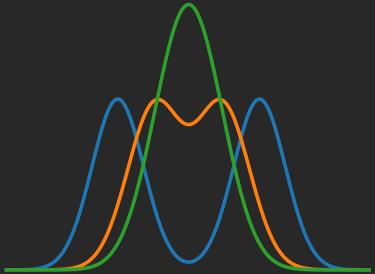
Unitary Renormalization Group Solution of the Single-Impurity Anderson model



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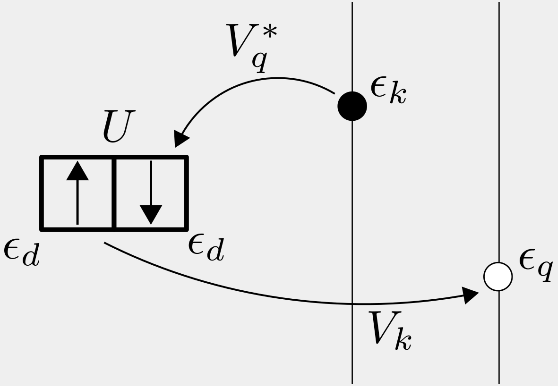
The Single-Impurity Anderson Model

The Single-Impurity Anderson Model

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



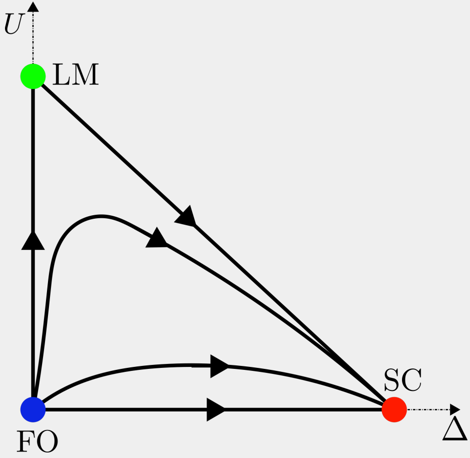
$$\rho(\epsilon) \approx \rho(\epsilon_F)$$

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

$$\epsilon_d = -\frac{1}{2} U \text{ (p-h symmetry)}$$

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.



Krishna-murthy, Wilson, and Wilkins 1975.

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- Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the spectral function?
- How does the renormalization affect the **many-particle entanglement** between the electrons?
- Are there any interesting **topological aspects** of the fixed points?

The Unitary Renormalization Group

Unitary Renormalization Group: Overview

The Short Version

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

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

$$\Big\Downarrow$$

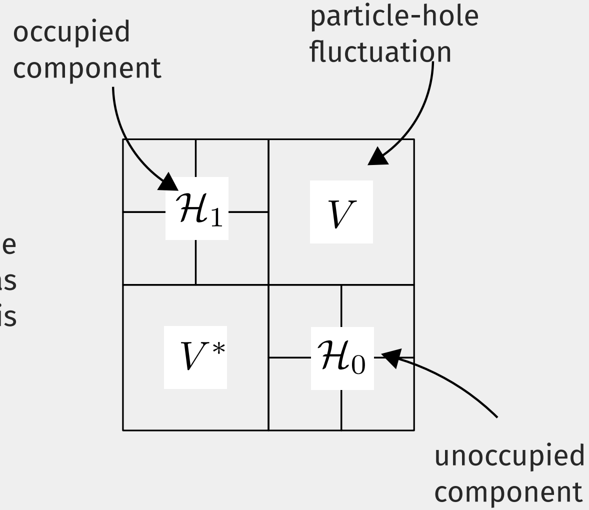
$$U\mathcal{H}(D)U^\dagger$$

$$\Big\Downarrow$$

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

Mukherjee and Lal 2020.

URG: Formalism

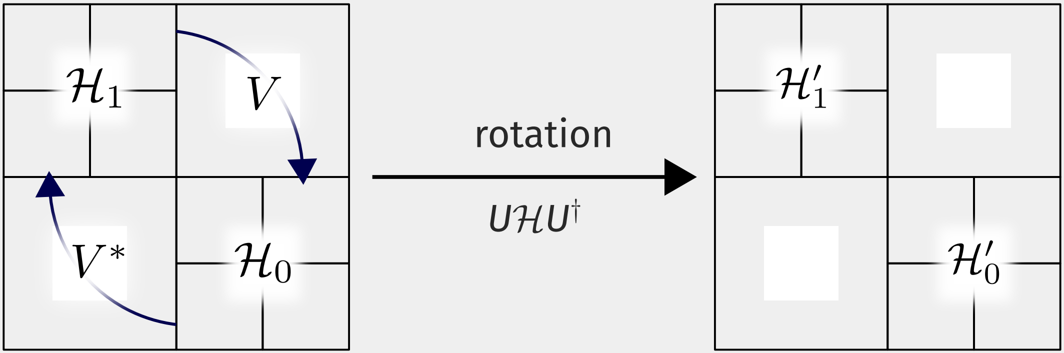


Step 1:

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

Step 2:

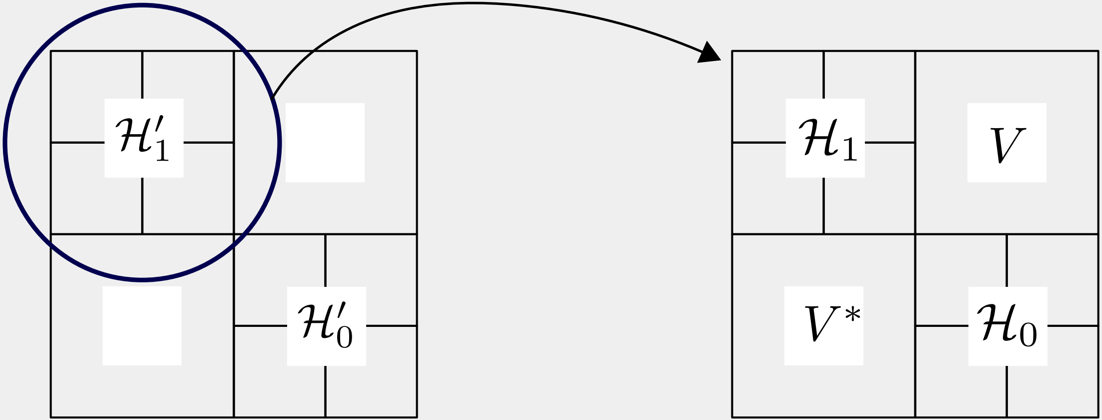
Rotate the Hamiltonian to kill the off-diagonal blocks.



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

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

Step 3:
Repeat the process with the new blocks.



URG: Salient Features

- Presence of the quantum fluctuation energy scale ω
- Presence of finite-valued fixed points
- Spectrum-preserving transformations
- Tractable low-energy effective Hamiltonians

Generalized SIAM

Model: Generalized SIAM

$$H = H_{\mathrm{SIAM}} + J\vec{S}_d \cdot \vec{s} + K\vec{C}_d \cdot \vec{c}$$

$$\vec{S}_d \equiv \frac{1}{2}\sum_{\alpha\beta} c^{\dagger}_{d\alpha}\vec{\sigma}_{\alpha\beta}c_{d\beta} \qquad \vec{s} \equiv \frac{1}{2}\sum_{\alpha\beta} c^{\dagger}_{0\alpha}\vec{\sigma}_{\alpha\beta}c_{0\beta}$$

$$\vec{C}_d \equiv \frac{1}{2}\sum_{\alpha\beta} \psi^{\dagger}_{d\alpha}\vec{\sigma}_{\alpha\beta}\psi_{d\beta} \qquad \vec{c} \equiv \frac{1}{2}\sum_{\alpha\beta} \psi^{\dagger}_{0\alpha}\vec{\sigma}_{\alpha\beta}\psi_{0\beta}$$

$$\vec{\psi}_d \equiv \begin{pmatrix} c_{d\uparrow} \\ c^{\dagger}_{d\downarrow} \end{pmatrix} \qquad \vec{\psi}_0 \equiv \sum_k \begin{pmatrix} c_{k\uparrow} \\ c^{\dagger}_{k\downarrow} \end{pmatrix}$$

Schrieffer and Wolff 1966.

RG Equations, Their Features and Fixed Points

RG Equations

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

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

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

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

Passage to Poor Man's Scaling Results

- $J = 0, K = 0$
- $\omega = -\frac{D}{2}$
- $U = -\frac{\epsilon_d}{2} \ll D$

$$\longrightarrow \qquad \delta U = \delta V = 0$$

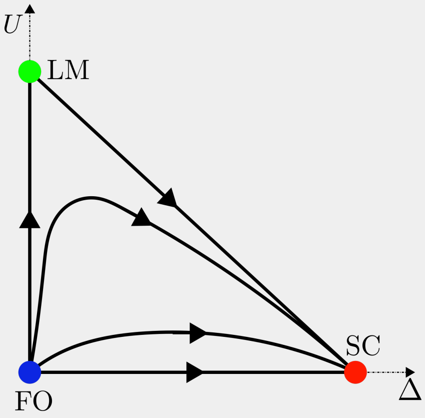
- $J = 0, K = 0$
- $\omega = -\frac{D}{2}$
- $U \gg D \gg \epsilon_d$

$$\longrightarrow \qquad \delta U = \delta V = 0$$

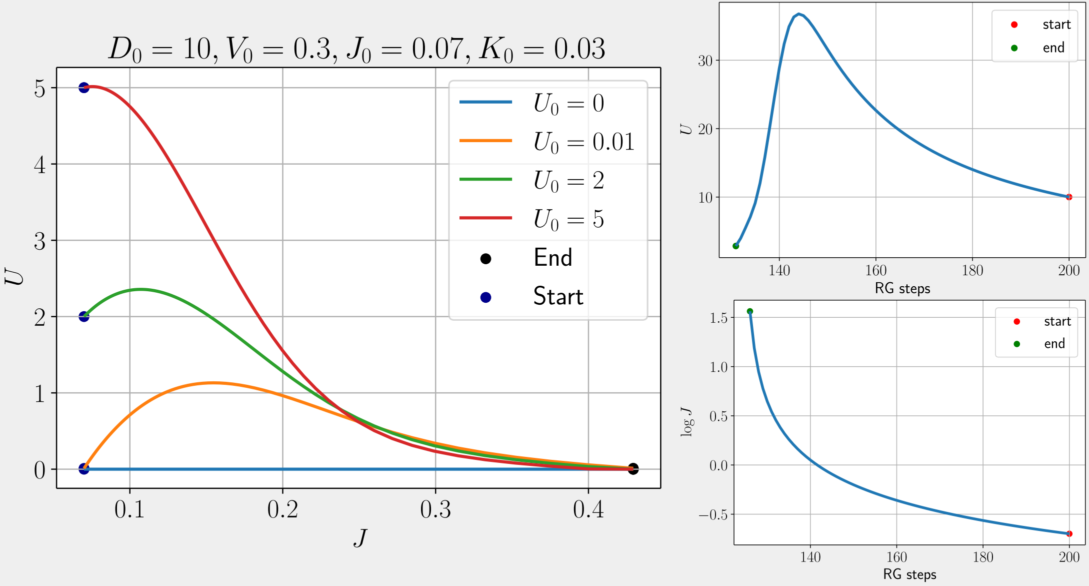
$$\delta \epsilon_d = \frac{\Delta}{\pi} \delta \ln D$$

Fixed Points

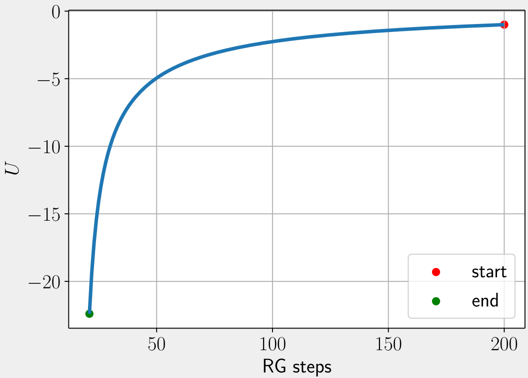
- $J = K = 0 \longrightarrow \Delta V = 0$
- $J, K, V = 0^{+} \longrightarrow (V^*, J^*, K^*) = \text{large}, U^* = 0$
  - **strong-coupling fixed point**
- $J = K = V = 0 \longrightarrow$ all couplings marginal
  - line of fixed points on y-axis
- $U = 0^{+} \longrightarrow$ **local moment fixed point**
  - ground-state is a decoupled impurity spin

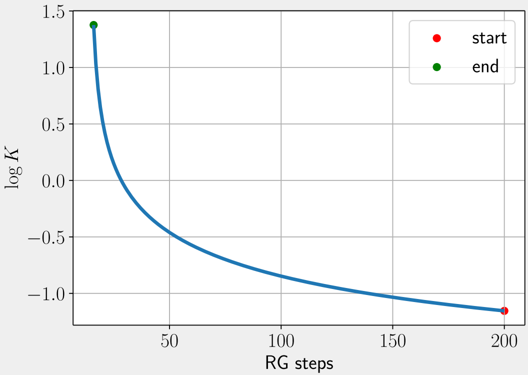


Results: $U > 0, J > K$



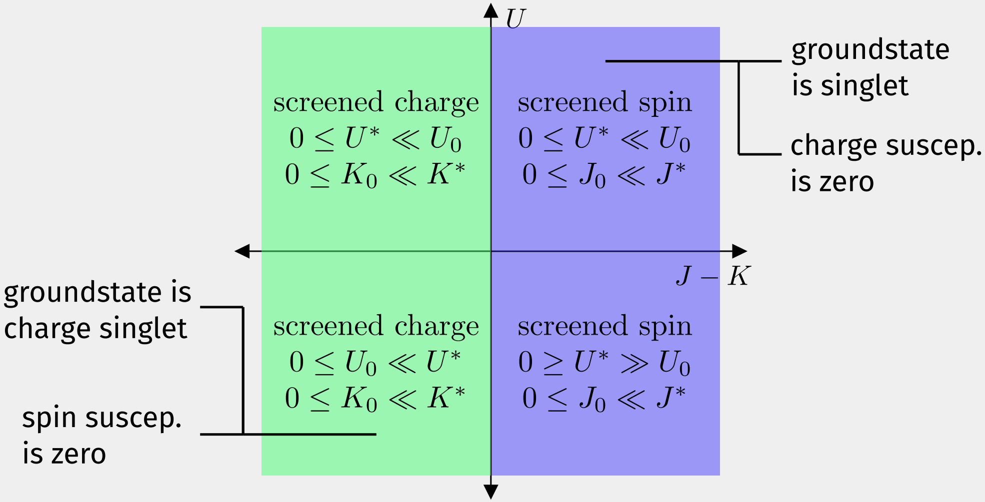
Results: $U < 0, J < K$





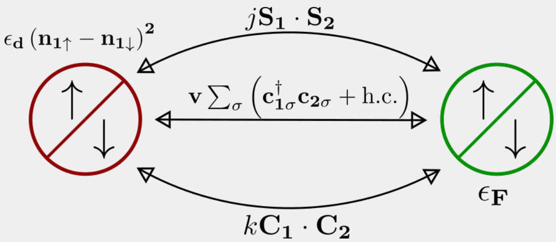
Low energy effective theory and ground state wavefunctions

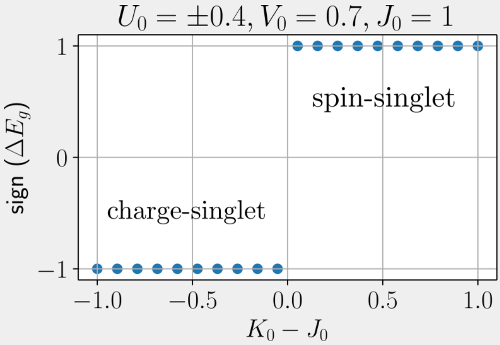
Results: Phase Diagram



Results: Effective Zero-mode Hamiltonian

$$H_{IR} = \epsilon_d^* \left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 + V^* \sqrt{N^*} \sum_\sigma \left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.}\right) + J^* N^* \vec{S_1} \cdot \vec{S_2} + K^* N^* \vec{C_1} \cdot \vec{C_2}$$



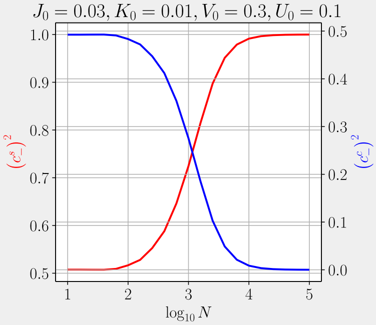


Wilson 1975; Krishna-murthy, Wilson, and Wilkins 1975; Taraphder and Coleman 1991.

Results: Ground State

$$J > K, U > 0$$

$$|\Psi\rangle_{GS} = c^s_- \left[|\uparrow, \Downarrow\rangle - |\downarrow, \Uparrow\rangle\right] + c^c_- \left[|\uparrow, \Downarrow\rangle + |\downarrow, \Uparrow\rangle\right]$$



$$c^s_- \to 1$$

$$c^c_- \to 0$$

$$|\Psi\rangle_{GS} \sim \left[|\uparrow, \Downarrow\rangle - |\downarrow, \Uparrow\rangle\right]$$

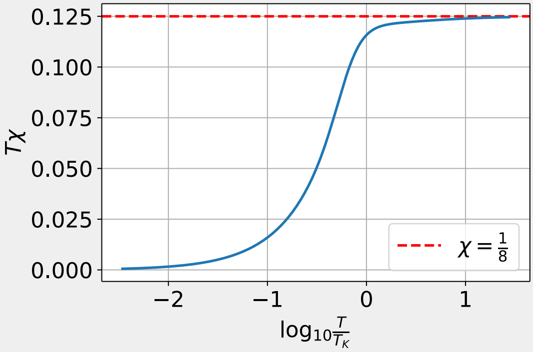
$$J < K, U < 0$$

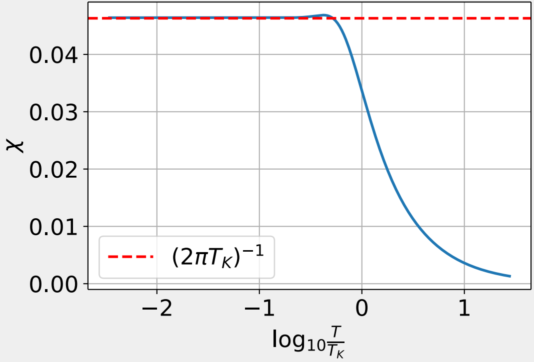
$$|\Psi\rangle_{GS} = \left[|\uparrow_c, \Downarrow_c\rangle - |\downarrow_c, \Uparrow_c\rangle\right]$$

Impurity Susceptibilities and Impurity spectral function

Results: Spin Susceptibility

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



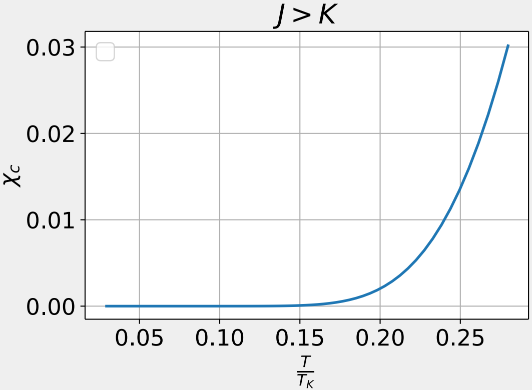


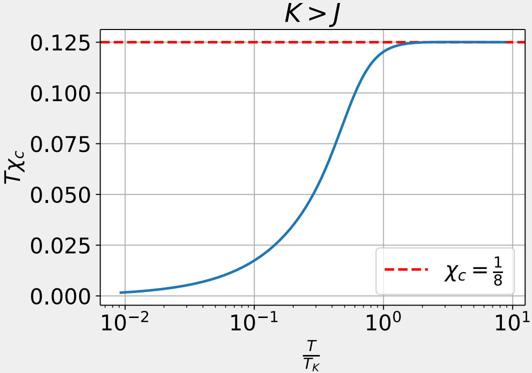
$(\chi \times T)(T \to 0) = \frac{1}{2j}$ $\quad T_K \equiv \frac{2N^*}{\pi}(D^* - 2\omega)$ $\quad \chi(T \to \infty) = \frac{1}{8}$

Wilson 1975; Krishna-murthy, Wilson, and Wilkins 1975.

Results: Charge Susceptibility

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



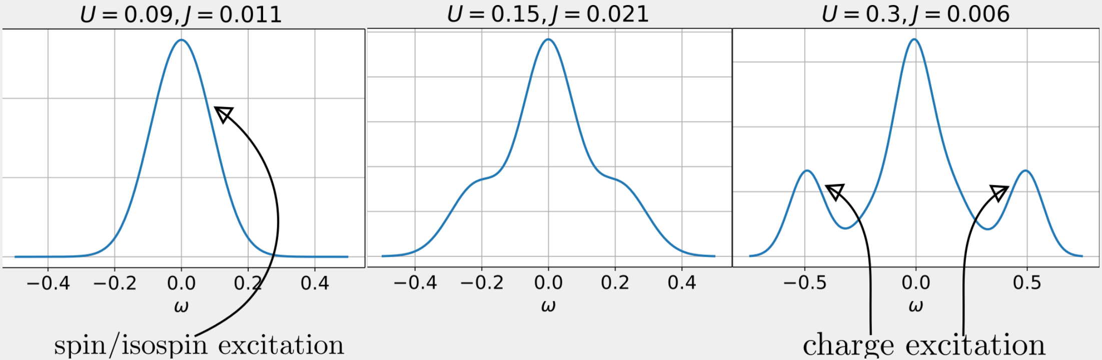


$$(\chi_c \times T)(T \to 0)\Big|_{K>J} = \frac{1}{2k} \qquad (\chi_c \times T)(T \to 0)\Big|_{J>K} = 0 \qquad \chi(T \to \infty) = \frac{1}{8}$$

Taraphder and Coleman 1991; Zitko and Bonca 2006.

Results: Impurity Spectral Function

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

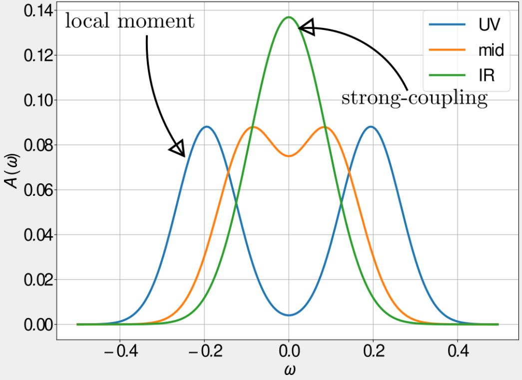


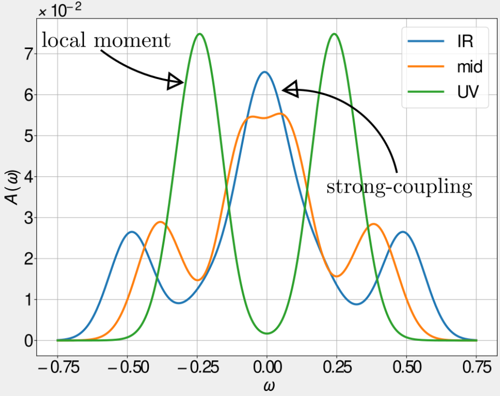
Hewson 1993; Bulla, Costi, and Pruschke 2008.

Results: Spectral Function Renormalization

$$\mathcal{A}(\omega) = -\frac{1}{\pi}\mathrm{Im}\ \left[G^{\sigma}_{dd}(\omega)\right]$$

$$G^{\sigma}_{dd}(t) = -i\theta(t)\left\langle\left\{c_{d\sigma}(t), c^{\dagger}_{d\sigma}\right\}\right\rangle$$



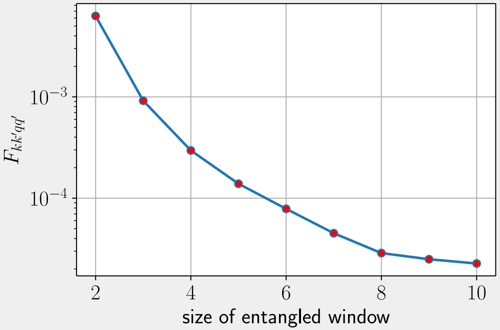


Entanglement measures and Topological Features of low energy theory

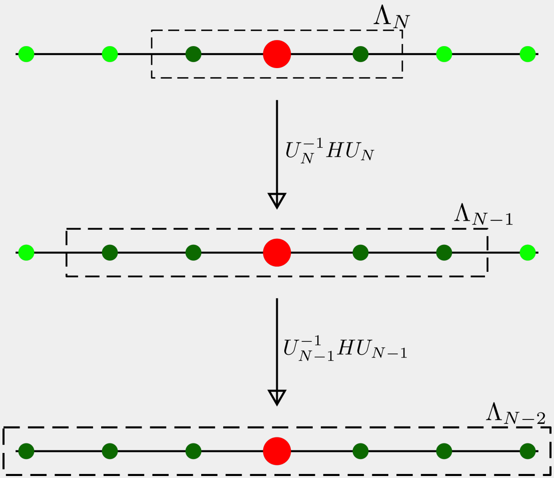
Results: Kondo Cloud Hamiltonian

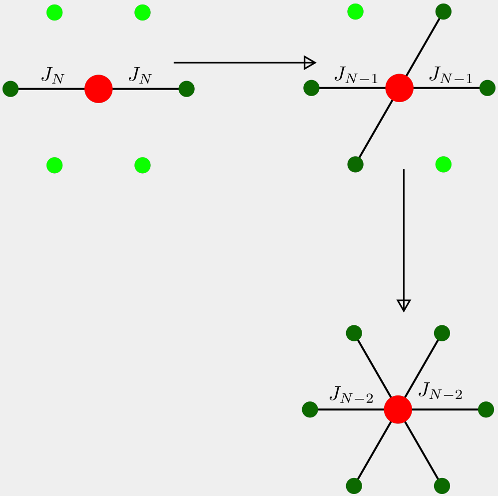
$$H^*(\text{d, cloud}) \xrightarrow{\text{solve for bath Hamiltonian}} H^*_{\text{cloud}}$$

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



Results: Reverse RG: Overview

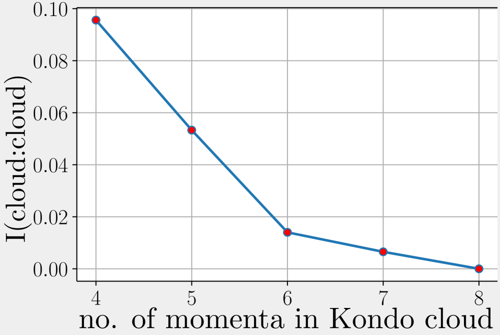


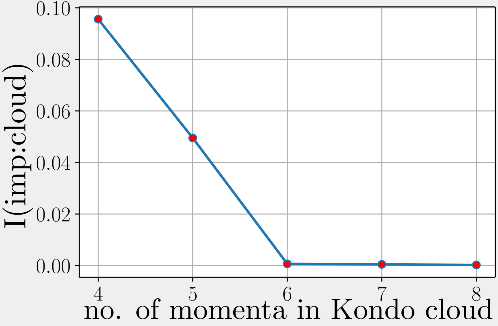


Mukherjee 2020.

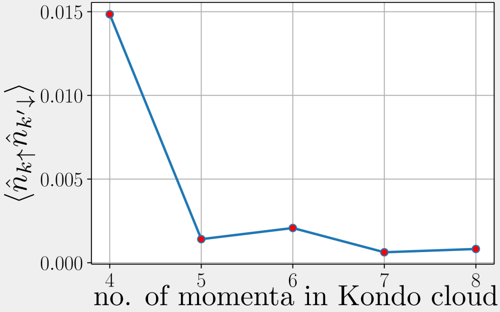
Results: Reverse RG: Mutual Information

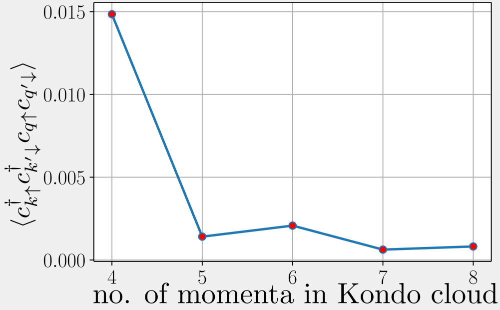
$$I(A:B) = S_A + S_B - S_{AB} \qquad S_A = -\mathrm{Tr}\left[\rho_A \ln \rho_A\right]$$





Results: Reverse RG: Correlations



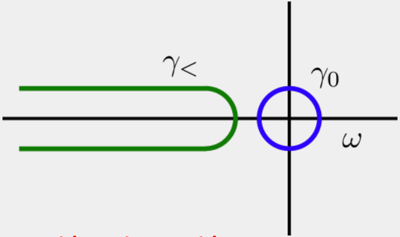


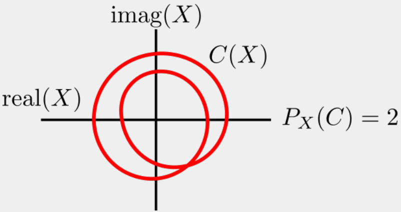
Results: Luttinger's Theorem

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

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

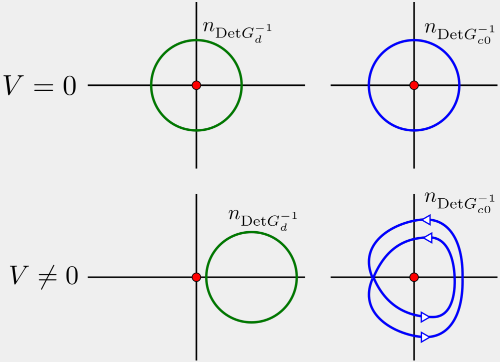
$$= \frac{1}{2\pi i}\oint_{C(X)} \frac{dX}{X} \quad = \text{winding number of } X \text{ around } X(C)$$





Seki and Yunoki 2017.

Results: Luttinger's Theorem



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

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

$$V_L = V_L^0 + 1$$

Martin 1982.

Results: Local Fermi Liquid

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

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

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

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

Nozières 1974.

Results: Wilson Ratio ($T = 0$)

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

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

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

$\longrightarrow$

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

$$R = \frac{\chi_s}{\frac{C_v}{T}} = 2$$

Hewson 1994.

Results: Relation between R and ΔV_L

- particle-hole symmetry
- strong-coupling fixed-point
- $T = 0$

$$\longrightarrow \qquad R = 1 + \sin^2 \delta(0)$$

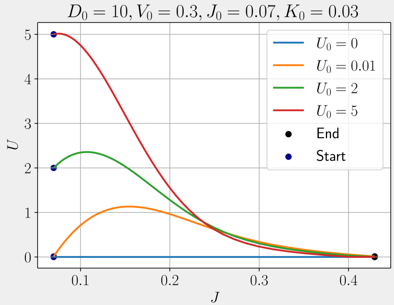
- Friedel's sum rule
- scattering theory arguments

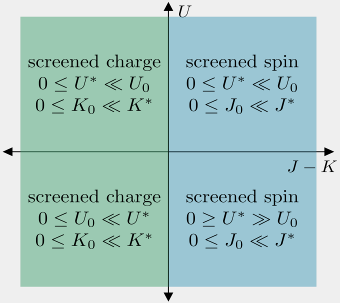
$$\longrightarrow \qquad \frac{1}{\pi}\delta(0) = \tilde{N} = \Delta V_L$$

$$R = 1 + \sin^2 (\pi \Delta V_L)$$

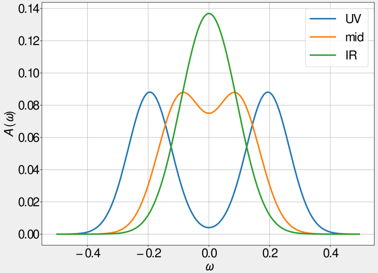
$$\Delta V_L = 1 \longrightarrow R = 2$$

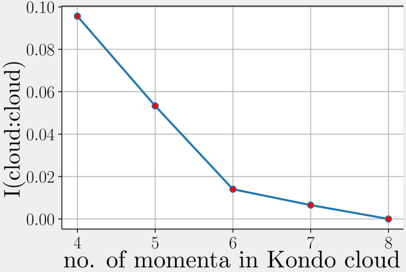
Summary of Results





$$H_{cloud} = H_0 + H_{FL} + H_{NFL}$$





$$R = 1 + \sin^2 \pi \Delta V_L = 2$$

$$\underset{\text{SC}}{\underset{\downarrow}{V_L}} = \underset{\text{LM}}{\underset{\downarrow}{V_L^0}} + 1$$

Future Directions

What's Next?

- Analytical expression for temperature-dependent Wilson ratio
- Separating the contributions of various parts of the Kondo cloud to the spectral function
- Suggested by the generalized double-bracket form of URG, we can try to see if URG can be used as an optimizer.
- Since the zero-mode low-energy theory is an Anderson molecule (which can be exactly solved), it would be interesting to see if there is a transformation which converts the Anderson molecule to the Hubbard molecule.
- We can also check how using more feature-full baths (with non-trivial self-energy) can change the phase diagram.
- extensions to the Kondo and Anderson lattices, and hence to the problem of heavy Fermions

Thanks for your attention!

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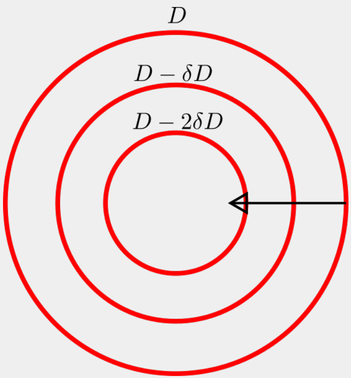
URG: Relation to Poor Man's Scaling

$$H = H_0 + \underbrace{V_+ + V_-}_{\text{off-diagonal terms we want to remove}}$$



Philosophy of Poor Man's scaling:

- Successively eliminate high-energy energy shells
- Write high energy excitations as second-order correction to low-energy scatterings
- Typically perturbative

Anderson 1970.

URG: Relation to Poor Man's Scaling

$$H = H_0 + \underbrace{V_+ + V_-}_{\substack{\text{off-diagonal terms} \\ \text{we want to remove}}}$$

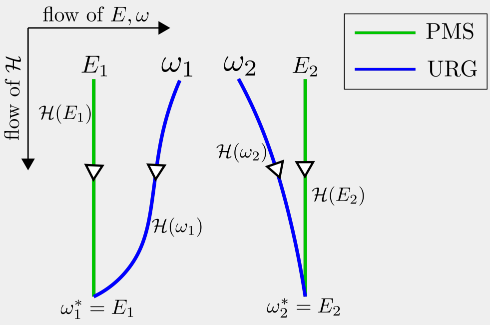
E = exact eigenvalue

ω = URG quantum fluctuation scale

$$\Delta H_{\text{PMS}} = V_- \frac{1}{E - H_0} V_+ + V_+ \frac{1}{E - H_0} V_-$$

$$\Big\downarrow E \to \omega$$

$$\Delta H_{\text{URG}} = V_- \frac{1}{\omega - H_0} V_+ + V_+ \frac{1}{\omega - H_0} V_-$$



URG: Relation to Continuous Unitary Transformation RG

$$H = \overbrace{H_d}^{\text{diagonal part}} + \overbrace{H_X}^{\text{off-diagonal part}}$$

$$\Delta H_{\text{CUT}} = \Delta l \left[\left[H_d(l), H_X(l) \right], H(l) \right]$$

$$V_{kq}(l) = V_{kq}(0) e^{(\epsilon_k - \epsilon_q) l}$$

- off-diagonal terms decay exponentially
- those that connect larger energy differences decay fastest

Głazek and Wilson 1993; Wegner 1994.

URG: Relation to Continuous Unitary Transformation RG

$$H = \overbrace{H_d}^{\text{diagonal part}} + \overbrace{H_X}^{\text{off-diagonal part}}$$

$$\Delta H_{\text{CUT}} = \Delta l \left[\left[H_d(l), H_X(l)\right], H(l)\right]$$

$$\Delta H_{\text{URG}} = \overbrace{\left[\left[H_d, \frac{1}{\omega_1 - \omega_0}\left(\hat{\omega} - H_d\right)^{-1} H_I\right], H\right]}^{\Delta H_0} - H^I$$

$$\Delta H_0 \xrightarrow{(\hat{\omega} - H_d)^{-1} \sim -H_d^{-1}} \Delta\lambda \times \left[\left[H_d, H_I\right], H\right]$$