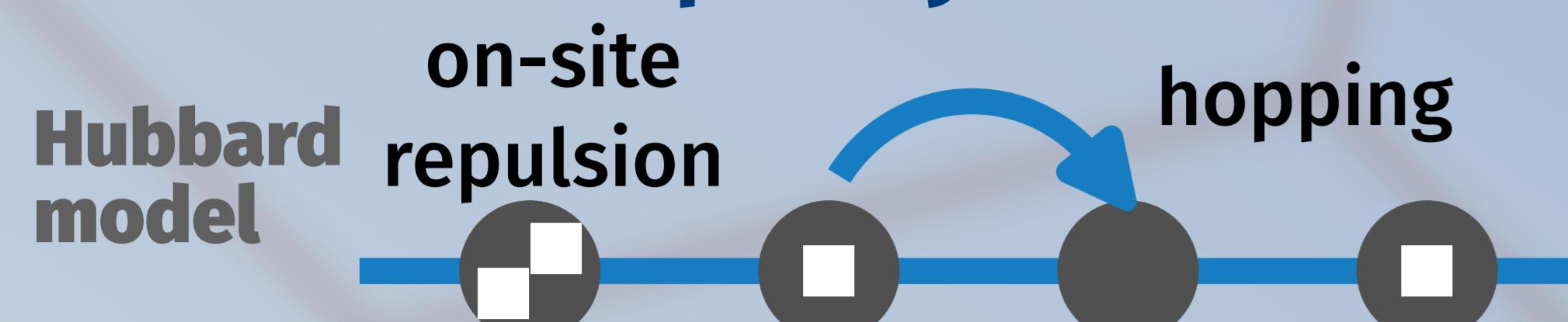


The Mott-Hubbard Transition: Search for a Self-Consistent Impurity Model



Metallic for $t \gg U$
Mott insulator for $U \gg t$
Metal-insulator transition separates the two phases

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

M Imada et al., RMP, 70(4): 1039, 1998

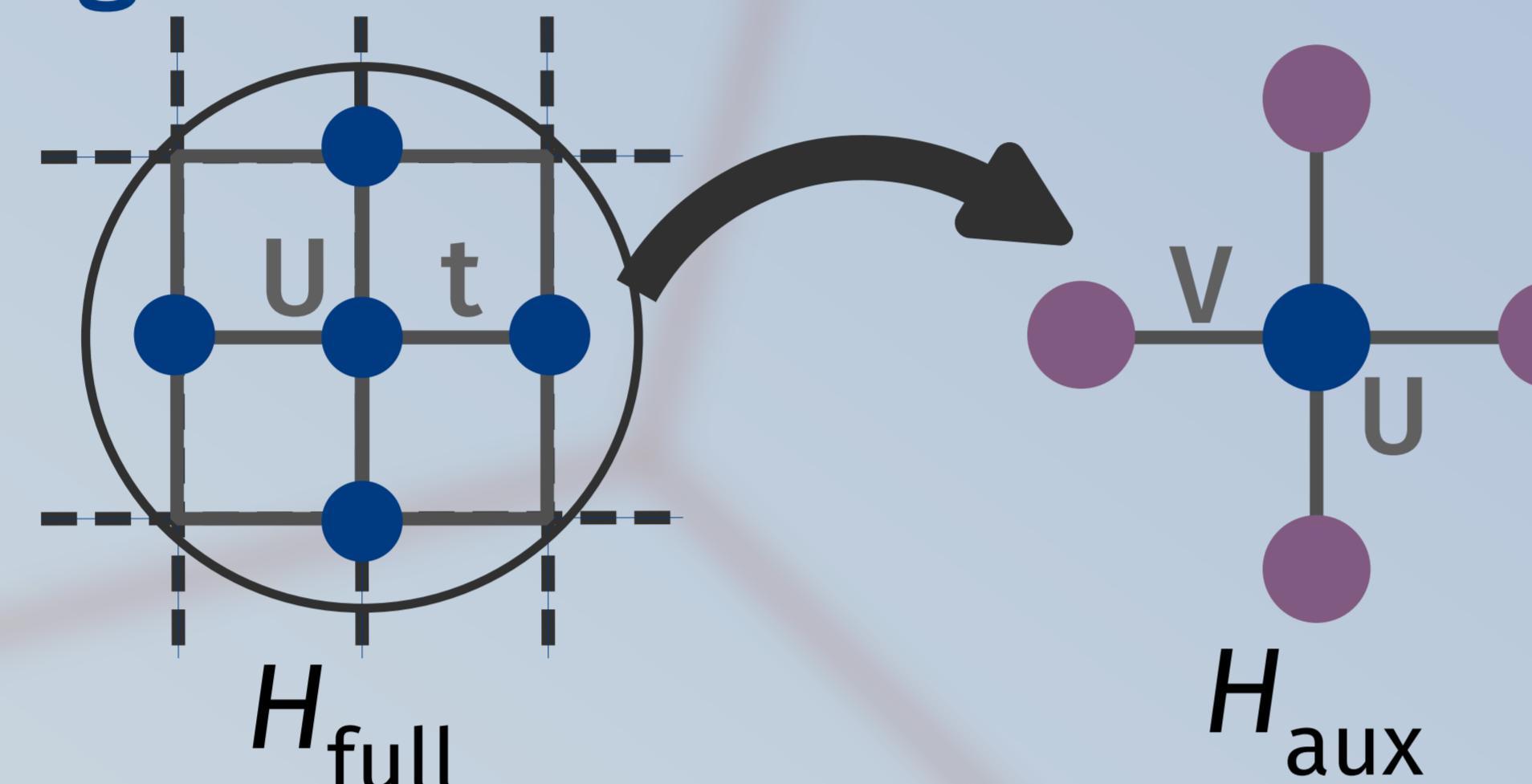
A. Georges et al., RMP 68, 13 (1996)

1. Is there a Hamiltonian-based description of the self-consistent model?
2. Can this be used to reconstruct the physics of the lattice model?
3. What additional insight will such a reconstruction provide beyond the physics of the impurity model?

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.

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

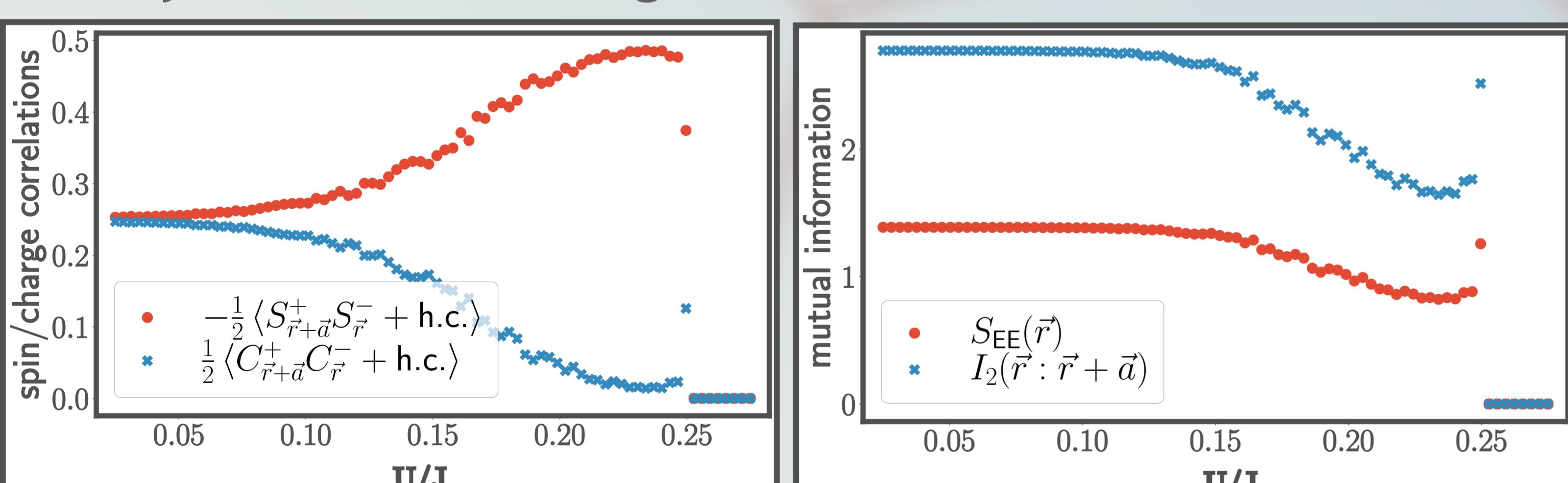
Translating over all sites leads to a Hubbard-Heisenberg model.

Transition from Fermi Liquid to Paramagnetic Mott Insulator

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.

Destruction of Fermi surface (leading to the transition) is driven by the growth of charge fluctuations that destroy the Kondo screening.

W Wu et al., PRX 8, 021048 (2018)



Critical Fermi Surface and 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 k-space 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 a **pseudogapped** spectral function.

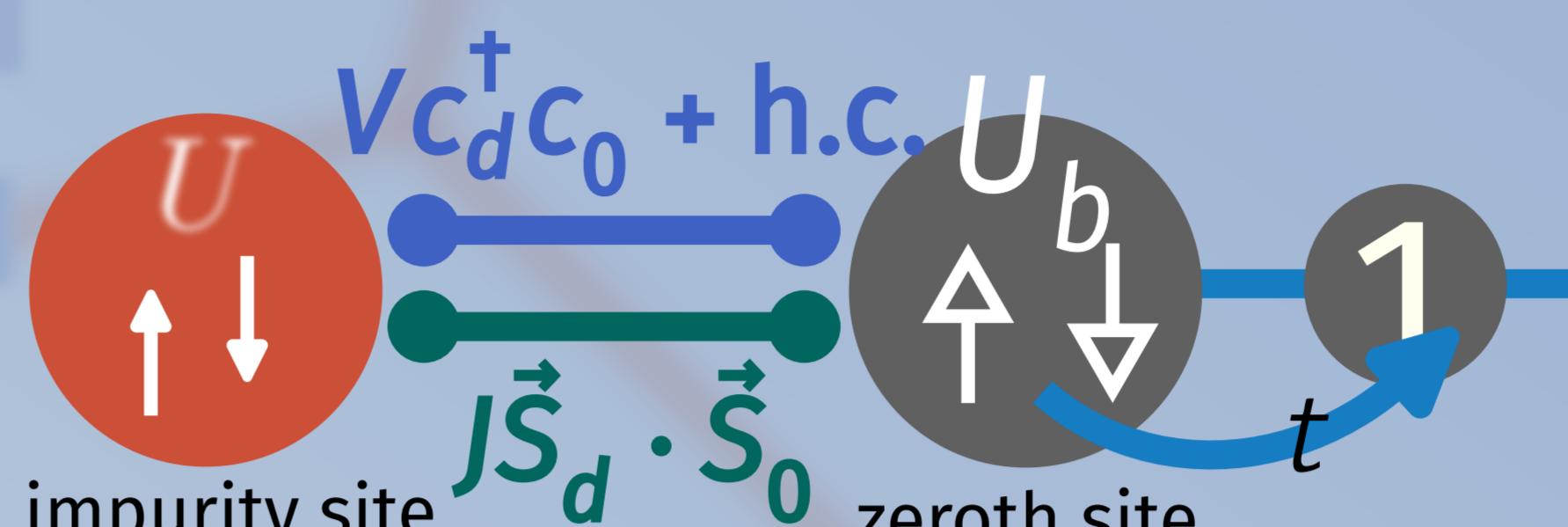
Q. Si et al., Nature 413, 804 (2001)

W Wu et al., PRX 8, 021048 (2018)

D=∞ Phase Transition in our Extended Model

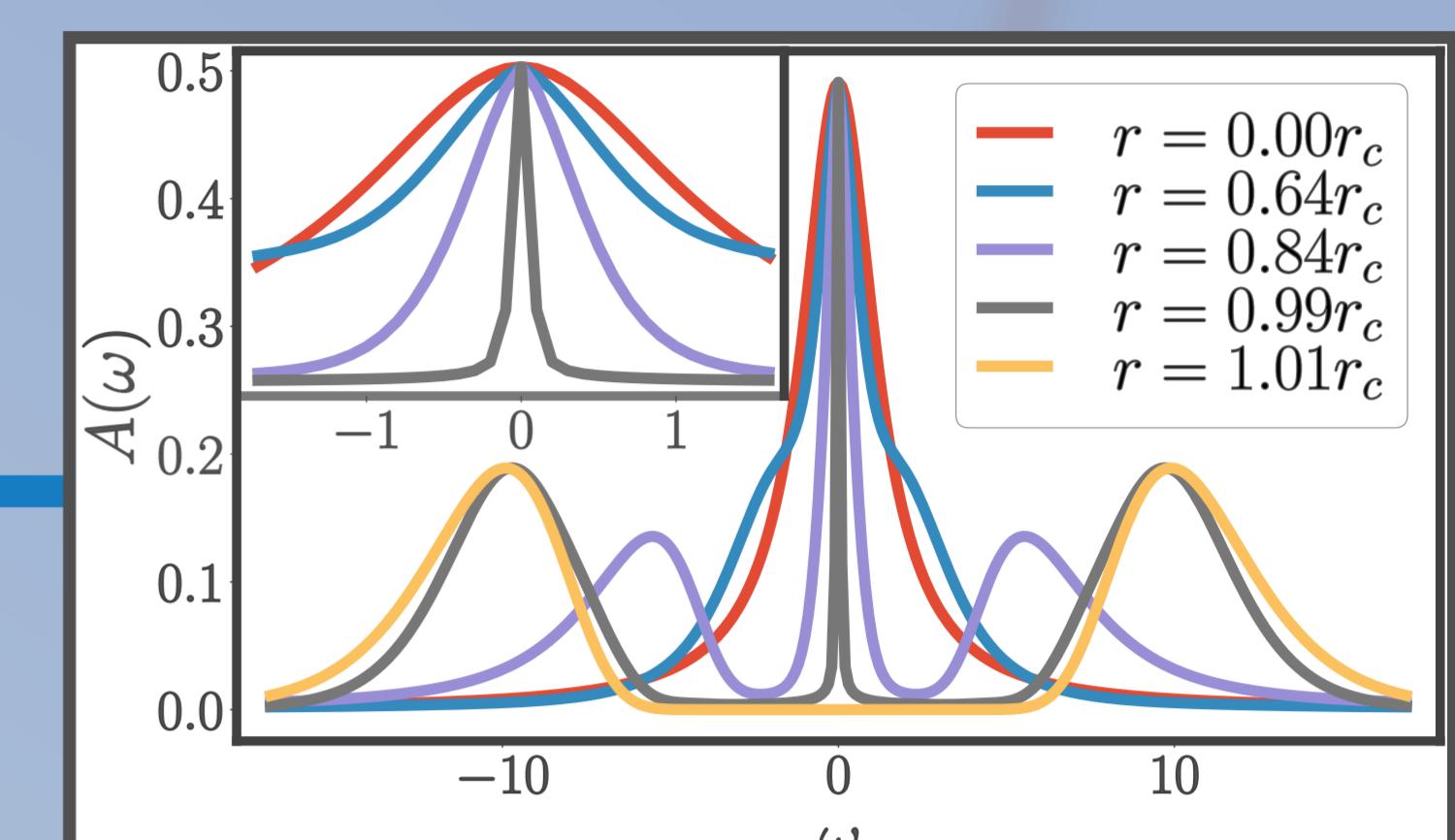
To find a self-consistent model, we extend the Anderson impurity model to **frustrate the Kondo screening**.

J: Kondo coupling
U_b: local bath correlation



A Mukherjee et al., NJP 25 113011 (2023)

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!

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

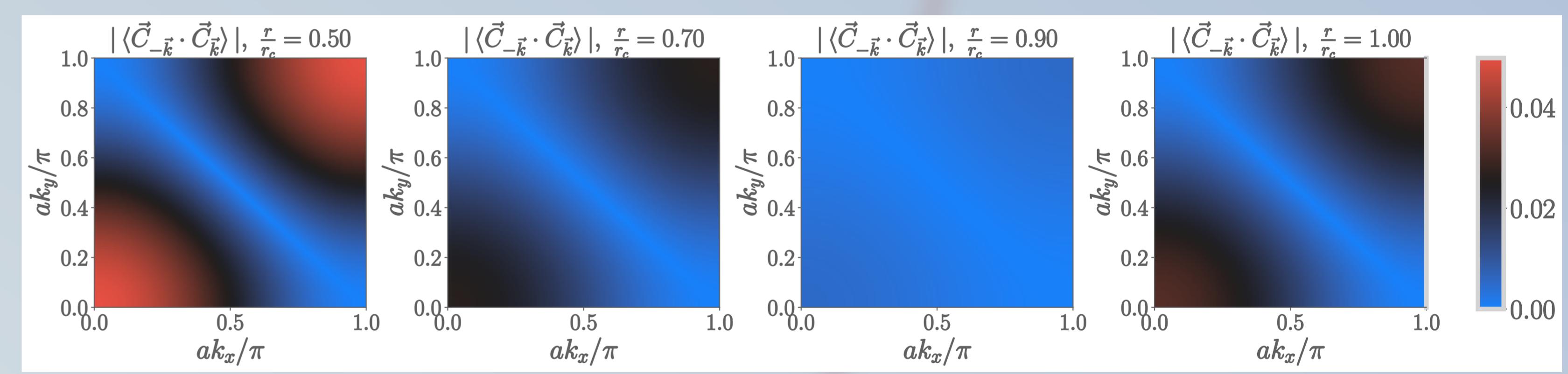
Greens functions acquire **momentum-dependence**. They can be used to obtain spectral functions. Static correlators can also be obtained.

C Yang et al., PRB 93, 081107(R) (2016)

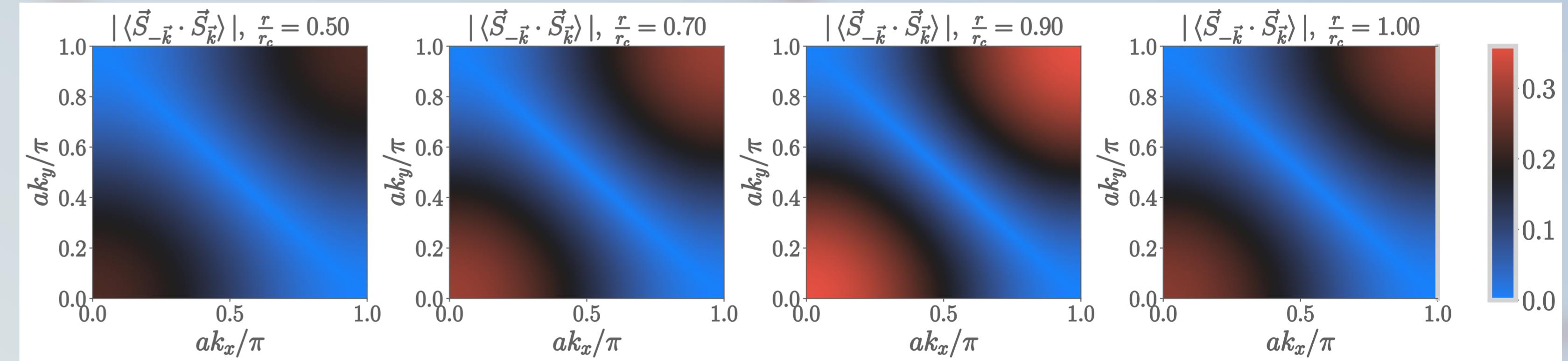
$$\langle \mathcal{O}_1(r) \mathcal{O}_2(r) \rangle = \frac{1}{2} \left(\langle \mathcal{O}_1(d) \mathcal{O}_2(d) \rangle_{\text{aux}} + \frac{1}{W} \langle \mathcal{O}_1(d) \mathcal{O}_2(z) \rangle_{\text{aux}} \right)$$

Similar relations hold for self-energies and **entanglement measures**.

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 ~ 1 is a bad (NFL) metal at the transition.



Conclusions and Perspectives

- Our method **connects lattice models to their impurity model** counterparts in terms of Greens functions, correlation functions and measures of entanglement.
- Such a method then allows the study of **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.

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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.

K. Sujan et al., PRB 107, 205104 (2023)