New Auxiliary Model Approach to the Mott MIT

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Brief Summary of Results

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- Promoting this impurity model to a bulk model using the tiling method creates a **Hubbard-Heisenberg model**.
- The impurity phase transition then leads to a **metal-insulator transition** in the bulk model.

Outline

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- description of the impurity model
- the unitary RG method
- renormalisation group results for the impurity model
- derivation of the present auxiliary model approach
- demonstration of a metal-insulator transition using this method
- some final remarks

The Model

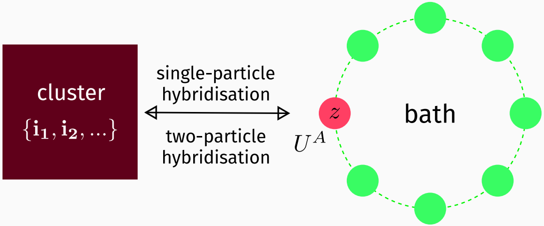
The Model

$$H = \overbrace{\sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2}^{\text{standard p-h symmetric Anderson impurity model}}$$

$$+ \underbrace{J \vec{S}_d \cdot \vec{s} - U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow} \right)^2}_{\text{additional terms}}$$

supplement 1-particle hybridisation with

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



Schrieffer and Wolff 1966; Anderson 1961.

The Unitary Renormalization Group Method

The General Idea

- Apply unitary many-body transformations to the Hamiltonian

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

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

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

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

The General Idea

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

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

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

Select a UV-IR Scheme

UV shell

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

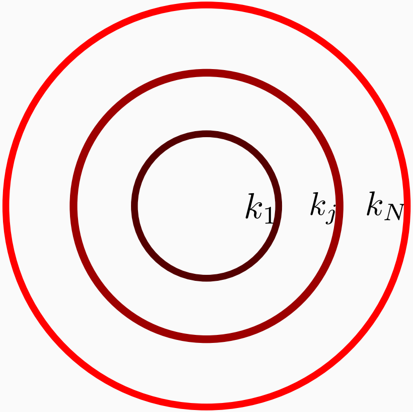
$\vdots$

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

$\vdots$

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

IR shell



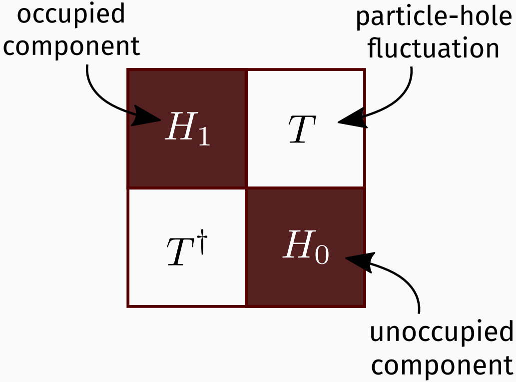
Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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



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

Rotate Hamiltonian and kill off-diagonal blocks

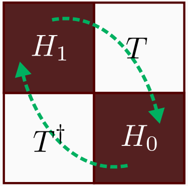
$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

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

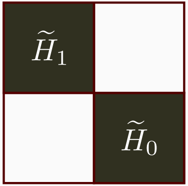
$$\left.\eta^{\dagger}_{(j)} = \frac{1}{\hat{\omega}_{(j)} - H_D} c^{\dagger}_j T \right\} \rightarrow \text{many-particle rotation}$$

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

(quantum fluctuation operator)



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



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

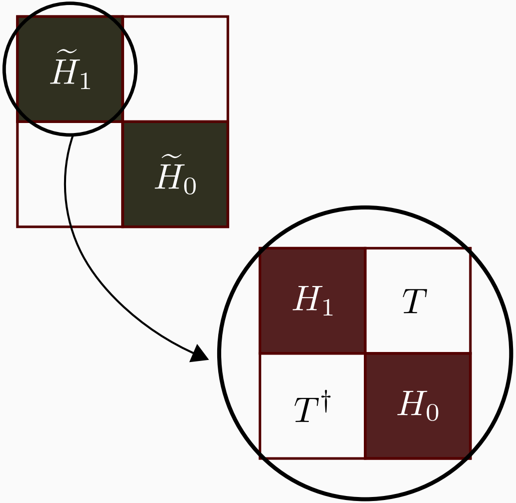
n_j becomes an
integral of motion
(IOM)

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

Repeat with renormalised Hamiltonian

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

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



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

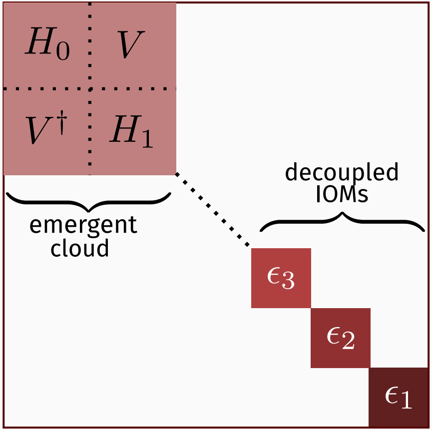
RG Equations and Denominator Fixed Point

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

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

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

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



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

Novel Features of the Method

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

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

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

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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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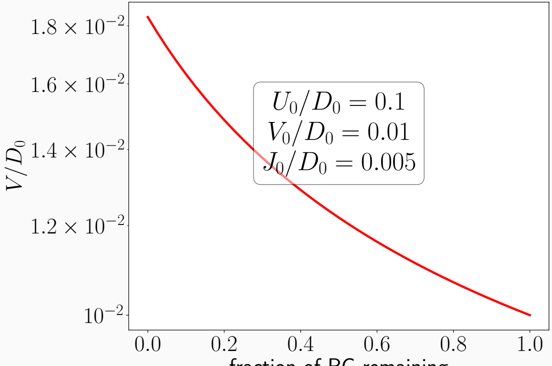
URG Analysis: $U_b = 0$

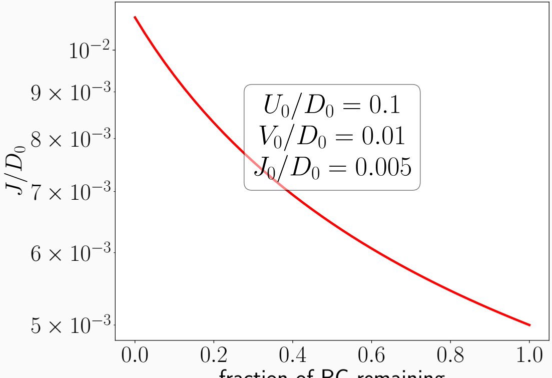
$U_b = 0$: Flow towards strong-coupling

$\mathbf{U > 0, J > 0}$

$$\Delta V = \frac{3 n_j V J}{8}\left(\frac{1}{|d_2|} + \frac{1}{|d_1|}\right) > 0, \qquad \Delta J = \frac{n_j J^2}{|d_2|} > 0$$

$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}$$



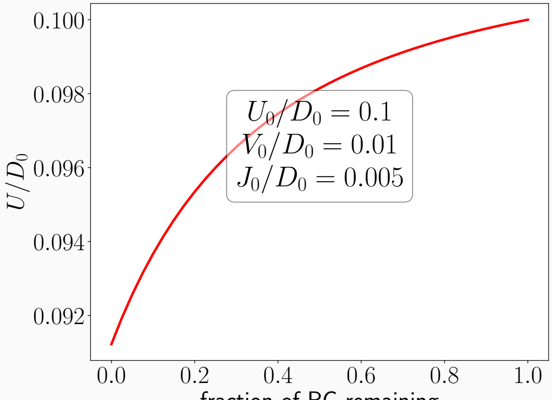


$U_b = 0$: Flow towards strong-coupling

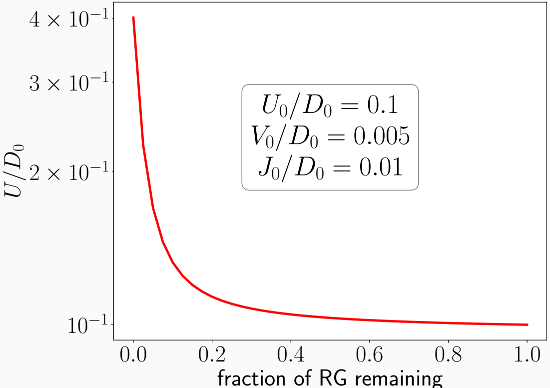
$\mathbf{U > 0, J > 0}$

$$\Delta U = 4V^2 n_j \left(\frac{1}{d_1} - \frac{1}{d_0}\right) - n_j \frac{J^2}{d_2}$$

$V > J$



$V < J$

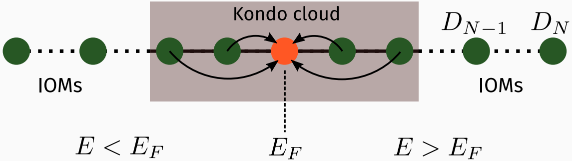


$U > 0$ Fixed point Hamiltonian

$$H^* = \sum_{k<k^*,\sigma} \epsilon_k \hat{n}_{k\sigma} + \frac{U^*}{2}\left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 + J^* \vec{S}_d \cdot \vec{s}_<$$

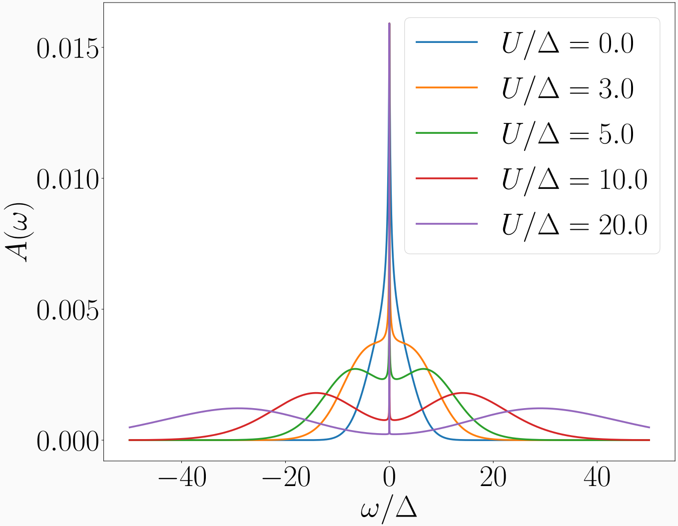
$$+ V^* \sum_{k<k^*,\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.}\right)$$

$$\vec{s}_< = \frac{1}{2} \sum_{k,k'<k^*} c^\dagger_{k\alpha} \vec{\sigma}_{\alpha\beta} c_{k',\beta}$$



Impurity Spectral Function

no gap at arbitrarily large U



URG Analysis: $U_b \neq 0$

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- Spin-exchange couling J can now be **driven irrelevant** by U_b:

$$\Delta J = -\frac{n_j J\left(J + 4U_b\right)}{d_2} \longrightarrow \begin{cases} \text{relevant when } J + 4U_b > 0 \\ \text{irrelevant when } J + 4U_b < 0 \end{cases}$$

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- Same can be said for the hybridisation V:

$$\Delta V = -\frac{3n_j V}{8}\left[\left(J + \frac{4U_b}{3}\right)\left(\frac{1}{d_2} + \frac{1}{d_1}\right) + \frac{4U_b}{3}\left(\frac{1}{d_3} + \frac{1}{d_0}\right)\right] \longrightarrow \begin{cases} \text{rel.}, J + 4U_b > 0 \\ \text{irrel.}, J + 4U_b < 0 \end{cases}$$

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- Same can be said for the hybridisation V:

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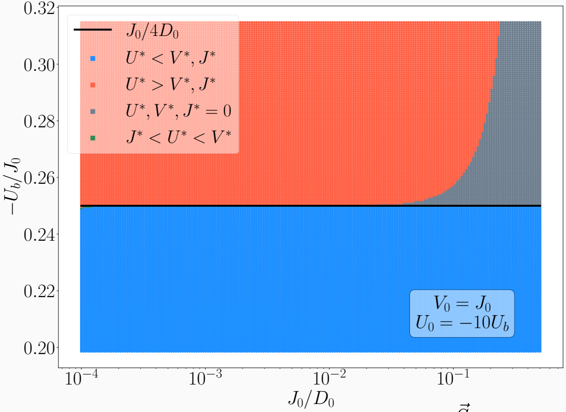
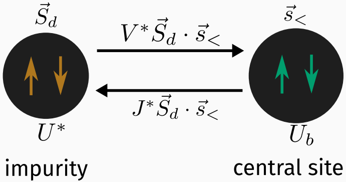
- ***U can be relevant if J decays slower than V***; needs to be checked numerically

$U > 0$ Phase Diagram



- black line: **critical points** at $U_b^* = -J^*/4$



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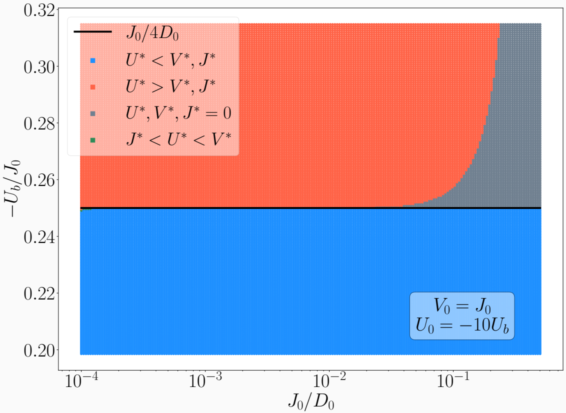

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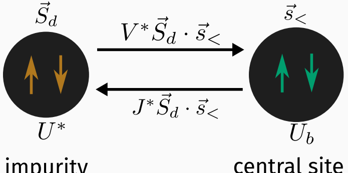
- blue: **screened** impurity (strong-coup.)



$$\Delta J > 0, \Delta V > 0, \Delta U < 0, \quad J^* \gg V^* \gg U^*$$

$$\frac{1}{\sqrt{2}} \left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \right)$$

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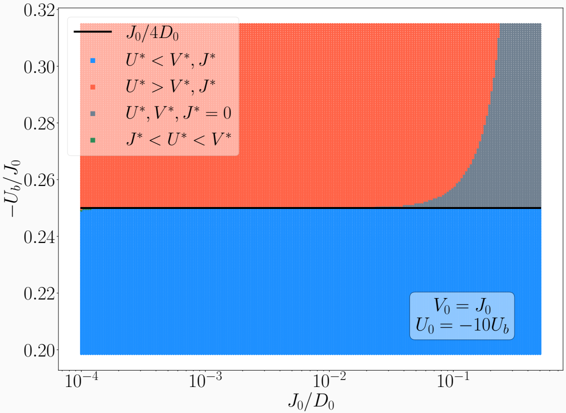

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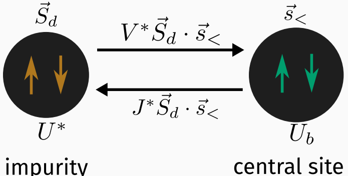
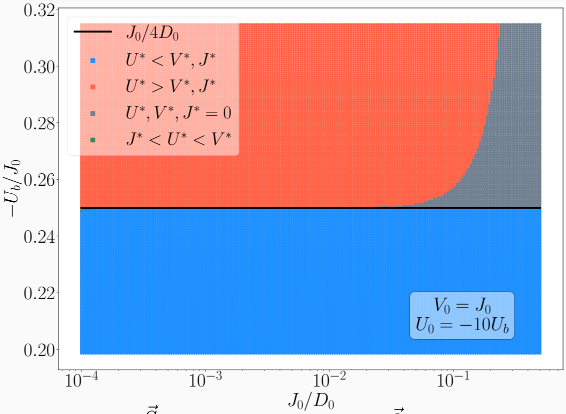


$$\Delta J < 0, \Delta V < 0, \Delta U > 0, \quad J^* = V^* = 0, U^* \geq 0$$

$$\{|\uparrow\rangle, |\downarrow\rangle\} \otimes \{|0\rangle, |2\rangle\}$$

$U > 0$ Phase Diagram



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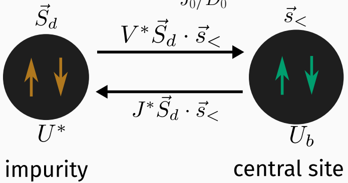

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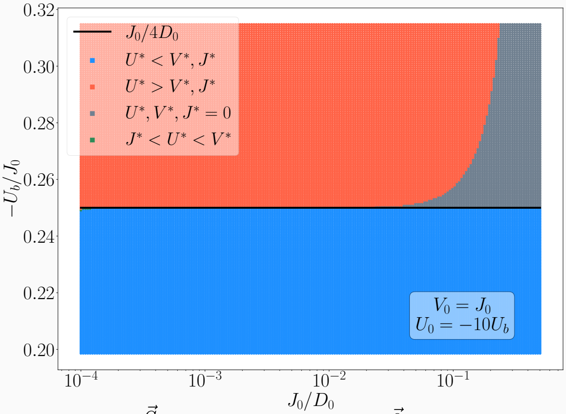

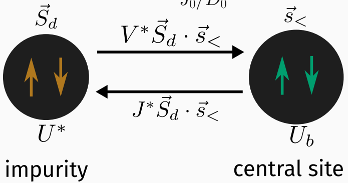

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- red: **unscreened** local mom. ($J = V = 0$)
- gray: imp. level absent ($U = J = V = 0$)
- green: J vanishes ($J < U$)

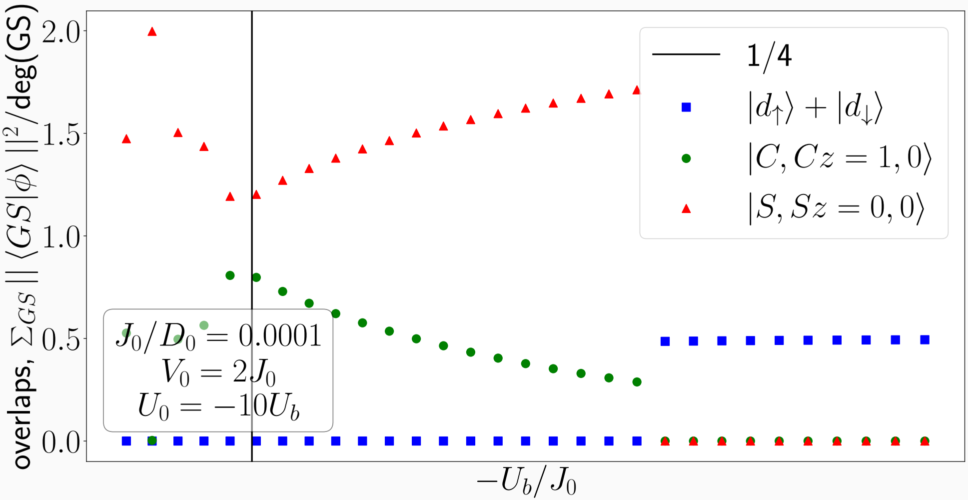
$$J^* < U^* < V^*$$

$$\frac{c}{\sqrt{2}} \left(|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle \right) + \frac{\sqrt{1 - c^2}}{\sqrt{2}} \left(|2, 0\rangle + |0, 2\rangle \right)$$

Evolution of two-site ground state and correlations across the transition

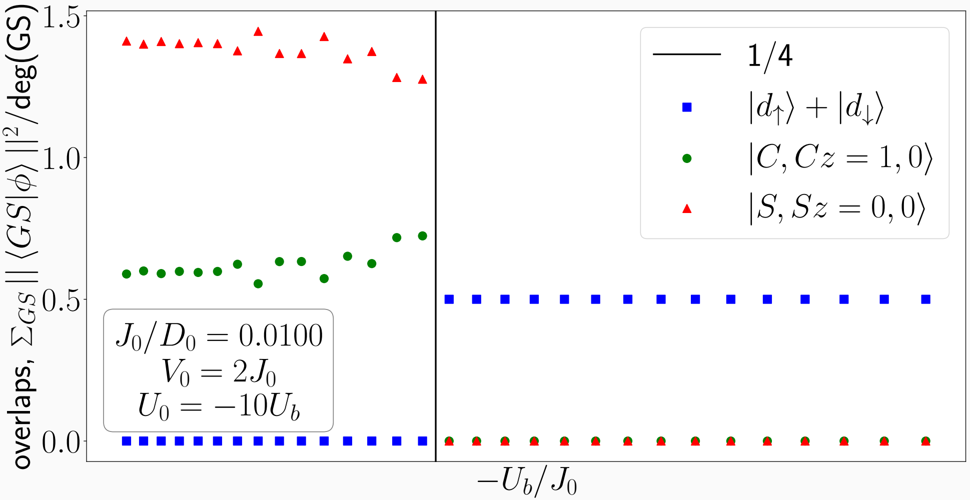
Overlap of ground state against spin singlet and charge triplet zero states

$J_0/D_0 = 10^{-4}$



Overlap of ground state against spin singlet and charge triplet zero states

$J_0/D_0 = 10^{-2}$



Overlap of ground state against spin singlet and charge triplet zero states

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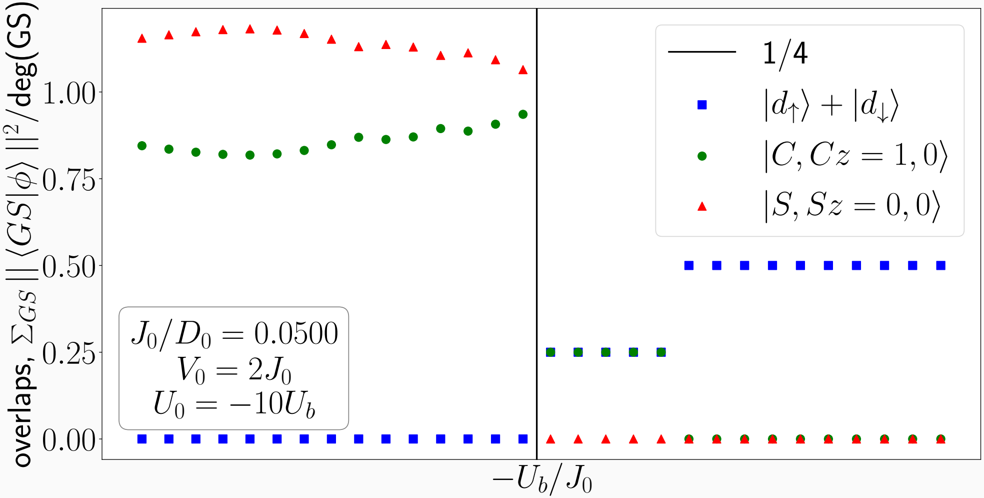

Spin and charge correlations in ground state

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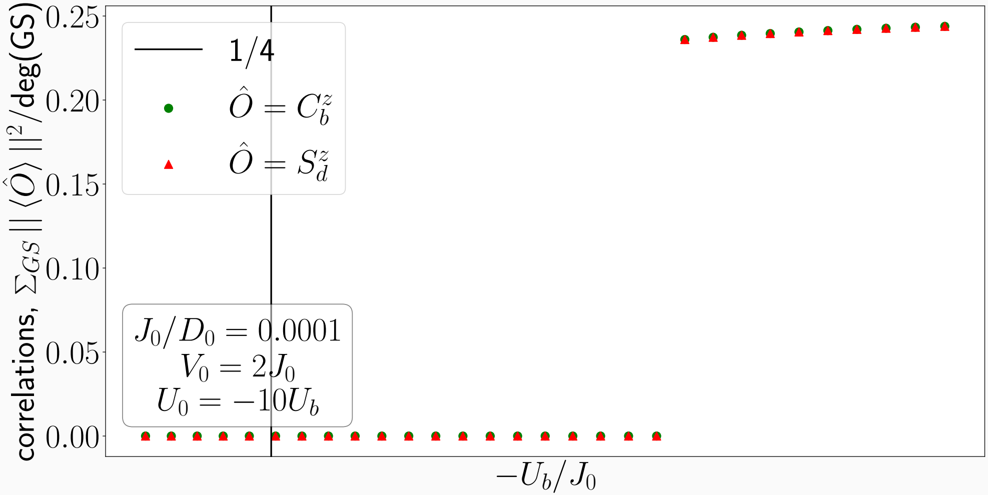

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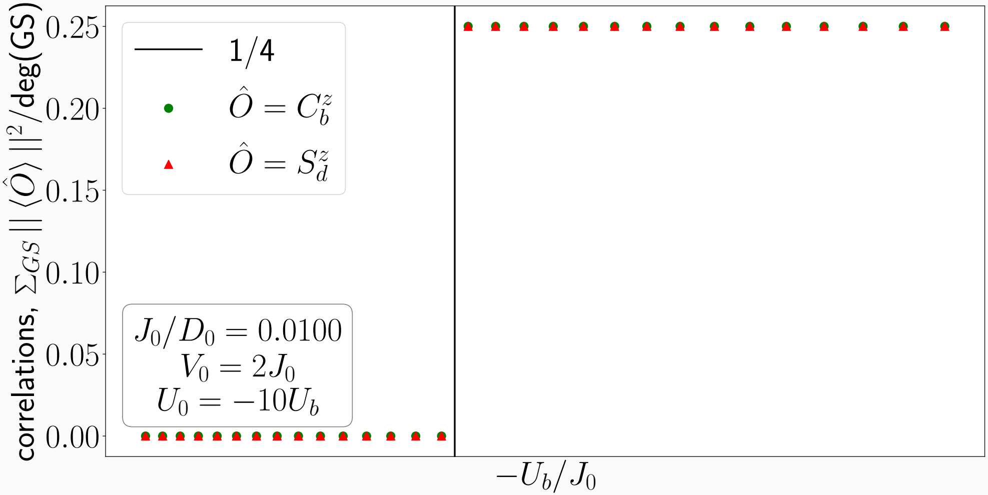

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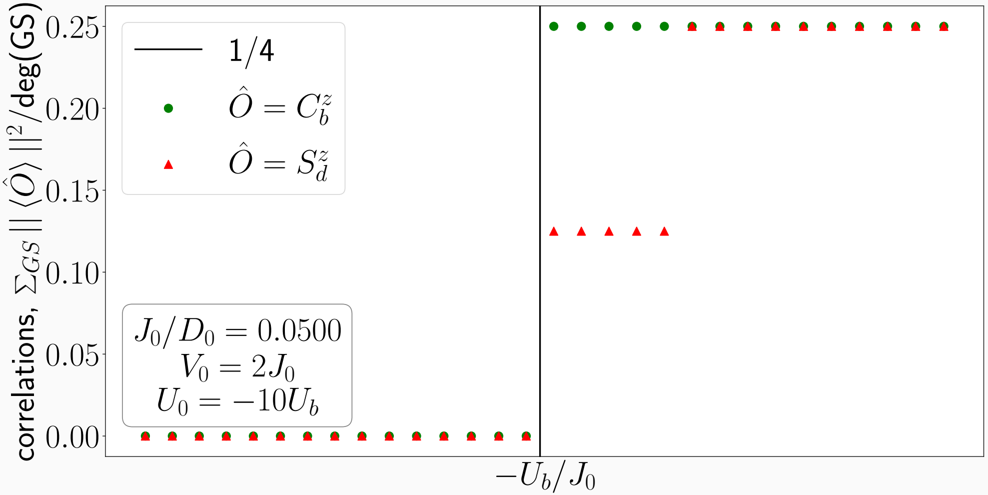
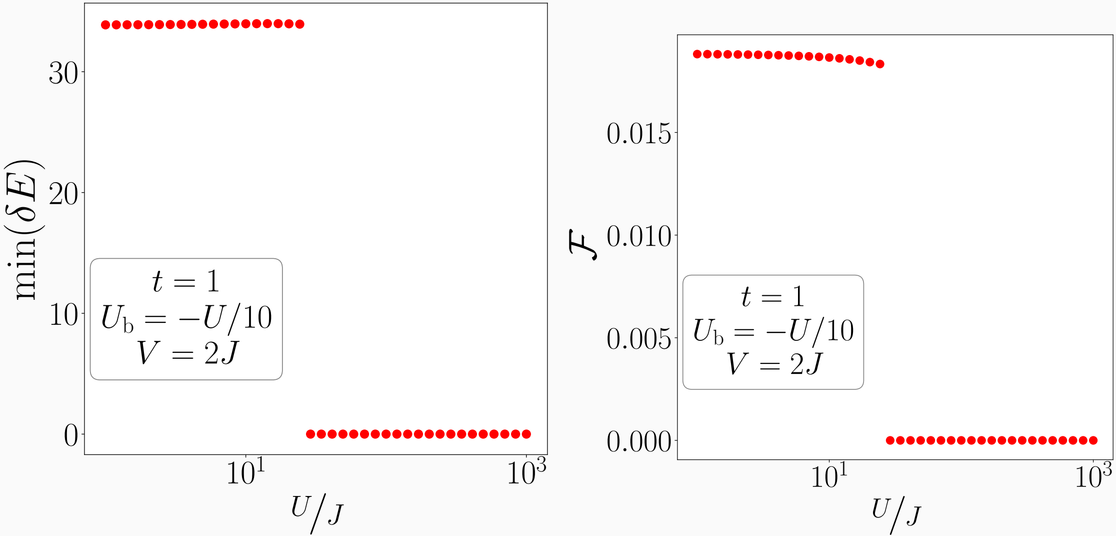
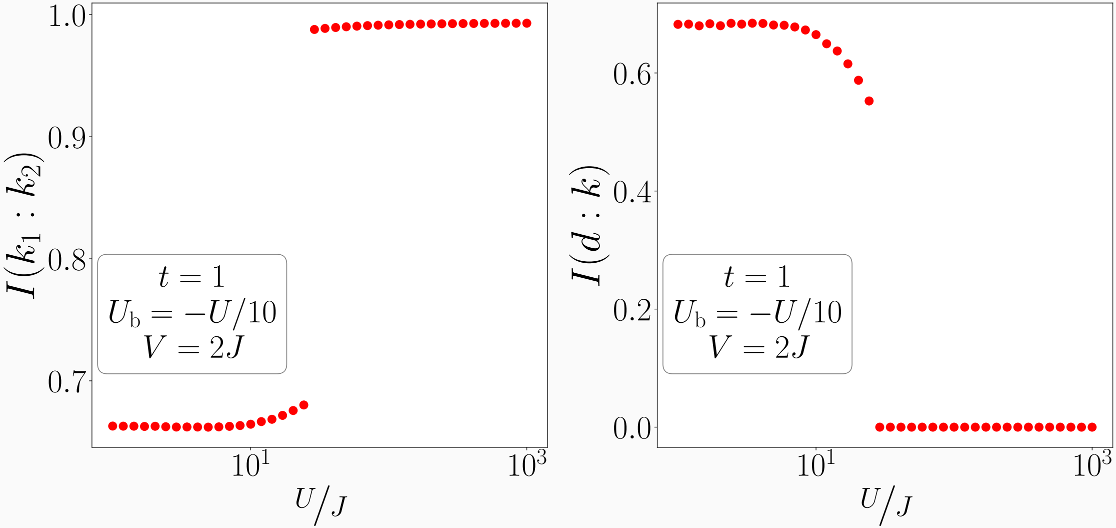


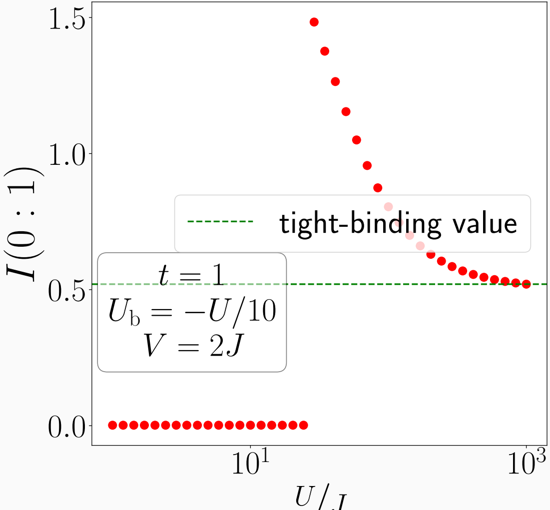
Correlation measures: Local Fermi liquid

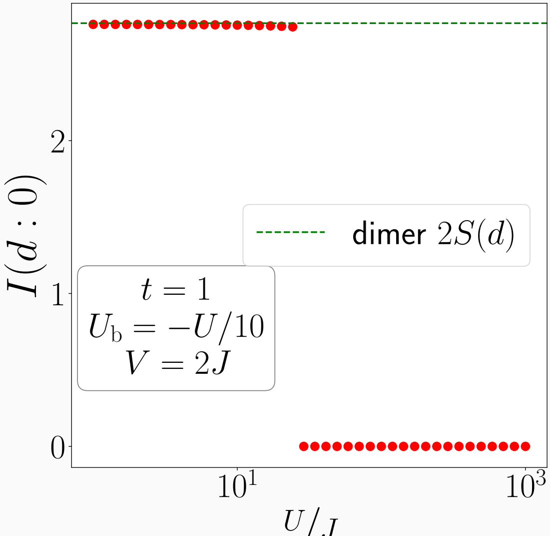


Correlation measures: Kondo cloud

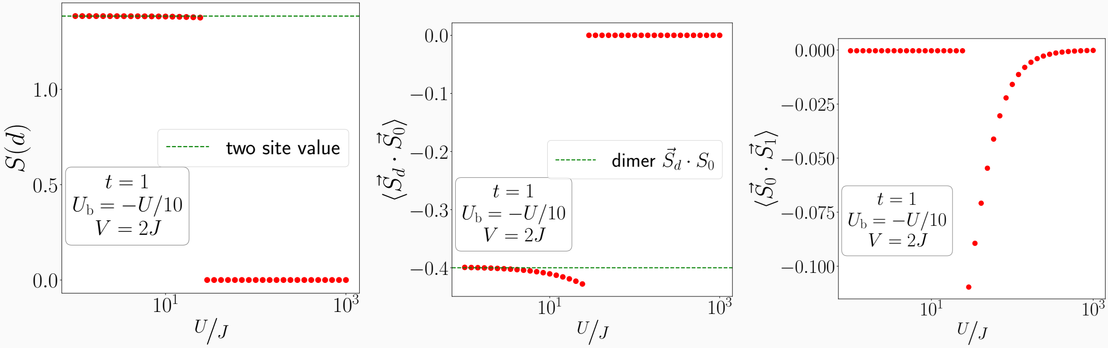


Correlation measures: Real space mutual information

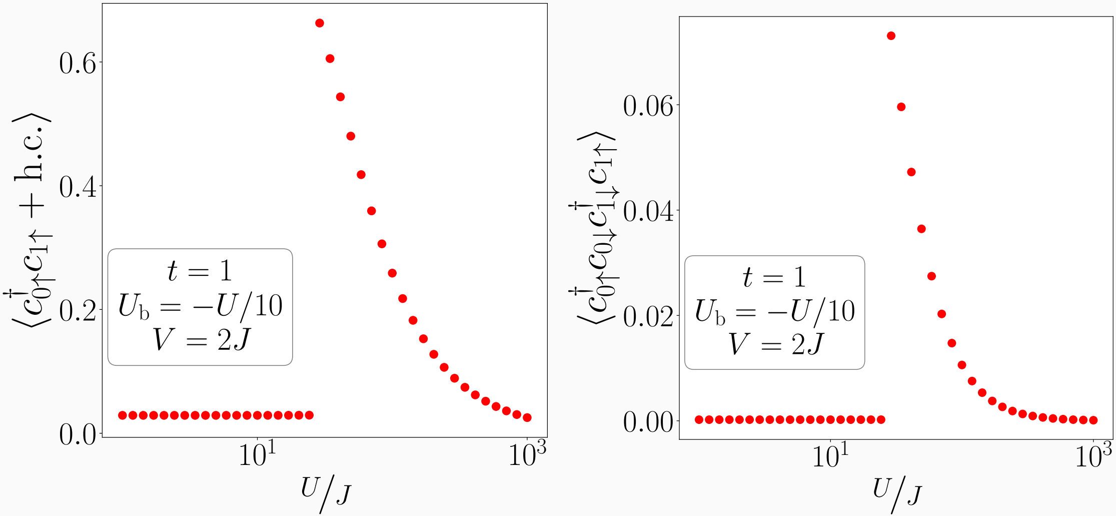




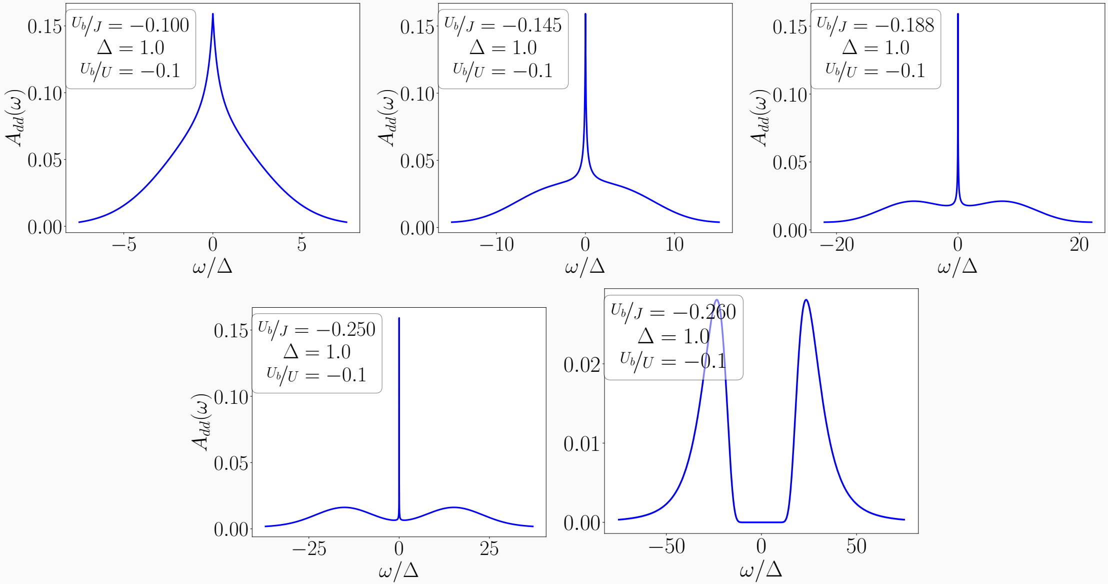
Correlation measures: Impurity entanglement entropy and spin-spin correlations



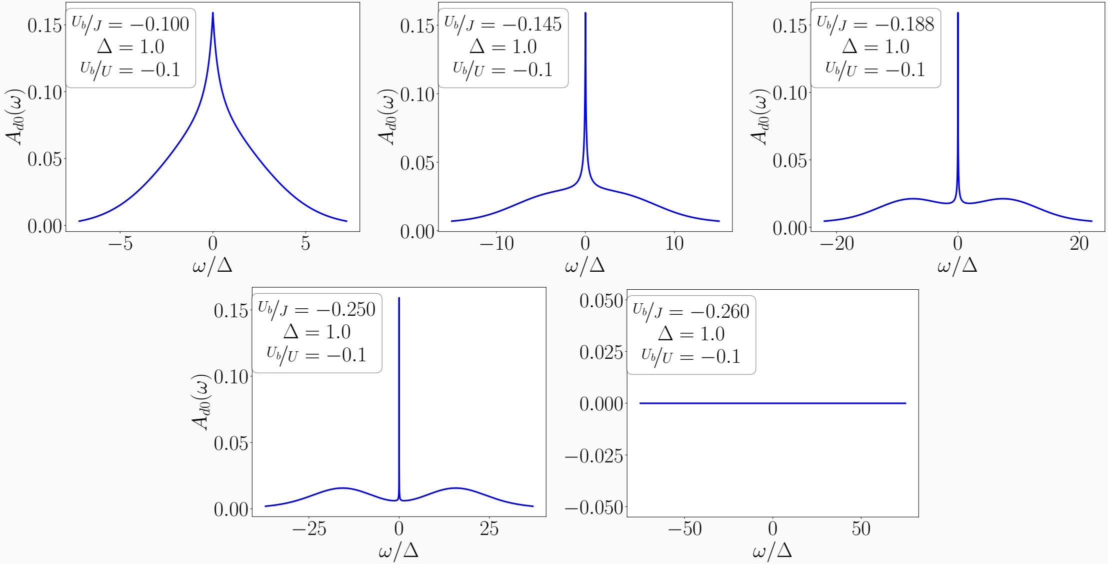
Correlation measures: Real-space correlations



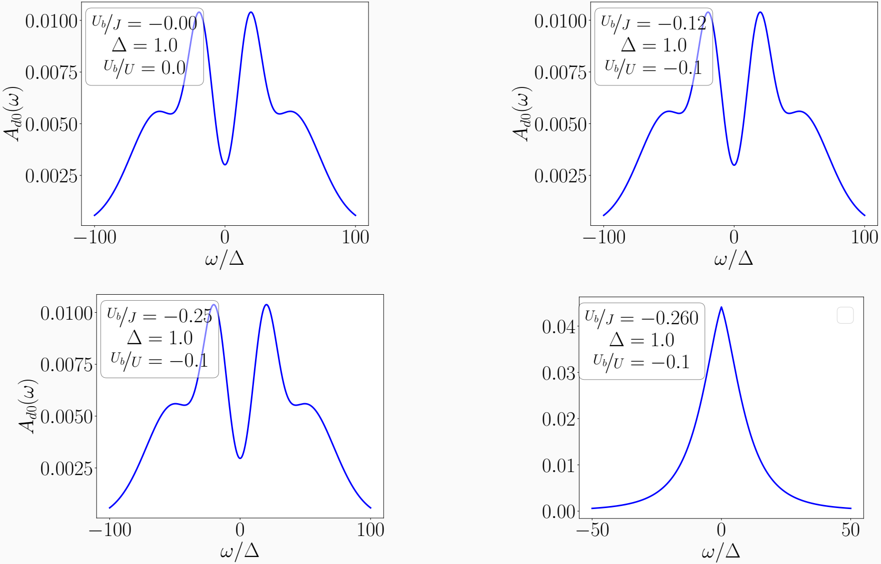
Correlation measures: Impurity spectral function



Correlation measures: Impurity-bath spectral function A_{d0}



Correlation measures: Bath spectral function A_{00}

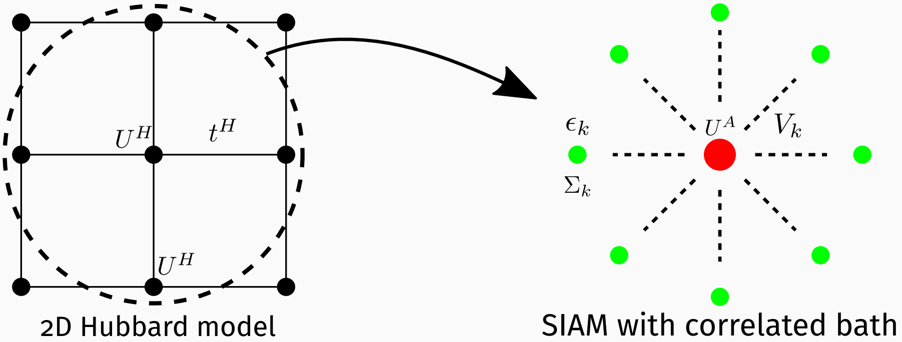


The Auxiliary Model Approach

General philosophy

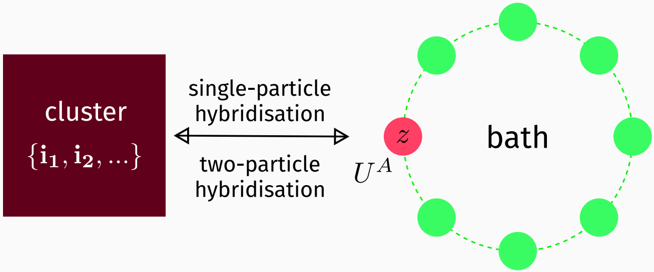
$$H = \overbrace{H_{\text{cluster}}}^{\text{simple}} + \underbrace{H_{\text{bath}} + H_{\text{cl-bath}}}_{\text{complicated}}$$

- find "appropriate" bath and then solve the cluster+bath problem
- appropriate = physical + solvable



The present method

- **Choose an auxiliary model** H_{aux} consisting of a correlated impurity interacting with a minimally correlated bath



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- **Solve** this impurity model H_{aux} using the unitary RG
- Create a **bulk lattice model** H_{bulk} from this auxiliary model H_{aux} by applying translation operators on the latter
- The relation hence obtained between the impurity and bulk models then allows us to **relate the physics** of the two.

The Tiling Process

Creating the unit of tiling

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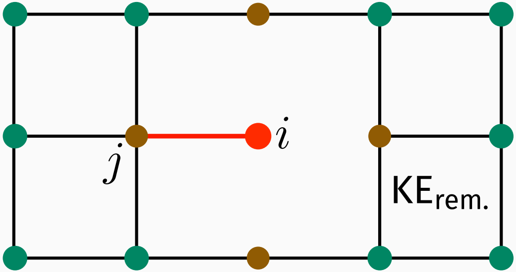
- Replace the zeroth site with one of the neighbours j of i

$$\mathcal{H}_{\text{aux}}(i,j) = \text{KE}_{\text{rem.}} - \frac{U}{2}\left(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right)^2 + V\sum_{\sigma}\left(c^\dagger_{j\sigma}c_{i\sigma} + h.c.\right) + J\vec{S}_i\cdot\vec{S}_j - U_b\left(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}\right)^2$$



Creating the bulk model

- Average over all w nearest neighbours

$$\mathcal{H}_{\mathsf{aux}}(i) = \frac{1}{w}\sum_{j}\mathcal{H}_{\mathsf{aux}}(i,j)$$

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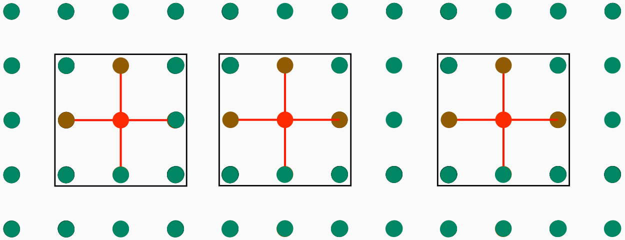
$$\mathcal{H}_{\text{aux}}(i) = \frac{1}{w}\sum_{j}\mathcal{H}_{\text{aux}}(i,j)$$

- Translate over all lattice sites i

$$\mathcal{H}_{\text{full}} = \sum_{i}\mathcal{H}_{\text{aux}}(i)$$



Result of tiling

We end up with a **Hubbard-Heisenberg** model.

$$\mathcal{H}_{H-H} = -\sum_{i} U_H \left(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}\right)^2 - t_H \sum_{<i,j>,\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + \text{h.c.}\right) + J_H \sum_{<i,j>} \vec{S}_i \cdot \vec{S}_j$$

The mapping between the parameters is

$$t_{H-H} = \left(2t(N-2) - \frac{2V}{N}\right), \quad U_{H-H} = \left(\frac{U}{2} + U_b\right), \quad J_{H-H} = \frac{2J}{w}$$

Greens functions, spectral functions and self-energy

Strategy

- Replace the Hamiltonian for inverse Greens operators
- Use equation to relate bulk and impurity inverse Greens operators
- Use spectral representation to invert them and obtain Greens functions
- Use Greens functions to compute the rest

Inverse Greens operator

Define inverse Greens operators:

$$\mathcal{G}_{\mathrm{aux}}(i) = \frac{1}{\omega - (H_{\mathrm{aux}}(i) - E_{\mathrm{gs}})}$$

$$\mathcal{G}_{H-H} = \frac{1}{N\omega - (H_{H-H} - NE_{\mathrm{gs}})}$$

Replace in tiling expression:

$$\mathcal{G}^{-1}_{H-H} = \sum_i \mathcal{G}^{-1}_{\mathrm{aux}}(i) = \frac{1}{w} \sum_{i,j \in \text{NN of i}} \mathcal{G}^{-1}_{\mathrm{aux}}(i,j)$$

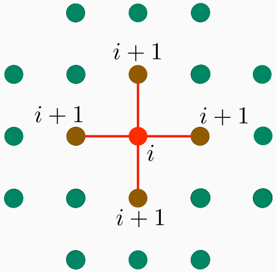
Matrix elements of $\mathcal{G}^{-1}_{\textbf{H-H}}$

Particle excitation on ground state of auxiliary model:

$$|i\rangle \equiv c^\dagger_{i\sigma}|\Phi_0\rangle$$

Local matrix elements $\left(\mathcal{G}^{-1}_{H-H}\right)^p_{ii}$ depend on the auxiliary model at i:

$$\left(\mathcal{G}^{-1}_{H-H}\right)^p_{ii} = \underbrace{w \times \frac{1}{w}\langle\Phi_0|c_{i\sigma}\mathcal{G}^{-1}_{\text{aux}}(i)c^\dagger_{i\sigma}|\Phi_0\rangle}_{w \text{ nearest neighbour pairs}} = \langle\Phi_0|c_{d\sigma}\mathcal{G}^{-1}_{\text{aux}}(d)c^\dagger_{d\sigma}|\Phi_0\rangle$$



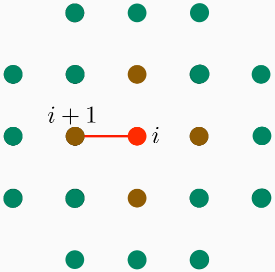
Matrix elements of $\mathcal{G}^{-1}_{\text{H-H}}$

Particle excitation on ground state of auxiliary model:

$$|i\rangle \equiv c^\dagger_{i\sigma} |\Phi_0\rangle$$

N-neighbour elements $\left(\mathcal{G}^{-1}_{H-H}\right)^p_{i,i+1}$ depend on the aux. model at i with 0^{th} site at $i+1$:

$$\left(\mathcal{G}^{-1}_{H-H}\right)^p_{i,i+1} = \underbrace{\frac{1}{w} \langle\Phi_0| c_{d\sigma} \mathcal{G}^{-1}_{\text{aux}}(d) c^\dagger_{z,\sigma} |\Phi_0\rangle}_{\text{one nearest-neighbour pair}}$$



Spectral representation of $\mathcal{G}^{-1}_{\textbf{H-H}}$ in eigenstates of $\mathcal{H}_{\textbf{aux}}$

Eigenstates of $\mathcal{H}_{\text{aux}}$: $|\Phi_n\rangle$

Insert $1 = \sum_m |m\rangle \langle m|$:

$$\left(\mathcal{G}^{-1}_{H-H}(\omega)\right)^p_{ii} = \sum_m |d^p_m|^2 \left(\mathcal{G}^{-1}_{\text{aux}}(d,\omega)\right)_{mm}$$

where d^p_m is the spectral weight factor:

$$d^p_m = \langle \Phi_m | \, c^\dagger_{d\sigma} \, | \Phi_0 \rangle$$

Spectral representation of $\mathcal{G}^{-1}_{\mathbf{H\text{-}H}}$ in eigenstates of $\mathcal{H}_{\mathbf{aux}}$

Eigenstates of $\mathcal{H}_{\text{aux}}$: $|\Phi_n\rangle$

Similarly, the off-diagonal matrix element also has a spectral representation:

$$\left(\mathcal{G}^{-1}_{H-H}\left(\omega\right)\right)^{p}_{i,i+1} = \frac{1}{w}\sum_{n}\left(d^{p}_{m}\right)^{*} z^{p}_{m}\left(\mathcal{G}^{-1}_{\text{aux}}(d,\omega)\right)_{mm}$$

where

$$z^{p}_{m} = \langle\Phi_m|c^{\dagger}_{z\sigma}|\Phi_0\rangle$$

Hole counterparts

- Hole excitations can be similarly obtained by considering states $|\tilde{i}\rangle = c_{i\sigma} |\Phi_0\rangle$
- Identical process but replace spectral weight factors with hole counterparts:

$$d_m^p = \langle \Phi_m | \, c_{d\sigma}^\dagger \, |\Phi_0\rangle \to d_m^h = \langle \Phi_m | \, c_{d\sigma} \, |\Phi_0\rangle$$

The corresponding relations are

$$\left(\mathcal{G}_{H-H}^{-1}(-\omega)\right)_{ii}^h = \sum_n |d_n^h|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d,-\omega)\right)_{nn}$$

$$\left(\mathcal{G}_{H-H}^{-1}\left(-\omega\right)\right)_{i,i+1}^h = \frac{1}{w} \sum_n \left(d_n^h\right)^* z_n^h \left(\mathcal{G}_{\text{aux}}^{-1}(d,-\omega)\right)_{nn}$$

Summary

- We have expressed matrix elements of the bulk in terms of those of the auxiliary model
- The spectral representation allows the right-hand side to have only diagonal matrix elements
- This makes it easier to invert them

Inversion and single-particle Greens functions

Since $\mathcal{G}_{\text{aux}}^{-1}(d, -\omega)$ is diagonal in the basis of $|\Phi_n\rangle$, we can simply write

$$\left(\mathcal{G}_{H-H}^{-1}(\omega)\right)_{ii}^{p} = \sum_m |d_m^p|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d, \omega)\right)_{mm} \implies \left(\mathcal{G}_{H-H}(\omega)\right)_{ii}^{p} = \sum_n |d_n^p|^2 \left(\mathcal{G}_{\text{aux}}(d, \omega)\right)_{nn}$$

The Greens function can be related to the Greens operator:

$$G(i, j, \omega) = \langle i| \mathcal{G}(\omega, H) |j\rangle - \langle \tilde{j}| \mathcal{G}(-\omega, H) |\tilde{i}\rangle$$

Using this, we can finally write down the Greens functions:

$$\left(G_{H-H}(\omega)\right)_{\text{loc}} = \sum_n \left[|d_n^p|^2 \left(\mathcal{G}_{\text{aux}}(d, \omega)\right)_{nn} - |d_n^h|^2 \left(\mathcal{G}_{\text{aux}}(d, -\omega)\right)_{nn}\right]$$

$$\left(G_{H-H}(\omega)\right)_{\text{n-n}} = \frac{1}{w} \sum_n \left[(d_n^p)^* z_n^p \left(\mathcal{G}_{\text{aux}}(d, \omega)\right)_{nn} - \left(z_n^h\right)^* d_n^h \left(\mathcal{G}_{\text{aux}}(d, -\omega)\right)_{nn}\right]$$

$k-$space Greens function, spectral function and self-energy

The $k-$space Greens function will be approximated by the local and nearest-neighbour Greens functions:

$$G_{H-H}(\vec{k},\omega) \simeq G_{H-H}(\omega)_{\text{loc}} + G_{H-H}(\omega)_{\text{n-n}} \sum_{i=1}^{w} e^{i\vec{k}\cdot\vec{a}_i} = G_{\text{aux}}(dd,\omega) + \frac{\xi_{\vec{k}}}{w} G_{\text{aux}}(d0,\omega)$$

Taking the imaginary part gives the **spectral function**:

$$A_{H-H}(\vec{k},\omega) = A_{\text{aux}}(dd,\omega) + \frac{\xi_{\vec{k}}}{w} A_{\text{aux}}(d0,\omega), \quad \xi_{\vec{k}} = \sum_{i=1}^{w} e^{i\vec{k}\cdot\vec{a}_i}$$

From Dyson's equation, we get **self-energy**:

$$\Sigma(\vec{k},\omega) = G_0(\vec{k},\omega)^{-1} - G(\vec{k},\omega)^{-1} = \omega + t^{H-H}\xi_{\vec{k}} - \left[G_{\text{aux}}(dd,\omega) + \frac{\xi_{\vec{k}}}{w} G_{\text{aux}}(d0,\omega) \right]^{-1}$$

Evidence for the Mott MIT

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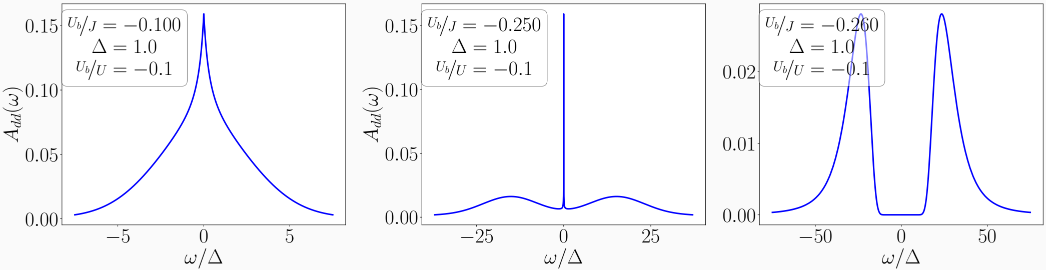
- **one-to-one mapping** between Greens functions of the bulk and the auxiliary models



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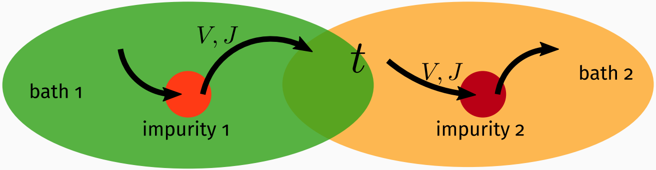

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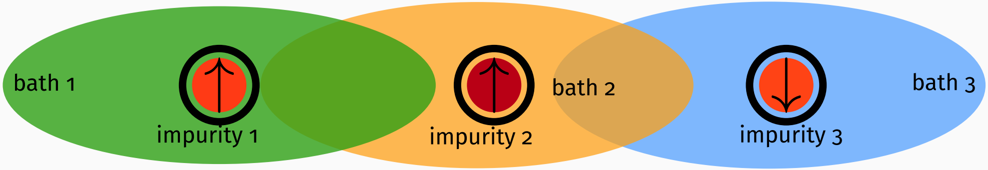

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- low energy resonance in the impurity excitations implies **propagation** of e^-s across lattice
- gap in the impurity excitations implies e^-s are "stuck" and **spectral flow is not possible**
- Constraining U_b to, say, $-U/10$, we get a critical ratio:

$$\frac{U^*_{\text{H-H}}}{J^*_{\text{H-H}}} = \frac{w}{4}\left(\frac{U^*}{J^*} - \frac{1}{2}\right) = 2$$

where we used $w = 4$ for a 2D square lattice.

Final Remarks

Conclusions

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- **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.

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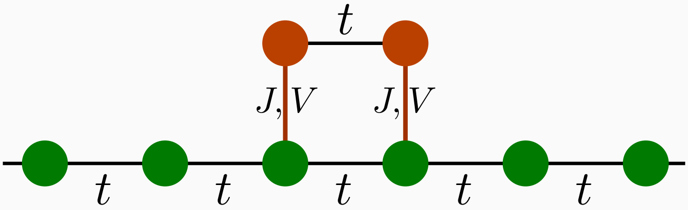
- Breaking particle-hole symmetry on the impurity will allow us to study bulk models **away from half-filling**.
- For more accurate results, one can consider **multiple impurities** in the cluster.



Thank you.