

A New Unitary RG-Based Auxiliary Model Approach: a Look into the Mott Metal-Insulator Transition

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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

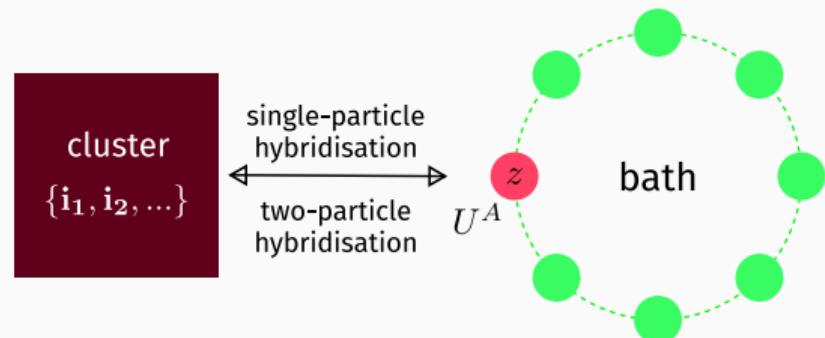
The Model

standard p-h symmetric Anderson impurity model

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

supplement 1-particle hybridisation with

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



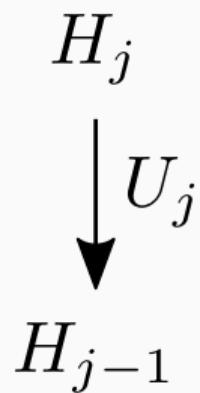
Schrieffer and Wolff 1966; Anderson 1961.

The Unitary Renormalization Group Method

The Unitary Renormalization Group Method

The General Idea

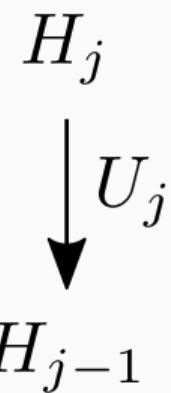
- Apply unitary many-body transformations to the Hamiltonian



The Unitary Renormalization Group Method

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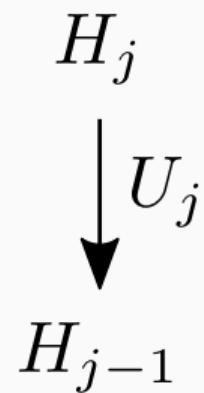
- Apply unitary many-body transformations to the Hamiltonian
- Successively decouple high energy states



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



The Unitary Renormalization Group Method

Select a UV-IR Scheme

UV shell

\vec{k}_N (zeroth RG step)

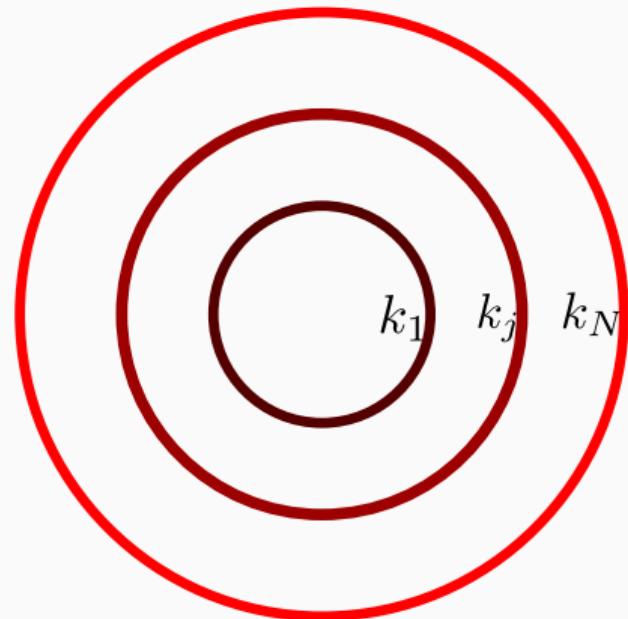
\vdots

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

\vdots

\vec{k}_1 (Fermi surface)

IR shell



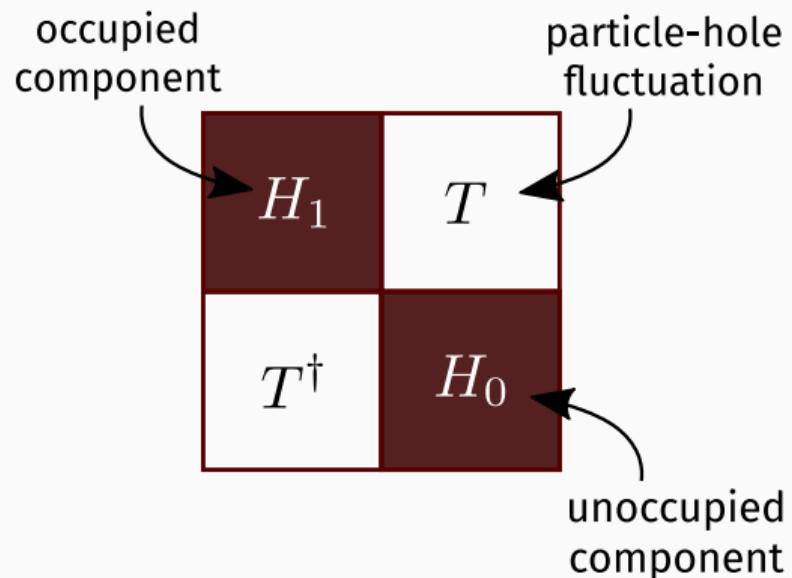
The Unitary Renormalization Group Method

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

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

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

(j) : j^{th} RG step



The Unitary Renormalization Group Method

Rotate Hamiltonian and kill off-diagonal blocks

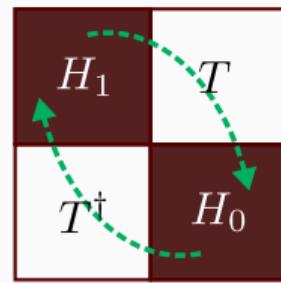
$$H_{(j-1)} = U_{(j)} H_{(j)} U_{(j)}^\dagger$$

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

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

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

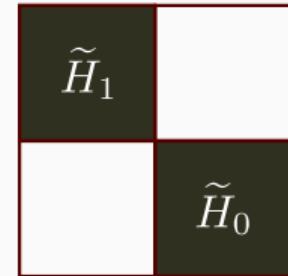
(quantum fluctuation operator)



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

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

n_j becomes an
integral of motion
(IOM)

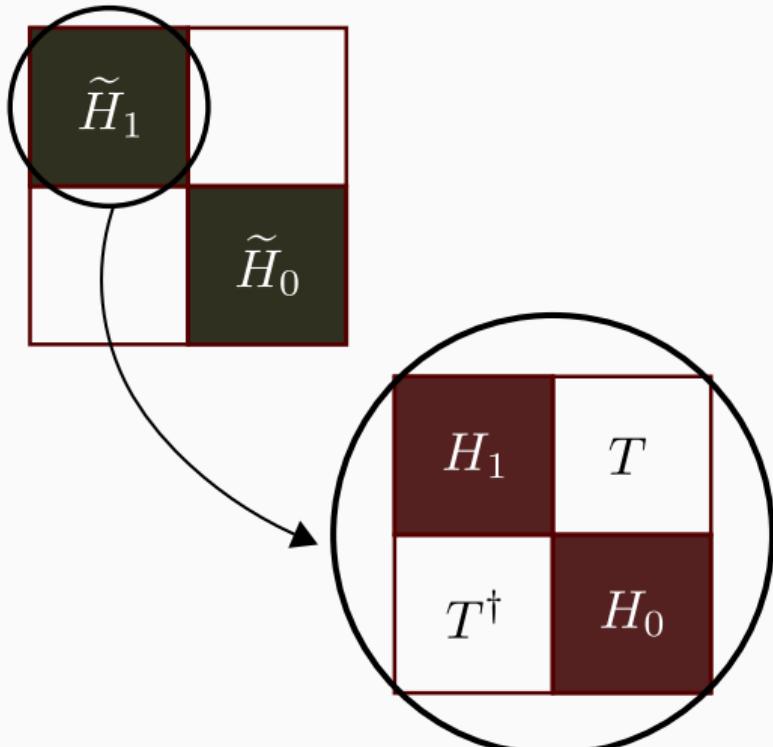


The Unitary Renormalization Group Method

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

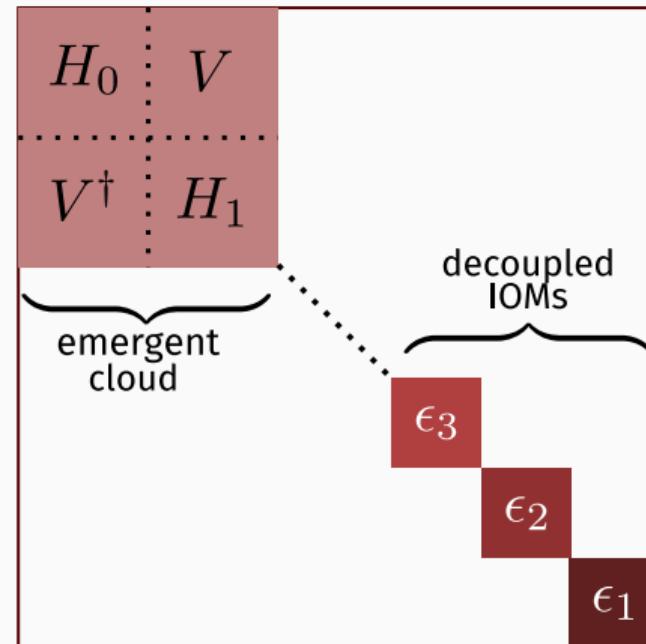
RG Equations and Denominator Fixed Point

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

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

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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- 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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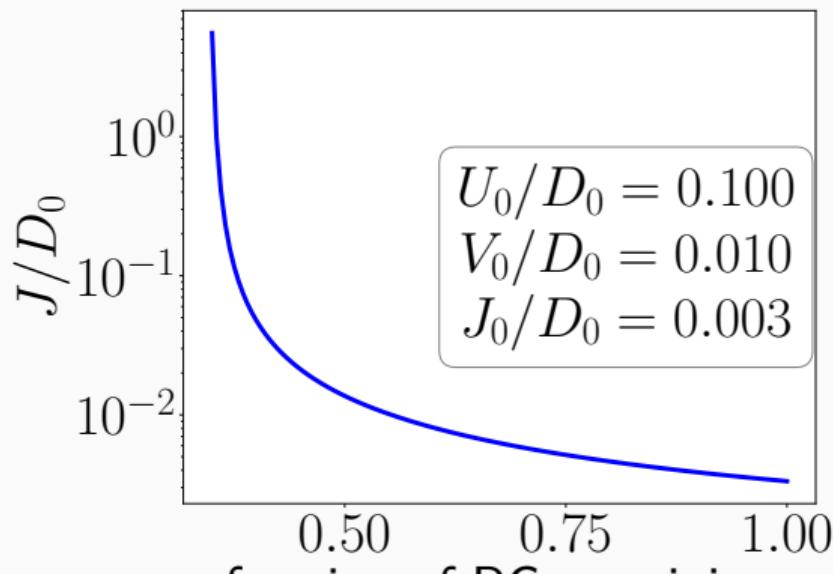
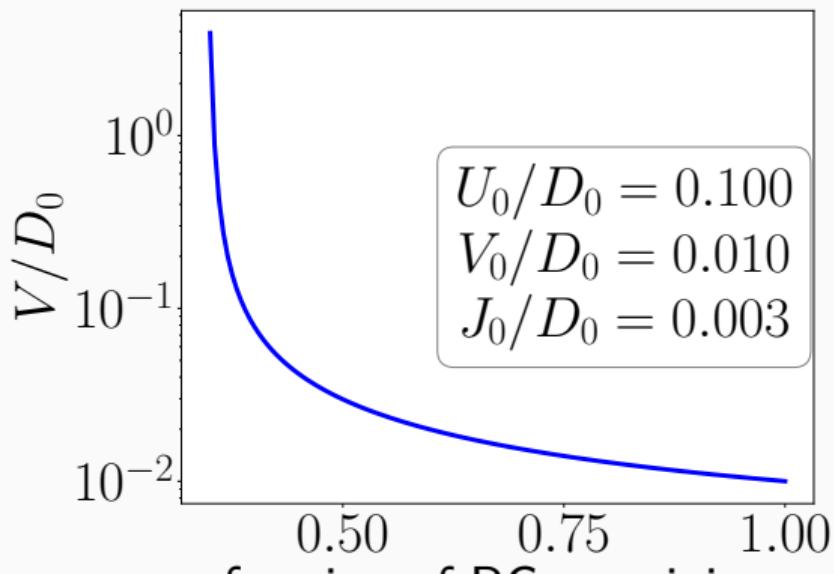
URG Analysis: $U_b = 0$

$U_b = 0$: Flow towards strong-coupling

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

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

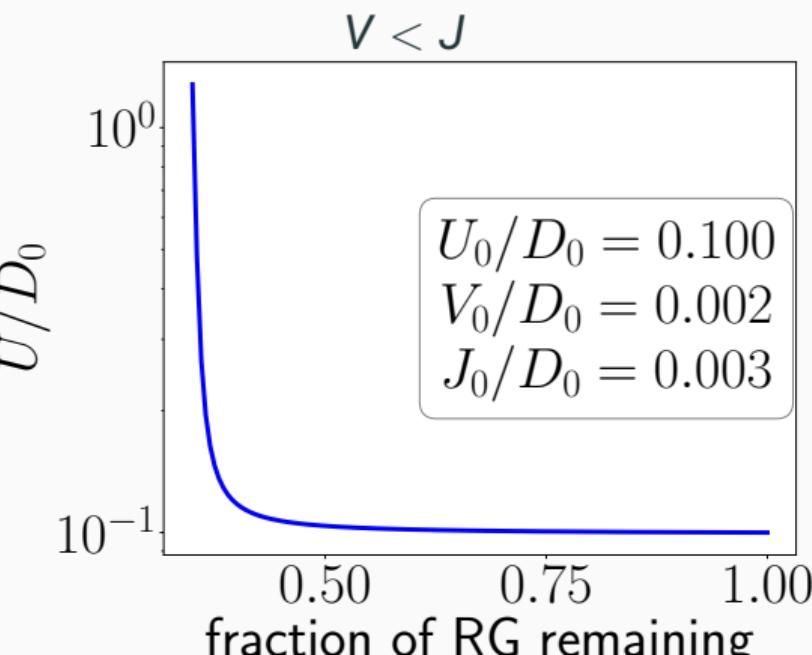
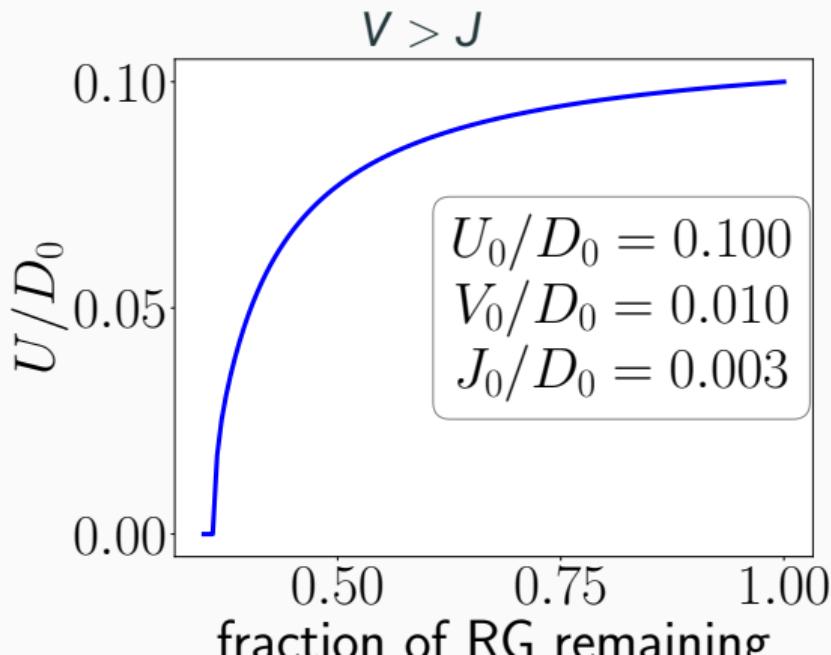
$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}$$



$U_b = 0$: Flow towards strong-coupling

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

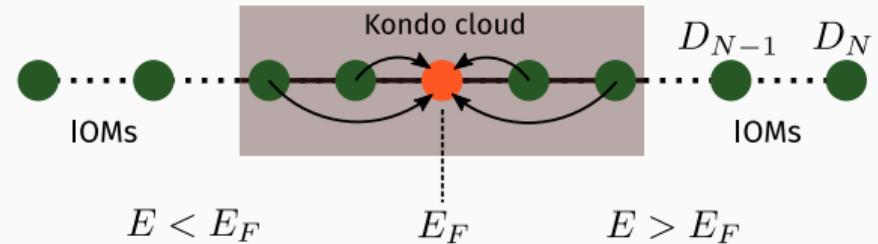


$U > 0$ Fixed point Hamiltonian

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

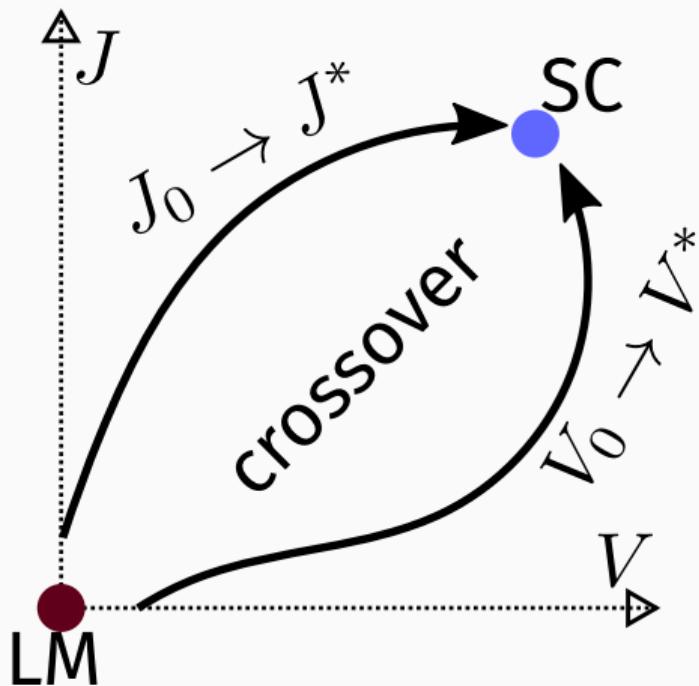
$$+ V^* \sum_{k < k^*, \sigma} (c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.})$$

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



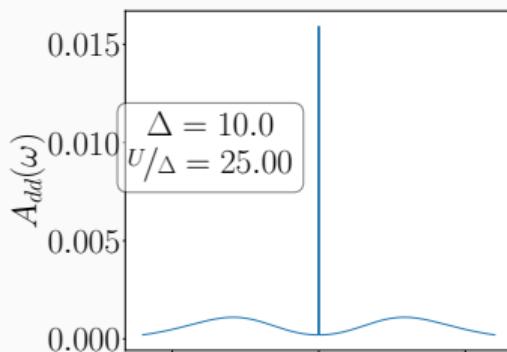
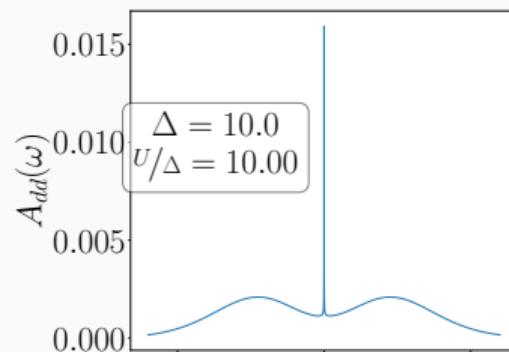
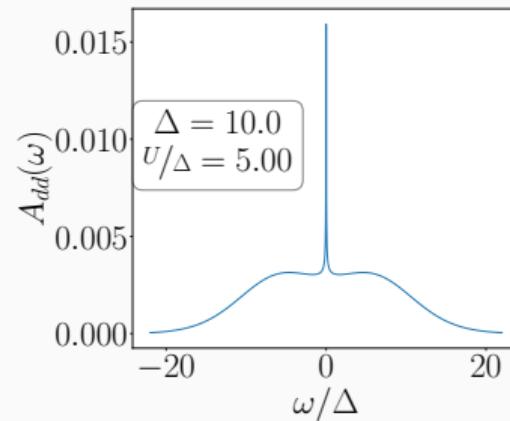
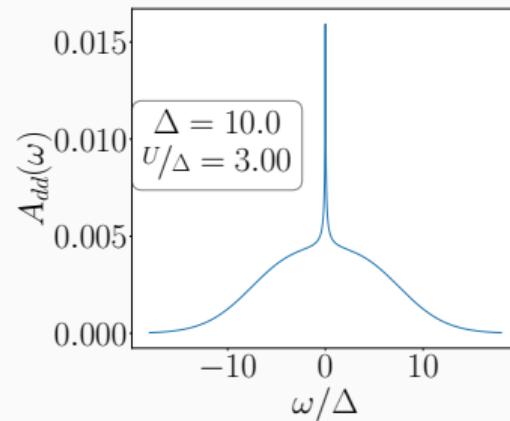
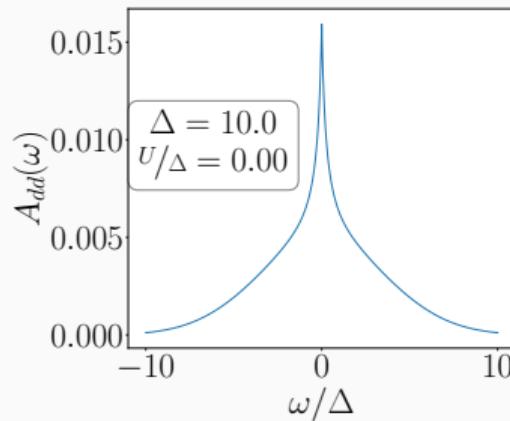
Phase Diagram

- only strong-coupling phase is stable
- impurity always screened
- no phase transition



Impurity Spectral Function

no gap at arbitrarily large U



URG Analysis: $U_b \neq 0$

$U > 0$ RG Equations

- U_b is **marginal**: $\Delta U_b = 0$

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- Same can be said for the hybridisation V :

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

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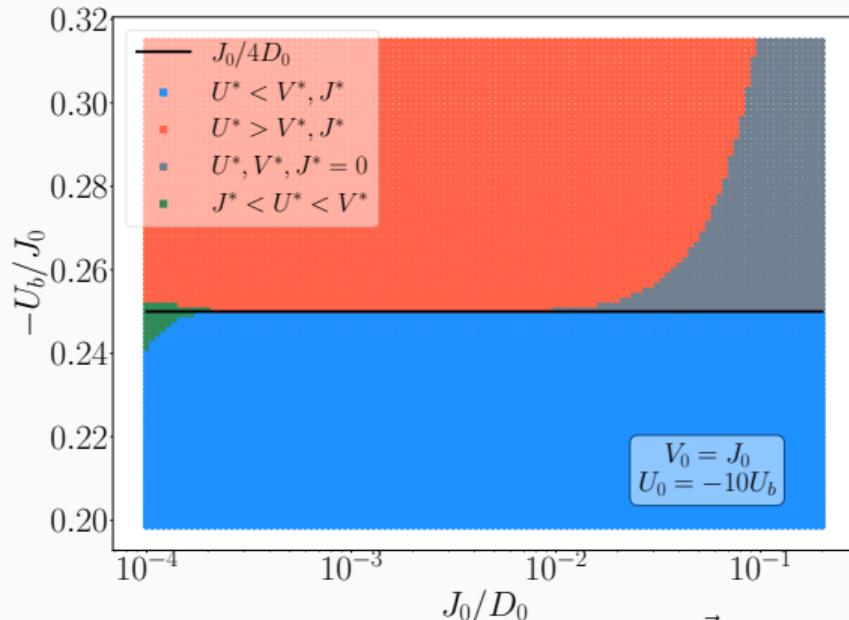
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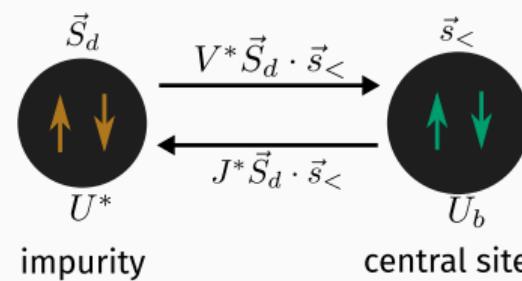
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- **U can be relevant if J decays slower than V** ; needs to be checked numerically

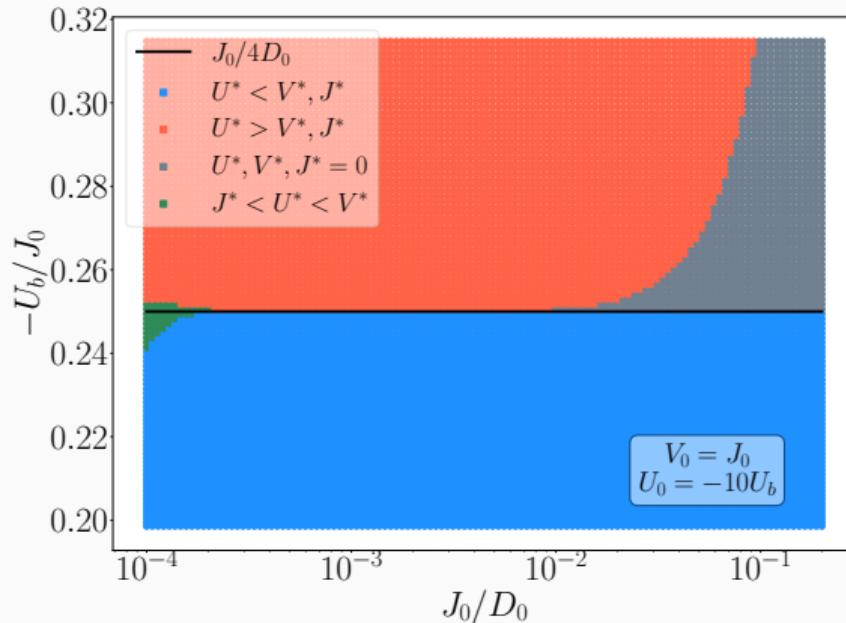
$U > 0$ Phase Diagram



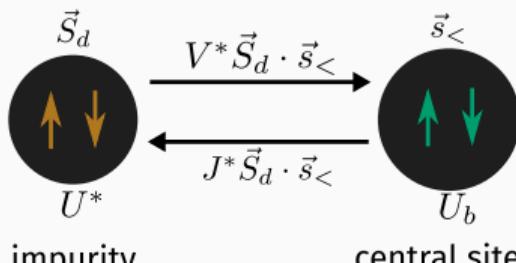
- black line: **critical points** at $U_b^* = -J^*/4$



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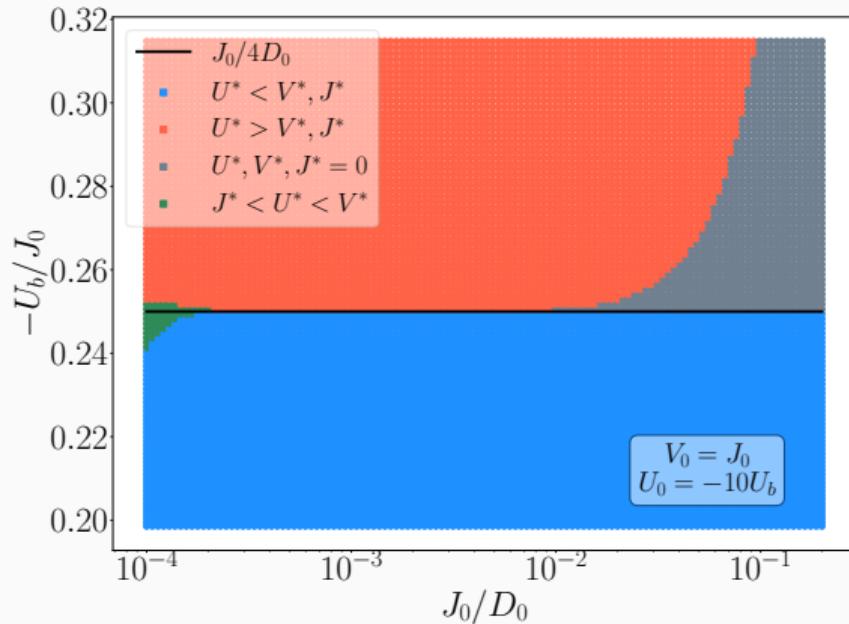
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- blue: **screened** impurity (strong-coup.)



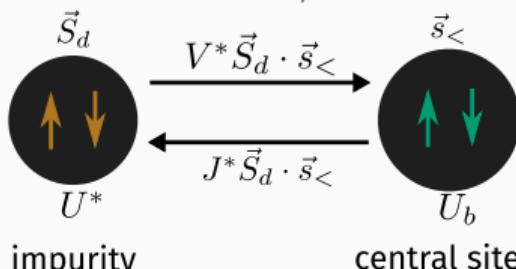
$$\Delta J > 0, \Delta V > 0, \Delta U < 0, \quad J^* \gg V^* \gg U^*$$

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

$U > 0$ Phase Diagram



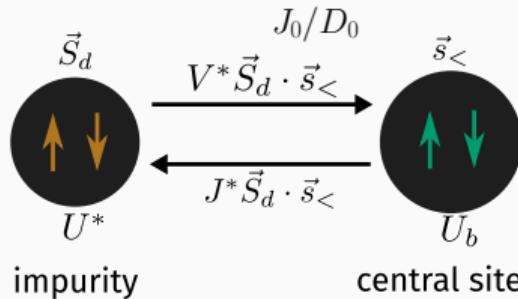
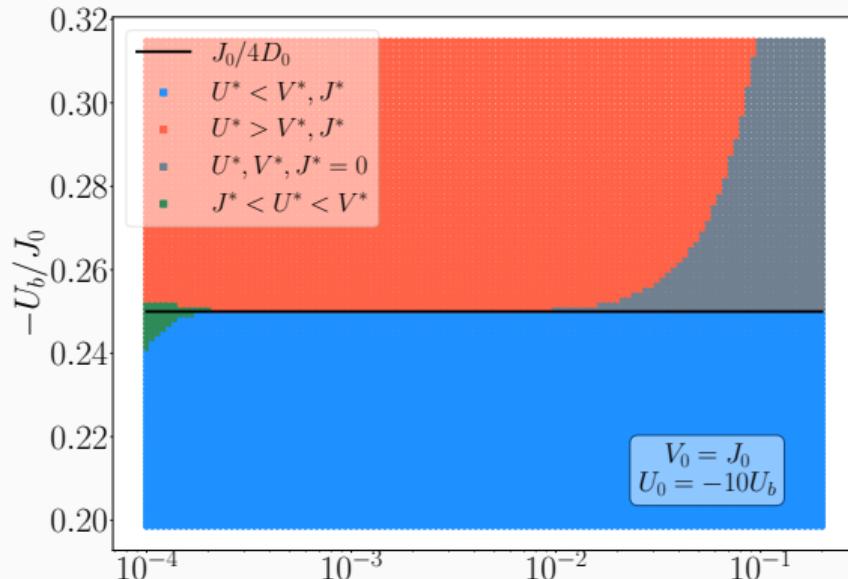
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- red: **unscreened** local mom. ($J = V = 0$)



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

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

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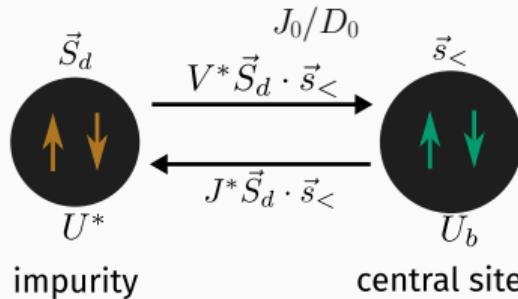
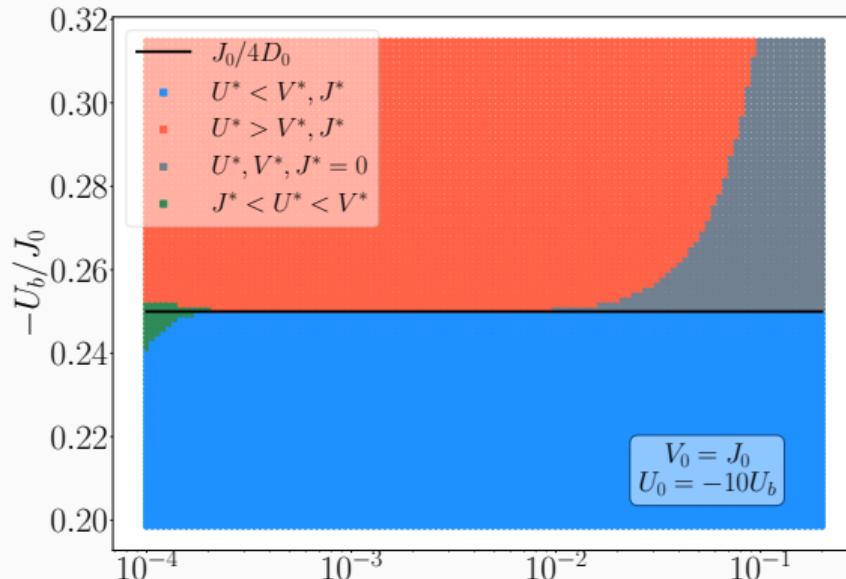


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- gray: imp. level absent ($U = J = V = 0$)

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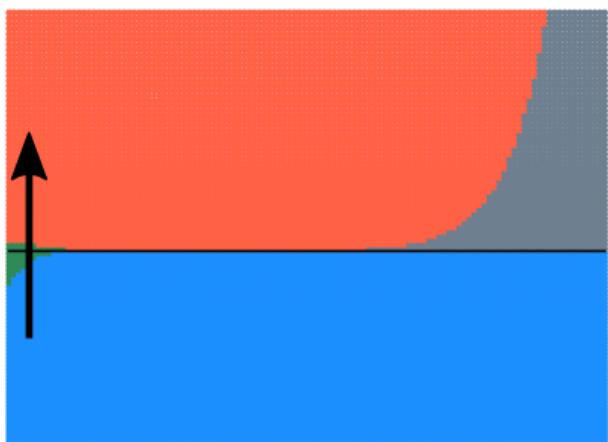
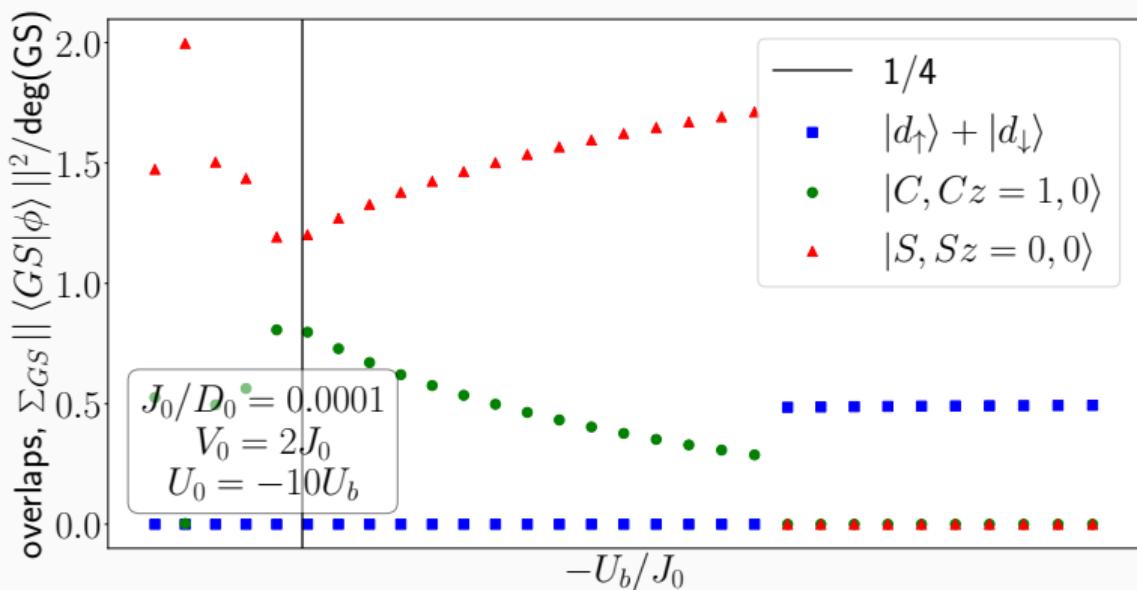
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- green: J vanishes ($J < U$)

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

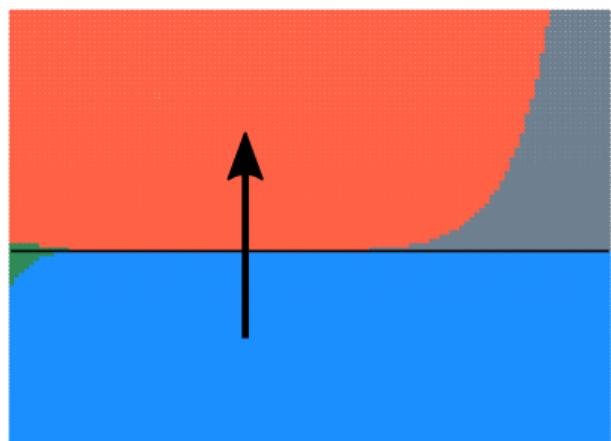
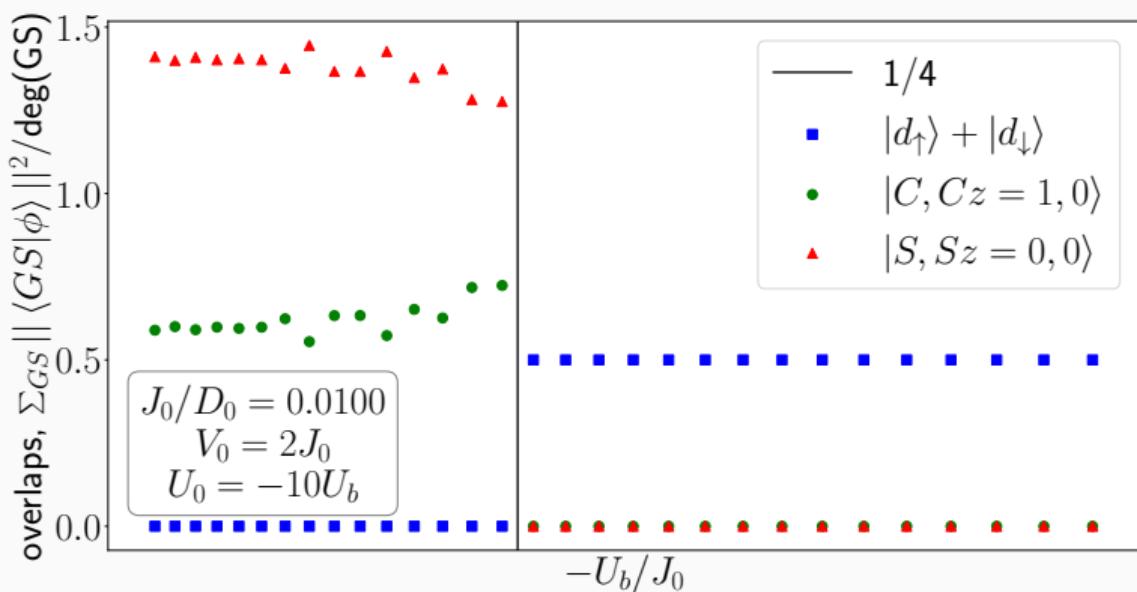
$$\frac{c}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{\sqrt{1-c^2}}{\sqrt{2}} (|2, 0\rangle + |0, 2\rangle)$$

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

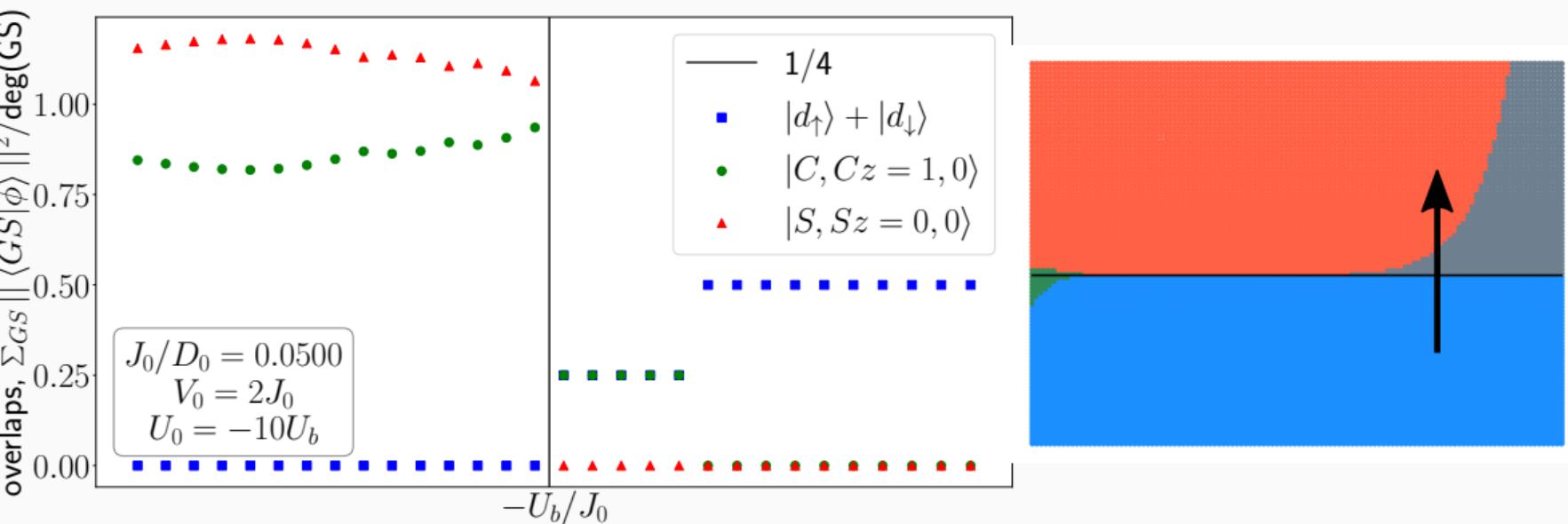
Overlap of ground state against spin singlet and charge triplet zero states



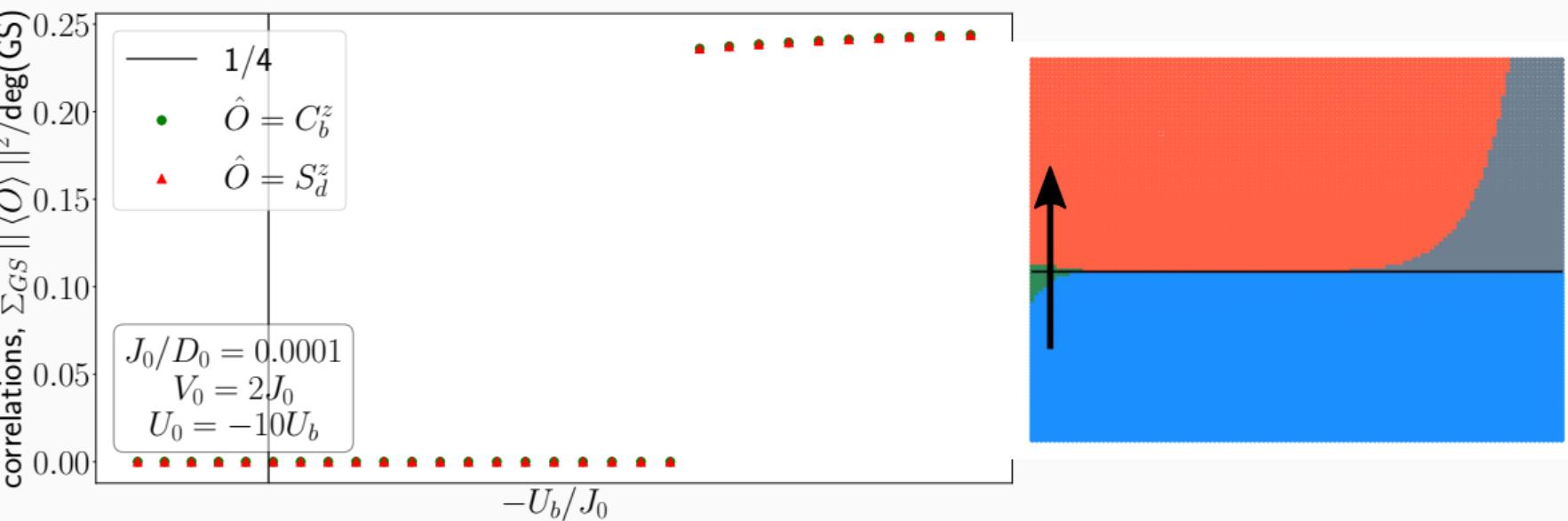
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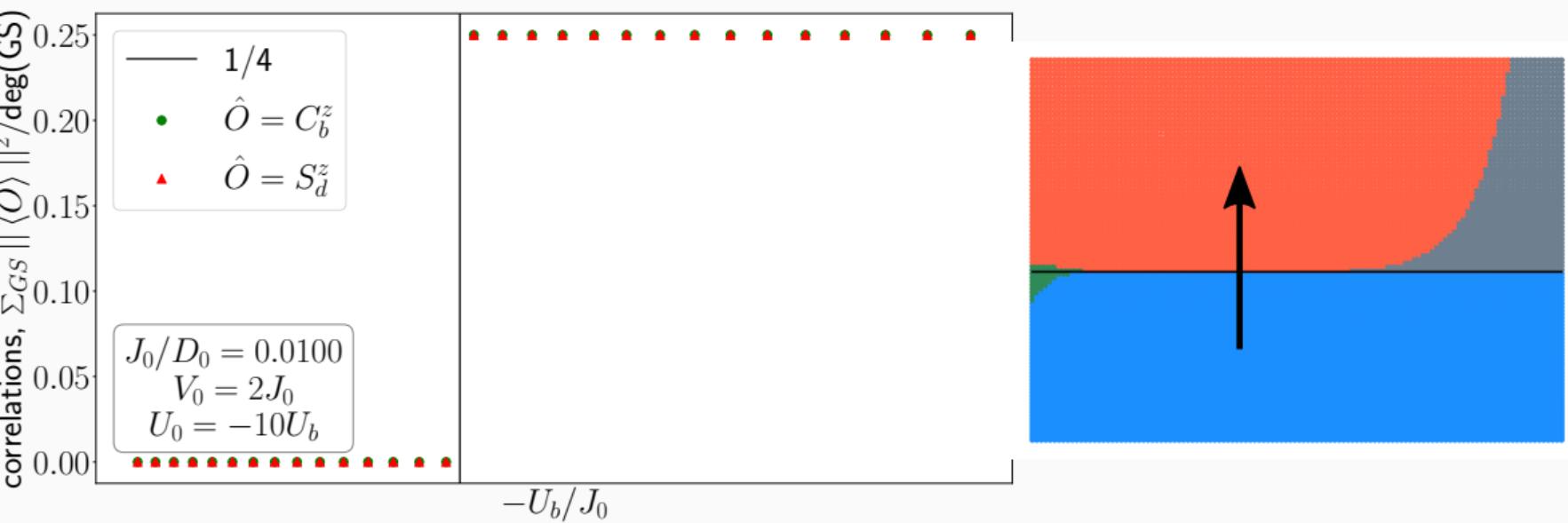
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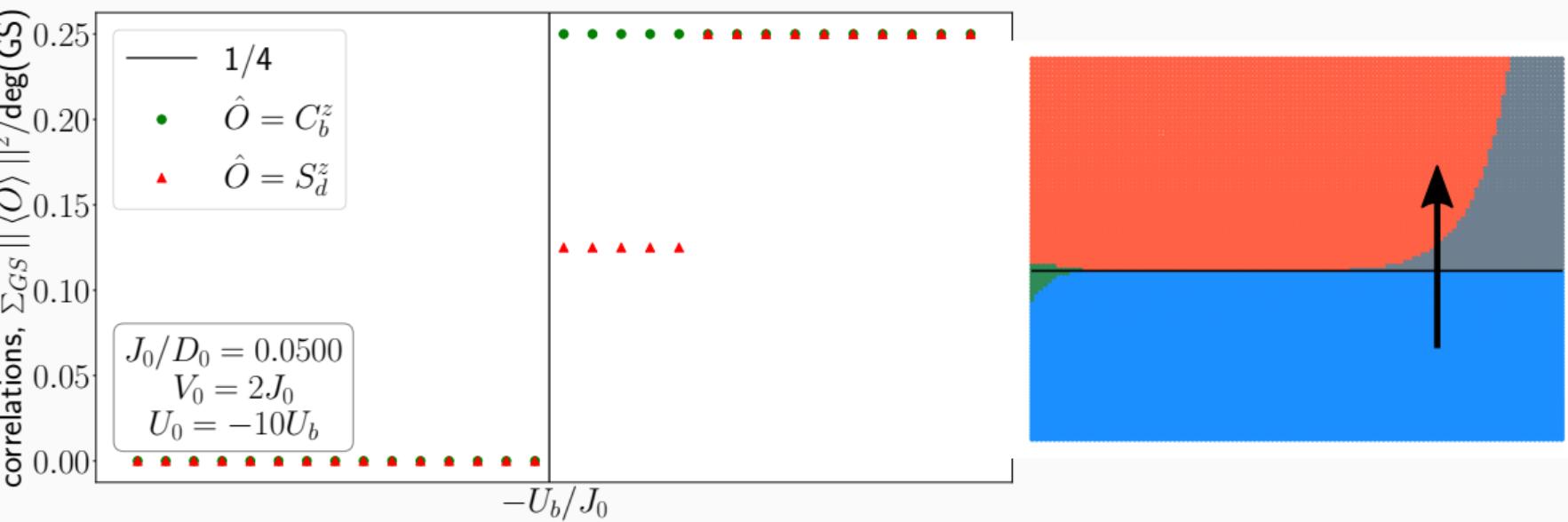
Spin and charge correlations in ground state



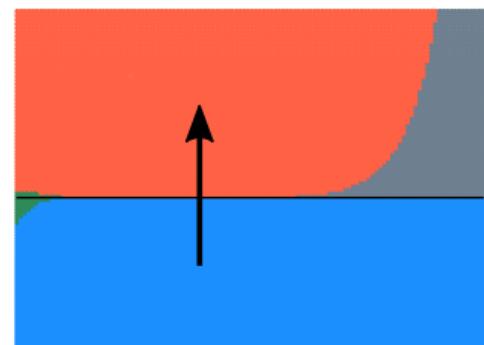
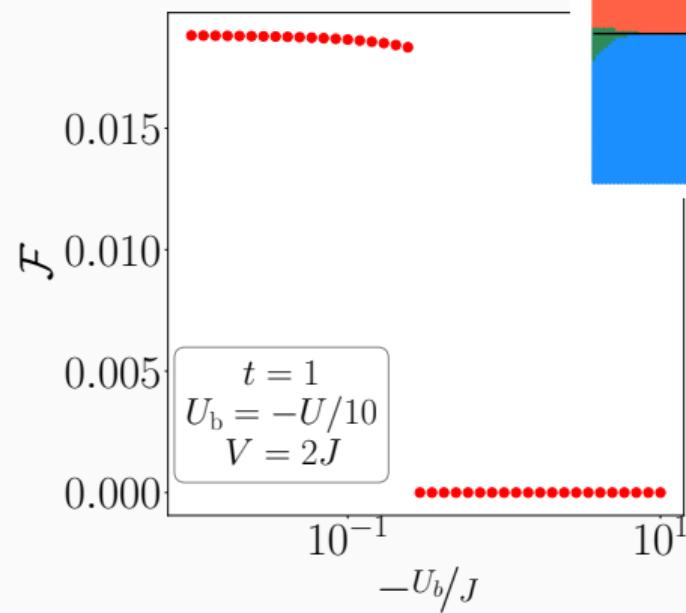
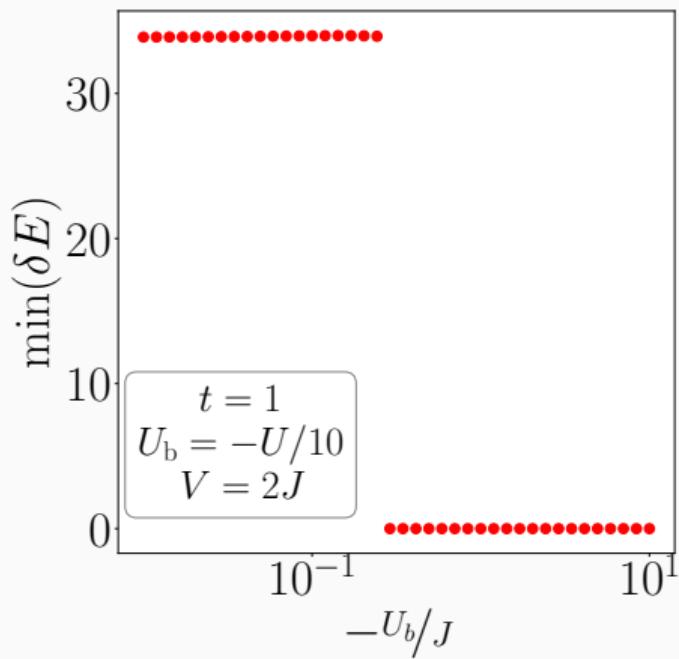
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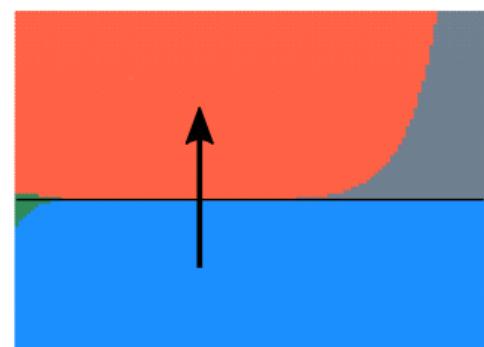
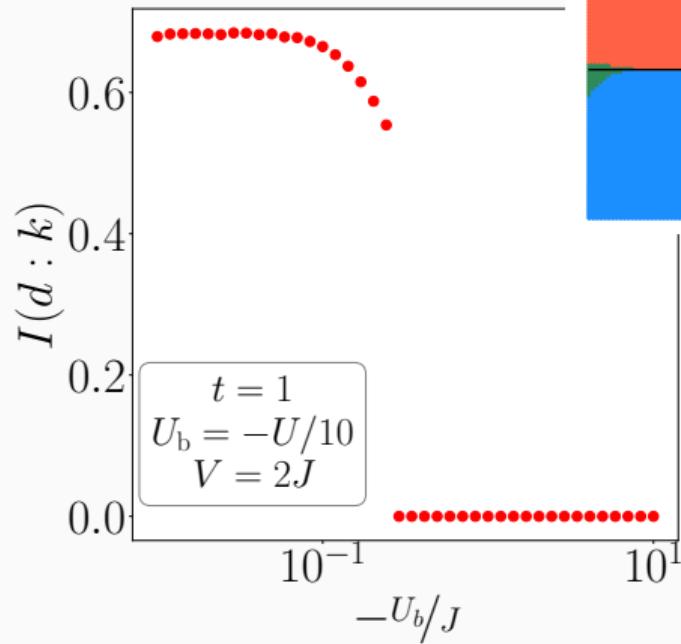
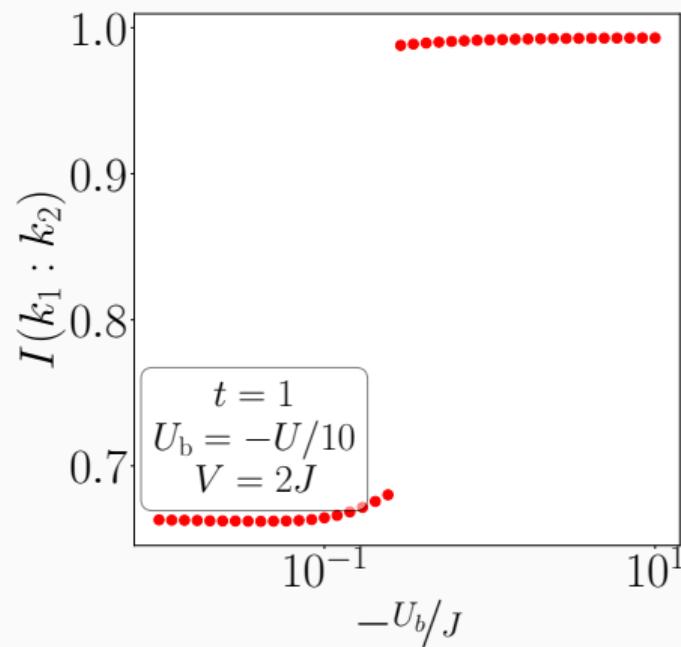
Spin and charge correlations in ground state



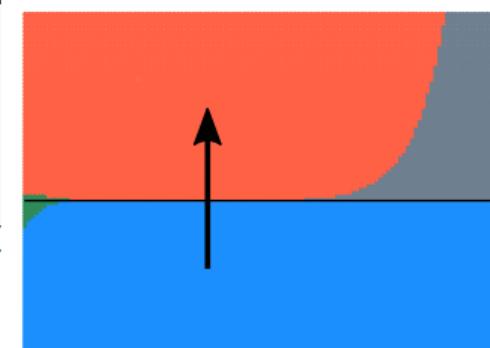
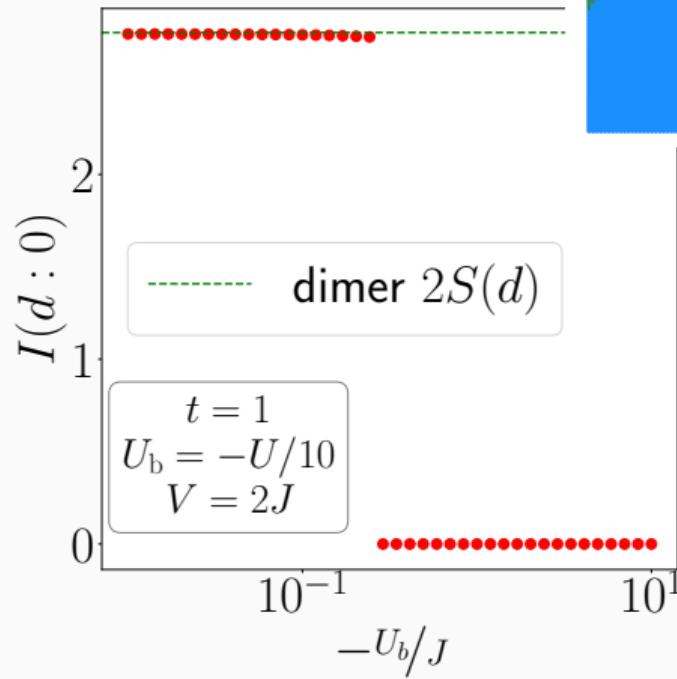
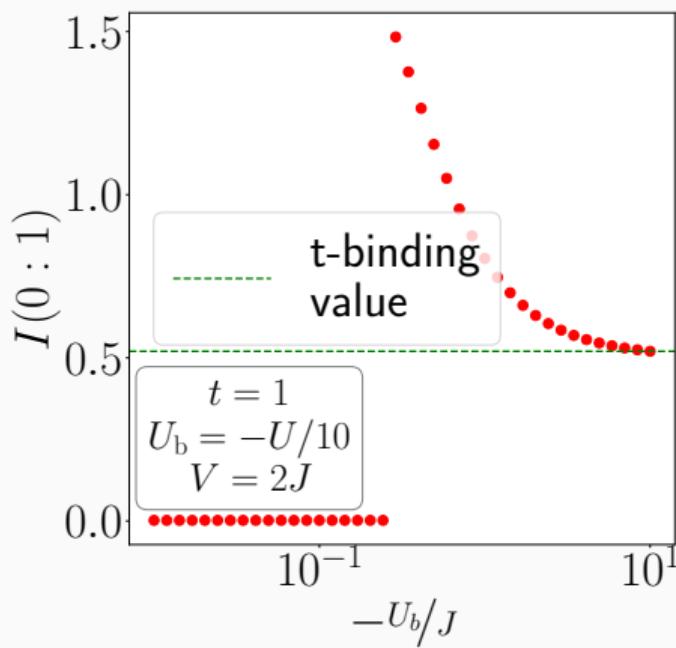
Correlation measures: Local Fermi liquid



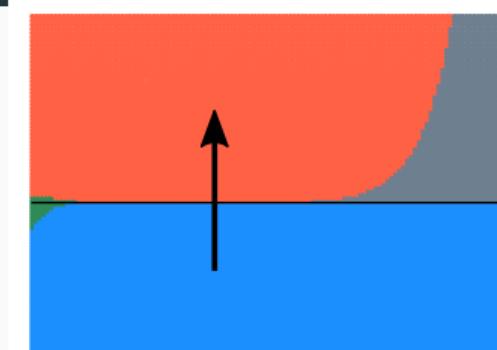
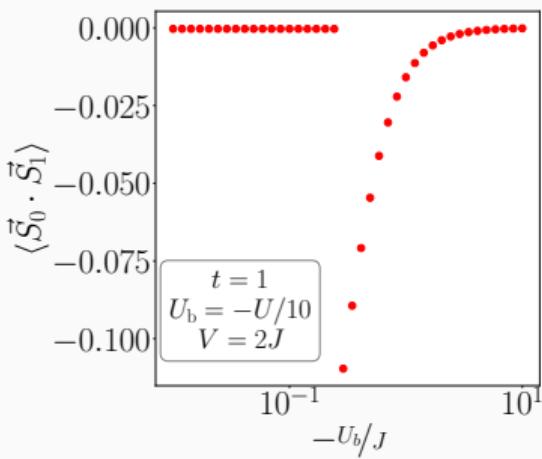
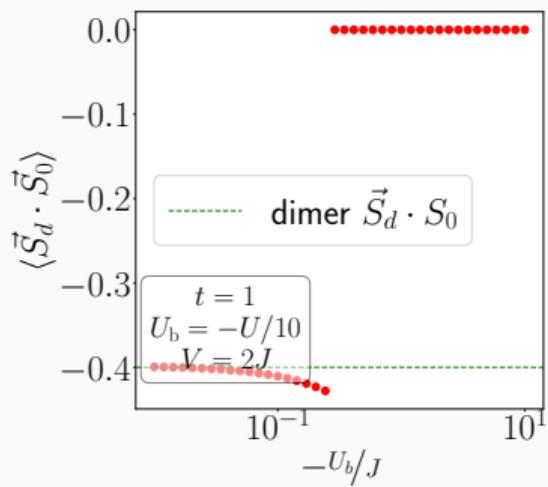
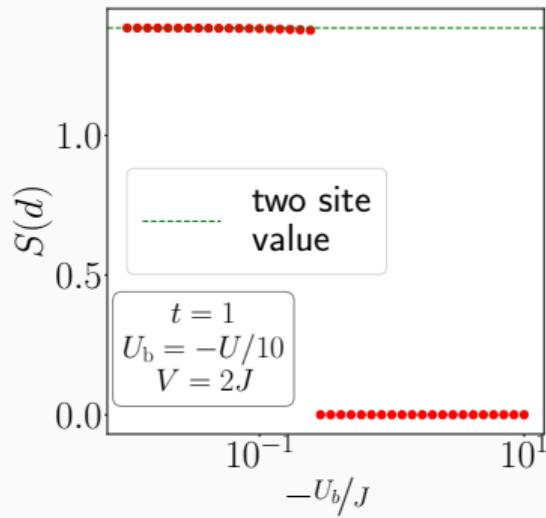
Correlation measures: Kondo cloud



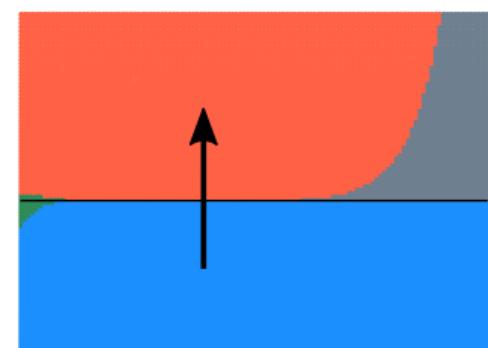
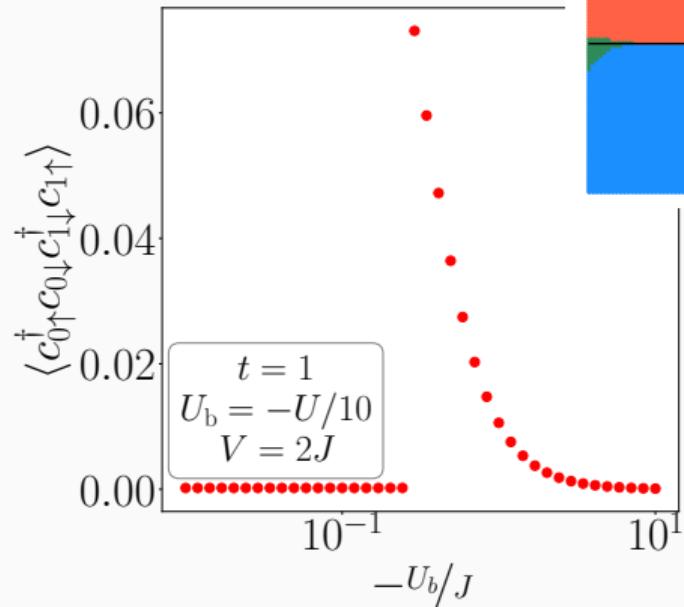
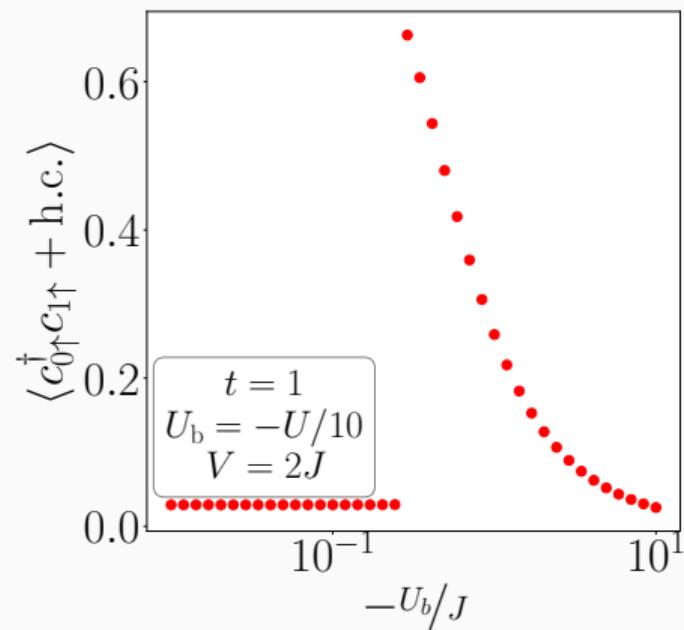
Correlation measures: Real space mutual information



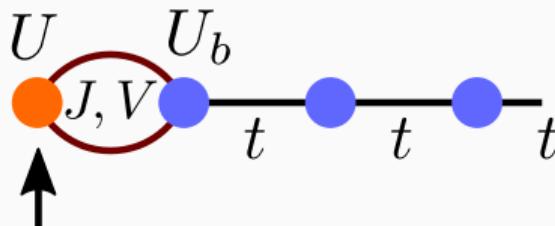
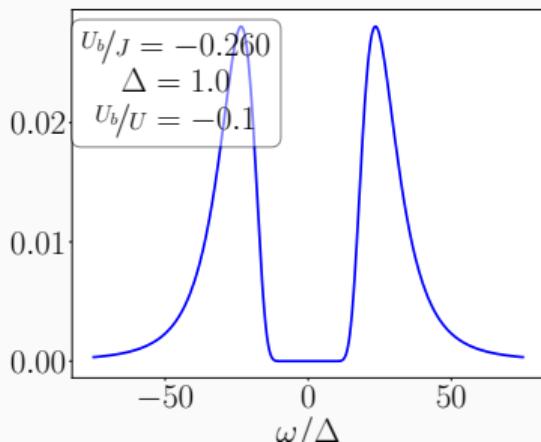
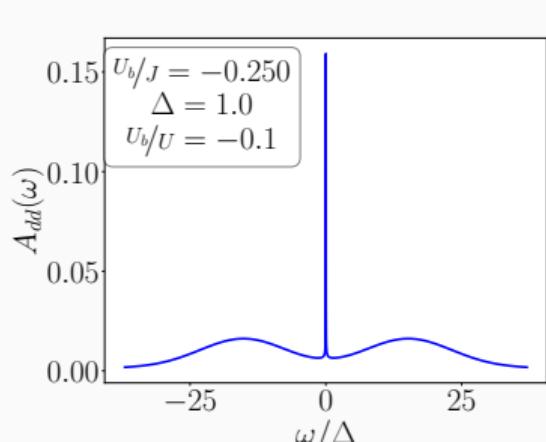
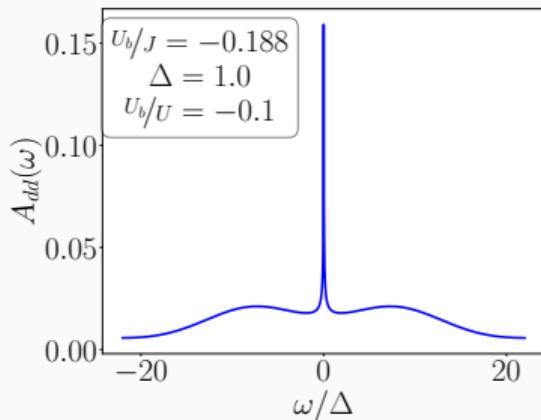
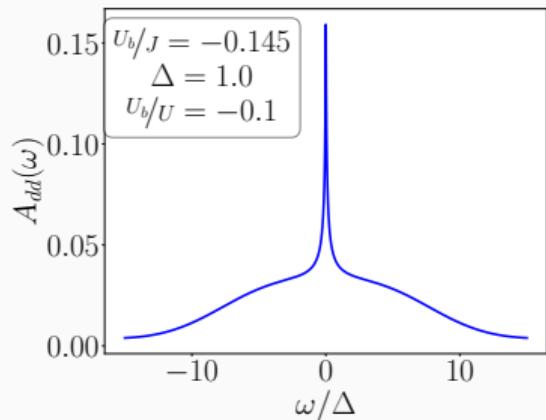
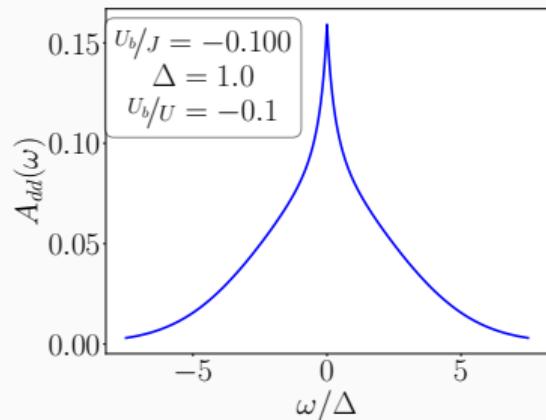
Correlation measures: Impurity entanglement entropy and spin-spin correlations



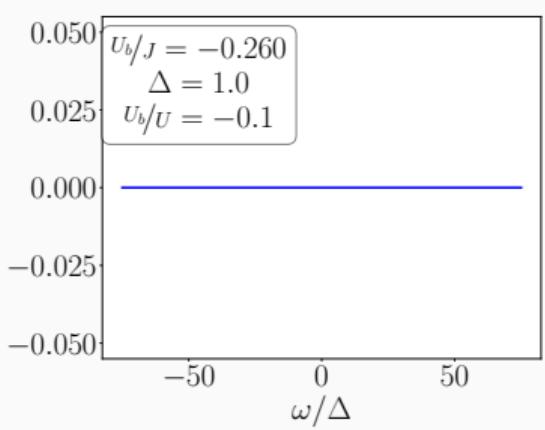
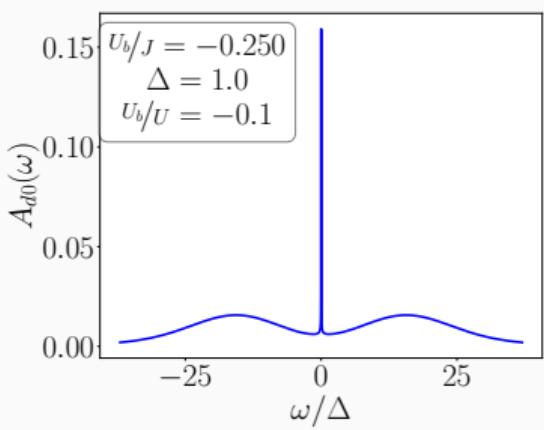
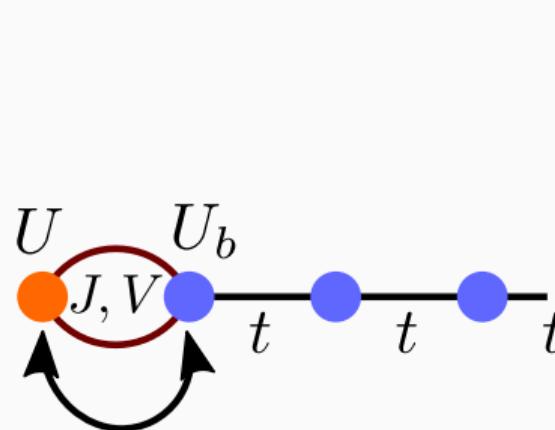
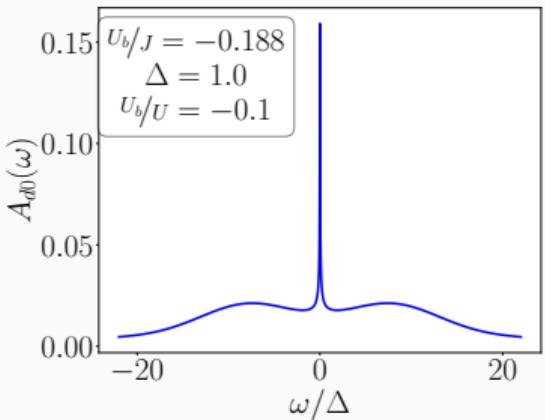
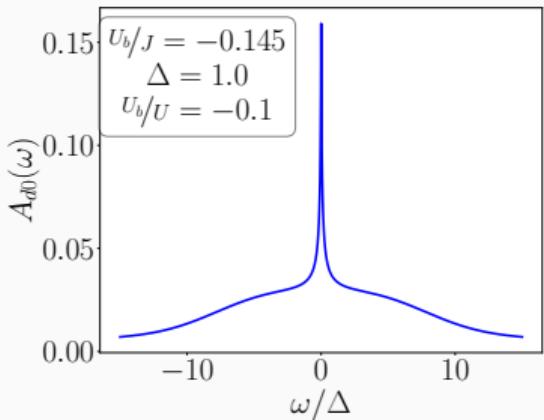
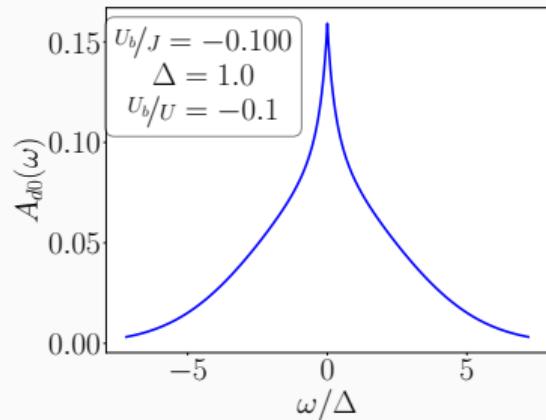
Correlation measures: Real-space correlations



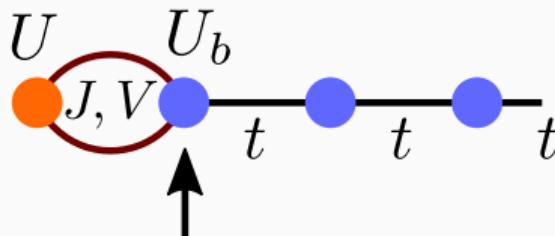
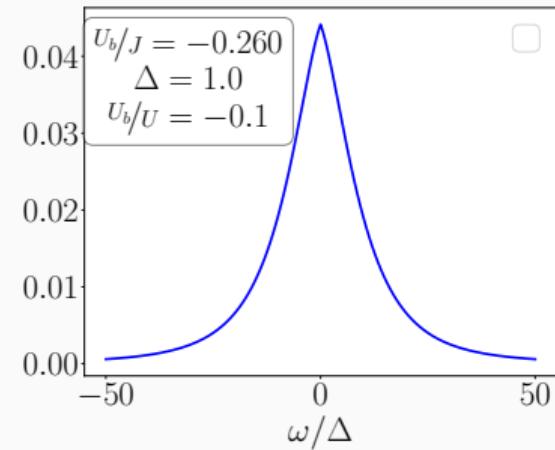
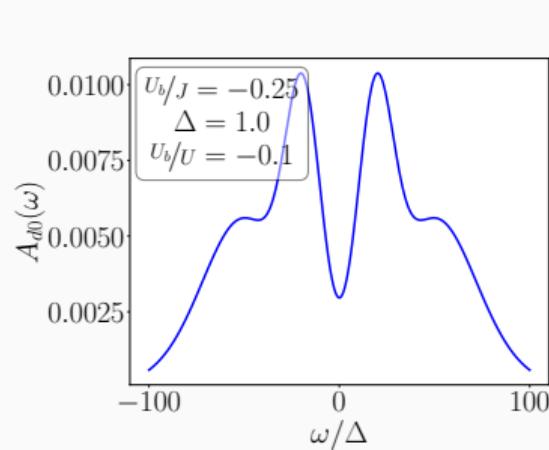
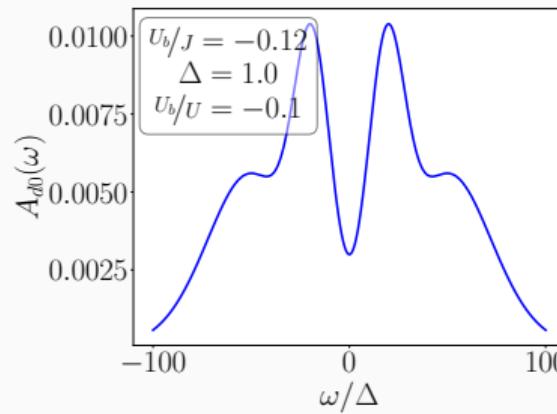
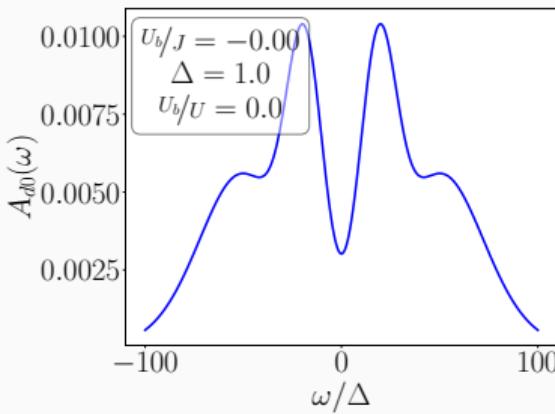
Correlation measures: Impurity spectral function



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



Correlation measures: Bath spectral function A_{00}

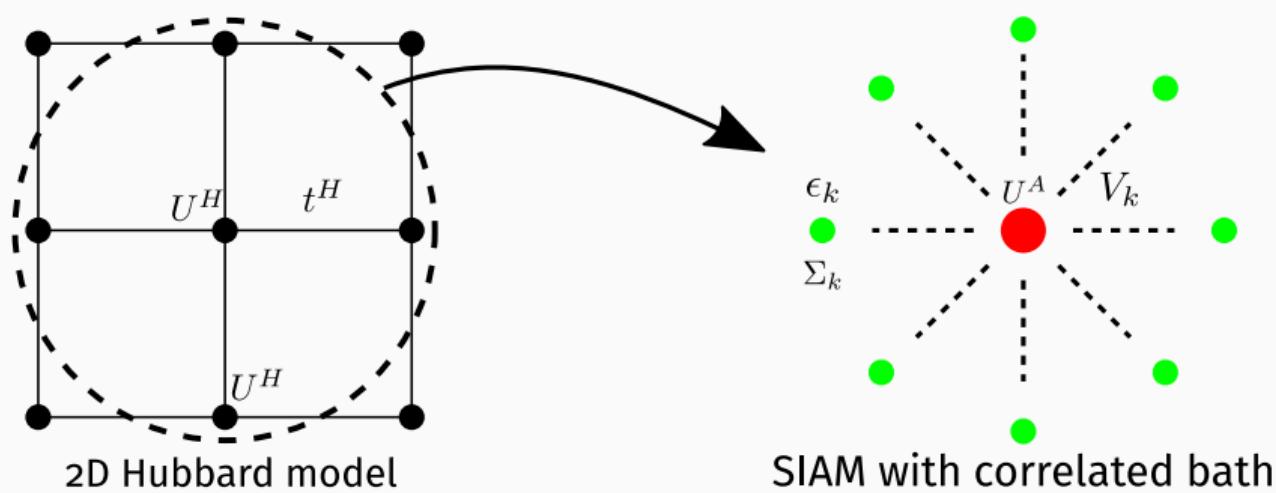


The Auxiliary Model Approach

General philosophy

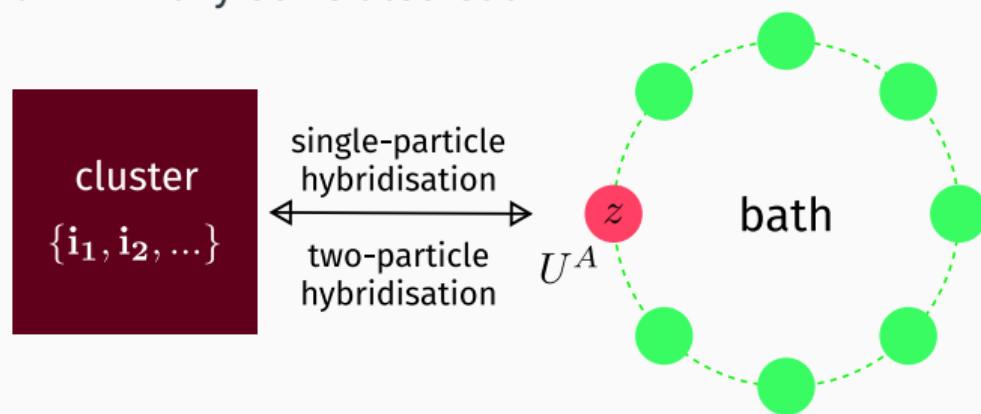
- find "appropriate" bath and then solve the cluster+bath problem
- appropriate = physical + solvable

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



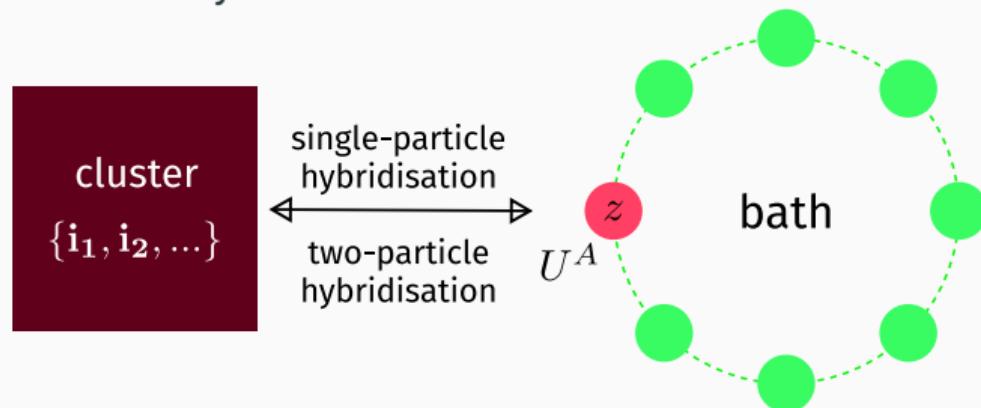
The present method

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



The present method

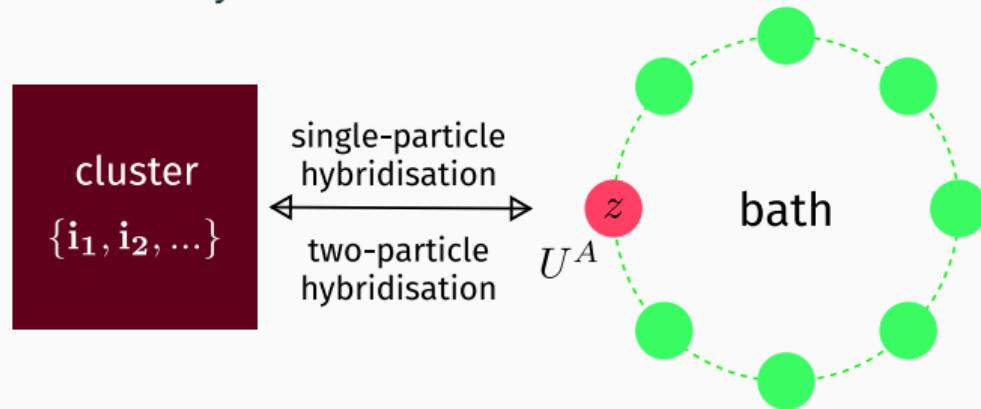
- Choose an auxiliary model H_{aux} consisting of a correlated impurity interacting with a minimally correlated bath



- Solve this impurity model H_{aux} using the unitary RG

The present method

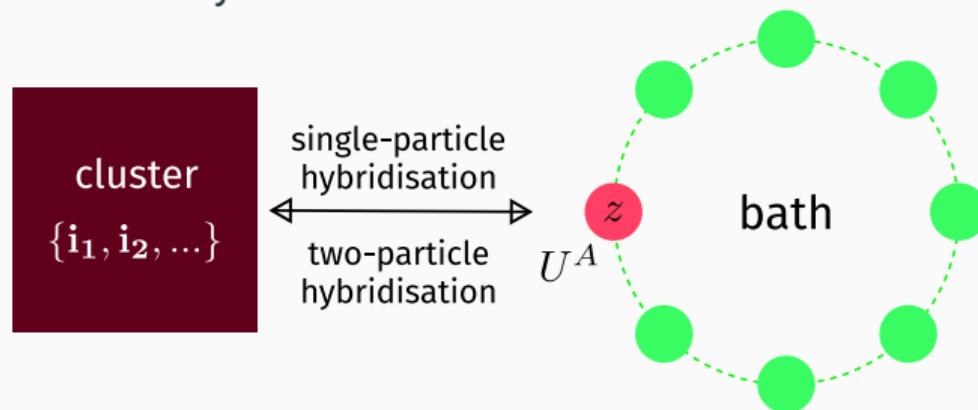
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- Create a **bulk lattice model** H_{bulk} from this auxiliary model H_{aux} by applying translation operators on the latter

The present method

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



- 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

- Replace impurity index with one particular lattice site i

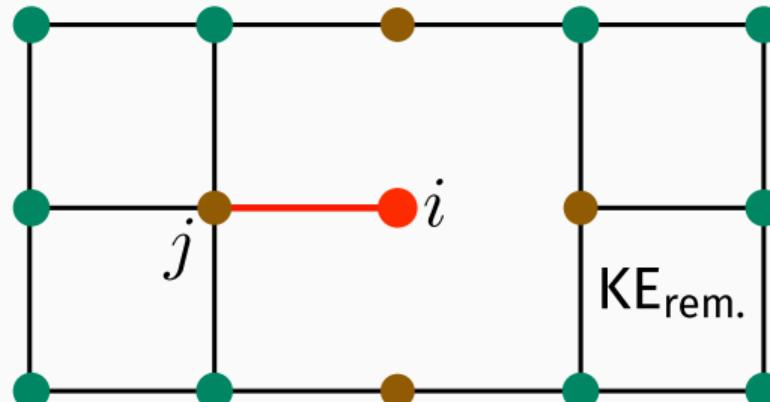
Creating the unit of tiling

- Replace impurity index with one particular lattice site i
- Replace bath with the remaining $N - 1$ sites of lattice

Creating the unit of tiling

- Replace impurity index with one particular lattice site i
- Replace bath with the remaining $N - 1$ sites of lattice
- Replace the zeroth site with one of the neighbours j of i

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



Creating the bulk model

- Average over all w nearest neighbours

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

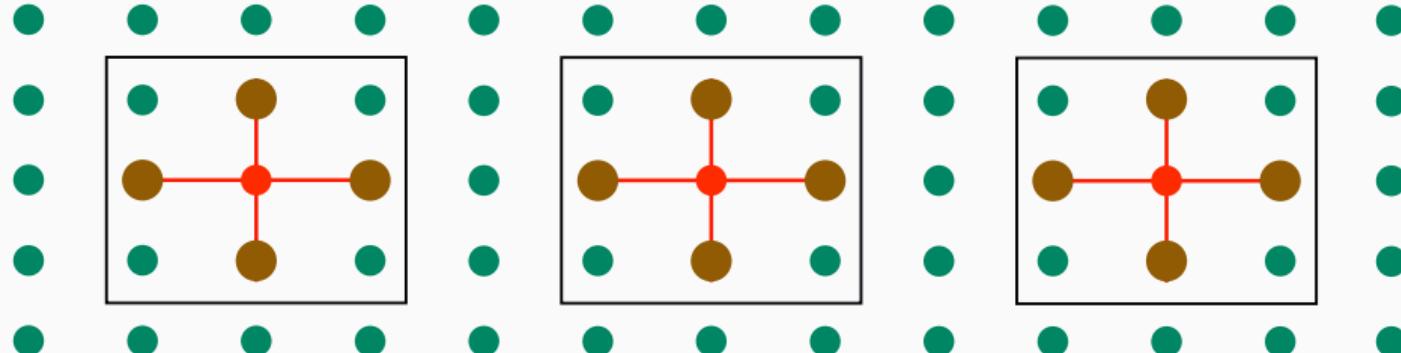
Creating the bulk model

- Average over all w nearest neighbours

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

- 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.

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

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:

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

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

Replace in tiling expression:

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

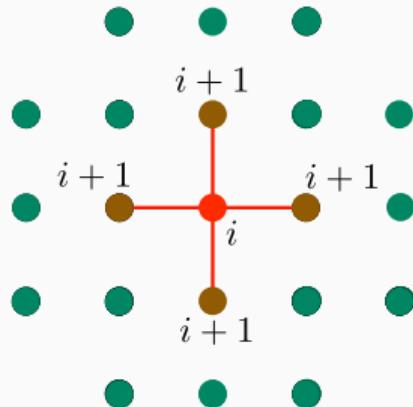
Matrix elements of $\mathcal{G}_{\text{H-H}}^{-1}$

Particle excitation on ground state of auxiliary model:

$$|i\rangle \equiv c_{i\sigma}^\dagger |\Phi_0\rangle$$

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

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



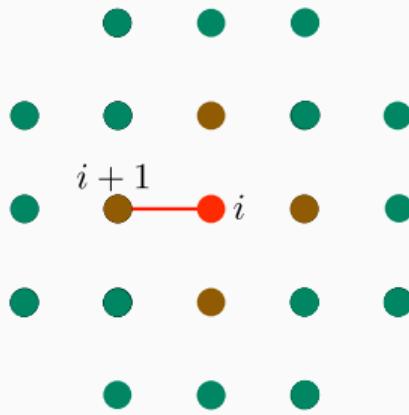
Matrix elements of \mathcal{G}_{H-H}^{-1}

Particle excitation on ground state of auxiliary model:

$$|i\rangle \equiv c_{i\sigma}^\dagger |\Phi_0\rangle$$

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

$$(\mathcal{G}_{H-H}^{-1})_{i,i+1}^p = \underbrace{\frac{1}{W} \langle \Phi_0 | c_{d\sigma} \mathcal{G}_{\text{aux}}^{-1}(d) c_{z,\sigma}^\dagger | \Phi_0 \rangle}_{\text{one nearest-neighbour pair}}$$



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

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

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

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

where d_m^p is the spectral weight factor:

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

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

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

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

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

where

$$z_m^p = \langle \Phi_m | c_{z\sigma}^\dagger | \Phi_0 \rangle$$

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:

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

The corresponding relations are

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

$$\left(\mathcal{G}_{H-H}^{-1}(-\omega) \right)_{i,i+1}^h = \frac{1}{w} \sum_m \left(d_m^h \right)^* z_m^h \left(\mathcal{G}_{\text{aux}}^{-1}(d, -\omega) \right)_{mm}$$

What's been achieved?

- 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 $|\Phi_m\rangle$, we can simply write

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

The Greens function can be related to the Greens operator:

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

Inversion and single-particle Greens functions

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

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

$$(G_{H-H}(\omega))_{n-n} = \frac{1}{w} \sum_m \left[(d_m^p)^* z_m^p (\mathcal{G}_{\text{aux}}(d, \omega))_{mm} - (z_m^h)^* d_m^h (\mathcal{G}_{\text{aux}}(d, -\omega))_{mm} \right]$$

$(G_{H-H}(\omega))_{n-n}$ vanishes on a **Bethe lattice** with infinite coordination number ($w \rightarrow \infty$)

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**:

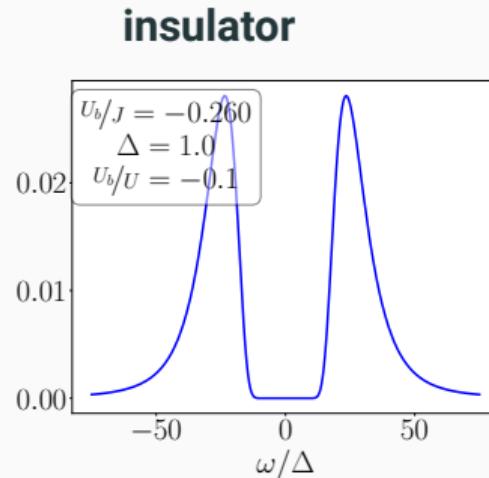
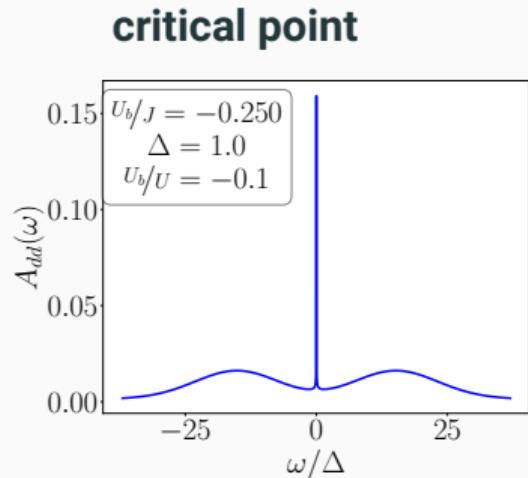
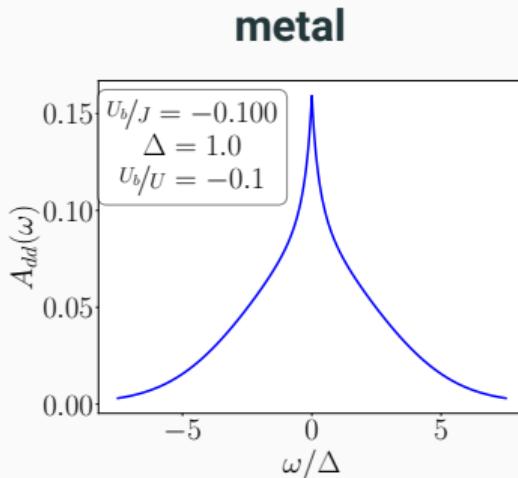
$$\Sigma(\vec{k}, \omega) = G_0(\vec{k}, \omega)^{-1} - G(\vec{k}, \omega)^{-1} = \omega + t^{H-H} \xi_{\vec{k}} - \left[G_{\text{aux}}(dd, \omega) + \frac{\xi_{\vec{k}}}{W} G_{\text{aux}}(d0, \omega) \right]^{-1}$$

Evidence for the Mott MIT

Evidence for Mott MIT

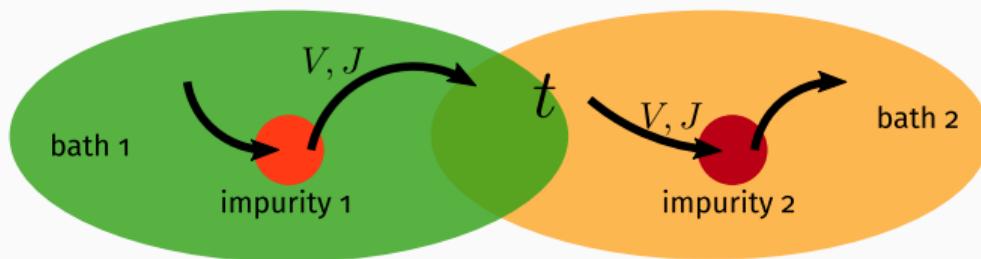
one-to-one mapping between Greens functions of the bulk and the auxiliary models, as well as spectral functions

$$A_{H-H}(\vec{k}, \omega) = A_{\text{aux}}(dd, \omega) + \frac{\xi_{\vec{k}}}{W} A_{\text{aux}}(d0, \omega)$$



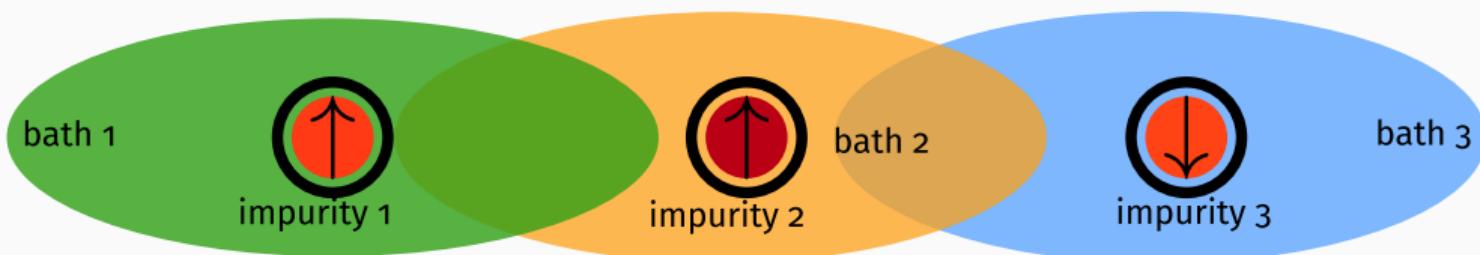
Evidence for Mott MIT

low energy resonance in the impurity excitations implies **propagation** of e^- s across lattice



Evidence for Mott MIT

gap in the impurity excitations implies e^- s are "stuck" and **spectral flow is not possible**



Evidence for Mott MIT

Choosing $U_b = -U/10$ and setting $w = 4$ for 2D square lattice, we get a critical ratio:

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

Final Remarks

Conclusions

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

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Conclusions

- The auxiliary model method described here provides a **constructionist**/bottoms-up 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** tendency on the partner site.

Moving forward

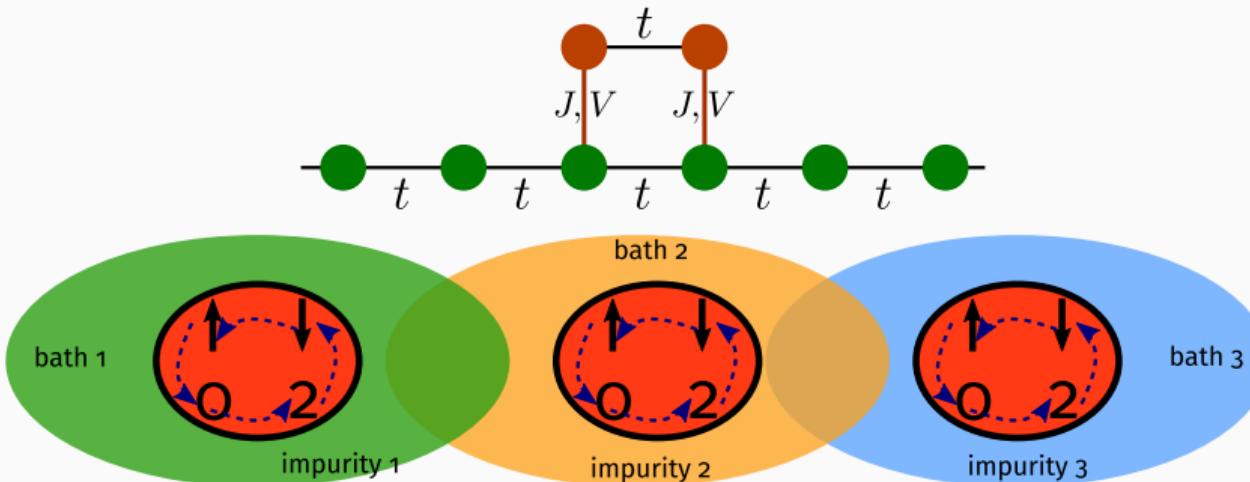
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- k -dependence of the self-energy: **electronic differentiation** and effects of Van Hove singularities?
- Breaking particle-hole symmetry on the impurity will allow us to study bulk models **away from half-filling**.
- For more accurate results, one can consider **multiple impurities** in the cluster.



Thank you.