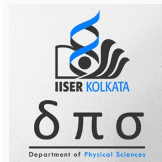


Local metal-insulator transition in a generalised Anderson impurity model

Abhirup Mukherjee, Siddhartha Lal

May 27, 2022

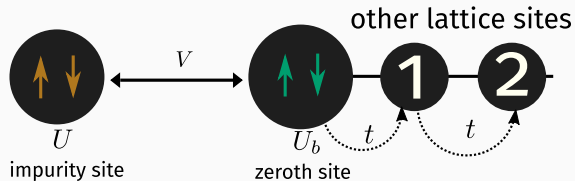
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Why another impurity model?

Anderson and Kondo impurity models - No transition!

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



Brief Summary of Results

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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

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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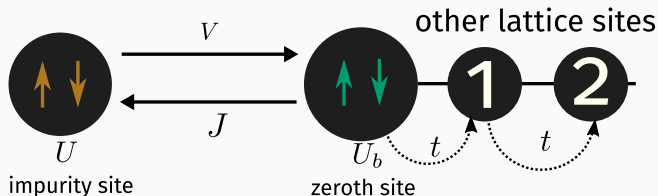
The Model

The Model

p-h symmetric Anderson impurity model

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

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



The Unitary Renormalization Group Method

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The General Idea

- Apply unitary many-body transformations to the Hamiltonian

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

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The Unitary Renormalization Group 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

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

The Unitary Renormalization Group Method

Select a UV-IR Scheme

UV shell

\vec{k}_N (zeroth RG step)

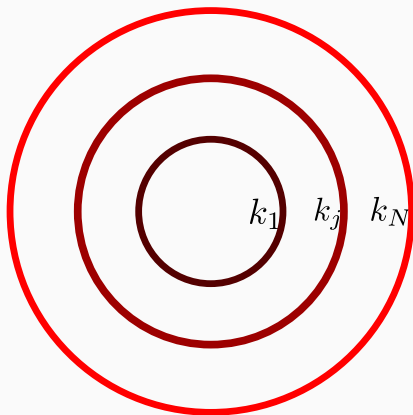
\vdots

\vec{k}_j (j^{th} RG step)

\vdots

\vec{k}_1 (Fermi surface)

IR shell



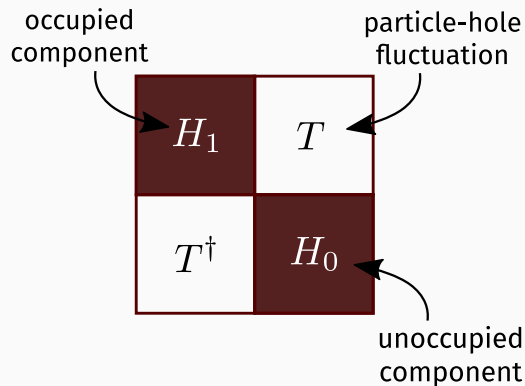
The Unitary Renormalization Group Method

Write Hamiltonian in the basis of \vec{k}_j

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

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

(j) : j^{th} RG step



The Unitary Renormalization Group Method

Rotate Hamiltonian and kill off-diagonal blocks

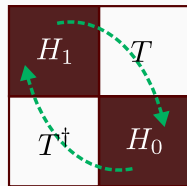
$$H_{(j-1)} = U_{(j)} H_{(j)} U_{(j)}^\dagger$$

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

$$\eta_{(j)}^\dagger = \frac{1}{\hat{\omega}_{(j)} - H_D} c_j^\dagger T \left\} \rightarrow \text{many-particle rotation}$$

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

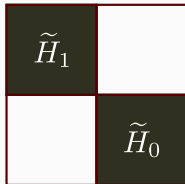
(quantum fluctuation operator)



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

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

n_j becomes an
integral of motion
(IOM)

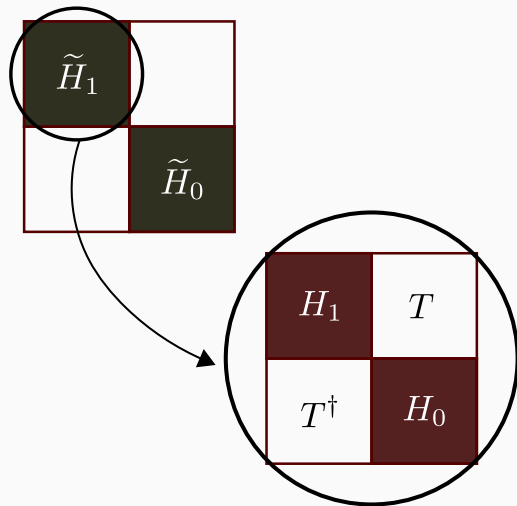


The Unitary Renormalization Group Method

Repeat with renormalised Hamiltonian

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

$$\tilde{H}_1 = H_1 \hat{n}_{j-1} + H_0 (1 - \hat{n}_{j-1}) + c_{j-1}^\dagger T + T^\dagger c_{j-1}$$



The Unitary Renormalization Group Method

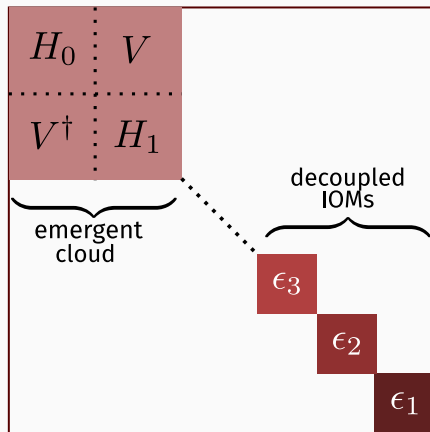
RG Equations and Denominator Fixed Point

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

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

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

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



The Unitary Renormalization Group Method

Novel Features of the Method

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

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- Tractable low-energy effective Hamiltonians - allows **renormalised perturbation theory** around them

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Final Remarks

Conclusions

- The auxiliary model method described here provides a **constructionist** approach to studying systems of strong correlations

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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

- k –dependence of the self-energy: **electronic differentiation** and effects of Van Hove singularities?

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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.