Local metal-insulator transition in an extended Anderson impurity model

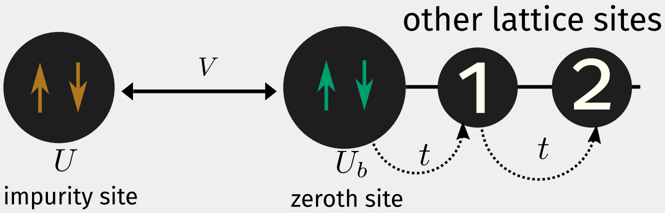
Abhirup Mukherjee, Siddhartha Lal

Department of Physical Sciences, IISER Kolkata, Mohanpur

May 29, 2022

Why another impurity model?

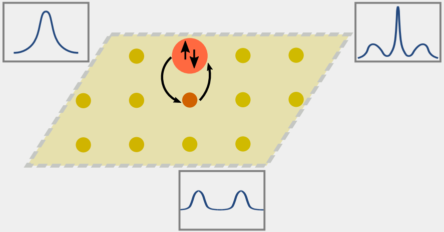
Anderson and Kondo impurity models - No transition!



- simplest impurity models - Anderson and Kondo
- localisation physics + hybridisation
- impurity is screened at low *T*

Anderson 1961; Anderson 1978; Kondo 1964; Wilson 1975; Krishna-murthy et al. 1980; Andrei et al. 1983.

DMFT AND THE MOTT MIT



- DMFT implementations use impurity models, exact in $d = \infty$
- Appropriate impurity model obtained through self-consistent equations
- Displays metal-insulator transition in Hubb. model at $\frac{1}{2}-$filling

Metzner et al. 1989; Georges et al. 1992; Hubbard 1963; Mott 1949.

Brief Summary of Results

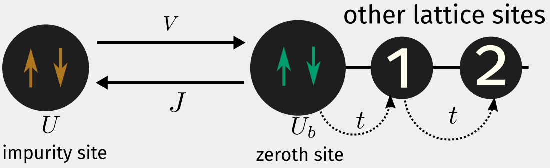
Brief Summary of Results

- Competition between Kondo interaction and local attractive interaction leads to multiple phases.
- Ground state interpolates between singlet and local moment, passing through spin+charge correlated state.
- Spectral function has 3-peak structure near critical point, develops gap beyond.
- Many-particle entanglement acts as an order parameter for the transition.

Extending the Anderson impurity model

$$H = \overbrace{\sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2}^{\text{p-h symmetric Anderson impurity model}} + \underbrace{J \vec{S}_d \cdot \vec{S}_0 - U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow} \right)^2}_{\text{additional terms}}$$

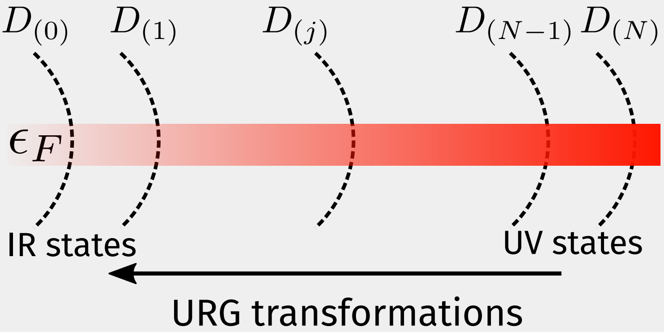
- spin-exchange J between impurity-bath
- correlation U_b on zeroth site of bath
- p-h symmetry is maintained
- J, U_b compete



$$r \equiv -U_b / J$$

The Unitary RG Method

The Unitary RG Method: Select a UV-IR Scheme



j^{th} RG step $\longrightarrow \vec{k}_{j\sigma}$

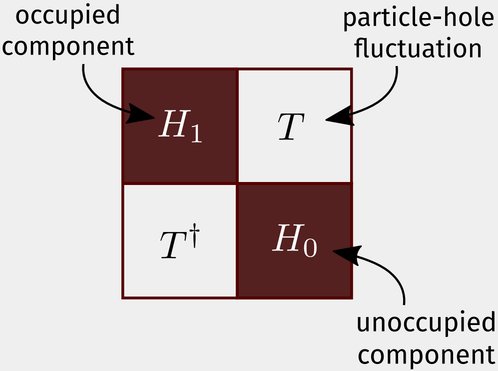
Mukherjee et al. 2020d; Mukherjee et al. 2020e.

The Unitary RG Method: Write Hamiltonian in the basis of $\vec{k}_j$

$$H_{(j)} = H_1 \hat{n}_j + H_0 \left(1 - \hat{n}_j\right) + c_j^\dagger T + T^\dagger c_j$$

$$2^{j-1}\text{-dim.} \longrightarrow \begin{cases} H_1, H_0 \longrightarrow \text{diagonal parts} \\ T \longrightarrow \text{off-diagonal part} \end{cases}$$

(j) : j^{th} RG step



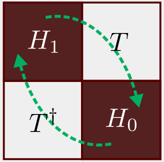
Mukherjee et al. 2020d; Mukherjee et al. 2020e.

The Unitary RG Method: Rotate and kill off-diagonal blocks

$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

$$U_{(j)} = \frac{1}{\sqrt{2}}\left(1 - \eta_{(j)} + \eta^{\dagger}_{(j)}\right)$$

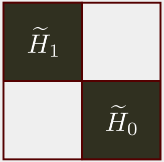
many-particle rotation of Hamiltonian



$$\left[H_{(j)}, n_j\right] \neq 0$$

$$\left[H_{(j-1)}, n_j\right] = 0$$

n_j becomes an
integral of motion
(IOM)



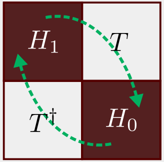
Mukherjee et al. 2020d; Mukherjee et al. 2020e.

The Unitary RG Method: Rotate and kill off-diagonal blocks

Fermionic: $\left\{\eta_{(j)}, \eta^\dagger_{(j)}\right\} = 1$

$$\left.\eta^\dagger_{(j)} = \frac{1}{\hat{\omega}_{(j)} - H_D} c^\dagger_j T \right\} \to \text{many-particle rotation}$$

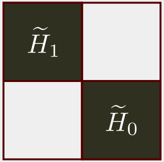
$\hat{\omega}$: quantum fluctuation operator



$\left[H_{(j)}, n_j\right] \neq 0$

$\left[H_{(j-1)}, n_j\right] = 0$

n_j becomes an **integral of motion** (IOM)

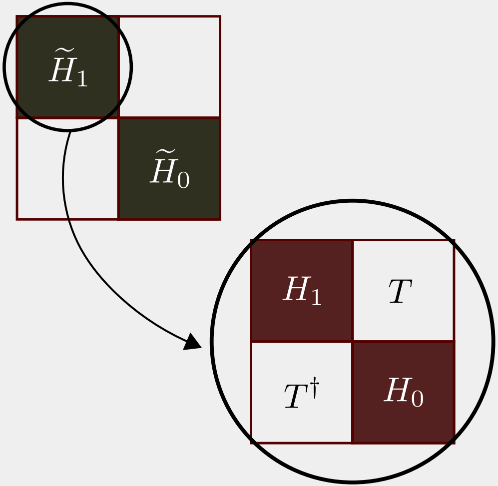


Mukherjee et al. 2020d; Mukherjee et al. 2020e.

The Unitary RG Method: Repeat with new Hamiltonian

$$H_{(j-1)} = \widetilde{H}_1 \hat{n}_j + \widetilde{H}_0 \left(1 - \hat{n}_j\right)$$

$$\widetilde{H}_1 = H_1 \hat{n}_{j-1} + H_0 \left(1 - \hat{n}_{j-1}\right) + c^\dagger_{j-1} T + T^\dagger c_{j-1}$$



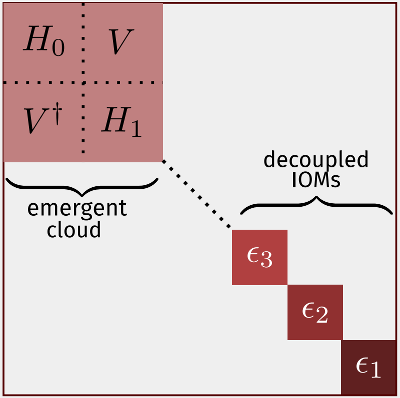
Mukherjee et al. 2020d; Mukherjee et al. 2020e.

$$\Delta H_{(j)} = \left(\hat{n}_j - \tfrac{1}{2}\right)\left\{c_j^\dagger T, \eta_{(j)}\right\}$$

$$\eta_{(j)}^\dagger = \frac{1}{\hat{\omega}_{(j)} - H_D} c_j^\dagger T$$

Fixed point: $\hat{\omega}_{(j^*)} - (H_D)^* = 0$

eigenvalue of $\hat{\omega}$ coincides with that of H



Mukherjee et al. 2020d; Mukherjee et al. 2020e.

The Unitary RG Method: Novel Features of the Method

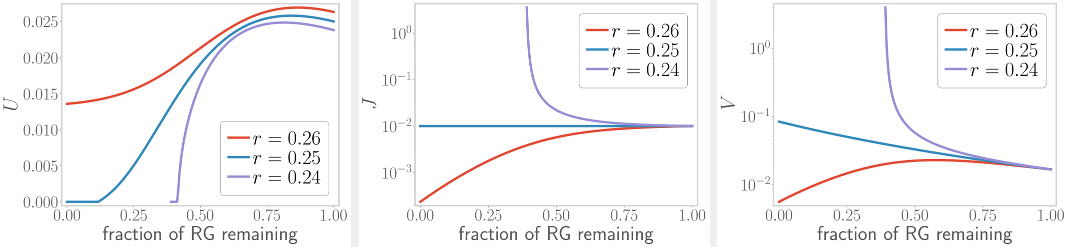
- Quantum fluctuation scale $\hat{\omega}$ that tracks all orders of renormalisation
- Finite-valued fixed points for finite systems - leads to emergent DOFs
- Spectrum-preserving unitary transformations - partition function left unchanged
- Tractable low-energy effective Hamiltonians - allows renormalised perturbation theory

Pal et al. 2019; Mukherjee et al. 2020b; Mukherjee et al. 2020c; Mukherjee et al. 2020a; Mukherjee et al. 2021; Patra et al. 2021; Mukherjee et al. 2022.

RG Flows & Phase Diagram

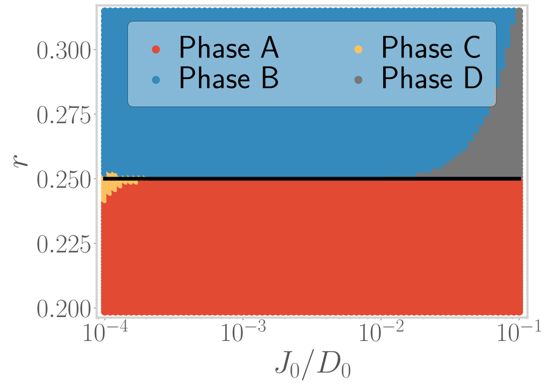
Coupling RG Flows

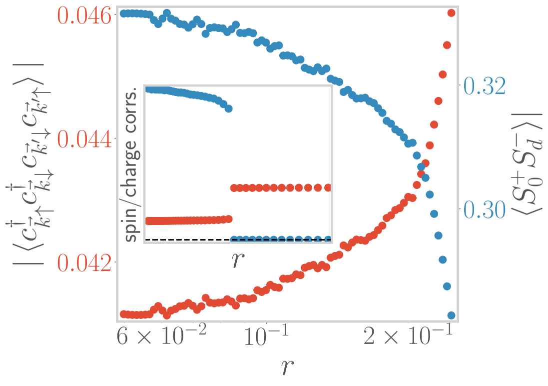
- U_b is marginal
- For $-U_b < J/4$: J, V are relevant, U is irrelevant
- For $-U_b > J/4$: J, V are irrelevant, U is "relevant"
- Transition at $r = -U_b/J = 1/4$



Phase diagram: $U_b = -U/10$

- **Red**: $V, J \uparrow$, $U \downarrow$: local FI
- **Yellow**: V, U survive: spin+charge
- **Blue**: $V, J \downarrow$, $U \uparrow$: local moment
- **Grey**: U, V, J all $\downarrow$



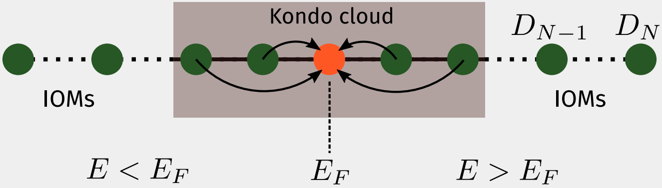


- Impurity is no longer screened
- $S_d^{\pm} S_0^{\mp}$ replaced by isospin flucts.
- Arises from U_b term

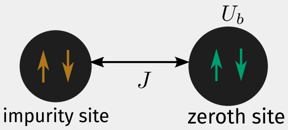
Low-energy effective Hamiltonian and the ground state

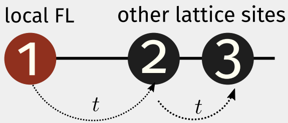
Fixed-point Hamiltonian

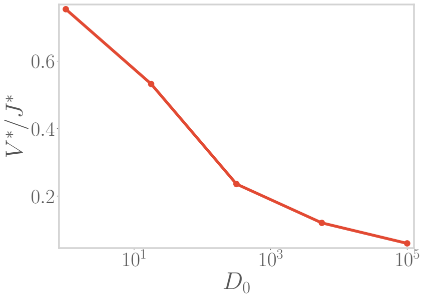
$$\mathcal{H}^* = -\frac{1}{2}U^* \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 + \sum_{\sigma,\vec{k}:|\epsilon_{\vec{k}}|<D^*} \epsilon_{\vec{k}}\tau_{\vec{k},\sigma} - U_b^*\hat{n}_{0\uparrow}\hat{n}_{0\downarrow} + V^*\sum_{\sigma}\left(c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}\right) + J^*\vec{S}_d\cdot\vec{S}_0$$



$$\mathcal{H}^{\text{sc}}_{\text{eff}} = J^*\vec{S}_d \cdot \vec{S}_0 - U_b \hat{n}_{0\uparrow}\hat{n}_{0\downarrow} + \sum_{\sigma,\vec{k}:|\epsilon_{\vec{k}}|<D^*} \epsilon_{\vec{k}} \tau_{\vec{k},\sigma}$$





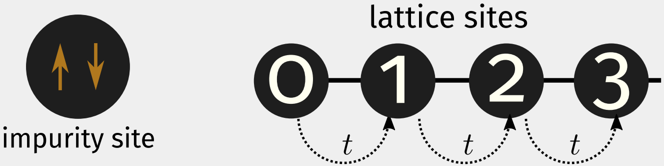


singlet ground state + local FL excitations

Wilson 1975; Nozieres 1974.

UNSCREENED REGIME: $-U_b > J/4$

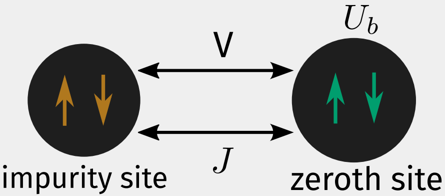
$$\mathcal{H}_{\text{eff}}^{\text{uns}} = -\frac{1}{2}U^* \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 - U_b \hat{n}_{0\uparrow}\hat{n}_{0\downarrow} + \sum_{\sigma,\vec{k}:|\epsilon_{\vec{k}}|<D^*} \epsilon_{\vec{k}} \tau_{\vec{k},\sigma}$$

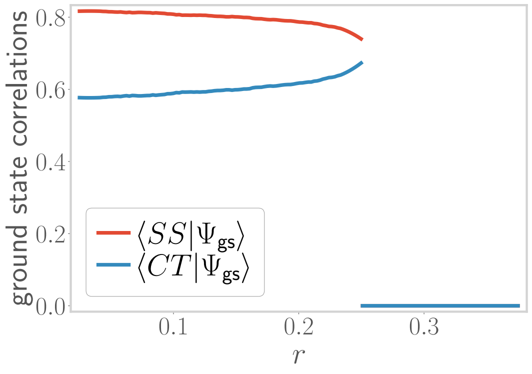


local moment ground state

NEAR THE CRITICAL POINT: $-U_b = J/4$

Both V, J survive



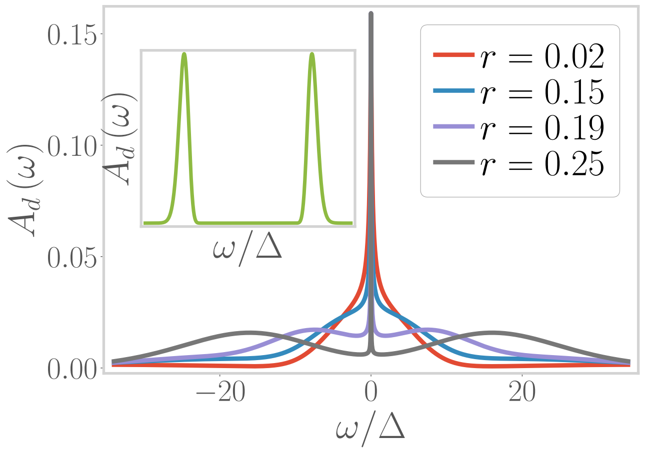


ground state has both spin and charge entanglement

Descriptors of the transition

Spectral function: Transfer of spectral weight along the transition

- single peak at $r \ll 1/4$, side peaks appear for $r \simeq 1/4$
- gap appears for $r > 1/4$
- pole in impurity Greens function is replaced by a zero



Hewson 1993.

Geometric entanglement: $\varepsilon\left(\psi_1, \psi_2\right) = 1 - \left| \langle \psi_1 | \psi_2 \rangle \right|^2$

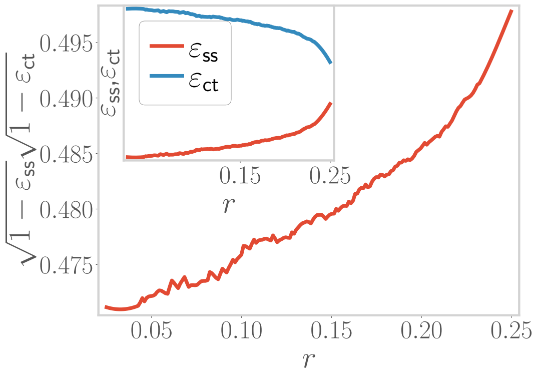
$$|\Psi\rangle_{\mathrm{gs}} \simeq |\Phi\rangle_{ss} \langle \mathrm{ss} | \Psi^{(2)}_{\mathrm{gs}} \rangle + |\Phi\rangle_{ct} \langle \mathrm{ct} | \Psi^{(2)}_{\mathrm{gs}} \rangle$$

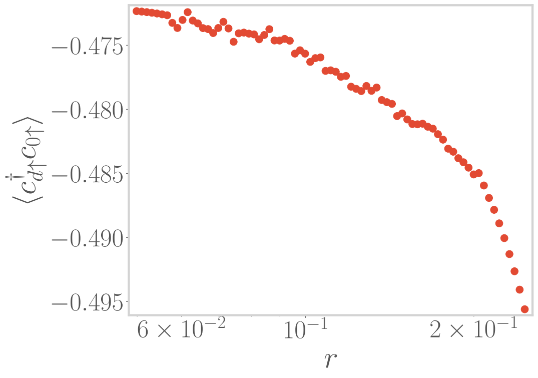
$$G_d(\omega) = \left(1 - \varepsilon_{\mathrm{ss}}\right) \mathcal{G}_{\mathrm{ss}} + \left(1 - \varepsilon_{\mathrm{ct}}\right) \mathcal{G}_{\mathrm{ct}} + \sqrt{\left(1 - \varepsilon_{\mathrm{ss}}\right)} \sqrt{\left(1 - \varepsilon_{\mathrm{ct}}\right)} \mathcal{G}_{\text{ss-ct}}$$

$\longrightarrow$ **relates** Green functions to a measure of entanglement

Shimony 1995; Wei et al. 2003; Horodecki et al. 2009.

Geometric entanglement as an order parameter for the transition

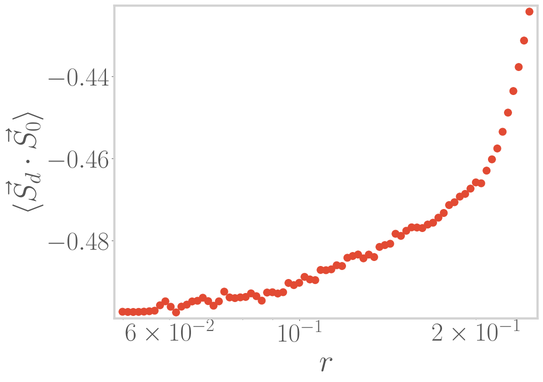




- Entanglement of spin increases towards the transition, that of charge decreases
- Cross-term $\sqrt{(1-\varepsilon_{ss})}\sqrt{(1-\varepsilon_{ct})}$ has an overall increase
- Increased mixing between spin and charge sectors (through 1-particle terms)

For general $T=0$ static correlation $\left\langle O_2 O_1^\dagger \right\rangle$:

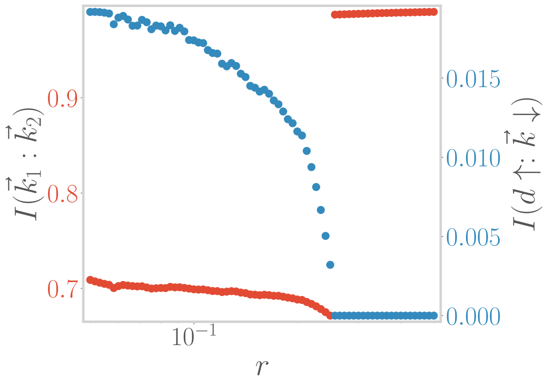
$$\left\langle O_2 O_1^\dagger \right\rangle = (1-\varepsilon_{\text{ss}}) \langle O_2 O_1^\dagger \rangle_{\text{ss}} + (1-\varepsilon_{\text{ct}}) \langle O_2 O_1^\dagger \rangle_{\text{ct}} + \sqrt{1-\varepsilon_{\text{ss}}}\sqrt{1-\varepsilon_{\text{ct}}} \langle O_2 O_1^\dagger \rangle_{\text{ss-ct}}$$



- compensation depends only on ε_{ss}
- ε_{ss} decreases towards transition
- explains increase in compensation

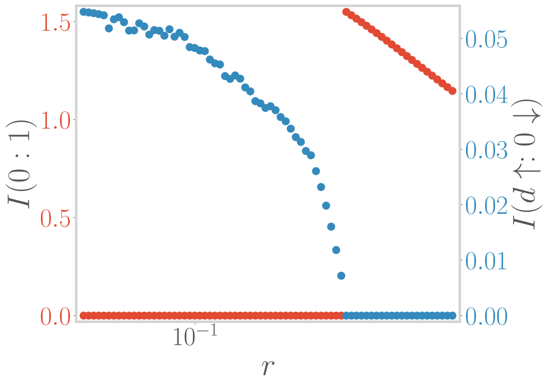
- ground state density matrix: $\rho = |\Psi_{\text{gs}}\rangle \langle\Psi_{\text{gs}}|$
- reduced density matrix - trace out certain DOFs : $\rho_A = \text{Tr}_A [\rho]$

- ground state **density matrix**: $\rho = |\Psi_{\text{gs}}\rangle \langle\Psi_{\text{gs}}|$
- reduced density matrix - **trace out** certain DOFs : $\rho_A = \text{Tr}_A[\rho]$
- **entanglement entropy** of A w.r.t. rest: $S(A) = -\text{Tr}[\rho_A \ln \rho_A]$
- **mutual information** between A and B: $I(A:B) = S(A) + S(B) - S(A \cup B)$



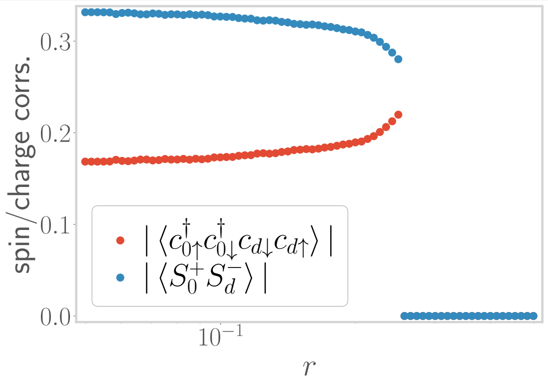
- MI within Kondo cloud as well as between impurity and $k-$states decreases
- signature of destruction of the Kondo cloud
- beyond the transition, $I(d : k)$ drops to zero, while $I(k : k')$ rises

Mutual information & spin-charge correlations: Fate of the Kondo cloud



- in real-space, impurity-zeroth site singlet gets decoupled into separable state
- this entanglement is transferred inot $0:1$ system
- shows the redistribution of entanglement from impurity site to the lattice

Mutual information & spin-charge correlations: Fate of the Kondo cloud



- lowering of spin-fluctuations explains destruction of Kondo cloud
- attractive U_b leads to pair-fluctuations between impurity and zeroth site

Final Remarks

Conclusions and Insights

- J and U_b lead to multiple phases under RG, with distinct eff. Hamiltonians and g.states
- Presence of subdominant pair fluctuations between d and 0 : reminiscent of subdominant Cooper-pairing tendency in URG study of $\mu = 0$ Hubbard model
- $\chi = \sqrt{1-\varepsilon_{\text{ss}}}\sqrt{1-\varepsilon_{\text{ct}}}$ is non-zero in screened phase and 0 in unscreened phase: acts as order parameter for the transition
- Discontinuous change in χ across the transition linked to the change in the topological Luttinger volume

Moving forward

- Changing the filling might lead to dominant fluctuations in pair formation
- $k-$space geometry effects can be captured by considering more impurities
- Restoring translation invariance using an appropriate translation algorithm can promote this local MIT to a bulk transition

References I

- Anderson, P. W. (1961). “Localized Magnetic States in Metals”. In: *Phys. Rev.* 124 (1), pp. 41–53.
- — (1978). “Local moments and localized states”. In: *Rev. Mod. Phys.* 50 (2), pp. 191–201.
- Andrei, N, K Furuya, and J H Lowenstein (1983). “Solution of the Kondo problem”. In: *Rev. Mod. Phys.* 55, p. 331.
- Georges, Antoine and Gabriel Kotliar (1992). “Hubbard model in infinite dimensions”. In: *Phys. Rev. B* 45 (12), pp. 6479–6483.
- Hewson, A. C. (1993). *The Kondo Problem to Heavy Fermions*. Cambridge University Press.
- Horodecki, Ryszard et al. (2009). “Quantum entanglement”. In: *Reviews of modern physics* 81.2, p. 865.
- Hubbard, John (1963). “Electron correlations in narrow energy bands”. In: *Proceedings of the royal society of london a: mathematical, physical and engineering sciences*. Vol. 276. 1365. The Royal Society, pp. 238–257.
- Kondo, Jun (1964). “Resistance minimum in dilute magnetic alloys”. In: *Progress of theoretical physics* 32.1, pp. 37–49.
- Krishna-murthy, H. R., J. W. Wilkins, and K. G. Wilson (1980). “Renormalization-group approach to the Anderson model of dilute magnetic alloys. I. Static properties for the symmetric case”. In: *Phys. Rev. B* 21 (3), pp. 1003–1043.
- Metzner, Walter and Dieter Vollhardt (1989). “Correlated Lattice Fermions in $d = \infty$ Dimensions”. In: *Phys. Rev. Lett.* 62 (3), pp. 324–327.
- Mott, N F (1949). “The Basis of the Electron Theory of Metals, with Special Reference to the Transition Metals”. In: *Proceedings of the Physical Society. Section A* 62.7, pp. 416–422.
- Mukherjee, Anirban and Siddhartha Lal (2020a). *Holographic entanglement renormalisation of topological order in a quantum liquid*.

- Mukherjee, Anirban and Siddhartha Lal (2020b). “Scaling theory for Mott–Hubbard transitions: I. T = 0 phase diagram of the 1/2-filled Hubbard model”. In: *New Journal of Physics* 22.6, p. 063007.
- — (2020c). “Scaling theory for Mott–Hubbard transitions-II: quantum criticality of the doped Mott insulator”. In: *New Journal of Physics* 22.6, p. 063008.
- — (2020d). “Unitary renormalisation group for correlated electrons-I: a tensor network approach”. In: *Nuclear Physics B* 960, p. 115170.
- — (2020e). “Unitary renormalisation group for correlated electrons-II: insights on fermionic criticality”. In: *Nuclear Physics B* 960, p. 115163.
- Mukherjee, Anirban, Siddhartha Patra, and Siddhartha Lal (2021). “Fermionic criticality is shaped by Fermi surface topology: a case study of the Tomonaga-Luttinger liquid”. In: *Journal of High Energy Physics* 04, p. 148.
- Mukherjee, Anirban et al. (2022). “Unveiling the Kondo cloud: Unitary renormalization-group study of the Kondo model”. In: *Phys. Rev. B* 105 (8), p. 085119.
- Nozieres, P (1974). “A “Fermi-liquid” description of the Kondo problem at low temperatures”. In: *Journal of Low Temperature Physics* 17, p. 31.
- Pal, Santanu, Anirban Mukherjee, and Siddhartha Lal (2019). “Correlated spin liquids in the quantum kagome antiferromagnet at finite field: a renormalization group analysis”. In: *New Journal of Physics* 21.2, p. 023019.
- Patra, Siddhartha and Siddhartha Lal (2021). “Origin of topological order in a Cooper-pair insulator”. In: *Phys. Rev. B* 104 (14), p. 144514.
- Shimony, Abner (1995). “Degree of entanglement”. In: *Annals of the New York Academy of Sciences* 755.1, pp. 675–679.

References III

- Wei, Tzu-Chieh and Paul M Goldbart (2003). “Geometric measure of entanglement and applications to bipartite and multipartite quantum states”. In: *Physical Review A* 68.4, p. 042307.
- Wilson, Kenneth G. (1975). “The renormalization group: Critical phenomena and the Kondo problem”. In: *Rev. Mod. Phys.* 47 (4), pp. 773–840.