Local metal-insulator transition in a generalised Anderson impurity model

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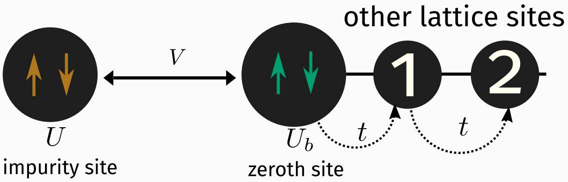
Why another impurity model?

Anderson and Kondo impurity models - No transition!

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



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- Transition involves growth of **charge content**, finally leading to local moment.
- **Spectral function** goes through a three-peak structure at the critical point, and develops a gap beyond that.
- Geometric **entanglement** acts as an order parameter for the transition.

Outline

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1. The generalised Anderson impurity model
2. Short description of the unitary RG method
3. RG equations, phase diagram and phase transition
4. Effective Hamiltonian and ground state
5. Description of phase transition through spectral functions and entanglement
6. Some concluding remarks

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The Model

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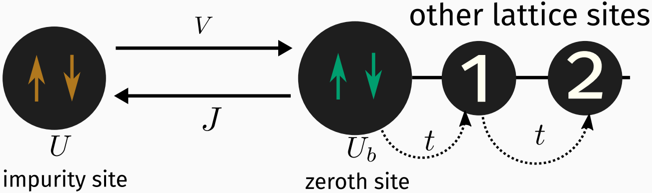
$$H = \overbrace{\sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2}^{\text{p-h symmetric Anderson impurity model}} + \underbrace{J \vec{S}_d \cdot \vec{S}_0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

- **spin-exchange** between impurity and bath
- **correlation** on zeroth site of bath



Schrieffer and Wolff 1966; Anderson 1961.

The Unitary Renormalization Group Method

The Unitary RG Method: The General Idea

- Apply unitary many-body transformations to the Hamiltonian

$$\begin{array}{c} H_j \\ \Big\downarrow{\scriptstyle U_j} \\ H_{j-1} \end{array}$$

Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple high energy states

$$\begin{tikzcd} H_j \arrow[d, "U_j"] \\ H_{j-1} \end{tikzcd}$$

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The Unitary RG Method: The General Idea

- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple high energy states
- Obtain sequence of Hamiltonians and hence scaling equations

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Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

The Unitary RG Method: Select a UV-IR Scheme

UV shell

$\vec{k}_N$ (zeroth RG step)

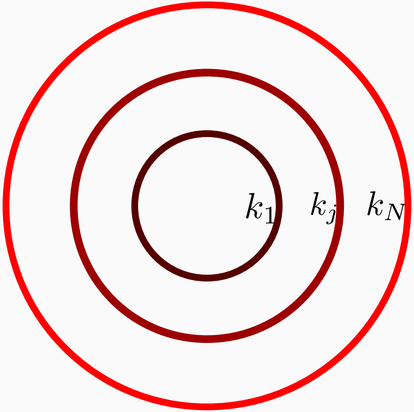
$\vdots$

$\vec{k}_j$ $\left(j^{\text{th}}\text{ RG step}\right)$

$\vdots$

$\vec{k}_1$ (Fermi surface)

IR shell

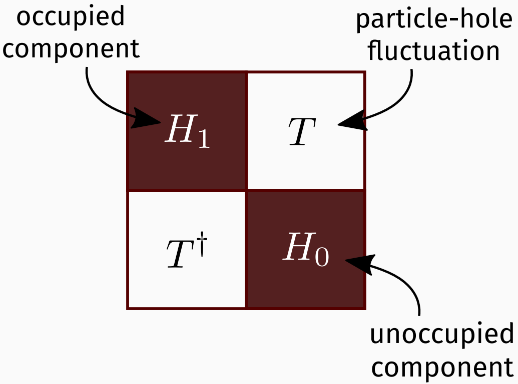


The Unitary RG Method: Write Hamiltonian in the basis of $\vec{k}_j$

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

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

(j) : j^{th} RG step



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

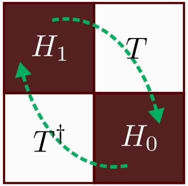
$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

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

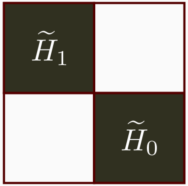
$$\left.\eta^{\dagger}_{(j)} = \frac{1}{\hat{\omega}_{(j)} - H_D} c^{\dagger}_j T \right\} \rightarrow \text{many-particle rotation}$$

$$\hat{\omega}_{(j)} = (H_1 + H_0)_{(j-1)} + \Delta T_{(j)}$$

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



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



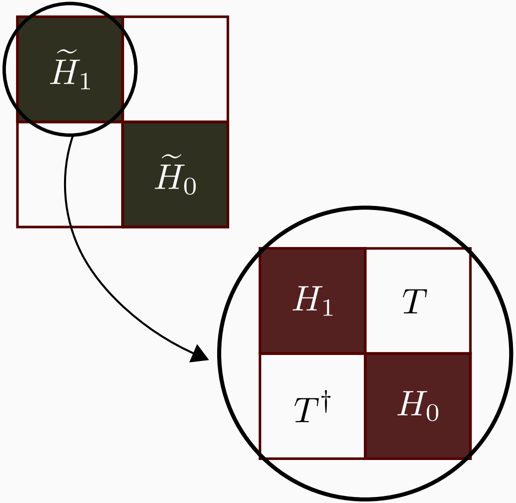
$$\left[H_{(j-1)}, n_j\right] = 0$$

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

The Unitary RG Method: Repeat with renormalised Hamiltonian

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

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



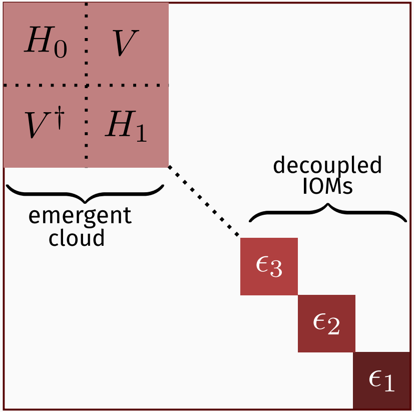
The Unitary RG Method: RG Equations and Denominator Fixed Point

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

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

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

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



The Unitary RG Method: Novel Features of the Method

- **Quantum fluctuation scale** $\hat{\omega}$ that tracks all orders of renormalisation

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- Finite-valued fixed points for finite systems - leads to **emergent degrees of freedom**
- **Spectrum-preserving** unitary transformations - partition function does not change
- Tractable low-energy effective Hamiltonians - allows **renormalised perturbation theory** around them

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Final Remarks

Conclusions

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- The auxiliary model method described here provides a **constructionist** approach to studying systems of strong correlations
- **Minimal attractive interaction** on bath leads to a metal-insulator transition in the Hubbard-Heisenberg model
- The transition derives from a competition between **Kondo** spin-flip physics and the physics of **pairing** instability.

Moving forward

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- Breaking particle-hole symmetry on the impurity will allow us to study bulk models **away from half-filling**.
- For more accurate results, one can consider **multiple impurities** in the cluster.

Thank you.