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

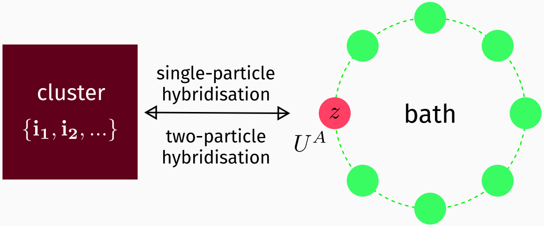
The Model

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

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

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

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

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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

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

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

Select a UV-IR Scheme

UV shell

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

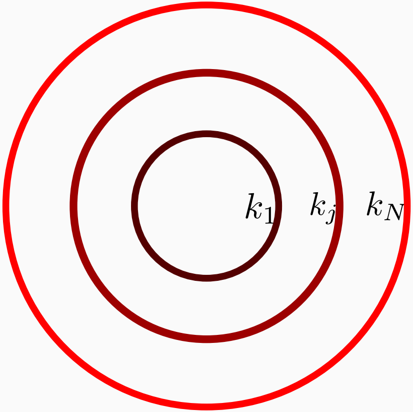
$\vdots$

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

$\vdots$

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

IR shell



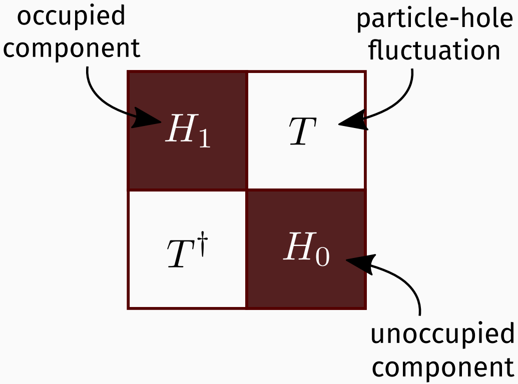
Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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

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

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

(j) : j^{th} RG step



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

Rotate Hamiltonian and kill off-diagonal blocks

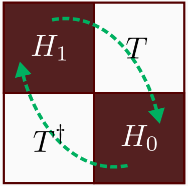
$$H_{(j-1)} = U_{(j)} H_{(j)} U^{\dagger}_{(j)}$$

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

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

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

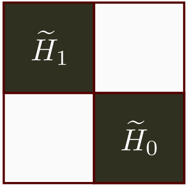
(**quantum fluctuation operator**)



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

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

n_j becomes an
integral of motion
(IOM)

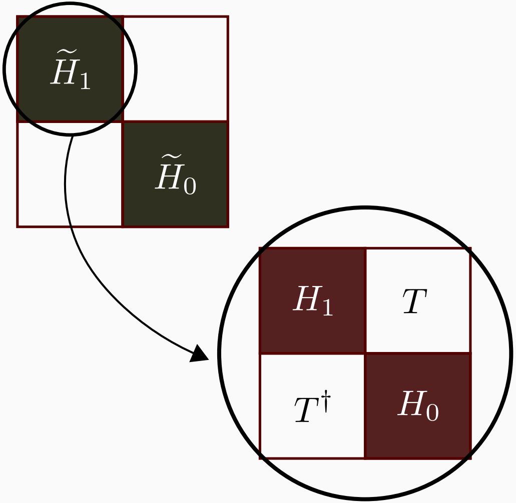


Mukherjee and Lal 2020a; Mukherjee and Lal 2020b.

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.

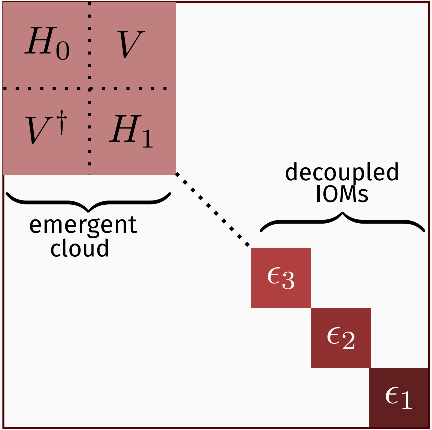
RG Equations and Denominator Fixed Point

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

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

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

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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- **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

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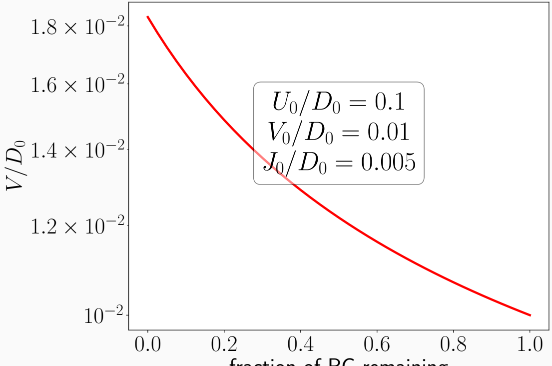
URG Analysis: $U_b = 0$

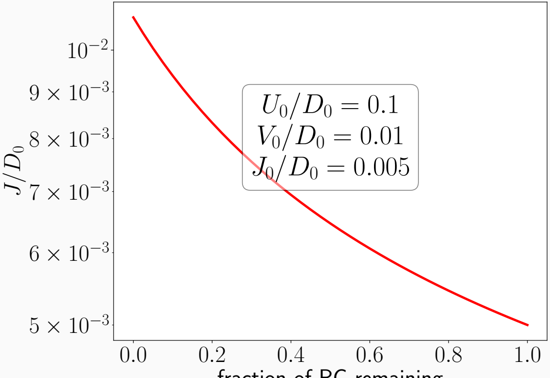
$U_b = 0$: Flow towards strong-coupling

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

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

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



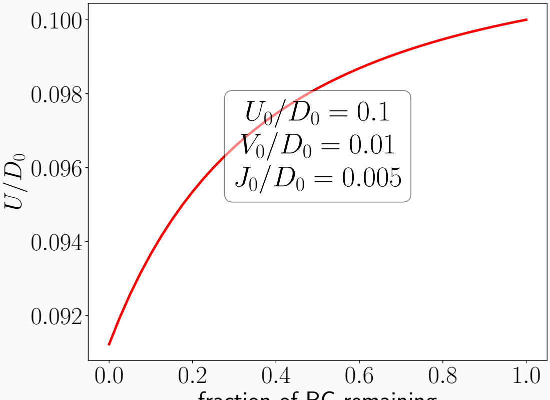


$U_b = 0$: Flow towards strong-coupling

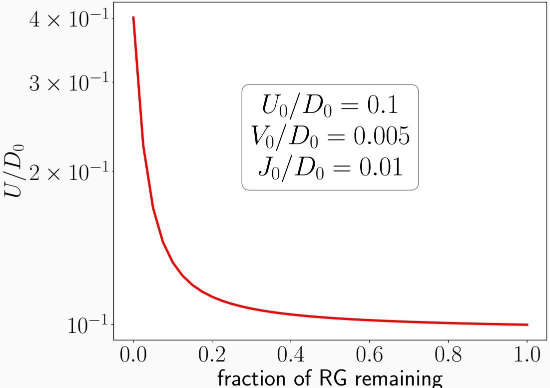
$\mathbf{U > 0, J > 0}$

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

$V > J$



$V < J$

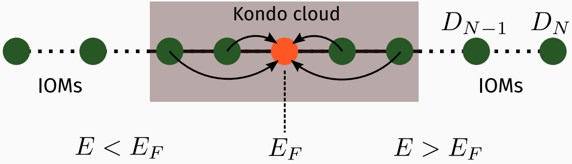


$U > 0$ Fixed point Hamiltonian

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

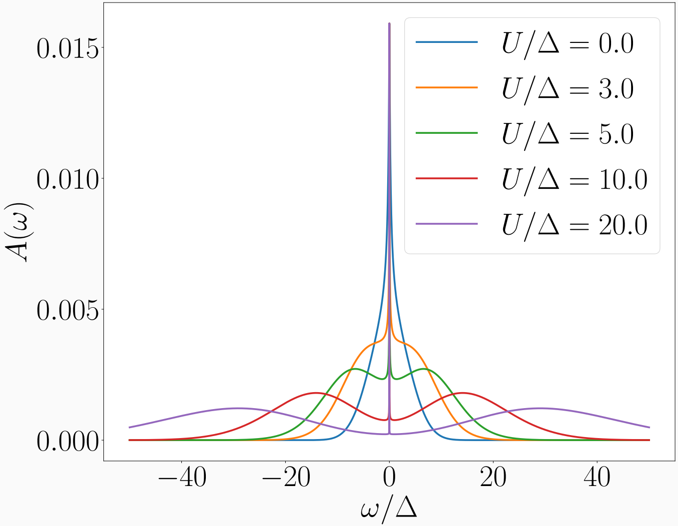
$$+ V^* \sum_{k<k^*,\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.}\right)$$

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



Impurity Spectral Function

no gap at arbitrarily large U



URG Analysis: $U_b \neq 0$

$U > 0$ RG Equations

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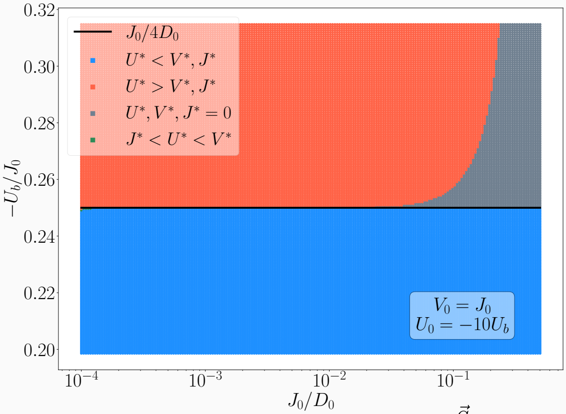
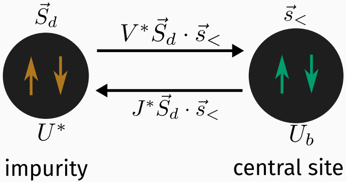
- ***U can be relevant if J decays slower than V***; needs to be checked numerically

$U > 0$ Phase Diagram



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



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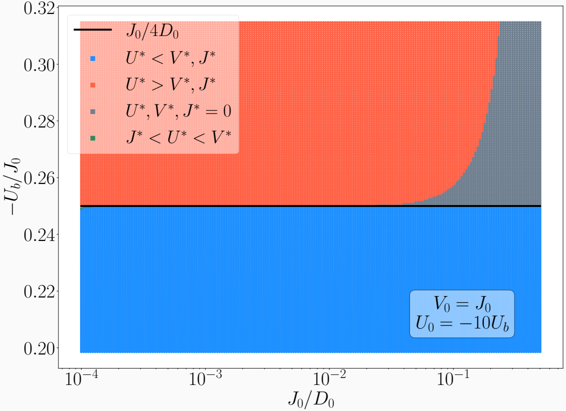

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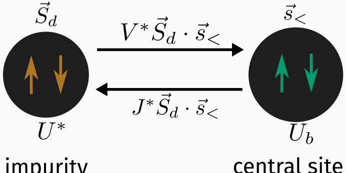
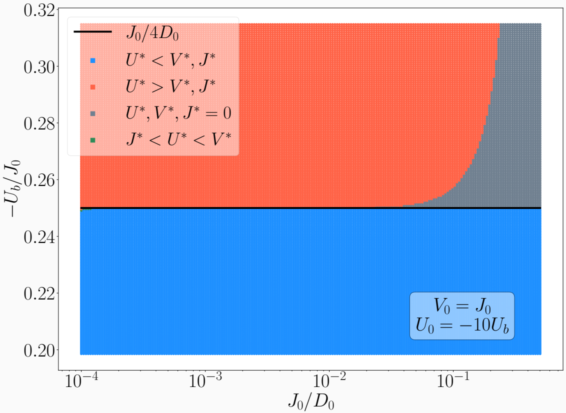
- blue: **screened** impurity (strong-coup.)



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

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

$U > 0$ Phase Diagram



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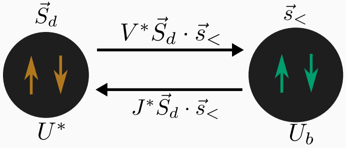


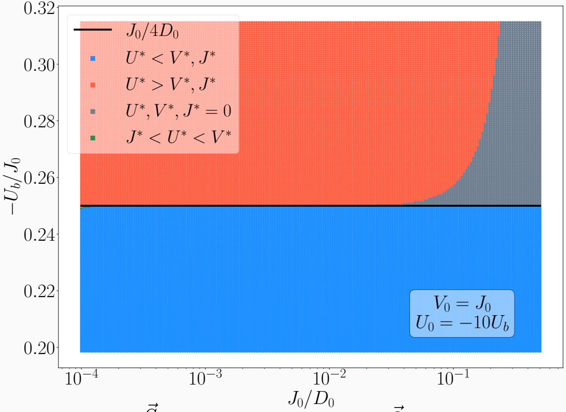
impurity

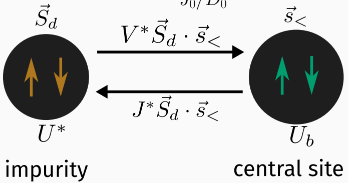
central site

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

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

$U > 0$ Phase Diagram





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- gray: imp. level absent $(U = J = V = 0)$

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

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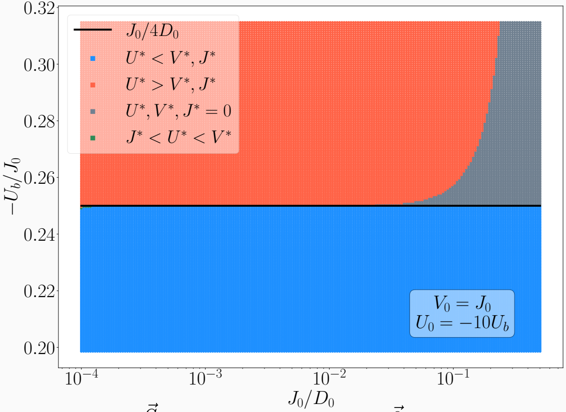

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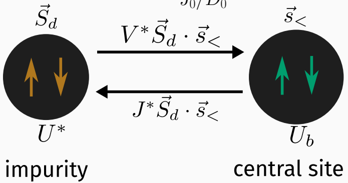
- green: J vanishes ($J < U$)



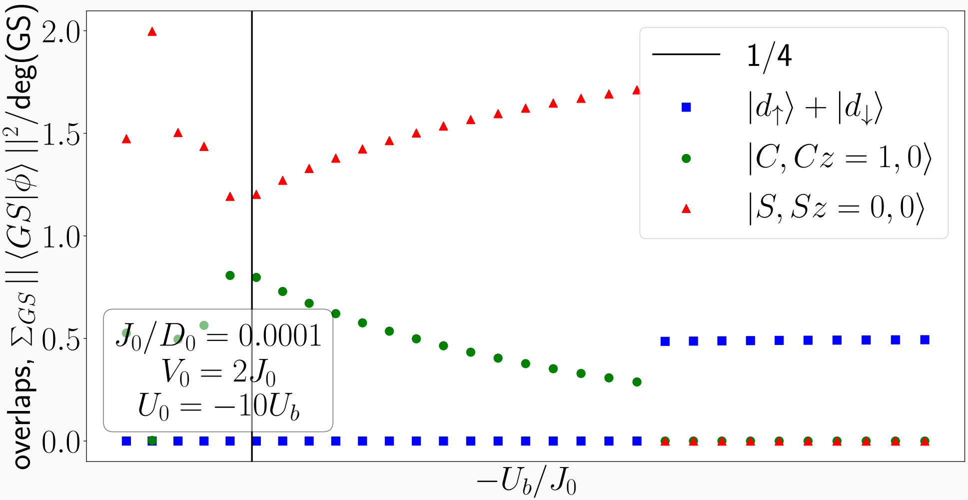
$$J^* < U^* < V^*$$

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

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

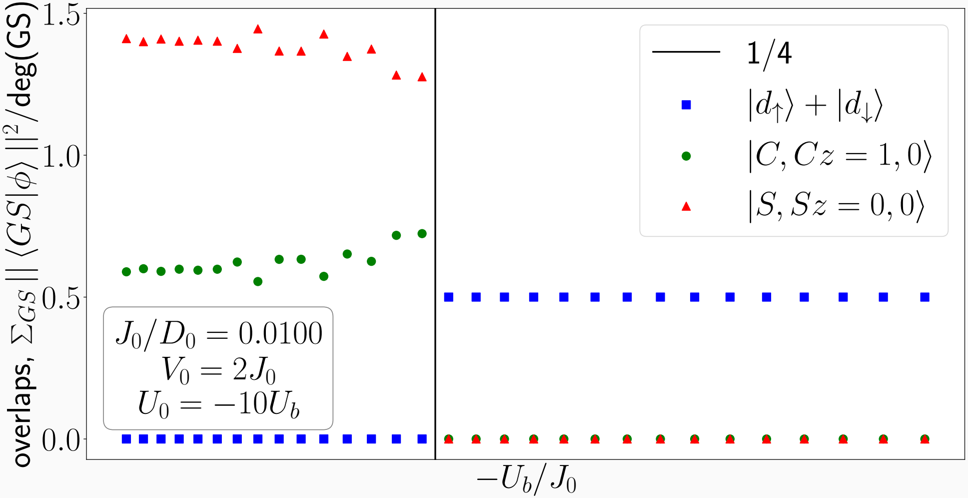
Overlap of ground state against spin singlet and charge triplet zero states

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



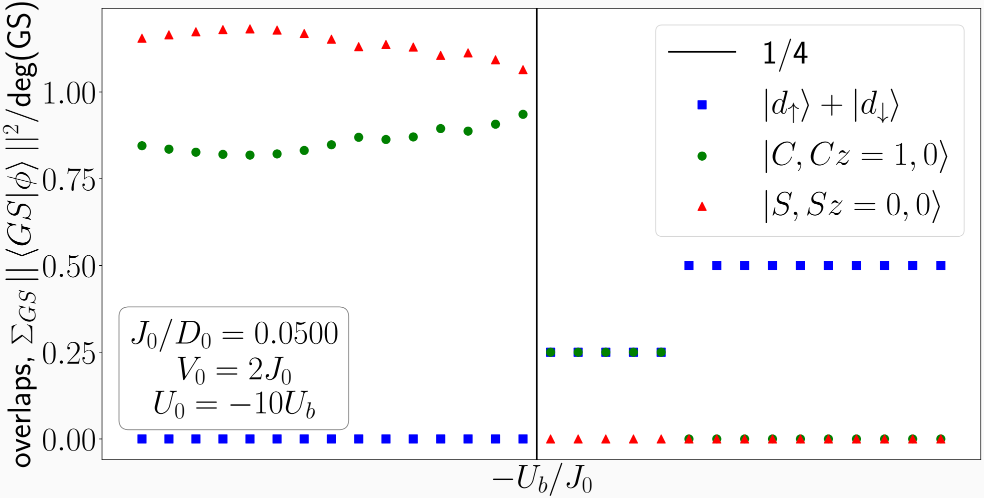
Overlap of ground state against spin singlet and charge triplet zero states

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



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

$J_0/D_0 = 10^{-1}$



Spin and charge correlations in ground state

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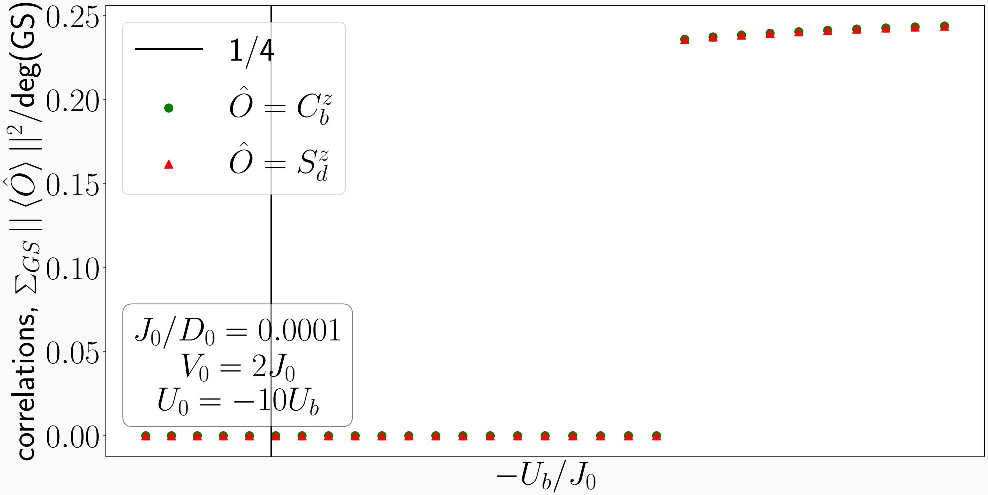

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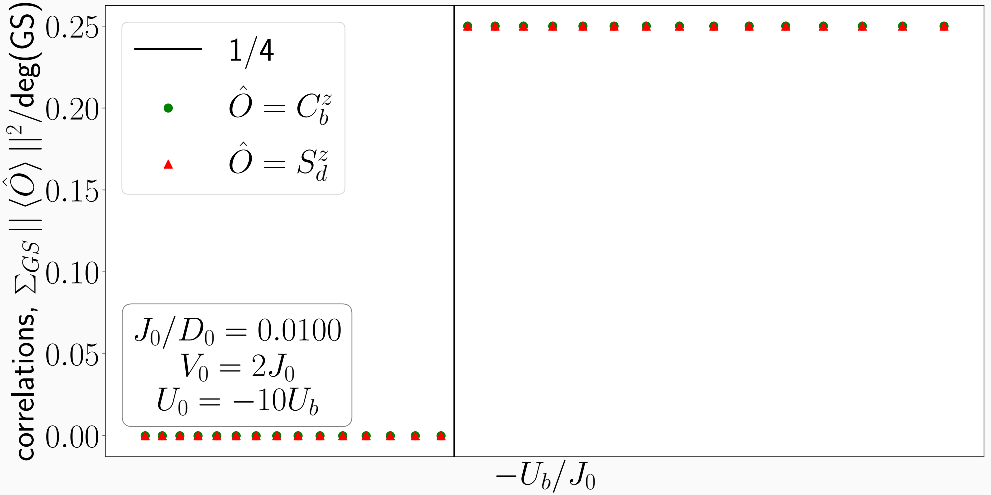

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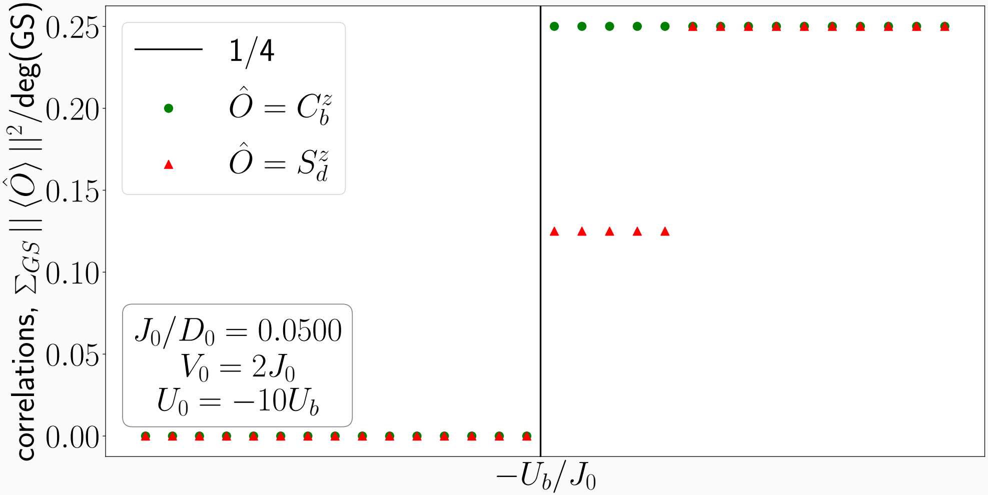
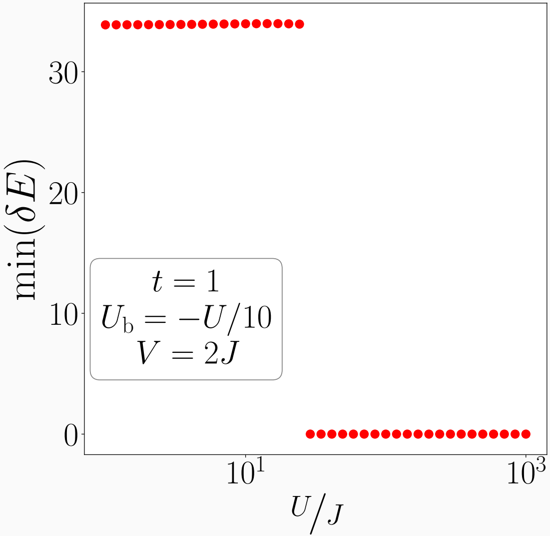
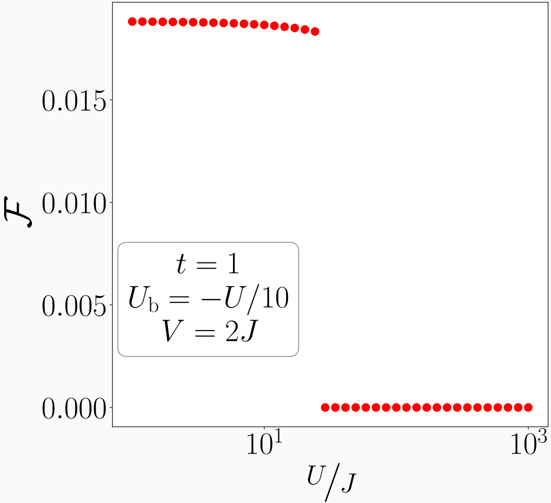
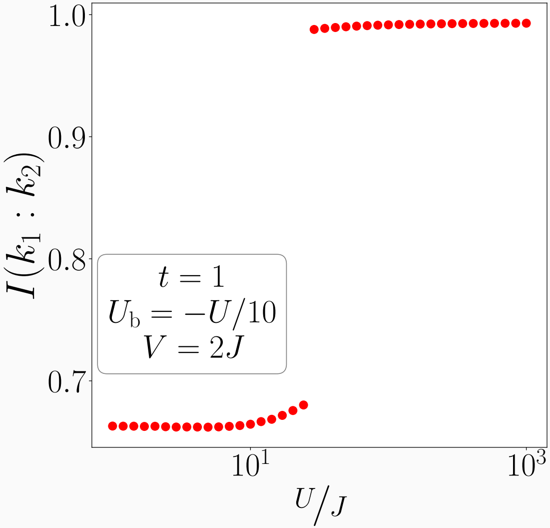


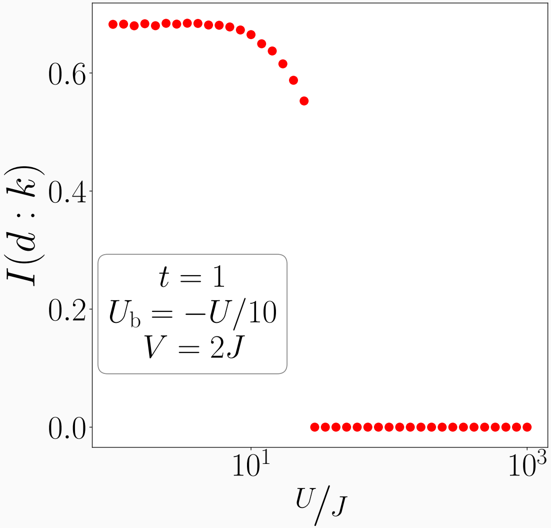
Correlation measures: Local Fermi liquid



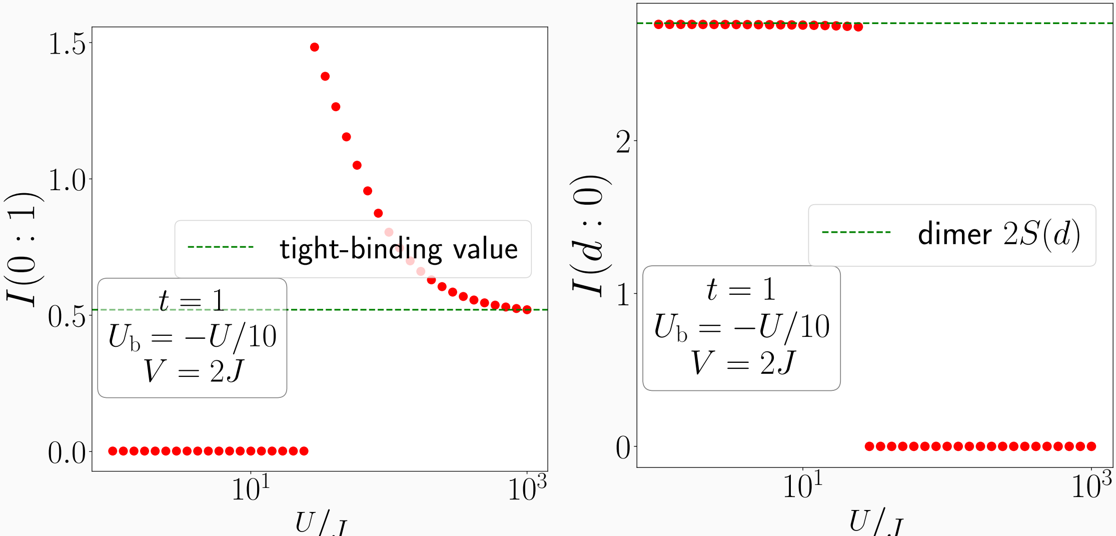


Correlation measures: Kondo cloud

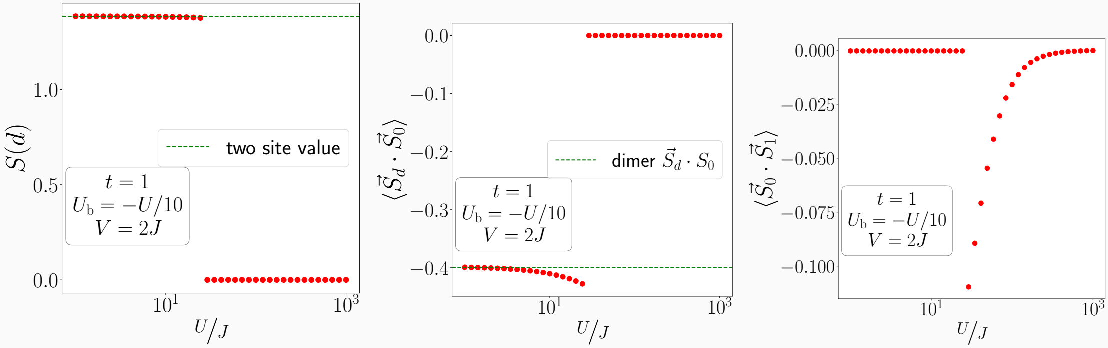




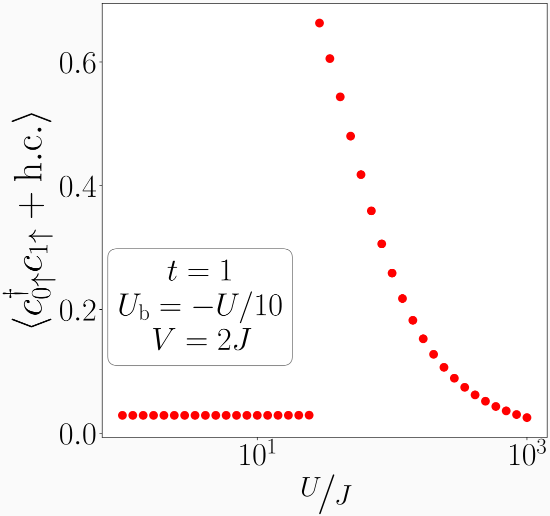
Correlation measures: Real space mutual information

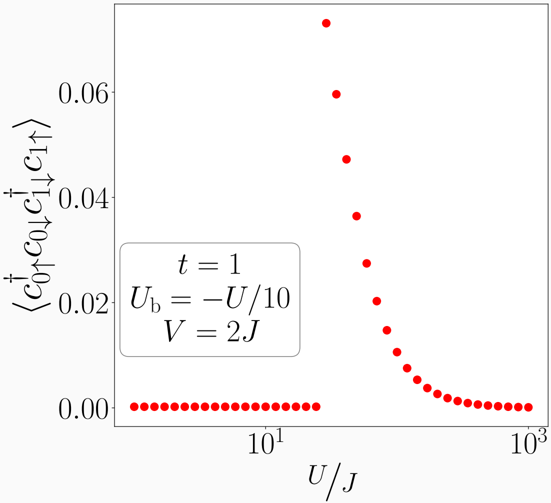


Correlation measures: Impurity entanglement entropy and spin-spin correlations

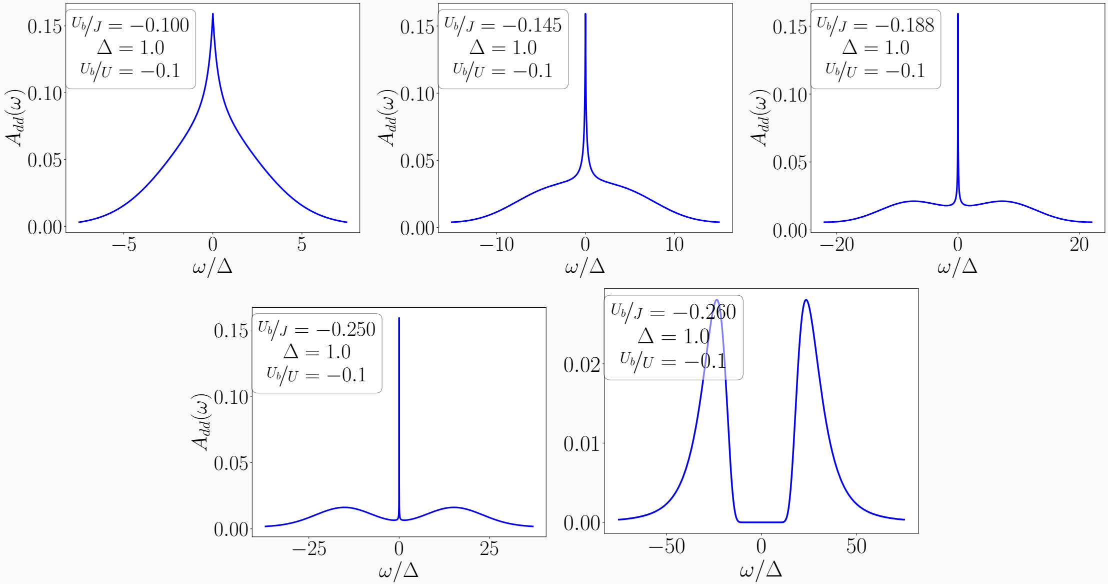


Correlation measures: Real-space correlations

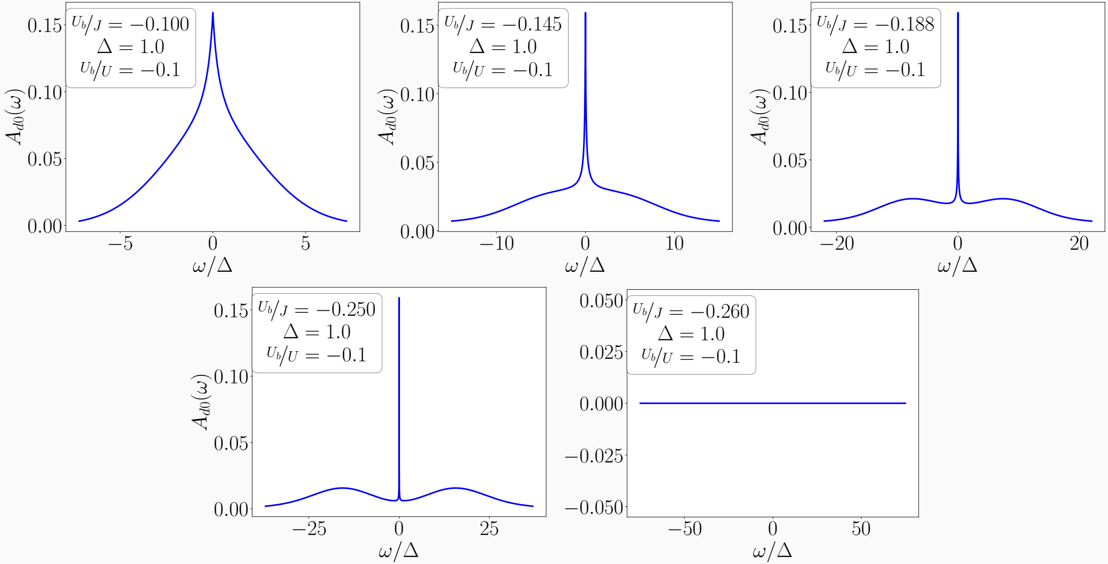




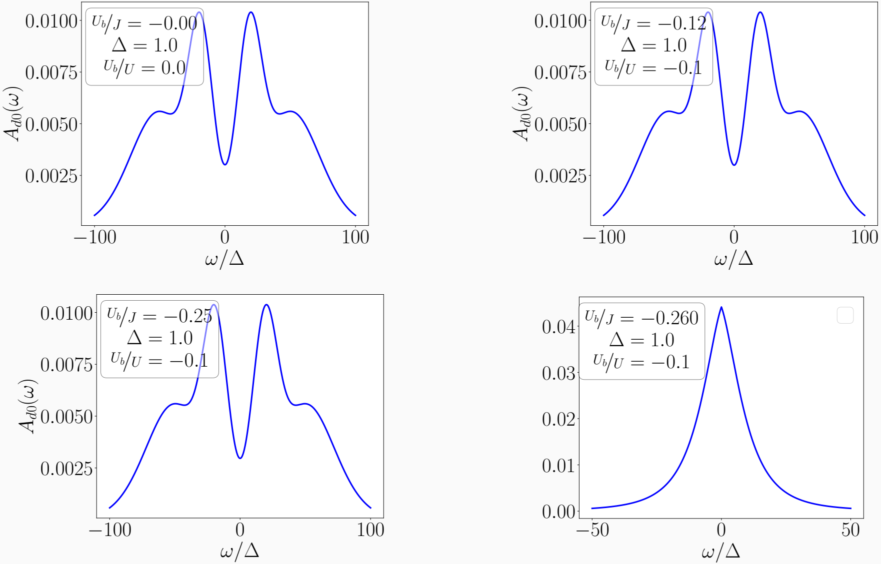
Correlation measures: Impurity spectral function



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



Correlation measures: Bath spectral function A_{00}



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.

Moving forward

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

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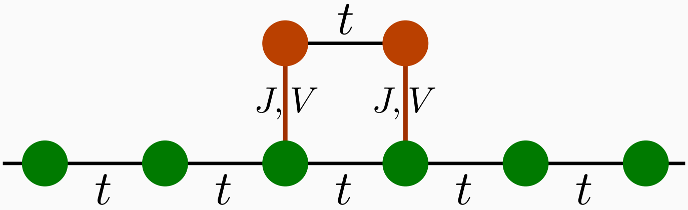
- Breaking particle-hole symmetry on the impurity will allow us to study bulk models **away from half-filling**.
- For more accurate results, one can consider **multiple impurities** in the cluster.



Thank you.