IISER Kolkata DPS Day 2023

Kondo breakdown drives the Mott-Hubbard MIT

Stabilising the Mott insulator via charge fluctuations

arXiv:2302.02328

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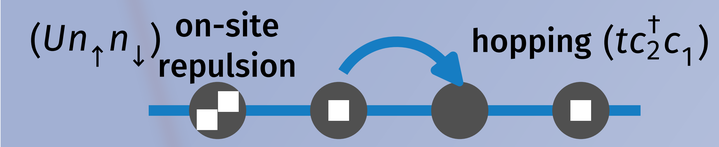
HUBBARD MODEL AND THE MOTT TRANSITION

Simplest lattice model for correlated electrons

Combines effects of kinetic energy and **local repulsion**

- **metallic** for $t \gg U$
- **Mott insulator** for $U \gg t$

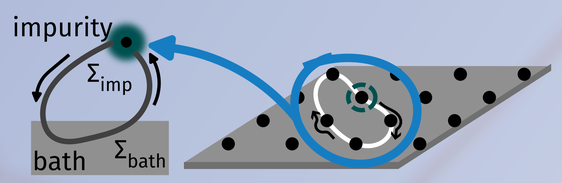
Two phases separated by a **metal-insulator transition**



DYNAMICAL MEAN-FIELD THEORY: MAPPING THE HUBBARD MODEL TO IMPURITY MODELS

DMFT maps local Greens func. of the Hubbard to that of a **self-consistent impurity model**

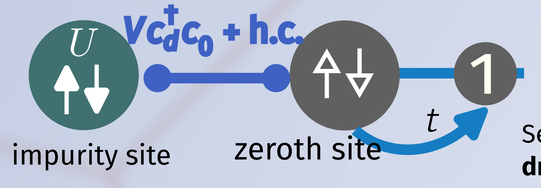
Ignores **non-local** contributions; exact in **infinite dimensions**



Shows metal-insulator transition at finite U

QUESTION: CAN WE EXTRACT THE SELF-CONSISTENT IMPURITY MODEL THAT SHOWS A TRANSITION ?

Anderson impurity model: correlated impurity hopping into and out of a bath



no transition, impurity always screened

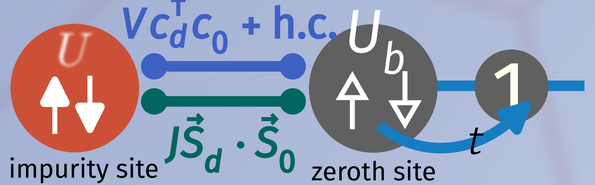
Self-consistency must lead to **drastic modification** of the bath;

What is this modified impurity model? What insight can it offer on the Mott MIT?

ADDING LOCAL INTERACTION IN THE BATH

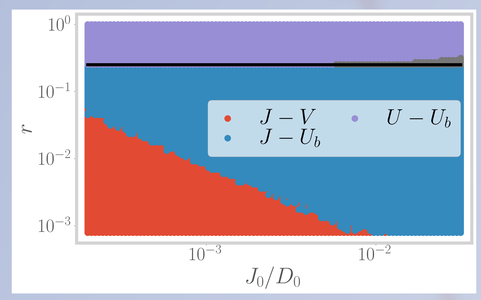
Kondo screening : **entanglement** of impurity & bath e⁻s
Mott MIT: **frustration** of Kondo screening

To see this, we **enhance** the Anderson impurity model



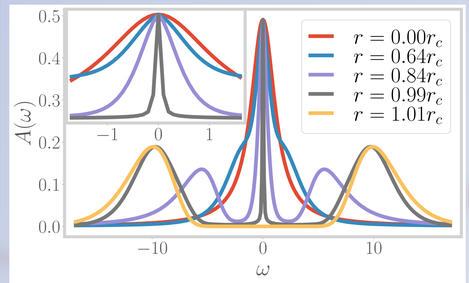
J: promotes spin-flip, **U_b**: local bath correlation

PHASE TRANSITION IN OUR EXTENDED IMPURITY MODEL



local Mott MIT: ground-state changes from **singlet to local moment** for r < 0

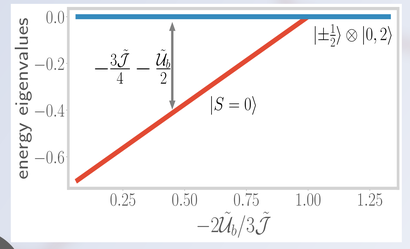
Unitary RG study shows presence of a **gapped phase** for r=U_b/J < 0



UNIVERSAL DESCRIPTION FOR THE MOTT MIT

Mott MIT involves two **competing tendencies:**

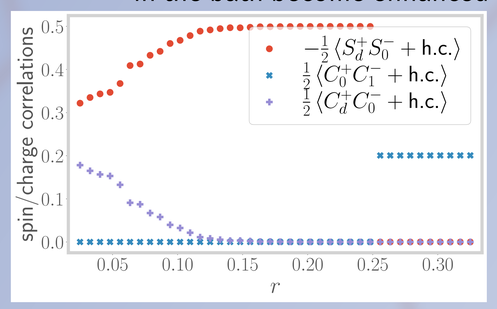
- correlated hopping $J\vec{S}_d \cdot \vec{S}_0$
- pairing tendency $-U_b \hat{n}_{0\uparrow} \hat{n}_{0\downarrow}$



PAIRING CORRELATIONS DRIVE THE TRANSITION

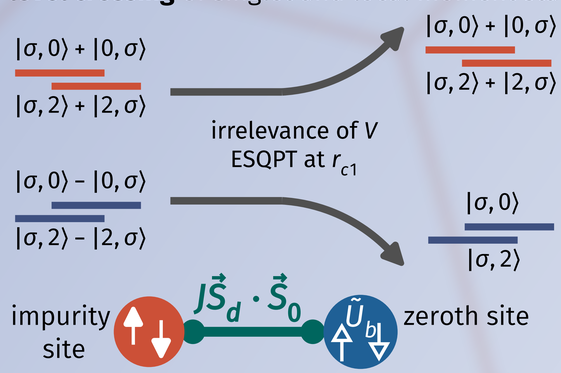
Vanishing spin correlations between impurity and bath

Pairing correlations in the bath become enhanced

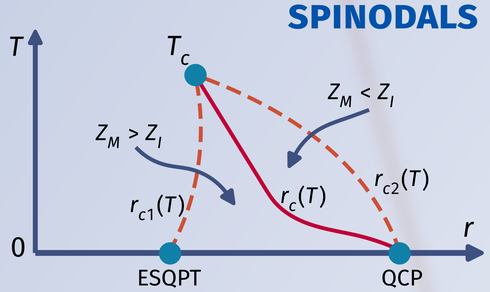


PRECURSOR: EXCITED STATE QPT

MIT found to occur in 2 steps:
1. **excited state transition**: loc. moment states emerge
2. **level crossing** of singlet and local moment states.



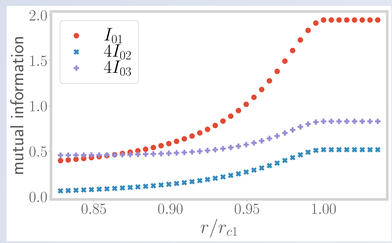
FIRST-ORDER PHYSICS & SPINODALS

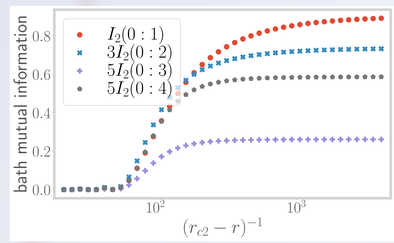


Between ESQPT and QPT, metal and insulator **coexist**.

Explains presence of **spinodals and coexistence region** in DMFT results

LONG-RANGED CRITICAL FLUCTUATIONS





Near ESQPT and QPT, **long-ranged correlations and entanglement** build up in the system.

Indicates the **critical nature** of the system.
Likely **source of critical fluctuations** observed in DMFT.

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CONCLUSIONS & OUTLOOK

1. **Pairing correlations** in the bath drive the Mott MIT.
2. Entire MIT occurs in 2 steps: an **ESQPT and a QPT**.
3. **Critical fluctuations** proliferate in both the steps.
4. Can be tested on mesoscopic quantum dots
5. Extensions include studying the role of **hole doping.**

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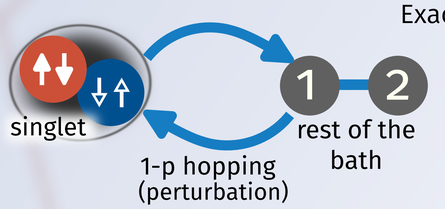
EMERGENCE OF NON-FERMI LIQUID EXCITATIONS AT THE MIT



Exactly at MIT, the excitations are of **non-Fermi liquid** kind:

- scatter between orthogonal states of the bath
- have vanishing 1-site quasiparticle residue
- power-law behaviour in self-energy and correlations
- fractional magnetisation and entanglement entropy