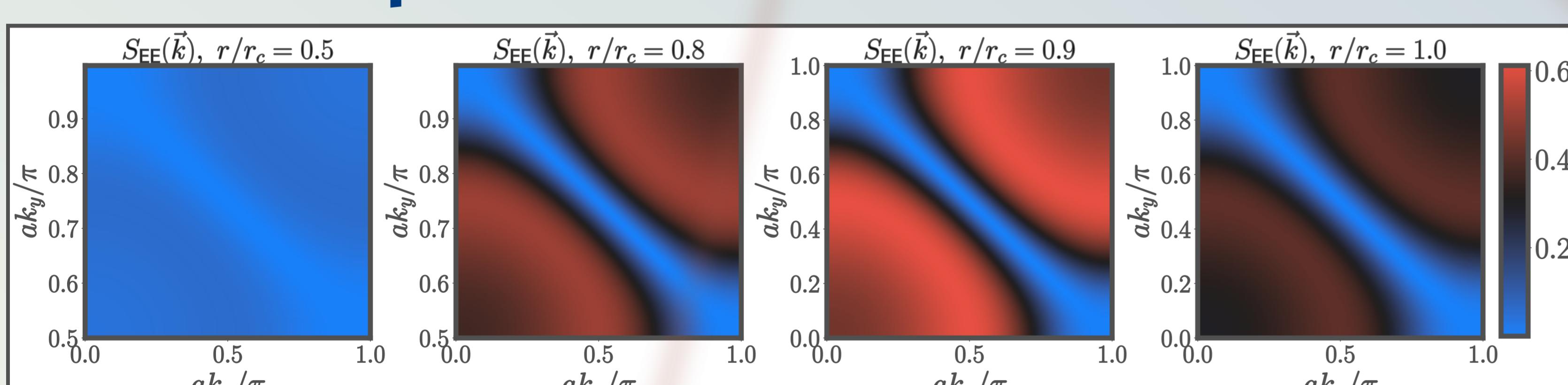
Nature of the Metal-Insulator transition

Gap appears in local spectral function for large U/J , indicating a Mott MIT from Fermi liquid metal to paramagnetic Mott insulator, through the vanishing of spin/charge fluctuations.

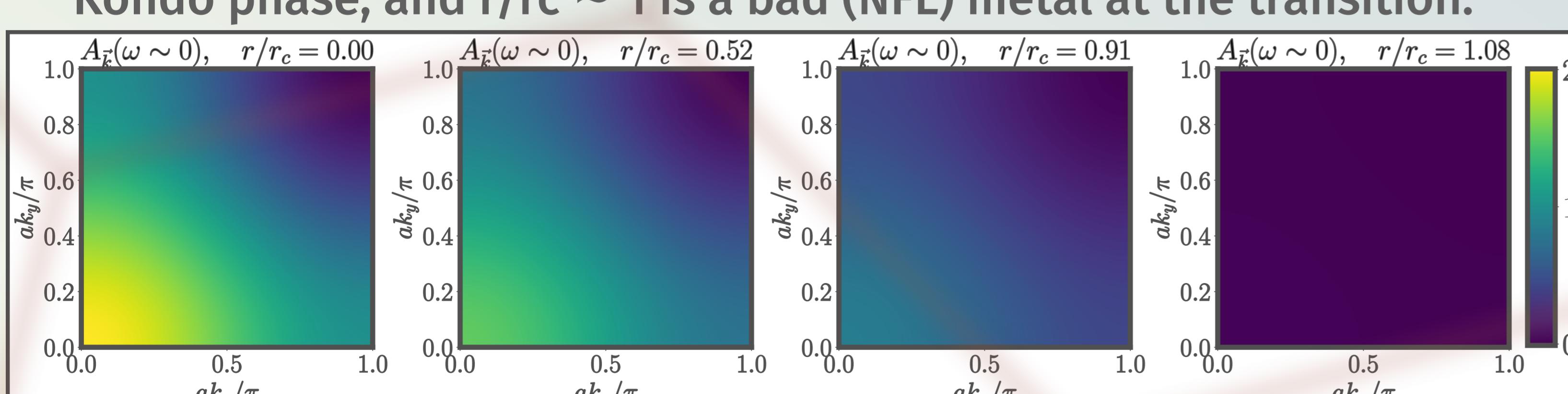
The transition itself seems to be driven by the growth of charge fluctuations that destroy the Kondo screening.



k-space Picture of the Transition



$r/r_c=0.5$ is a good metal, $r/r_c=0.8, 0.9$ is a correlated metal in the Kondo phase, and $r/r_c \sim 1$ is a bad (NFL) metal at the transition.



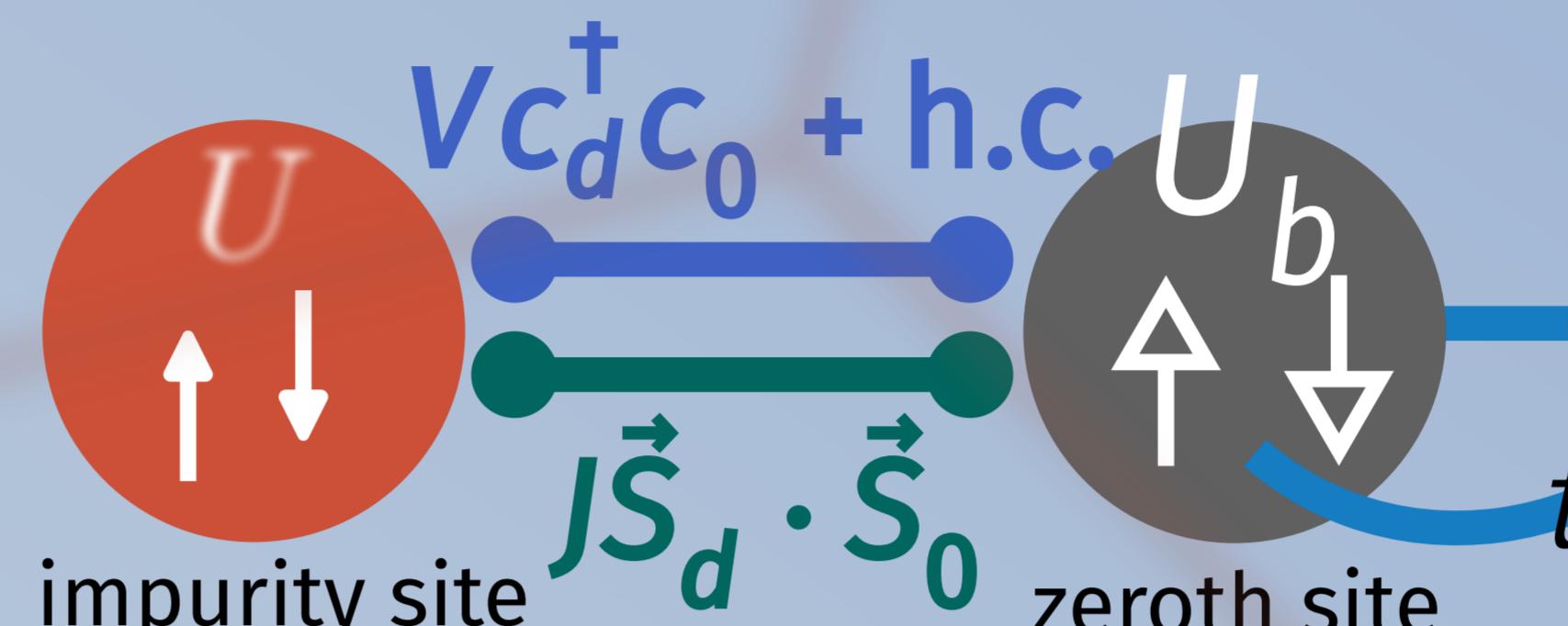
Conclusions and Perspectives

- Our method connects lattice models to their impurity model counterparts, allowing us to study non-local features like electronic differentiation within the k-space Brillouin zone.
- For the 2D Hubbard-Heisenberg model, the metal at the MIT appears pseudogapped away from the Fermi surface.
- Possible extensions include studying other geometries and considering clusters of impurities in the auxiliary model.

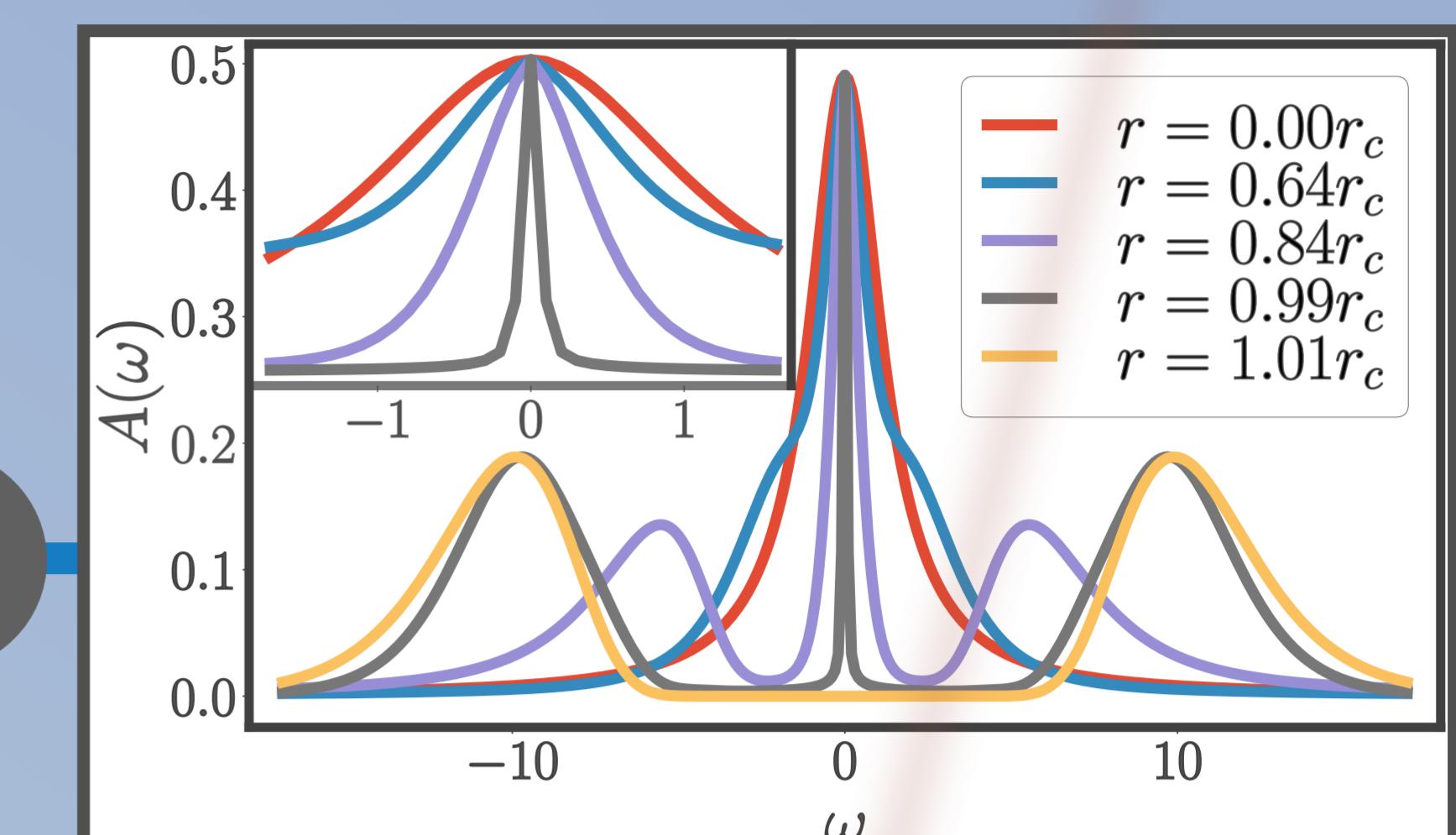
D=∞ Phase Transition in our Extended Model

To find a self-consistent model, we extend the Anderson impurity model to frustrate the Kondo screening mechanism.

J : Kondo coupling
 U_b : local bath correlation



Unitary RG study shows transition between Kondo screened phase and local moment phase.



Mapping Green's functions and other correlators

We use Bloch's theorem to express full eigenstates in terms of local eigenstates. This then allows us to relate Greens functions of the auxiliary model with those of the lattice model!

$$G_{\text{loc}} \sim G_{dd}, \quad G_{\text{n.n.}} \sim \frac{1}{W} G_{dz}, \quad G(k) \sim G_{dd} + G_{dz} \sum_a \frac{e^{ika}}{W}$$

Greens functions acquire momentum-dependence. Can be used to obtain spectral functions. Static correlators can also be obtained.

$$\langle \mathcal{O}_1(r) \mathcal{O}_2(r) \rangle = \frac{1}{2} \left(\langle \mathcal{O}_1(d) \mathcal{O}_2(d) \rangle_{\text{aux}} + \frac{1}{W} \langle \mathcal{O}_1(d) \mathcal{O}_2(z) \rangle_{\text{aux}} \right)$$

Similar relations hold for self-energies and entanglement measures.

Local Quantum Critical Metal at the MIT

We find that local self-energy vanishes while nearest-neighbour self-energy diverges as $\omega \rightarrow 0$:

$$\Sigma_{\text{loc}} \sim \omega^{1+3\alpha/8}, \quad \Sigma_{\text{n.n.}} \sim \omega^{-3\alpha/4}, \quad \alpha > 0$$

This results in the vanishing of the self-energy at the Fermi surface, but its divergence elsewhere:

$$\Sigma_k(\omega) \approx \Sigma_{\text{loc}} + \xi_k \Sigma_{\text{n.n.}} = \begin{cases} 0 & \text{if } k = k_F \\ \infty & \text{if } k \neq k_F \end{cases}$$

This corresponds to a gapless non-Fermi liquid metal with Landau quasiparticles surviving on the Fermi surface but destroyed everywhere else.

References

- M Imada et al., RMP, 70(4): 1039, 1998
- A. Georges et al., RMP 68, 13 (1996)
- A Mukherjee et al NJP 25 113011 (2023)
- Q. Si et al., Nature 413, 804 (2001)
- K. Sujan et al., PRB 107, 205104 (2023)
- W Wu et al., PRX 8, 021048 (2018)
- C. Walsh et al., PRL 122, 067203 (2019)
- C Yang et al., PRB 93, 081107(R) (2016)

Acknowledgements

AM thanks IISER Kolkata for funding this work through a JRF and an SRF fellowship. S L thanks the SERB for funding through MATRICS Grant MTR/2021/000141 and Core Research Grant CRG/2021/000852.