Unitary Renormalization Group Approach to the Single-Impurity Anderson model

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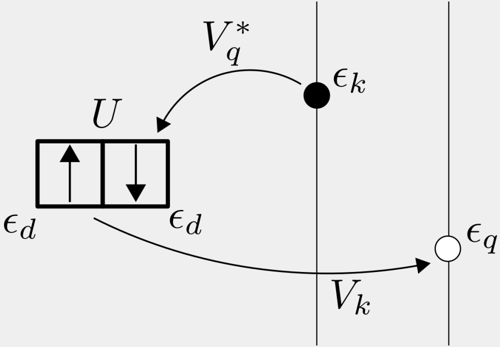
The Single-Impurity Anderson Model

$$\mathcal{H} = \overbrace{\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}}^{\text{conduction bath}} + \overbrace{\sum_{k\sigma} \left[V(k) c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right]}^{\text{hybridisation}} + \overbrace{\epsilon_d \sum_{\sigma} \hat{n}_{d\sigma}}^{\text{impurity site energy}} + \overbrace{U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}^{\text{d-d repulsion}}$$



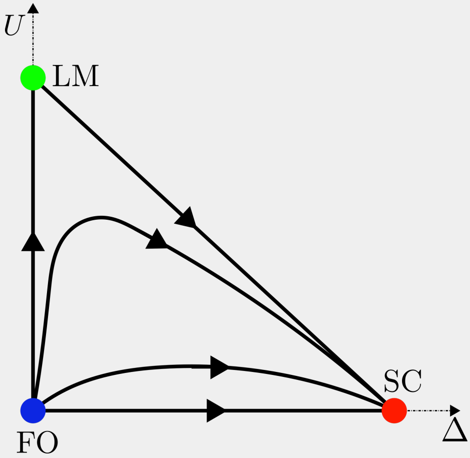
$$\rho(\epsilon) \approx \rho(\epsilon_F)$$

$$\Delta = \rho V^2$$

$$\epsilon_d = -\frac{1}{2} U$$

NRG Results - Symmetric Model

- the **free-orbital** fixed point ($U = \Delta = 0$) - unstable
- the **local moment** fixed point ($U = \infty, \Delta = 0$) - saddle point, and
- the **strong-coupling** fixed point ($\Delta = \infty, U =$ finite) - stable.



Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?

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- How does the renormalization affect the **many-particle entanglement** between the electrons?
- Are there any interesting **topological aspects** of the fixed points?

The Short Version

Apply *unitary many-body transformations* to the Hamiltonian so as to successively *decouple* high energy states and hence obtain scaling equations.

$$\mathcal{H}(D)$$

$$\Downarrow$$

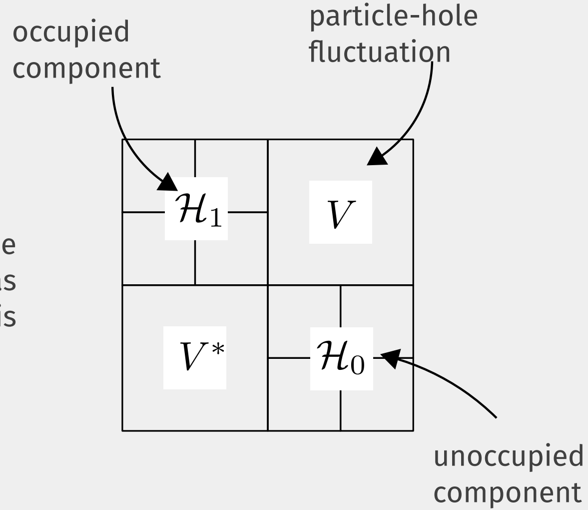
$$U\mathcal{H}(D)U^\dagger$$

$$\Downarrow$$

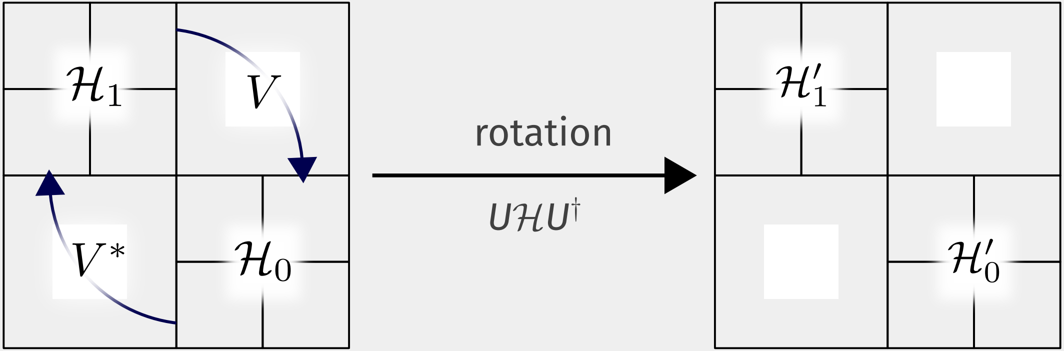
$$H(D) + \mathcal{H}'(D - \delta D)$$

Step 1:

Start with the electrons farthest from the Fermi surface. Write the Hamiltonian as *diagonal and off-diagonal terms* in this basis.



Step 2:
Rotate the Hamiltonian to kill the off-diagonal blocks.

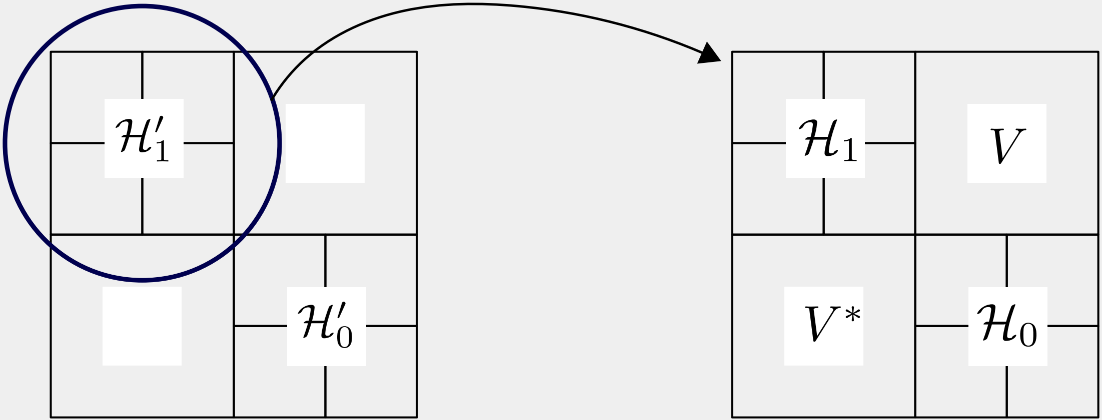


$[\mathcal{H}, \hat{n}] \neq 0$

$[\mathcal{H}, \hat{n}] = 0$

Step 3:

Repeat the process with the new blocks.



Model: Generalized SIAM

$$H = H_{\mathrm{SIAM}} + J\vec{S_d} \cdot \vec{s} + K\vec{C_d} \cdot \vec{c}$$

$$\vec{S_d} \equiv \frac{1}{2}\sum_{\alpha\beta} c^\dagger_{d\alpha}\vec{\sigma}_{\alpha\beta}c_{d\beta}$$

$$\vec{s} \equiv \frac{1}{2}\sum_{\alpha\beta} c^\dagger_{0\alpha}\vec{\sigma}_{\alpha\beta}c_{0\beta}$$

$$\vec{C_d} \equiv \frac{1}{2}\sum_{\alpha\beta} \psi^\dagger_{d\alpha}\vec{\sigma}_{\alpha\beta}\psi_{d\beta}$$

$$\vec{c} \equiv \frac{1}{2}\sum_{\alpha\beta} \psi^\dagger_{0\alpha}\vec{\sigma}_{\alpha\beta}\psi_{0\beta}$$

$$\vec{\psi}_d \equiv \begin{pmatrix} c_{d\uparrow} \\ c^\dagger_{d\downarrow} \end{pmatrix}$$

$$\vec{\psi}_0 \equiv \sum_k \begin{pmatrix} c_{k\uparrow} \\ c^\dagger_{k\downarrow} \end{pmatrix}$$

Results: RG Equations

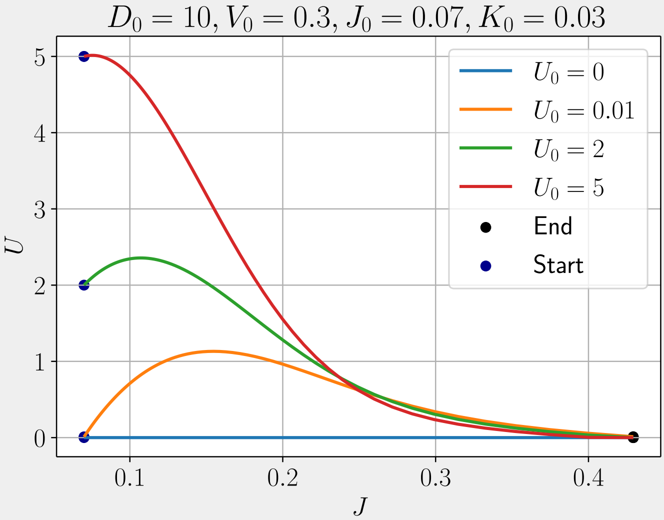
$$\Delta U = 4|V|^2 \left[\frac{1}{\omega - \frac{1}{2}D + \frac{U}{2} + \frac{1}{2}J} - \frac{1}{\omega - \frac{1}{2}D - \frac{U}{2} + \frac{1}{2}K}\right] + \sum_{k<\Lambda_j} \frac{3}{4}\frac{K^2 - J^2}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}$$

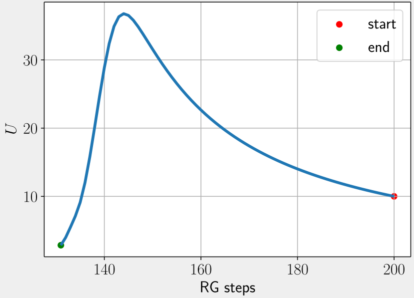
$$\Delta V = \frac{VK}{16}\left(\frac{1}{\omega - \frac{1}{2}D - \frac{U}{2} + \frac{1}{2}K} + \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}\right) - \frac{3VJ}{4}\left(\frac{1}{\omega - \frac{1}{2}D + \frac{U}{2} + \frac{1}{2}J} + \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}\right)$$

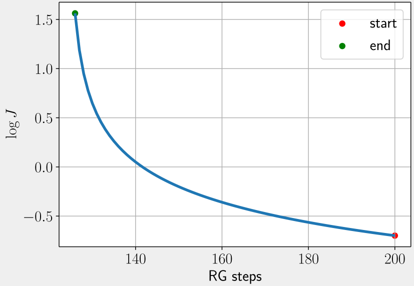
$$\Delta J = -J^2\left(\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K\right)^{-1}$$

$$\Delta K = -K^2\left(\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K\right)^{-1}$$

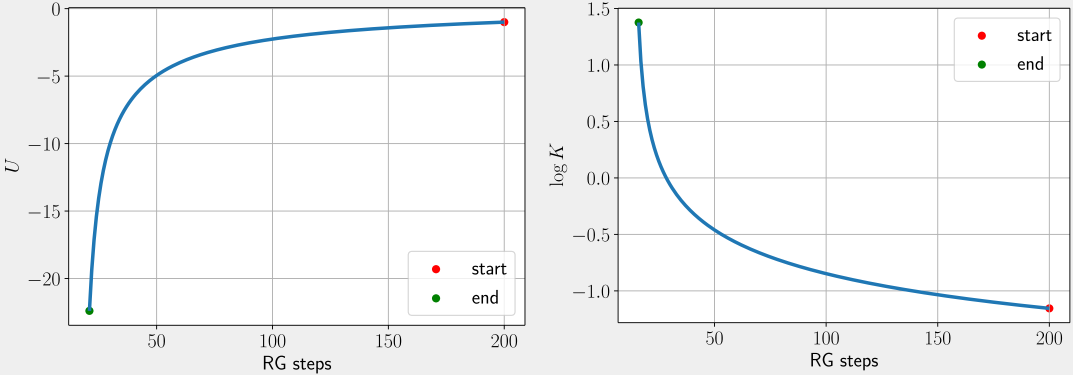
Results: $U > 0, J > K$



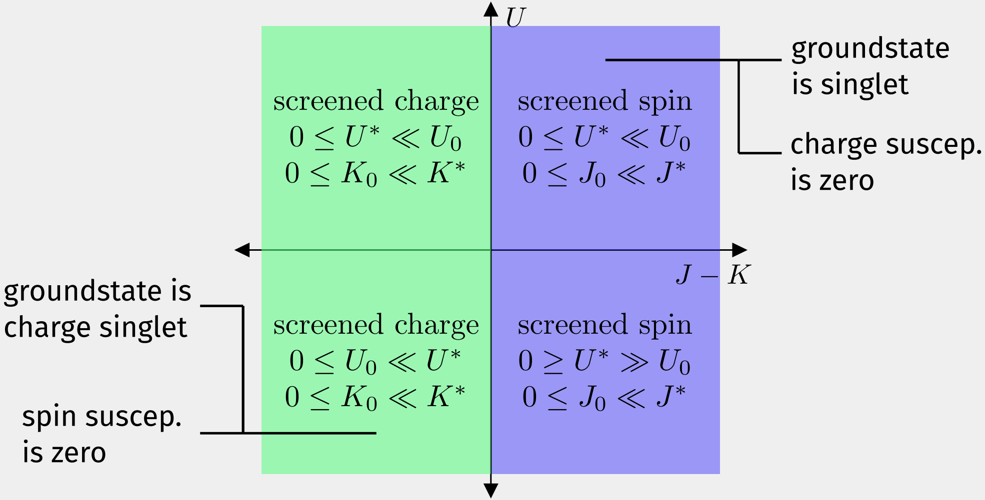




Results: $U < 0, J < K$

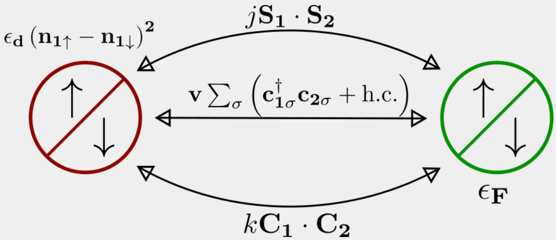


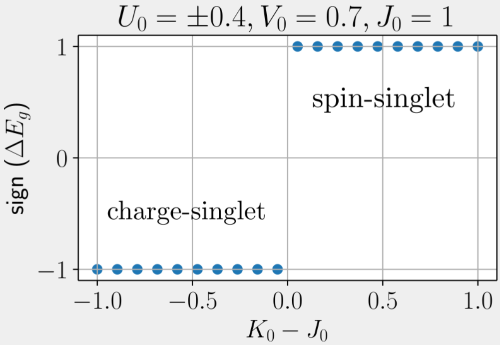
Results: Phase Diagram



Results: Effective Zero-mode Hamiltonian

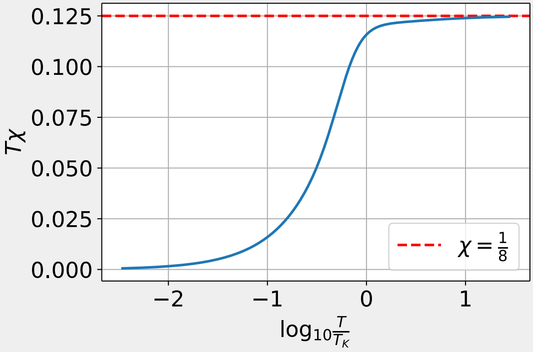
$$H_{IR} = \epsilon_d^* \left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 + V^* \sqrt{N^*} \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + \text{h.c.}\right) + J^* N^* \vec{S}_1 \cdot \vec{S}_2 + K^* N^* \vec{C}_1 \cdot \vec{C}_2$$

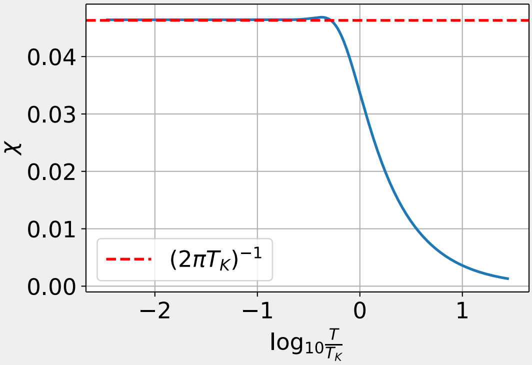




Results: Spin Susceptibility

$$\chi_s = \lim_{B \to 0} \frac{\partial m}{\partial B}$$

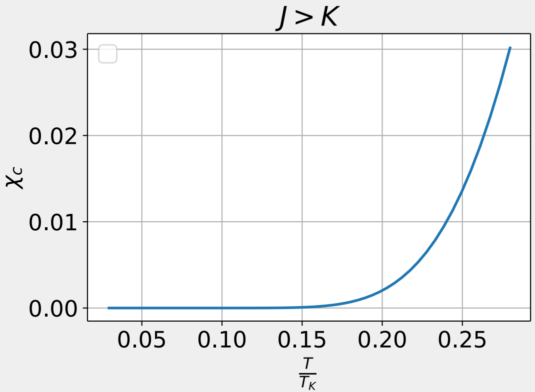


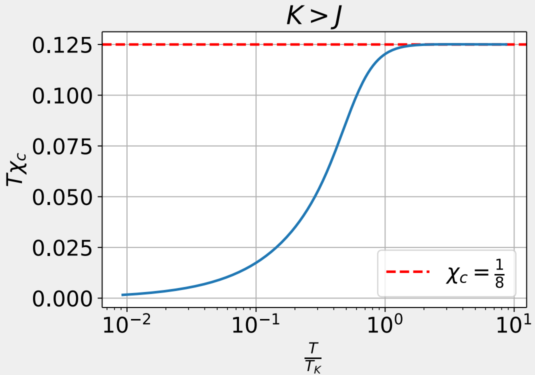


$(\chi \times T)(T \to 0) = \frac{1}{2j}$ $\qquad T_K \equiv \frac{2N^*}{\pi}(D^* - 2\omega)$ $\qquad \chi(T \to \infty) = \frac{1}{8}$

Results: Charge Susceptibility

$$\chi_c = \lim_{\mu \to 0} \frac{\partial N}{\partial \mu}$$

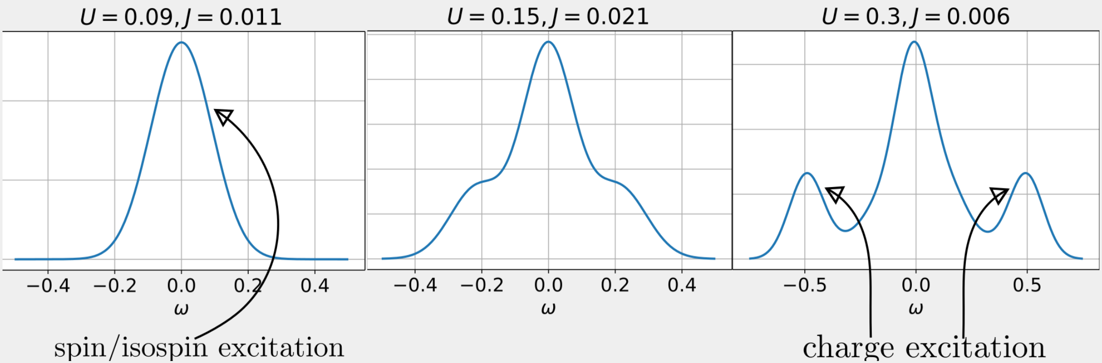




$$(\chi_c \times T)(T \to 0)\Big|_{K>J} = \frac{1}{2k} \qquad (\chi_c \times T)(T \to 0)\Big|_{J>K} = 0 \qquad \chi(T \to \infty) = \frac{1}{8}$$

Results: Impurity Spectral Function

$$\mathcal{A}(\omega) = -\frac{1}{\pi}\mathrm{Im}\ \left[G^{\sigma}_{dd}(\omega)\right] \qquad G^{\sigma}_{dd}(t) = -i\theta(t)\left\langle\left\{c_{d\sigma}(t), c^{\dagger}_{d\sigma}\right\}\right\rangle$$



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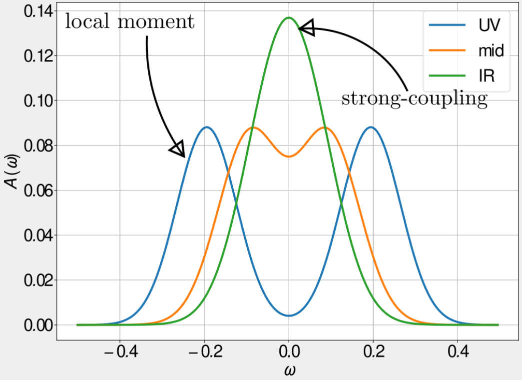
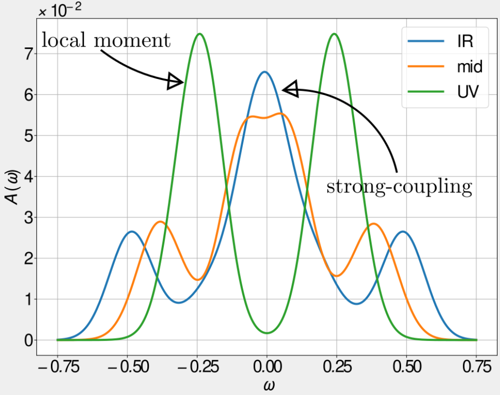
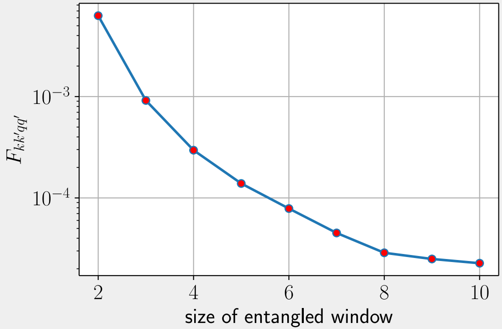




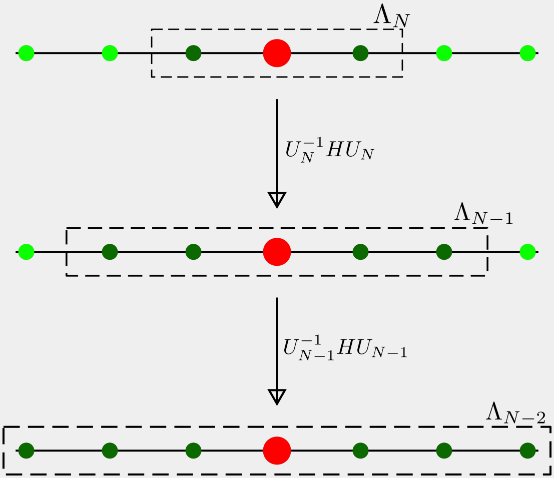
Results: Kondo Cloud Hamiltonian

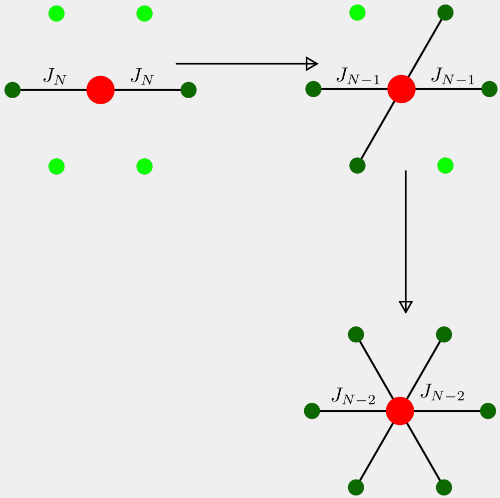
$$H^*(\mathrm{d}, \mathrm{cloud}) \xrightarrow{\text{solve for bath Hamiltonian}} H^*_{\mathrm{cloud}}$$

$$H^*_{\mathrm{cloud}} = \overbrace{H^*_0}^{\text{kinetic energy}} + \overbrace{\sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'}}^{\text{Fermi liquid-type interaction}} + \overbrace{\sum_{kk'qq'} F_{kk'qq'} c^\dagger_{k\uparrow} c^\dagger_{k'\downarrow} c_{q\uparrow} c_{q'\downarrow}}^{\text{non-Fermi liquid-type interaction}}$$

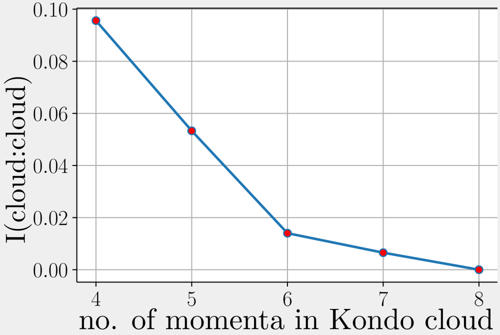


Results: Reverse RG: Overview

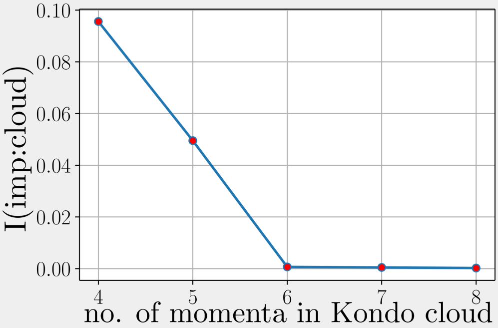


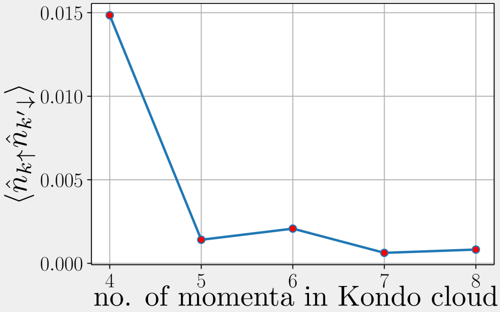


$$I(A:B) = S_A + S_B - S_{AB}$$

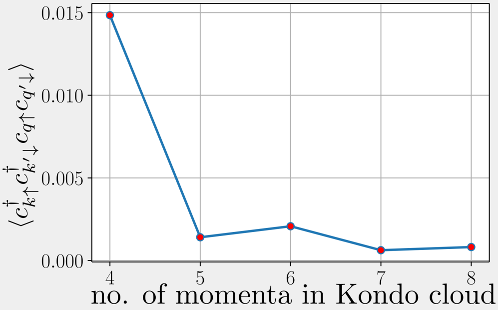


$$S_A = -\mathrm{Tr}\,\left[\rho_A \ln \rho_A\right]$$





$\langle \hat{n}_{k\uparrow}\hat{n}_{k'\downarrow}\rangle$
0.015
0.010
0.005
0.000
4
5
6
7
8
no. of momenta in Kondo cloud



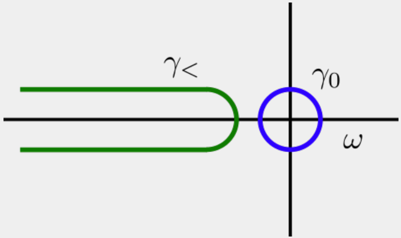
$\langle c^\dagger_{k\uparrow}c^\dagger_{k'\downarrow}c_{q\uparrow}c_{q'\downarrow}\rangle$
0.015
0.010
0.005
0.000
4
5
6
7
8
no. of momenta in Kondo cloud

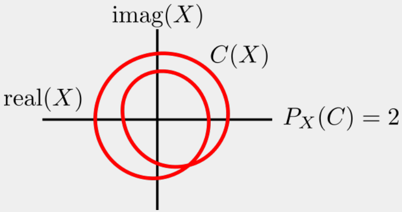
Results: Luttinger's Theorem

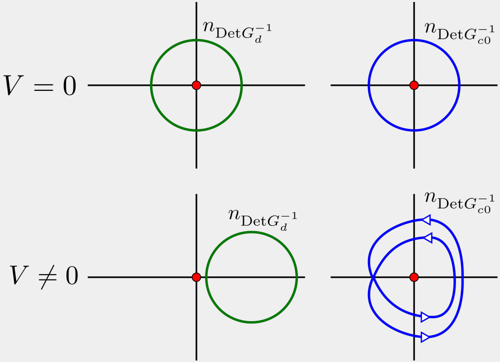
$$\overbrace{N}^{\text{total no. of particles}} = \overbrace{P_{\mathrm{Det}\,G_d}(\Gamma_<) + \frac{1}{2}P_{\mathrm{Det}\,G_d}(\Gamma_0)}^{\text{no. of poles of imp. Greens func.}} + \overbrace{V_L}^{\text{no. of poles of cbath Greens func}}$$

$$P_X(C) \equiv \frac{1}{2\pi i}\oint_C dz \frac{\partial \ln X}{\partial z} = \text{no. of poles of } X \text{ enclosed by curve } C$$

$$= \frac{1}{2\pi i}\oint_{C(X)} \frac{dX}{X} = \text{winding number of } X \text{ around } X(C)$$







$$n_{\mathrm{Det}\ G_d^{-1}} = 1$$

$$n_{\mathrm{Det}\ G_d^{-1}} = 0$$

$$V_L = V_L^0 + 1$$

$$H^* = \overbrace{J^*\vec{S_d}\cdot\vec{s} + K^*\vec{C_d}\cdot\vec{c} + V^*\left(c^\dagger_{d\sigma}c_{0\sigma} + \text{h.c.}\right)}^{\text{solve exactly}} + \overbrace{t\sum_{\langle i,j\rangle} c^\dagger_{i\sigma}c_{j\sigma}}^{\text{treat as perturbation}}$$

$$\Big\downarrow \; 4^{\text{th}} \text{ fourth order pert.}$$

$$E_1^{(4)} = -\frac{16t^4}{3J^{*3}}, E_2^{(4)} = -\frac{16t^4}{9J^{*3}}$$

$$H^* \sim J^*\vec{S_d}\cdot\vec{s} + K^*\vec{C_d}\cdot\vec{c} + V^*\left(c^\dagger_{d\sigma}c_{0\sigma} + \text{h.c.}\right) + \overbrace{\frac{t^4}{J^{*3}}\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}}^{\text{local Fermi liquid}}$$

$$\langle\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}\rangle \xrightarrow[]{\substack{\text{mean field}\\ \text{approximation}}} \langle\hat{n}_{1\uparrow}\rangle\langle\hat{n}_{1\downarrow}\rangle$$

Results: Wilson Ratio ($T = 0$)

$$\epsilon_{k\sigma} = \epsilon_k^0 + \sum_q f_{kq} \langle n_{q\overline{\sigma}} \rangle$$

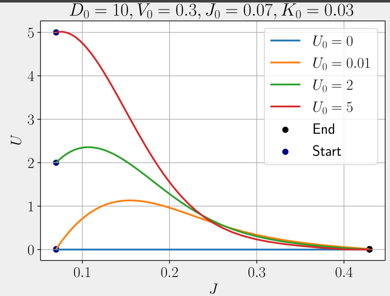
- $f_{\uparrow\uparrow} = 0$
- $\chi_c(T \to 0) = 0$

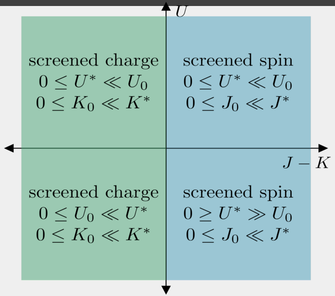
$$\longrightarrow$$

- $C_v(T \to 0) = \rho_{\text{imp}} T$
- $\chi_s(T \to 0) = 2\rho_{\text{imp}}$

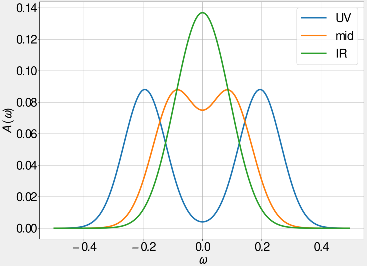
$$R = \frac{\chi_s}{\gamma} = 2$$

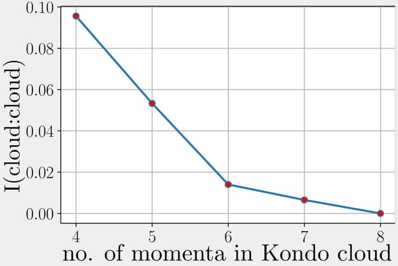
Summary of Results





$$H_{\text{cloud}} = H_0^* + H_{Fl} + H_{NFL}$$





$$V_L = V_L^0 + 1$$

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What's Next?

We have barely scratched the surface of the problem.

- Asymmetric model and valence fluctuations
- effective Hamiltonians and wavefunctions.
- entanglement measures and dynamic quantities like susceptibility
- use as impurity solver in DMFT
- extensions to the Kondo and Anderson lattices, and hence to the problem of heavy Fermions

Thank You!