Local metal-insulator transition in a generalised Anderson impurity model

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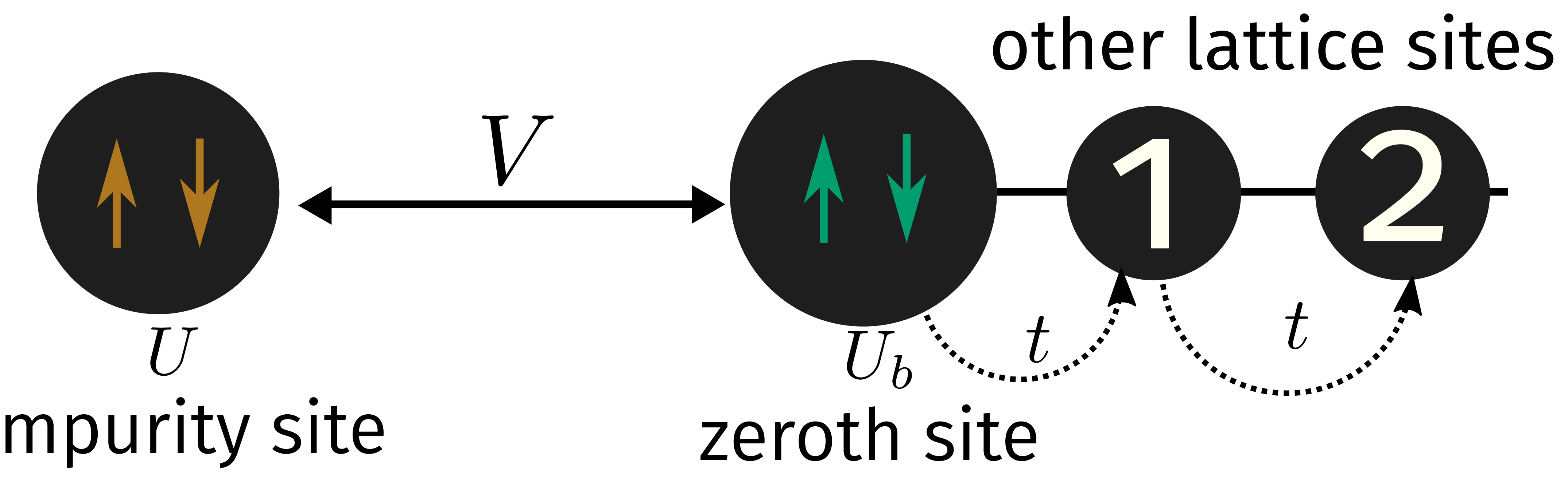
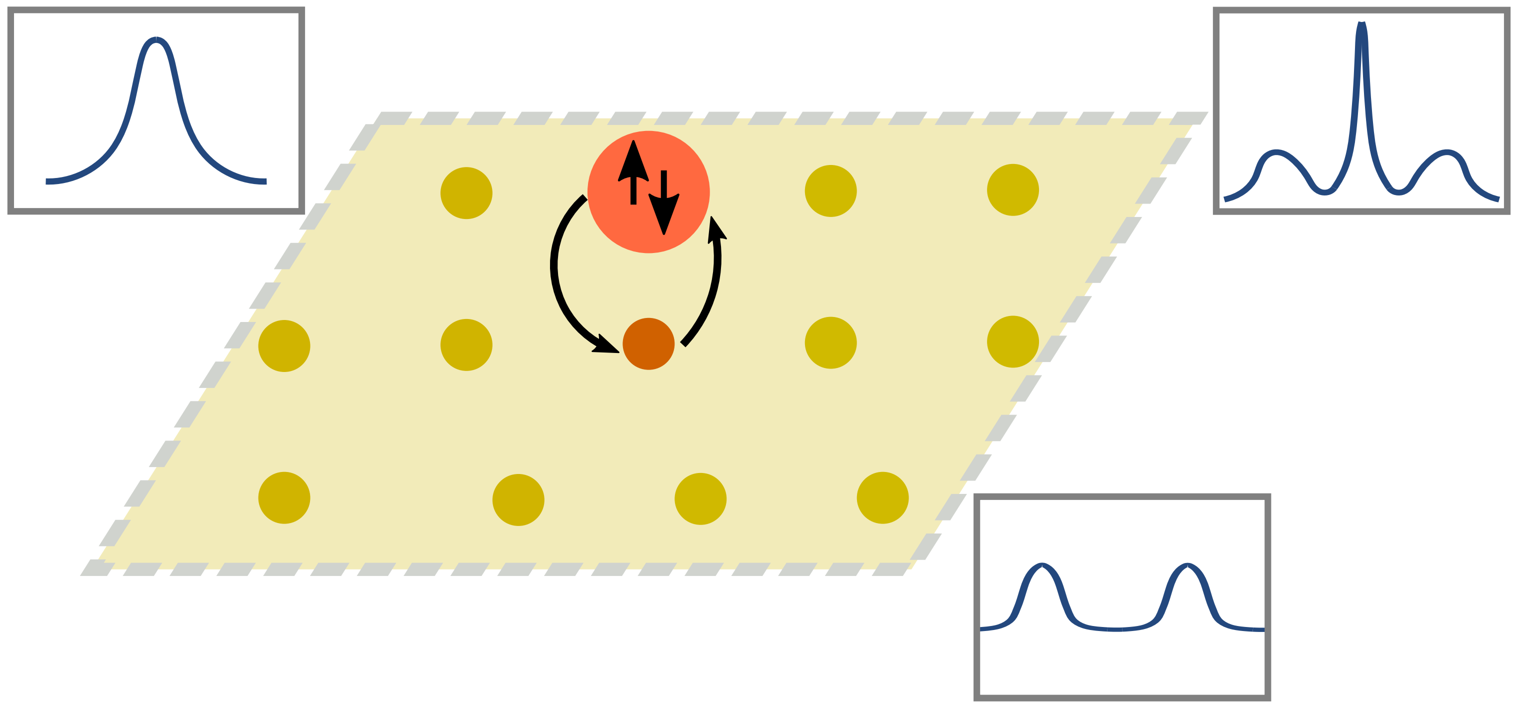
Why another impurity model ?

Anderson and Kondo impurity models - no transition!



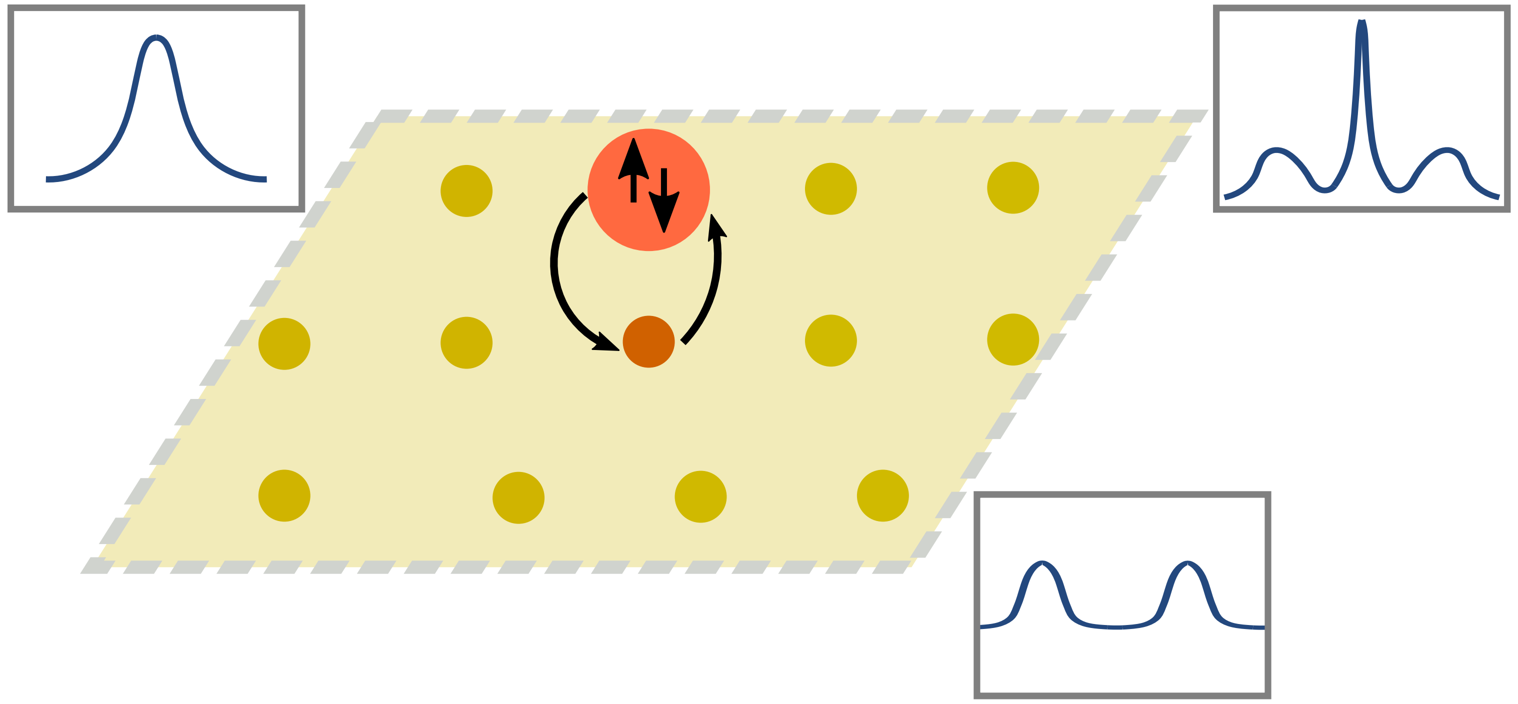
- simplest models - Anderson and Kondo
- localisation physics + hybridisation
- impurity is **screened** at low T

DMFT and the Mott MIT



- DMFT implementations use impurity models
- Determine correct impurity model **self-consistently**
- Exact in $d = \infty$ limit
- Displays **metal-insulator** transition in Hubbard model at $\frac{1}{2}$–filling

Some outstanding questions



- Which single impurity model shows such a transition?
- Can we relate impurity thermodynamics to that of the bulk?
- Which fluctuations lead to the MIT?

A Brief Summary of the Results

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- Introducing spin-exchange coupling and local attractive correlation in the bath leads to multiple phases under RG.

- Ground state interpolates from singlet to local moment, passing through a spin-charge correlated state.

- Many-particle entanglement acts as order parameter for the transition.

- Impurity spectral function has three-peak structure at critical point, becomes gapped beyond.

The Generalised Anderson Impurity model

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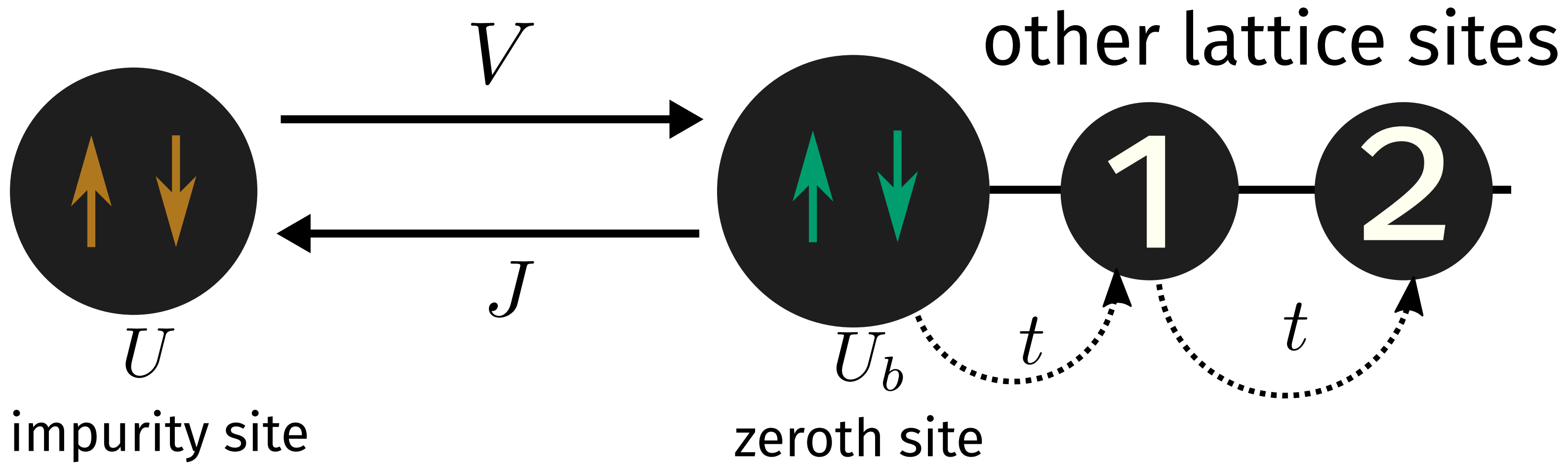
$$H = \overbrace{\sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2}^{\text{p-h symmetric Anderson impurity model}} + \underbrace{J \vec{S}_d \cdot \vec{S}_0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

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



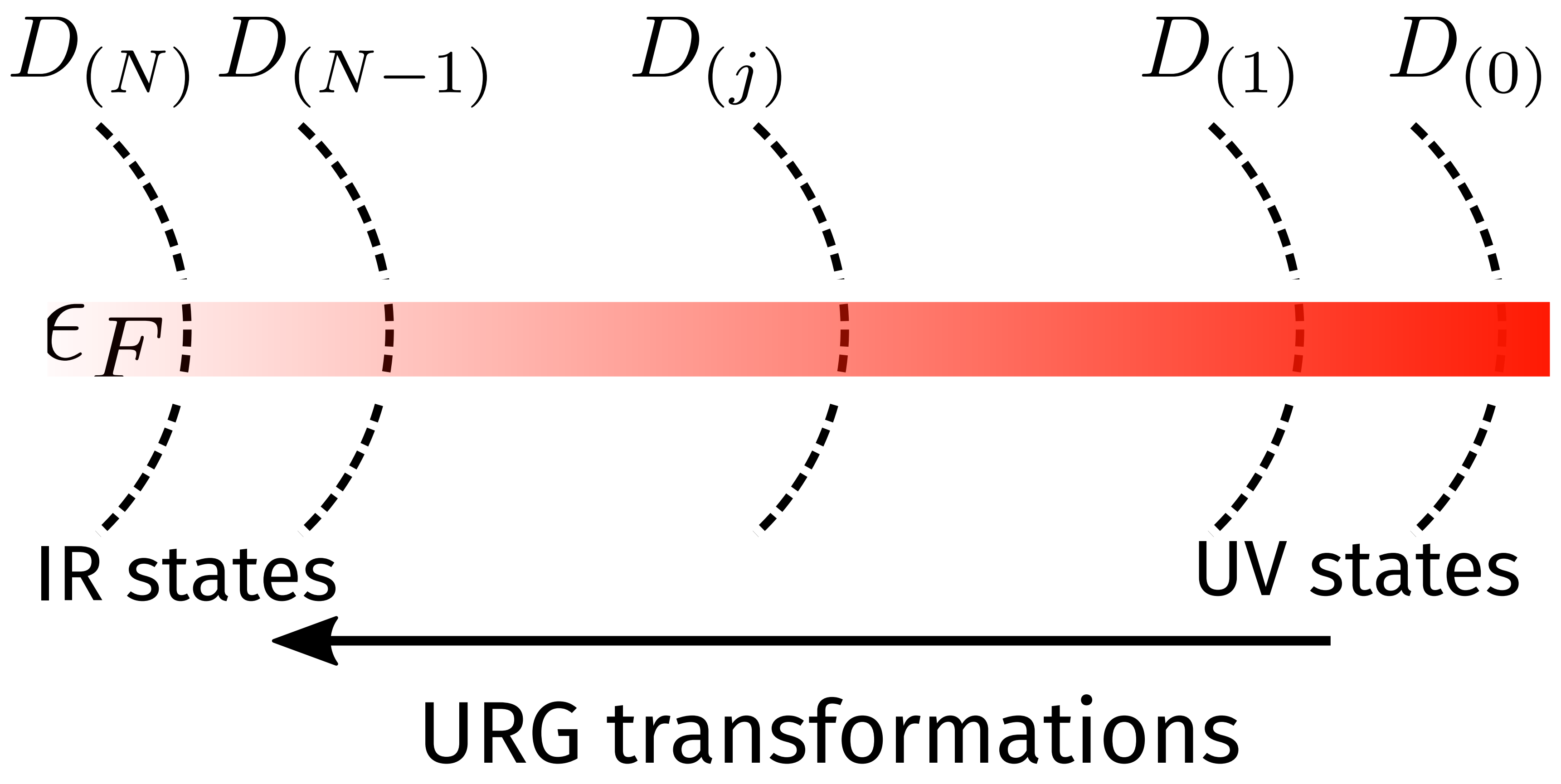
The Unitary RG method

The Unitary RG method: General Idea

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

$$H_j \xrightarrow{U_j} H_{j-1}$$

The Unitary RG method: Step 1 - Select UV-IR Scheme



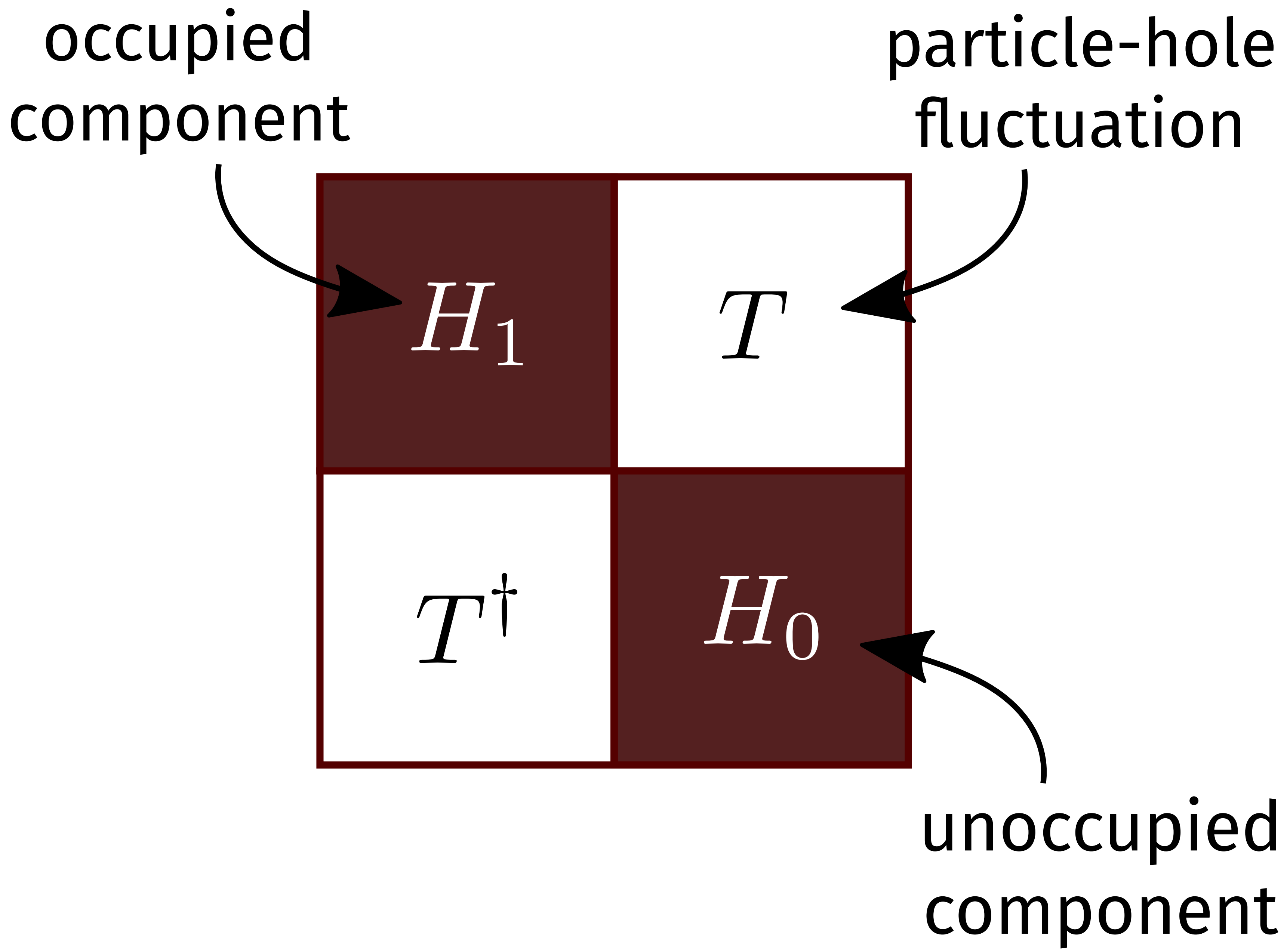
$$j^{\text{th}}\ \text{RG step} \longrightarrow \vec{k}_{j\sigma}$$

The Unitary RG method: Step 2 - 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: Step 3 - Rotate and kill off-diagonal blocks

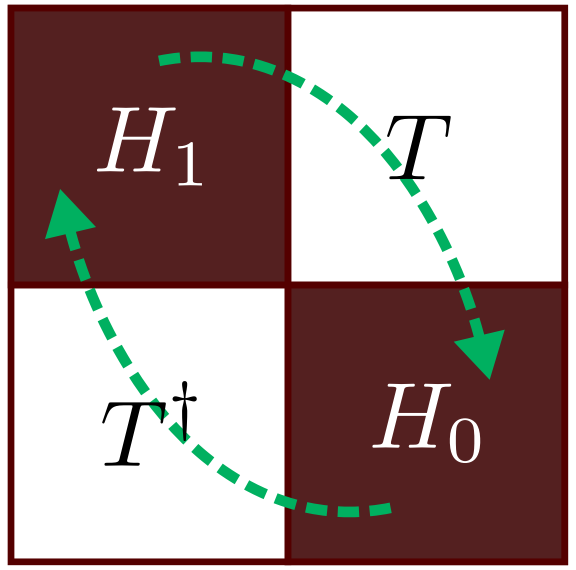
$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

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

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

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

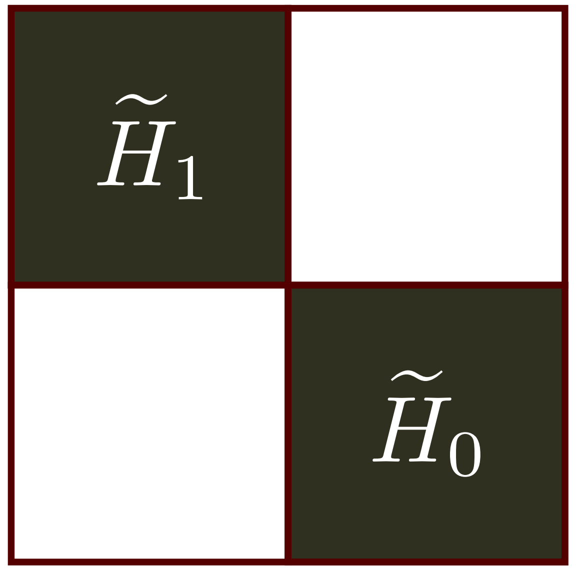
(quantum fluctuation operator)



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

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

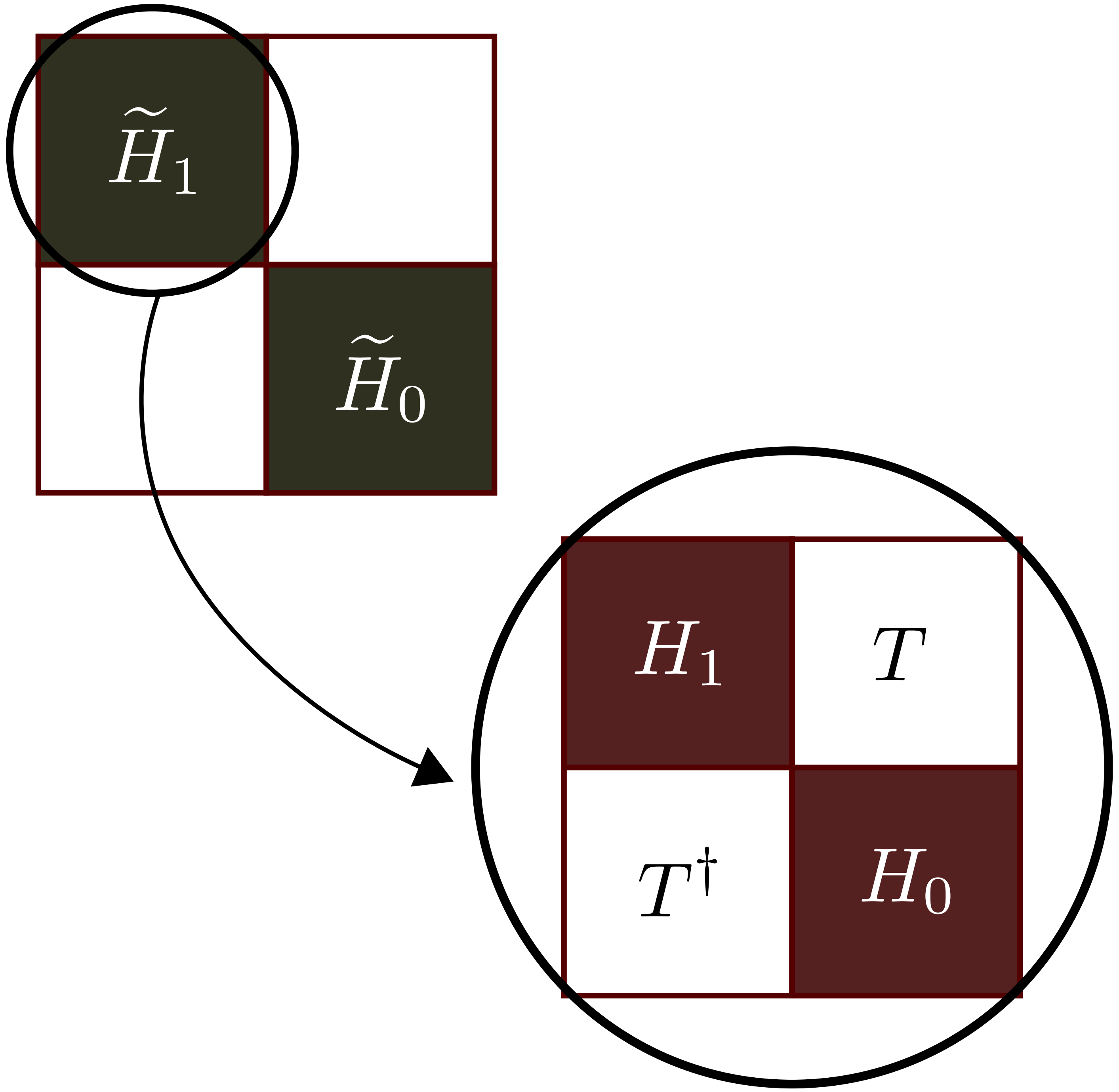
n_j becomes an
integral of motion
(IOM)



The Unitary RG method: Step 4 - Repeat with renormalised Hamiltonian

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

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



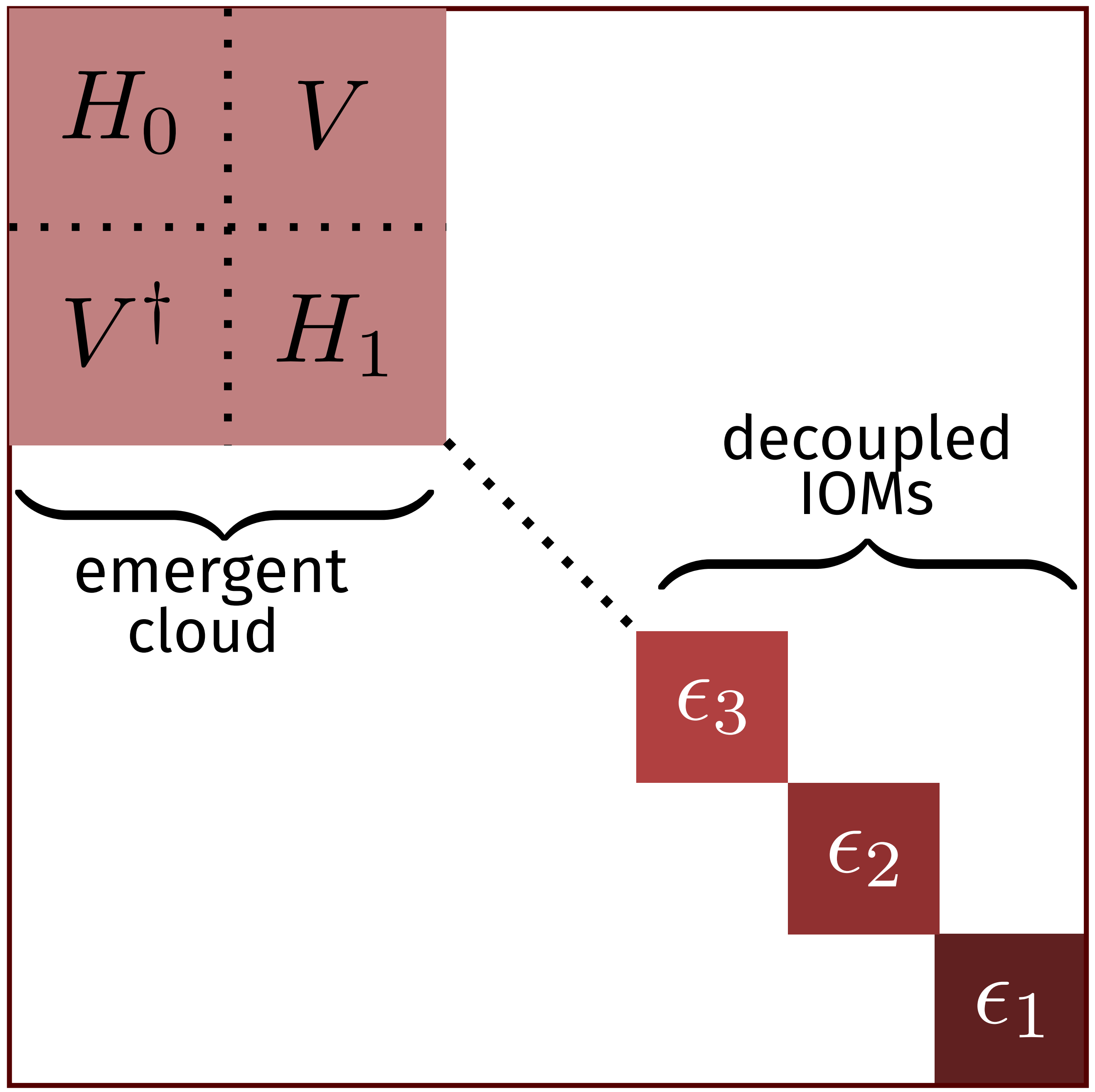
The Unitary RG method: RG Equations and Denominator Fixed Point

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

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

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

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
- 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

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

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

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

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