Destruction of the Kondo cloud in the generalised SIAM: Unitary RG perspective

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Abhirup Mukherjee [1], Siddhartha Lal [1]

[1]Department of Physical Sciences,IISER Kolkata

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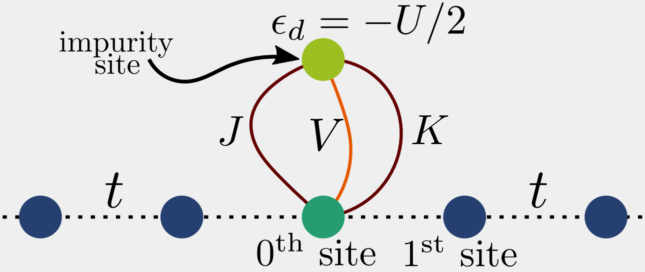
The Generalised SIAM Model

The Model

$$H = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + J \vec{S}_d \cdot \vec{s} + K \vec{C}_d \cdot \vec{C}$$

supplement 1-particle hybridisation with **spin-exchange** and **charge isospin-exchange**



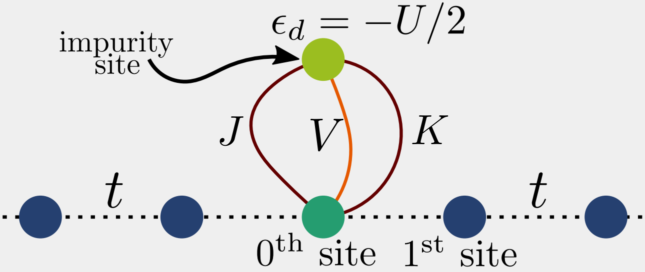
Schrieffer and Wolff 1966; Anderson 1961.

$$H = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + V \sum_{k\sigma} \left(c^\dagger_{d\sigma} c_{k\sigma} + \text{h.c.} \right) - \frac{1}{2} U \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + J \vec{S}_d \cdot \vec{s} + K \vec{C}_d \cdot \vec{C}$$

$$C^z_d = \frac{1}{2} \left(\hat{n}_d - 1 \right)$$

$$C^+_d = c^\dagger_{d\uparrow} c^\dagger_{d\downarrow}$$

$$C^-_d = c_{d\downarrow} c_{d\uparrow}$$



Schrieffer and Wolff 1966; Anderson 1961.

URG of Generalised SIAM

$U > 0$ $(J > 0, K < 0)$: Flow towards strong-coupling

$J \rightarrow$ **AFM,** $\quad K \rightarrow$ **FM**

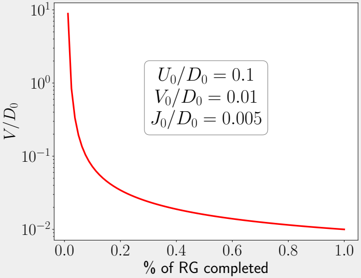
$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{K}{4}$$

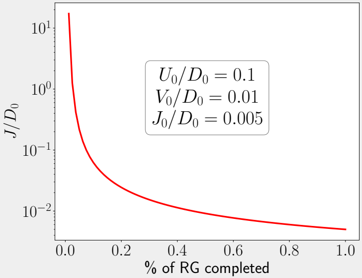
$$\Delta V = \frac{3 n_j V J}{8} \left(\frac{1}{|d_2|} + \frac{1}{|d_1|} \right) > 0$$

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

$$\Delta K = \frac{n_j K^2}{|d_3|} > 0$$

(K is irrelevant)



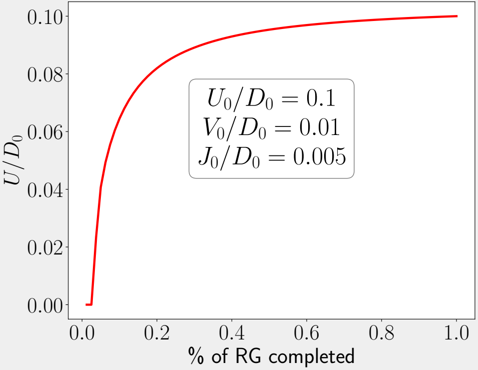


$U > 0$ ($J > 0, K < 0$) : Flow towards strong-coupling

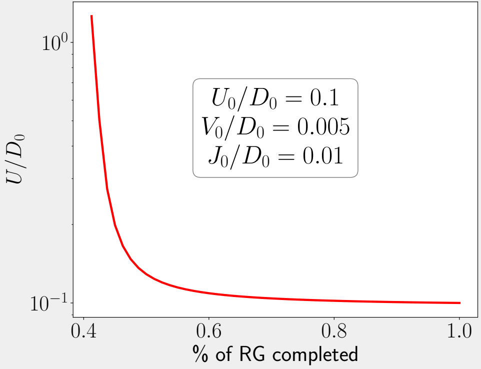
$J \to$ **AFM,** $K \to$ **FM**

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

$V > J$



$V < J$

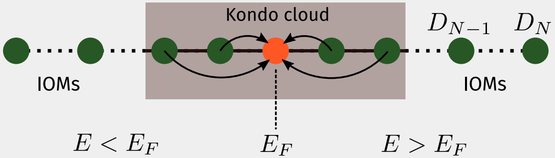


$U > 0$ Fixed point Hamiltonian

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

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

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



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**

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

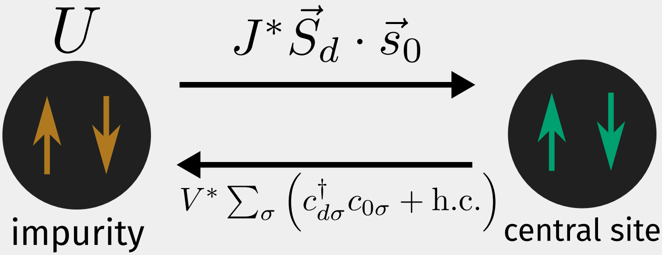
(center of motion)

- 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

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



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

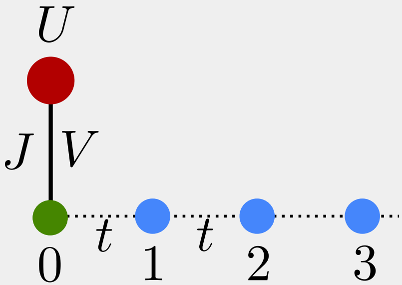
Local Fermi liquid excitations

Local Fermi liquid excitations

Effective Hamiltonian in singlet subspace

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

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

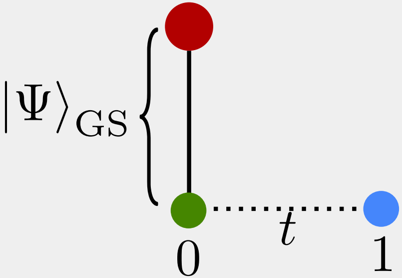


Effective Hamiltonian in singlet subspace

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

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

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

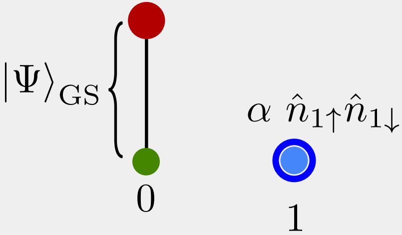


Effective Hamiltonian in singlet subspace

Upto **fourth order**, effective Hamiltonian is

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

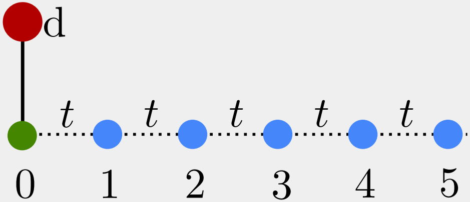
$$\mathcal{P}_{\text{charge}} \longrightarrow \text{projector onto } \hat{n}_1 \neq 1$$

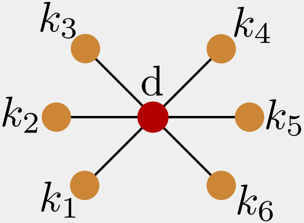


- For $U \ll V \ll J$, we get $0 < \alpha \ll 1$
- a **very weak local FL** on 1st site

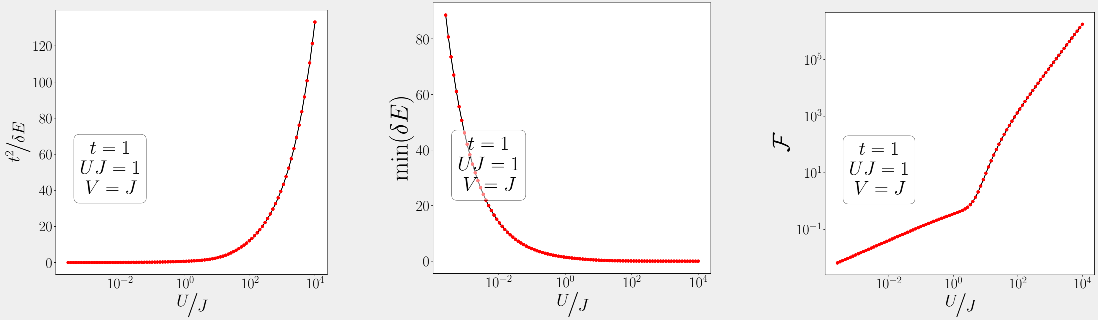
Signatures of breakdown of screening - Journey towards local moment phase

- 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



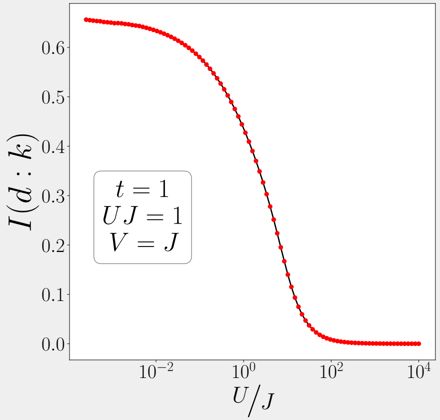


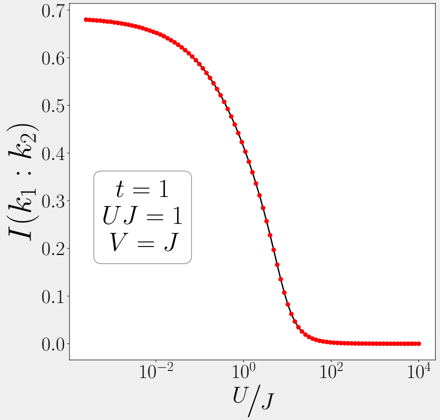
Perturbation parameter, zero mode gap and local FL strength



closing of gap, breakdown of p. theory, extremely **correlated** LFL

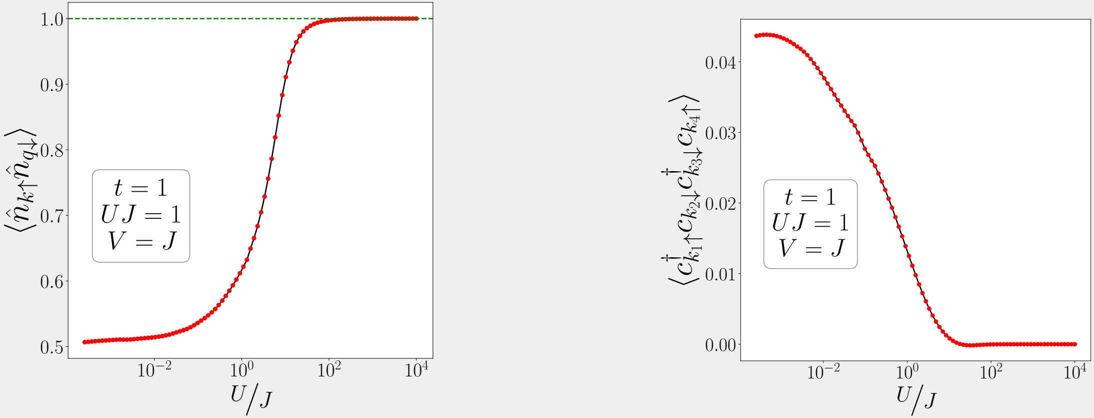
Mutual information within the Kondo cloud





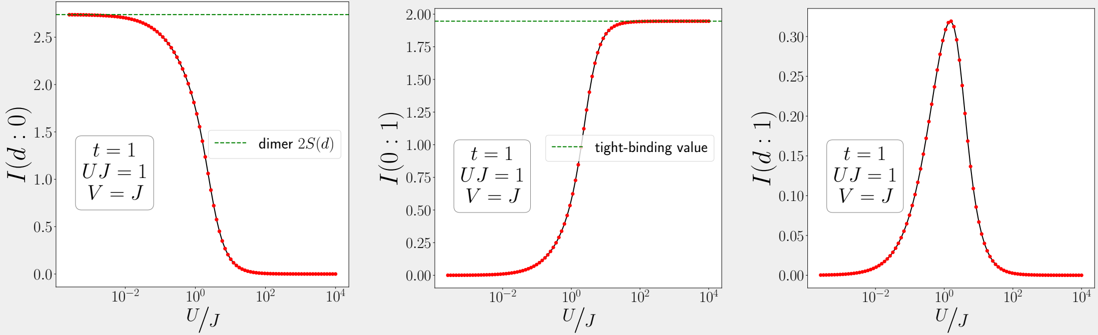
- loss of spin-flip scattering and **disappearance of Kondo cloud**

Many-particle correlations in $k-$space



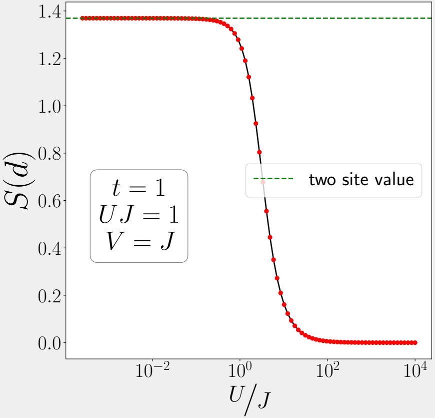
- loss of entanglement within the K cloud, **breakdown of screening**

Mutual information in real space



- *d* and 0 disentangle, 0 gets entangled with the lattice

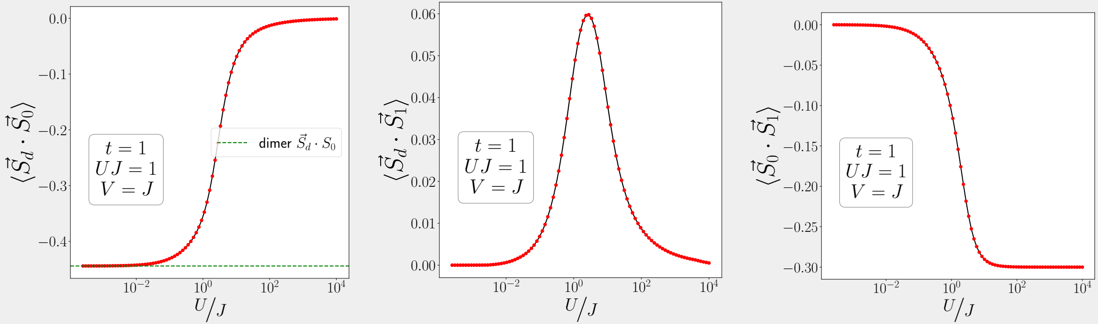
Impurity entanglement entropy



- impurity site **disentangles from the lattice**

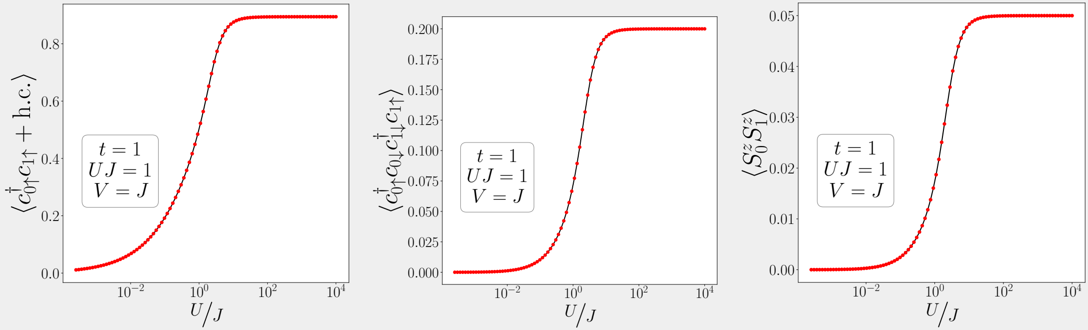
Decoupling of impurity site from lattice

Real space spin-spin correlations



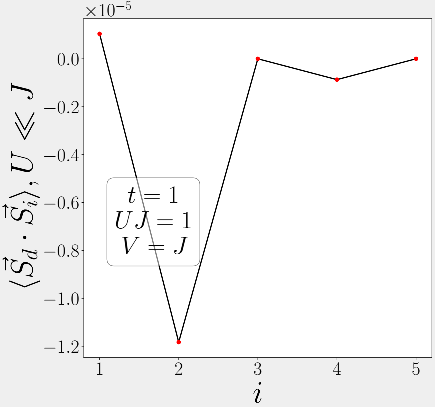
- impurity **spin compensation vanishes** (loss of screening)
- Spin correlation between 0 and 1 increases

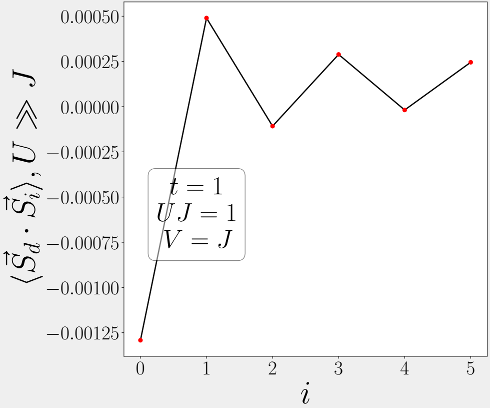
Real space diagonal and off-diagonal correlations



- **Correlations between 0 and 1 increase**
- Result of tight-binding hopping **breaking the singlet**

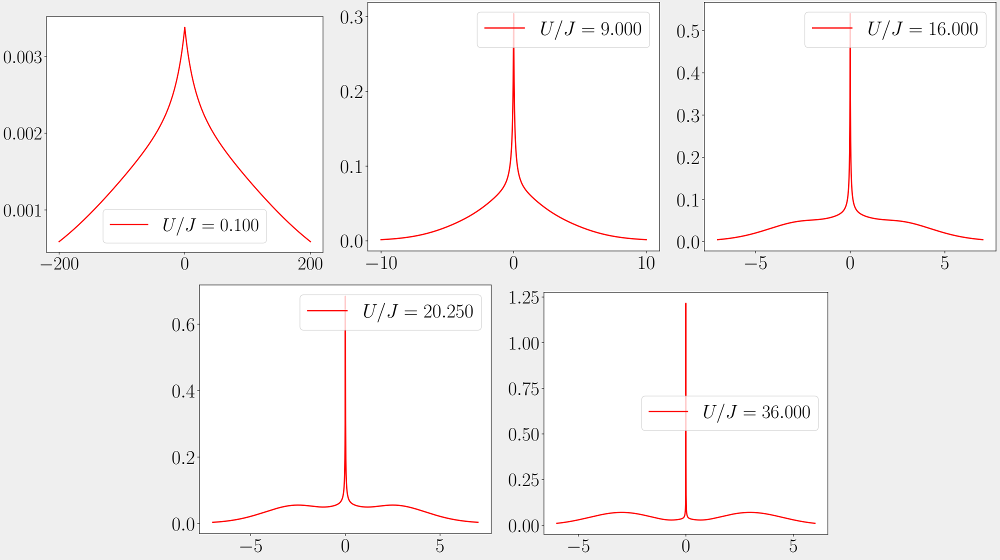
Variation of real-space correlations with distance





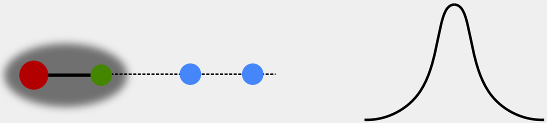
- Correlations **fall off with distance**
- Even sites are AFM in correlation, odd sites are FM

Variation of spectral function

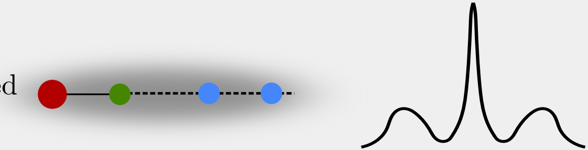


What's happening?

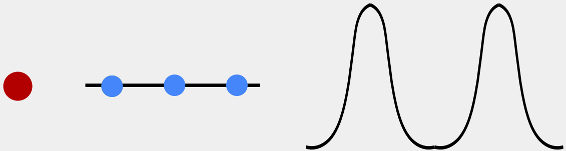
$J, V \gg U, t$: weak LFL



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



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



Discussions & Further Work

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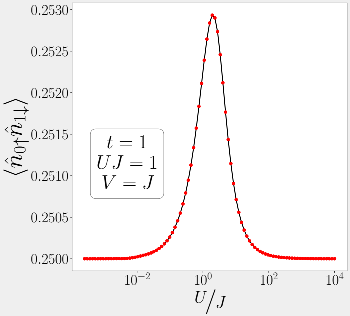
- Stabilising the insulating phase under RG **still remains to be done**.

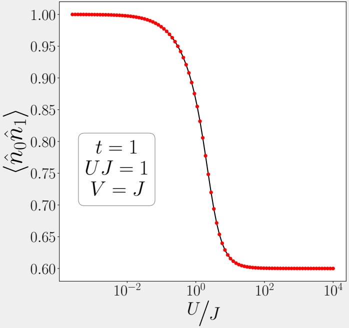
Discussions & Further Work

- 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.

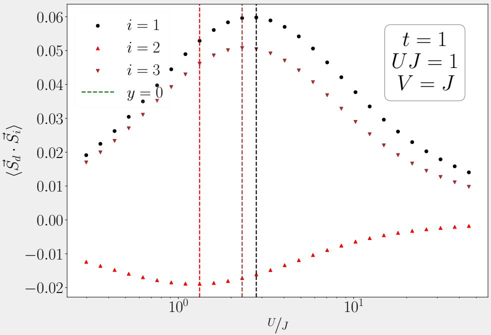
Other measures of correlation in gen. SIAM

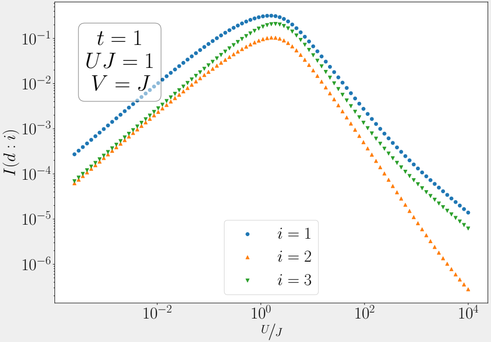
Real space correlations





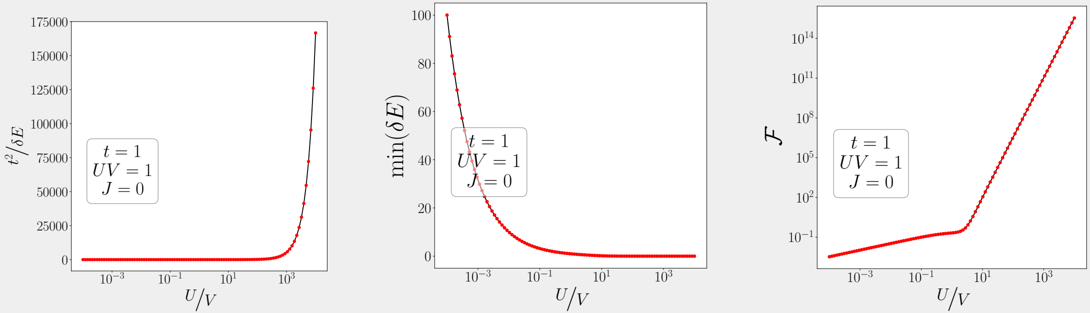
Real space correlations as functions of distance



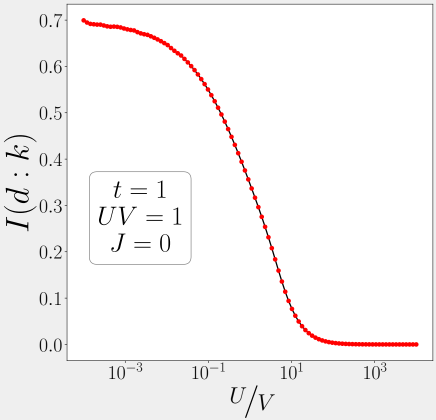


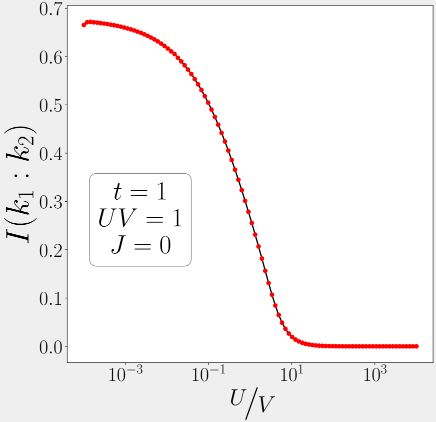
Measures of correlation in pure SIAM

Perturbation parameter, zero mode gap and local FL strength

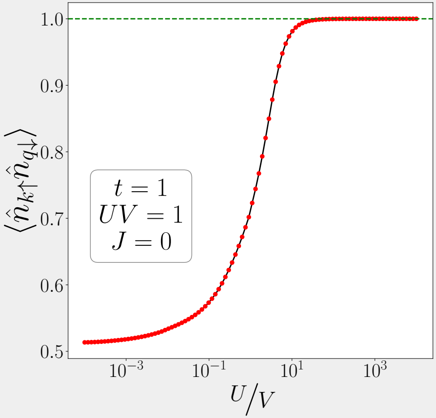


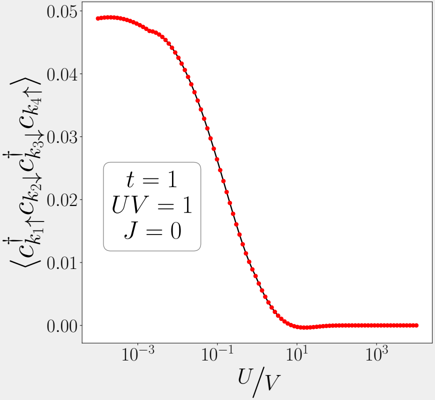
Mutual information within the Kondo cloud



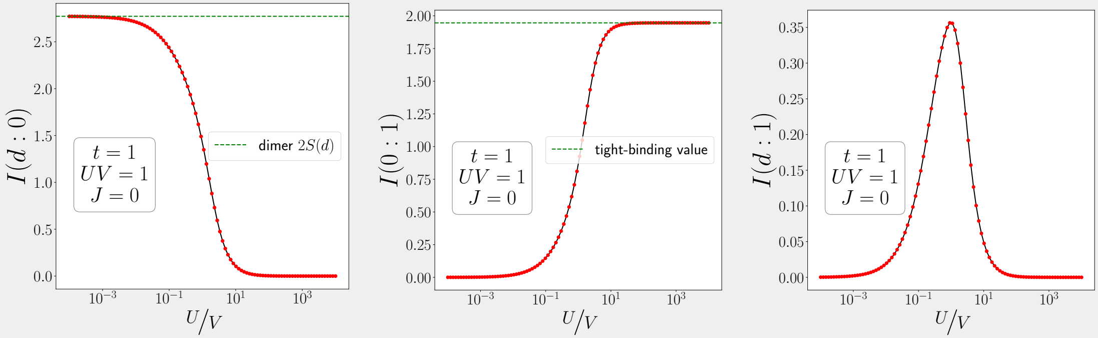


Many-particle correlations in $k-$space

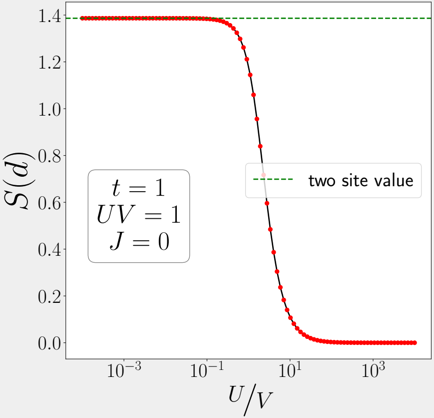




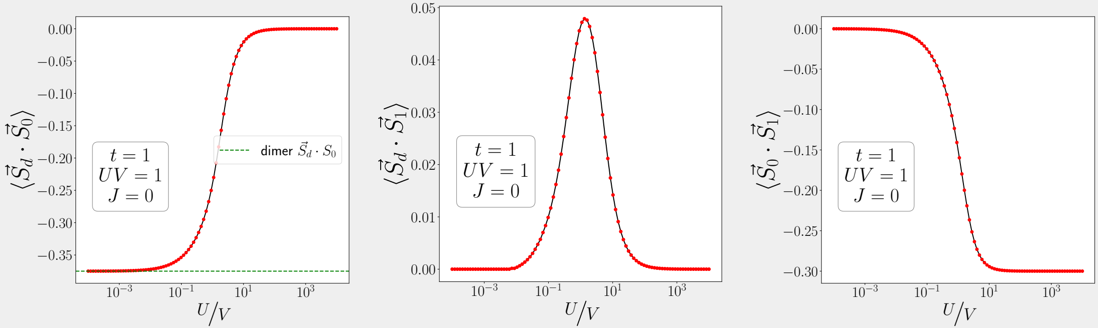
Mutual information in real space



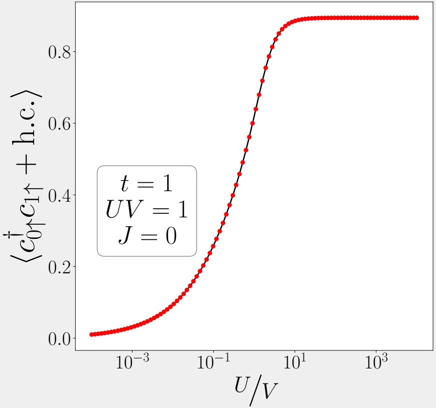
Impurity entanglement entropy

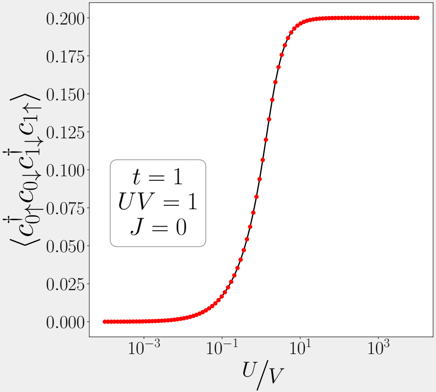


Real space spin-spin correlations

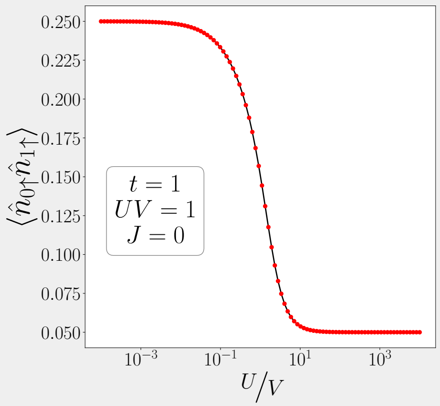


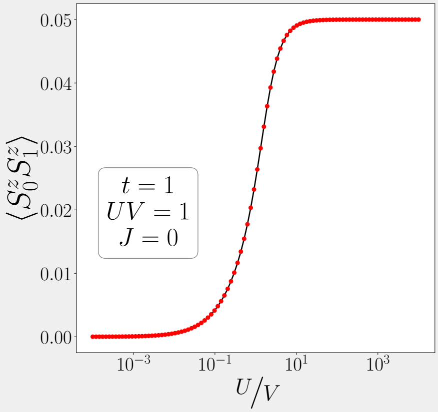
Real space off-diagonal 1-particle and 2-particle correlations





Real space diagonal correlations





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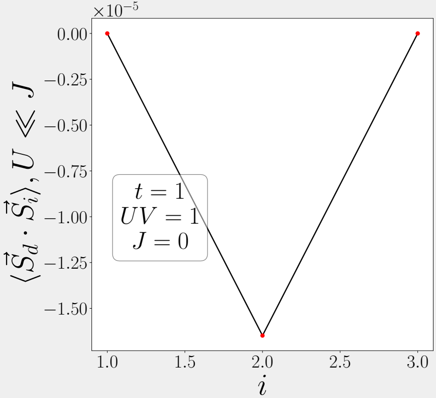
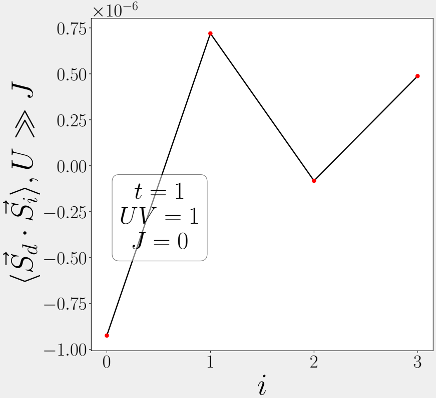
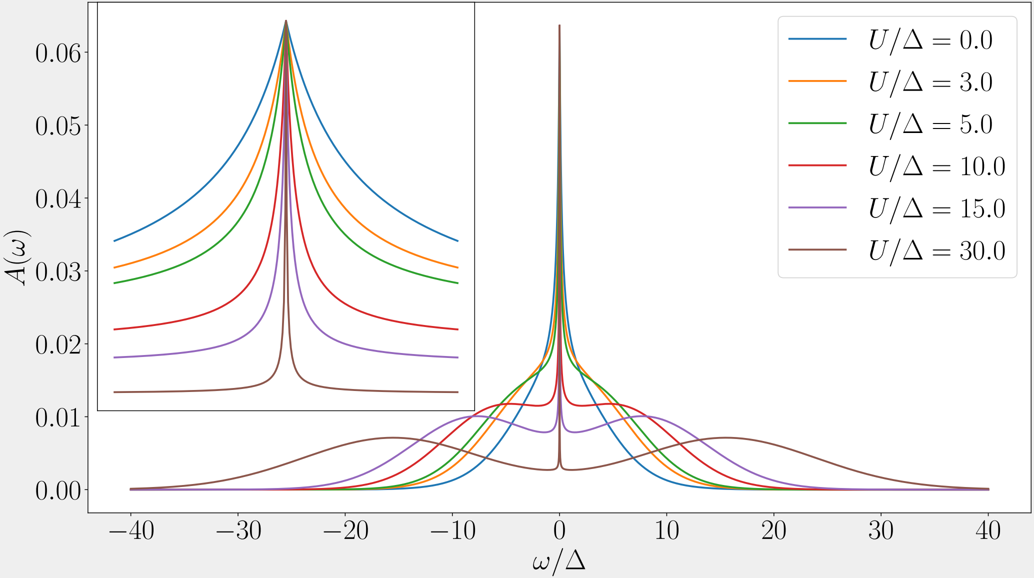




Impurity spectral function (Gen. SIAM)



Form of Kondo cloud Hamiltonian

$$H_{\text{eff}} = 2h S_0^z + \frac{2}{J^*} h^2 S_0^z + \sum_{1234} V_{1234}\, c^\dagger_{k_4\uparrow} c_{k_3\downarrow} c^\dagger_{k_2\downarrow} c_{k_1\uparrow}$$

$$V_{1234} = \left(\epsilon_{k_1} - \epsilon_{k_3}\right)\left[1 - \frac{2}{J^*}\left(\epsilon_{k_3} - \epsilon_{k_1} + \epsilon_{k_2} + \epsilon_{k_4}\right)\right]$$

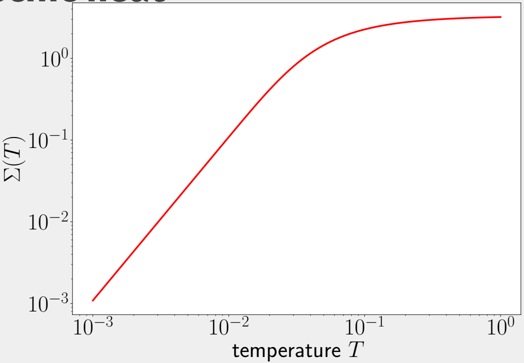
- Mixture of **Fermi liquid** and **two-particle off-diagonal scattering term**
- Fermi liquid part: **result of Ising scattering**
- 2P off-diagonal term: **Non-Fermi liquid** in character - **result of spin-flip scattering**
- NFL part **leads to screening** and formation of singlet

Impurity specific heat

- Fermi-liquid part renormalises one-particle **self-energy**

$$\bar{\epsilon}_k = \epsilon_k + \Sigma_k$$

$$\Sigma_k = \sum_{k'\sigma'} \frac{\epsilon_{k'}\epsilon_k}{J^*} \delta n_{k',\sigma'}$$



Impurity specific heat

- Fermi-liquid part renormalises one-particle **self-energy**

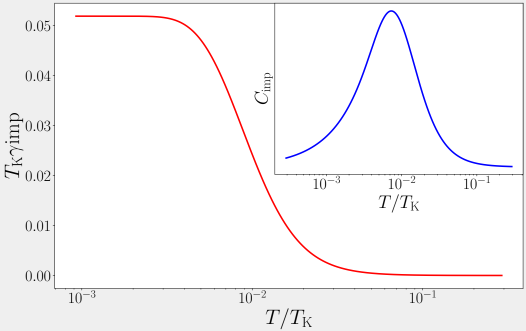
$$C_V = \gamma \times T$$

$$\bar{\epsilon}_k = \epsilon_k + \Sigma_k$$

$$\Sigma_k = \sum_{k'\sigma'} \frac{\epsilon_{k'}\epsilon_k}{J^*} \delta n_{k',\sigma'}$$

- Compute renormalisation in C_V:

$$C_{\mathrm{imp}} = \sum_{k,\sigma} \frac{1}{T^2} \left[\frac{(\bar{\epsilon}_k)^2 e^{\beta\bar{\epsilon}_k}}{(e^{\beta\bar{\epsilon}_k}+1)^2} - \frac{(\epsilon_k)^2 e^{\beta\epsilon_k}}{(e^{\beta\epsilon_k}+1)^2} \right]$$



Wilson 1975; Andrei, Furuya, and Lowenstein 1983; Wiegmann 1981.

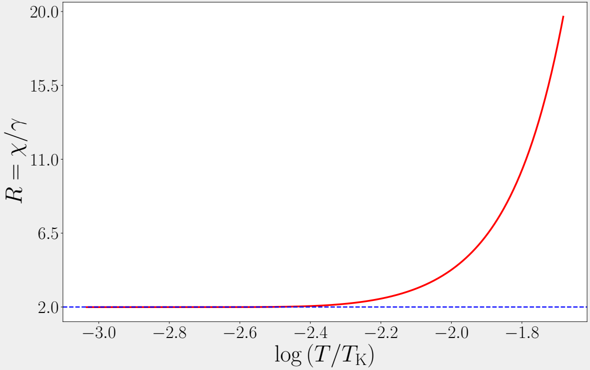
Wilson ratio

$R = \frac{\chi}{\gamma}$

$\chi(T \to 0) = \frac{1}{2J^*}$

$\gamma(T \to 0) = \frac{1}{4J^*}$

R saturates to 2 as $T \to 0$



Wilson 1975; Andrei, Furuya, and Lowenstein 1983; Wiegmann 1981.