New Auxiliary Model Approach to the Mott MIT

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The Model

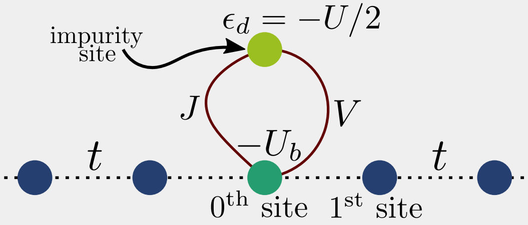
The Model

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

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

supplement 1-particle hybridisation with

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



Schrieffer and Wolff 1966; Anderson 1961.

URG Analysis: $U_b = 0$

$U_b = 0$: Flow towards strong-coupling

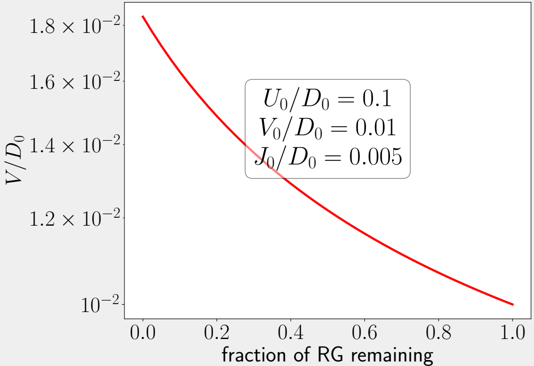
$U > 0, J > 0$

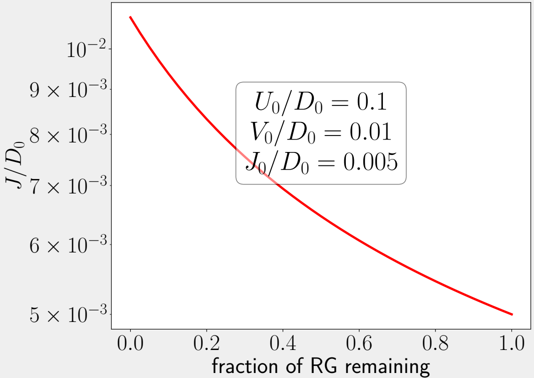
$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}$$

$$d_2 = \omega - \frac{D}{2} + \frac{J}{4}$$

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

$$\Delta J = \frac{n_j J^2}{|d_2|} > 0$$



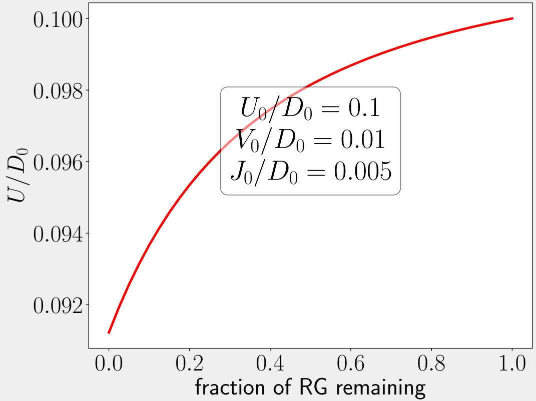


$U_b = 0$: Flow towards strong-coupling

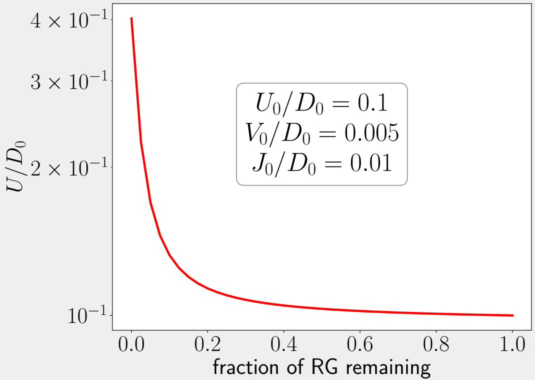
$U > 0, J > 0$

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

$V > J$



$V < J$

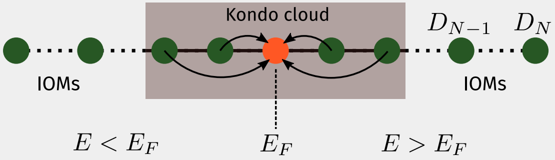


$U > 0$ Fixed point Hamiltonian

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

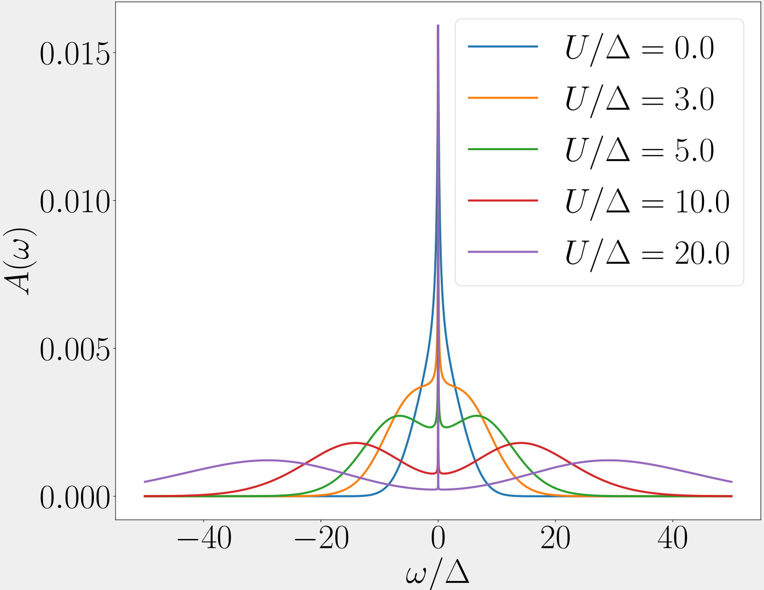
$$+ V^* \sum_{k<k^*,\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.}\right)$$

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



Impurity Spectral Function

no gap at arbitrarily large *U*



URG Analysis: $U_b \neq 0$

$U > 0$ RG Equations

- U_b is **marginal**: $\Delta U_b = 0$
- Spin-exchange couling J can now be **driven irrelevant** by U_b:

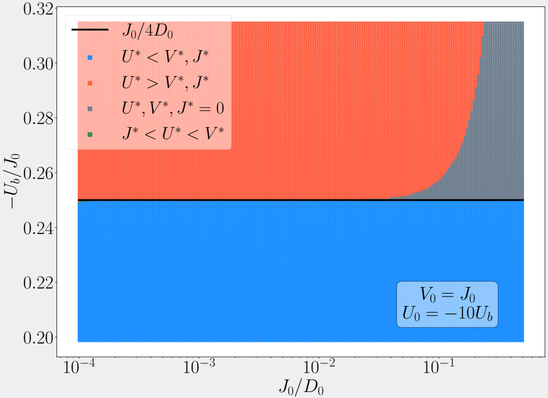
$$\Delta J = -\frac{n_j J\left(J + 4U_b\right)}{d_2} \longrightarrow \begin{cases} \text{relevant when } J + 4U_b > 0 \\ \text{irrelevant when } J + 4U_b < 0 \end{cases}$$

- Same can be said for the hybridisation V:

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

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

$U > 0$ Phase Diagram

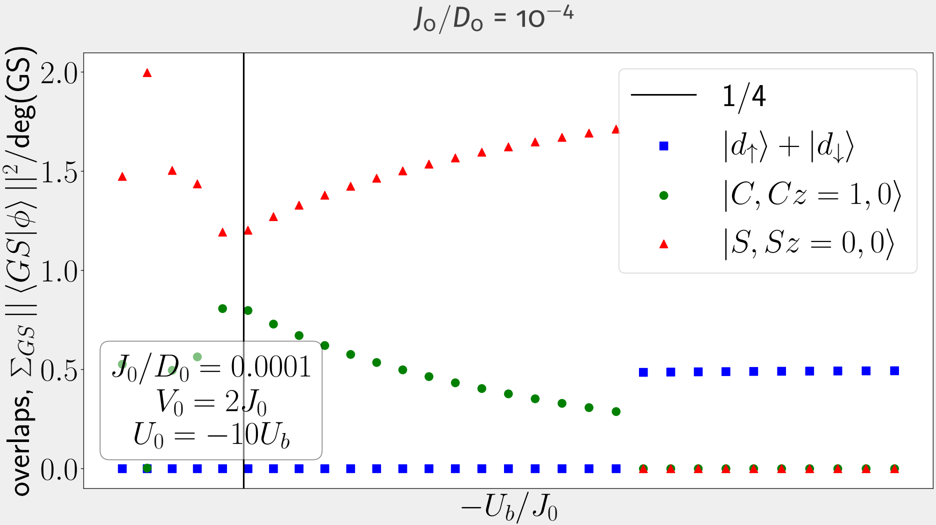


- black line represents line of **critical points** at $U_b^* = -J^*/4$
- blue: screened impurity (strong-coup.)
- red: unscreened local mom. ($J = V = 0$)
- gray: imp. level absent ($U = J = V = 0$)
- green: J vanishes ($J < U$) (this region vanishes in therm. limit)

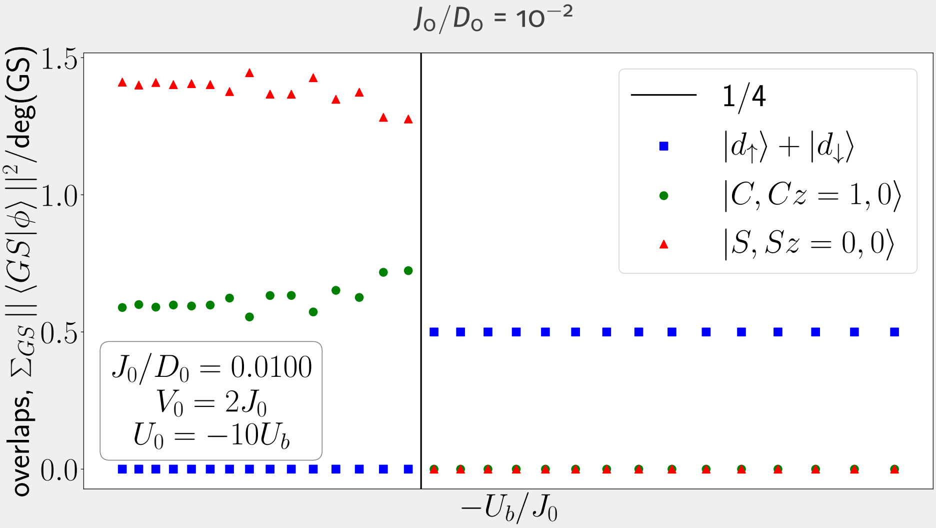
phase	RG flow	fixed point	GS	2-site GS
blue	$\Delta U < 0, \Delta J, \Delta V > 0$	$U^* \ll V^* \ll J^*$	SS	$\|SS\rangle = \|\uparrow, \downarrow\rangle - \|\downarrow, \uparrow\rangle$
green	$\Delta U < 0, \Delta J < 0, \Delta V > 0$	$J^* < U^* \ll V^*$	SS + CT-0	$c\,\|SS\rangle + \sqrt{1 - c^2}\,\|CT - 0\rangle$
red	$\Delta U > 0, \Delta J, \Delta V < 0$	$U^* \gg 1, V^* = J^* = 0$	loc. mom	$\{\|\uparrow\rangle, \|\downarrow\rangle\} \otimes \{\|0\rangle, \|2\rangle\}$
gray	$\Delta U, \Delta J, \Delta V < 0$	$U^* = V^* = J^* = 0$	bath	$\{\|\uparrow\rangle, \|\downarrow\rangle, \|0\rangle, \|2\rangle\} \otimes \{\|0\rangle, \|2\rangle\}$

Evolution of two-site groundstate and correlations across the transition

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



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



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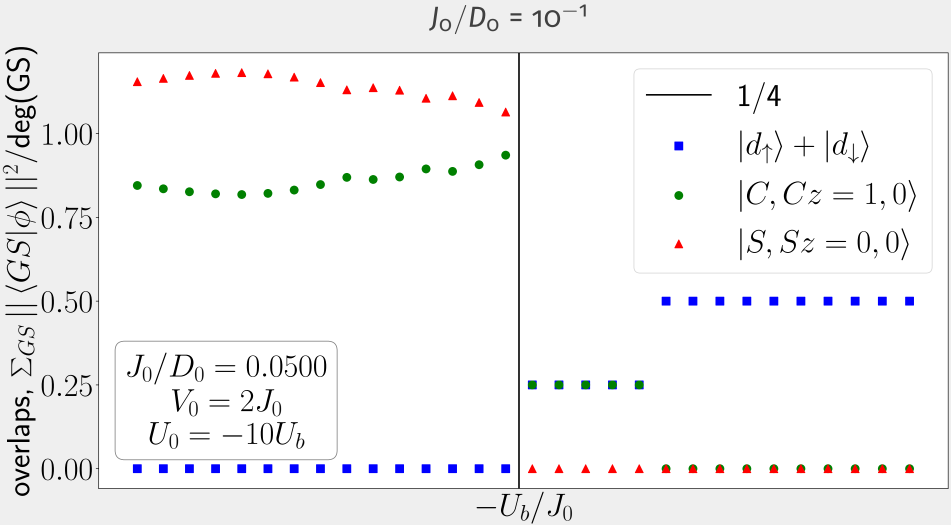
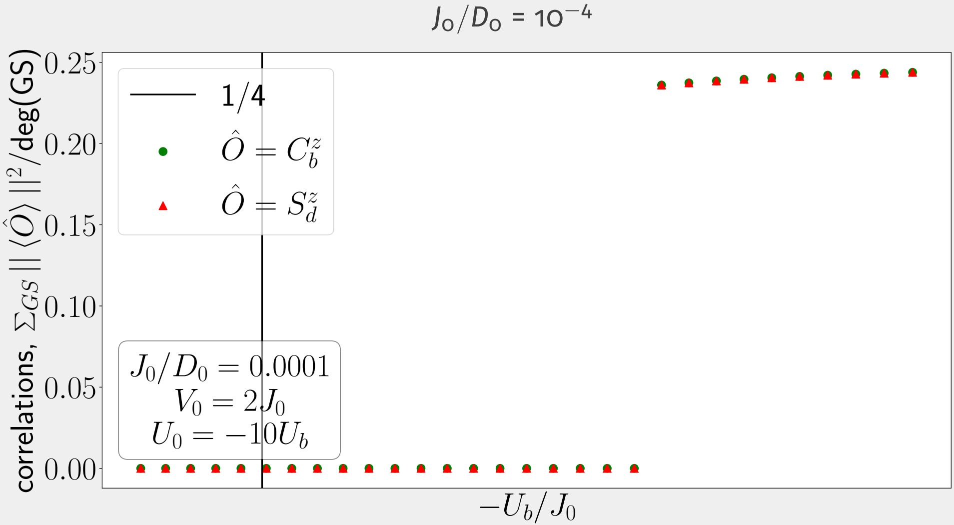
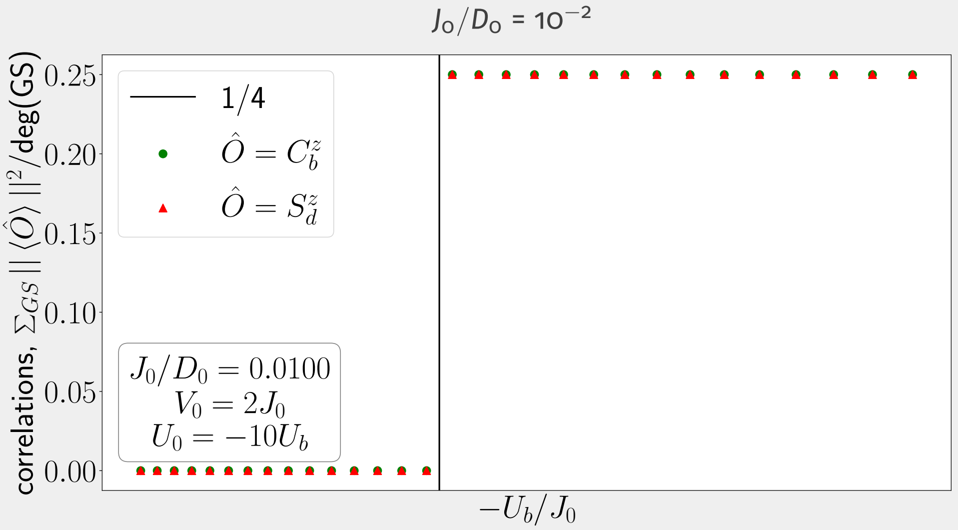


Spin and charge correlations in ground state



Spin and charge correlations in ground state



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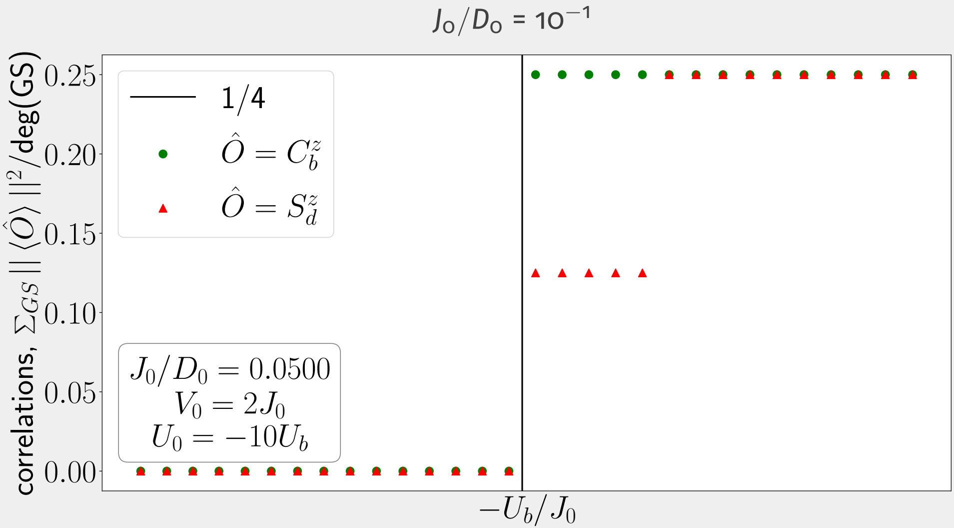
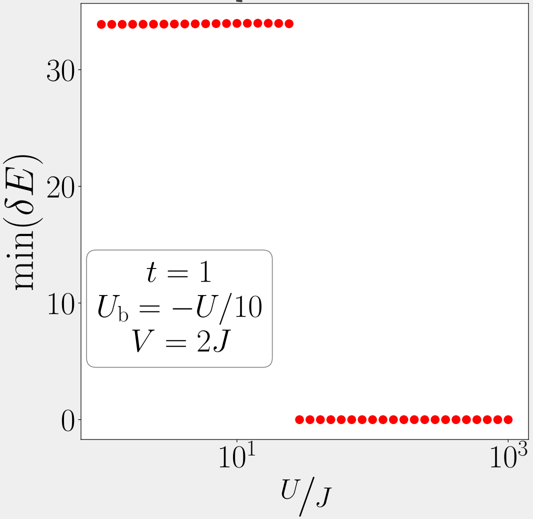
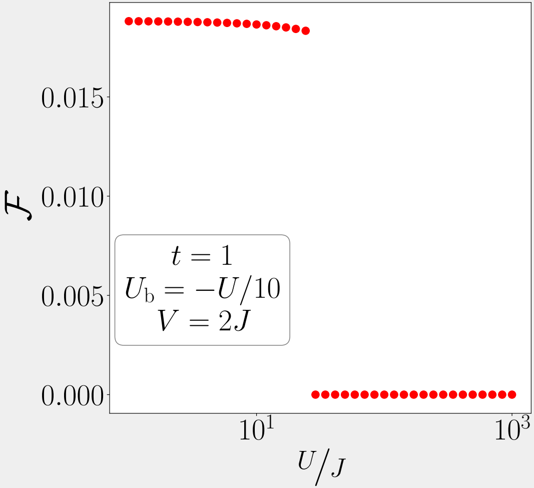
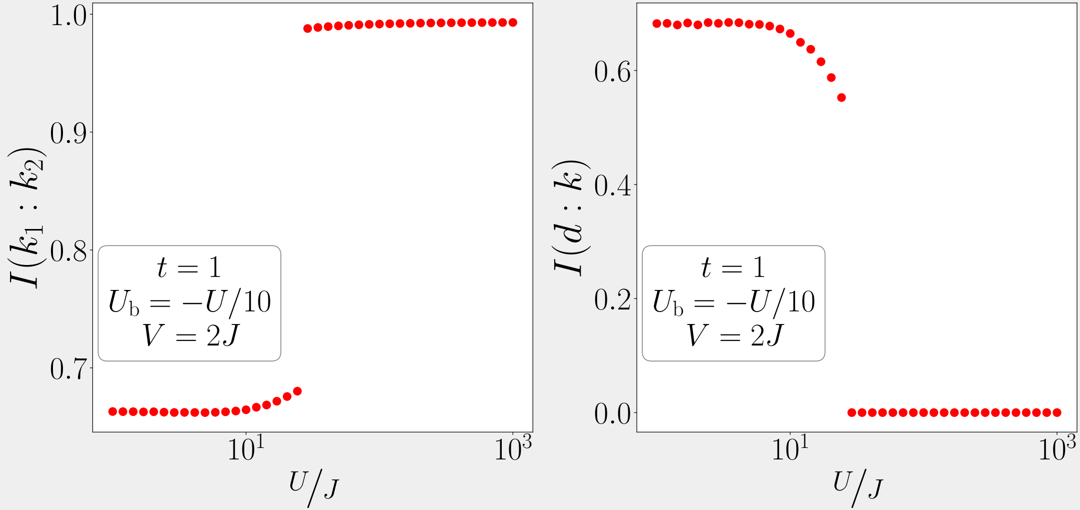


Local Fermi liquid

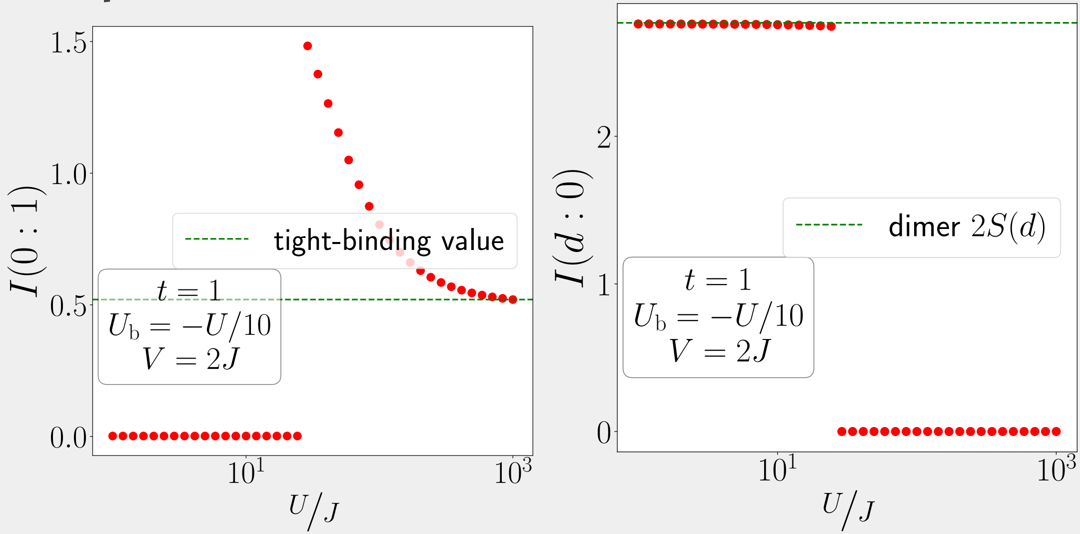




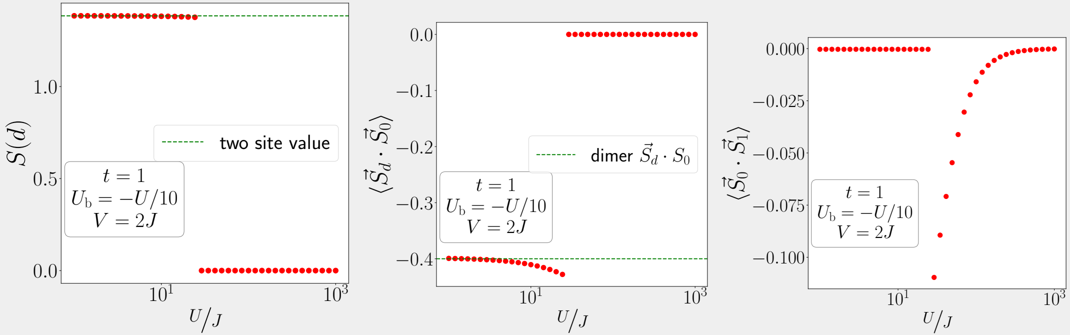
Kondo cloud


1.0
0.9
0.8
0.7
$I(k_1 : k_2)$
$t = 1$
$U_b = -U/10$
$V = 2J$
10^1
10^3
U/J
0.6
0.4
0.2
0.0
$I(d : k)$
$t = 1$
$U_b = -U/10$
$V = 2J$
10^1
10^3
U/J

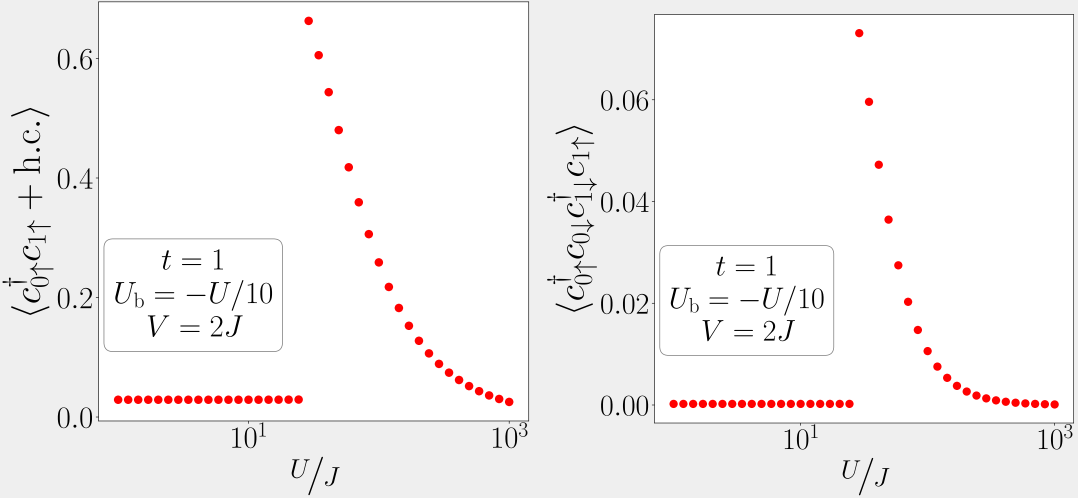
Real space mutual information



Impurity entanglement entropy and spin-spin correlations



Real-space correlations



Zero-bandwidth limit of fixed point Hamiltonian

Route to the zero-bandwidth model

At strong-coupling fixed point,

- kinetic energy acts as a perturbation
- **compress the bandwidth to just the Fermi surface**

$$H^*_{\text{zero bw}} = (\epsilon_F - \mu)\, \hat{n}_{k_F} + \frac{U^*}{2}\left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 + V^* \sum_\sigma \left(c^\dagger_{d\sigma} c_{0\sigma} + \text{h.c.}\right) + J\vec{S}_d \cdot \vec{s}_0$$

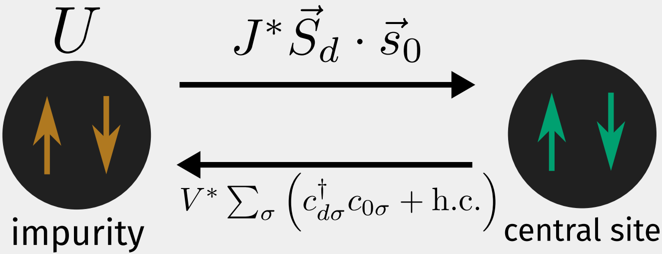
(center of motion)

- Setting $\mu = \epsilon_F$ gives a **two-site model**

$$H^*_{\text{zero}} = \frac{U^*}{2}\left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 + V^* \sum_\sigma \left(c^\dagger_{d\sigma} c_{0\sigma} + \text{h.c.}\right) + J\vec{S}_d \cdot \vec{s}_0$$

Effective two-site problem

$$H^*_{\text{zero}} = J^* \vec{S}_d \cdot \vec{s}_< + H^*_{\text{IOMS}}$$



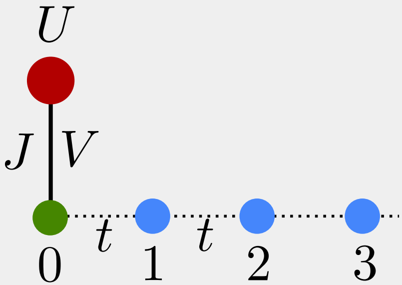
$$|\Psi\rangle_{\text{gs}} = \frac{c_s}{\sqrt{2}} \left(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle\right) + \frac{\sqrt{1-c_s^2}}{\sqrt{2}} \left(|2,0\rangle + |0,2\rangle\right), \quad c_s \to 1 \text{ as } D \to \infty$$

Local Fermi liquid excitations

Effective Hamiltonian in singlet subspace

We treat the dispersion as a **real-space nearest neighbour hopping**.

$$H^* = -\frac{U}{2}\left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow}\right)^2 + J^*\vec{S}_d \cdot \vec{s}_0$$
$$+V\sum_\sigma \left(c^\dagger_{d\sigma}c_{0\sigma} + \text{h.c.}\right)$$
$$-t\sum_{i\sigma}\left(c^\dagger_{i\sigma}c_{i+1,\sigma} + \text{h.c.}\right)$$

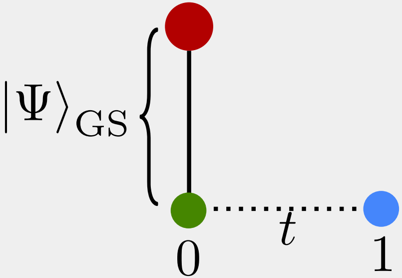


Effective Hamiltonian in singlet subspace

Initially consider **just the first site**. Treat **hopping as perturbation**:

$$|\Psi\rangle^*_{GS} = c_S\,|SS\rangle + \sqrt{1-c_S^2}\,|CT,0\rangle$$

$$V = -t\sum_\sigma \left(c^\dagger_{0\sigma}c_{1,\sigma} + \text{h.c.}\right)$$

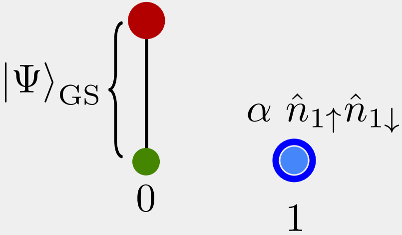


Effective Hamiltonian in singlet subspace

Upto **fourth order**, effective Hamiltonian is

$$H^*_{\text{eff}} = \text{constant} + \alpha \mathcal{P}_{\text{charge}}$$

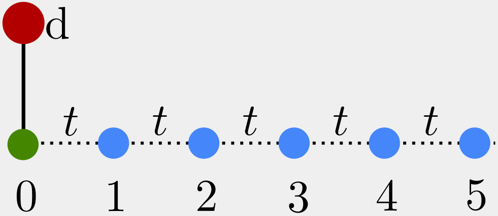
$$\mathcal{P}_{\text{charge}} \longrightarrow \text{projector onto } \hat{n}_1 \neq 1$$

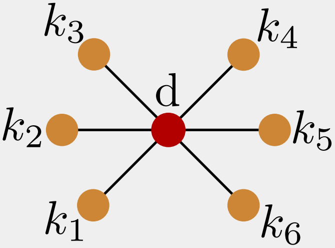


- For $U \ll V \ll J$, we get $0 < \alpha \ll 1$
- a **very weak local FL** on 1st site

Signatures of breakdown of screening - Journey towards local moment phase

- We will work with a Hilbert space of (6+1=) **7 sites**
- **Recreate RG flow** by tuning the parameters U, V, J
- **Observe various measures** of entanglement and correlation along this variation



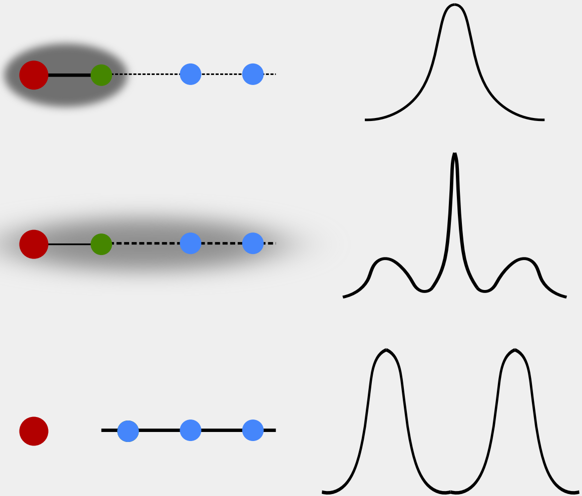


What's happening?

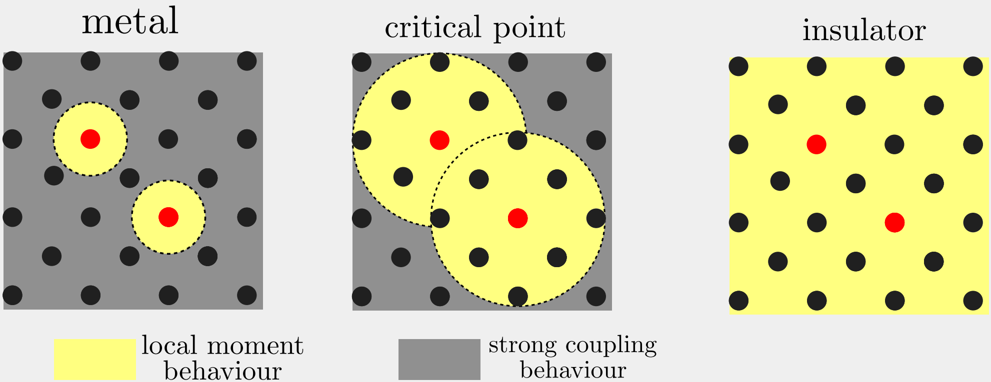
$J, V \gg U, t$: weak LFL

$U \gg J, V \sim t$: highly correlated metal

$U > 0; J, V = 0$: insulator



Auxiliary Model → bulk



- At large J, V, we have **large overlapping** Kondo clouds (gray regions)
- As we go towards the local moment phase, the **Kondo clouds shrink**
- At $V, J \sim 0$, the Kondo **length scale diverges** and the system becomes insulating

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- Rewinding the RG flow shows the **decoupling** of the impurity site.
- When used as an auxiliary model, this a **metal-insulator transition**.
- Stabilising the insulating phase under RG **still remains to be done**.
- For this, we will insert a **Hubbard term on the zeroth site**, and check the RG flows.