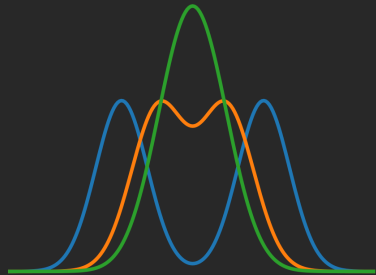


# UNITARY RENORMALIZATION GROUP SOLUTION OF THE SINGLE-IMPURITY ANDERSON MODEL



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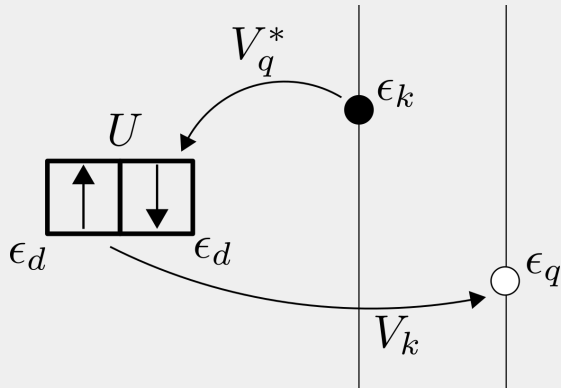
JULY 11, 2021



# **THE SINGLE-IMPURITY ANDERSON MODEL**

# THE SINGLE-IMPURITY ANDERSON MODEL

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



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

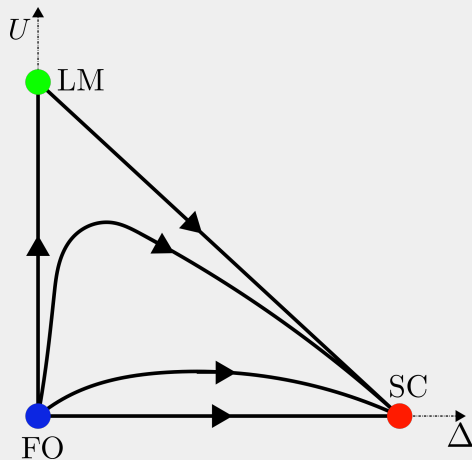
$$\Delta = \rho V^2$$

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

# THE SINGLE-IMPURITY ANDERSON MODEL

## 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 ( $\Delta = \infty, U = \text{finite}$ ) - stable.



## **SOME OUTSTANDING QUESTIONS**

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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

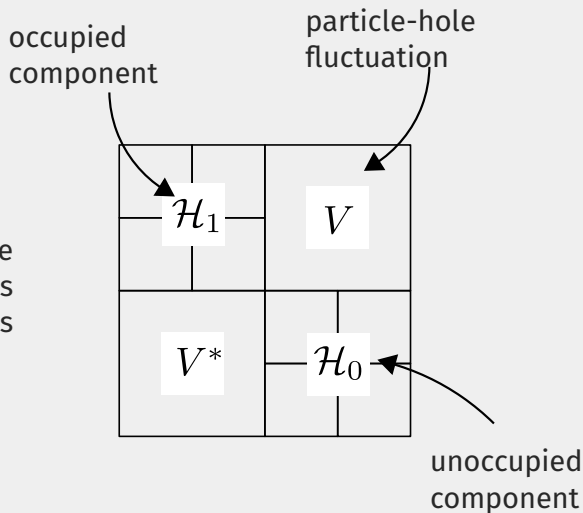
## The Short Version

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

$$\begin{array}{c} \mathcal{H}(D) \\ \Downarrow \\ U\mathcal{H}(D)U^\dagger \\ \Downarrow \\ H(D) + \mathcal{H}'(D - \delta D) \end{array}$$

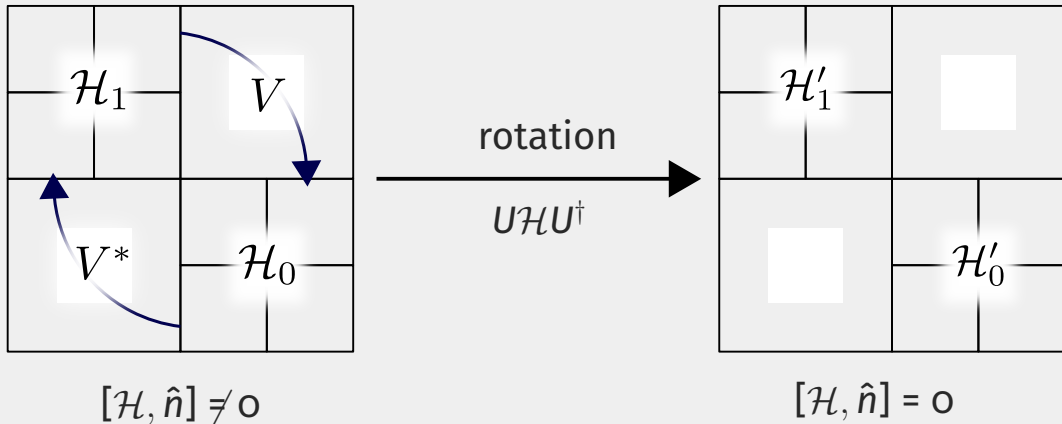
## Step 1:

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



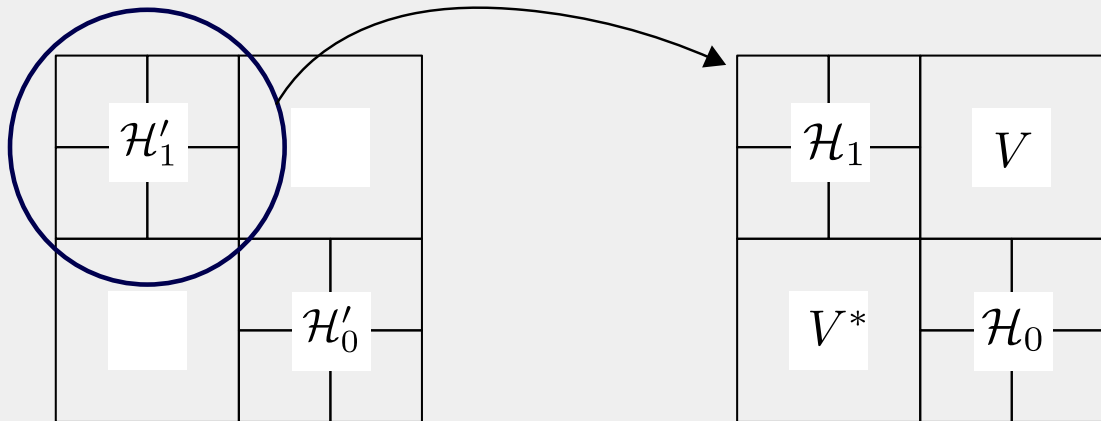
## Step 2:

Rotate the Hamiltonian to kill the off-diagonal blocks.



## Step 3:

Repeat the process with the new blocks.

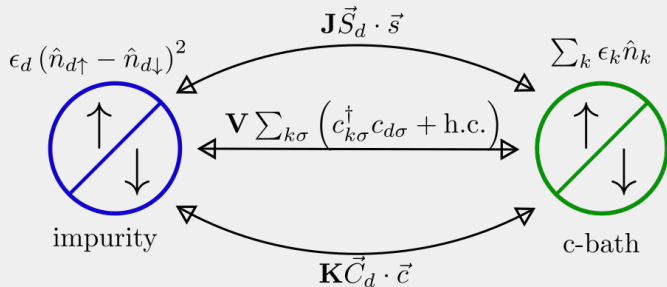


# GENERALIZED SIAM



# MODEL: GENERALIZED SIAM

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



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

$$\vec{S} \equiv \frac{1}{2} \sum_{\alpha\beta} c_{0\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{0\beta}$$

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

$$\vec{C} \equiv \frac{1}{2} \sum_{\alpha\beta} \psi_{0\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{0\beta}$$

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

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

## Symmetric SIAM

$$\blacksquare J = 0, K = 0$$

$$\blacksquare \omega = -\frac{D}{2}$$

$$\blacksquare U = -\frac{\epsilon_d}{2} \ll D$$



$$\delta U = \delta V = 0$$

# PASSAGE TO POOR MAN'S SCALING RESULTS

## Asymmetric SIAM

- $J = 0, K = 0$

- $\omega = -\frac{D}{2}$

- $U \gg D \gg \epsilon_d$



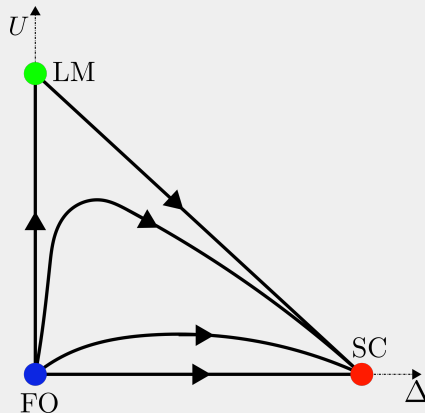
$$\delta U = \delta V = 0$$

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

# FIXED POINTS

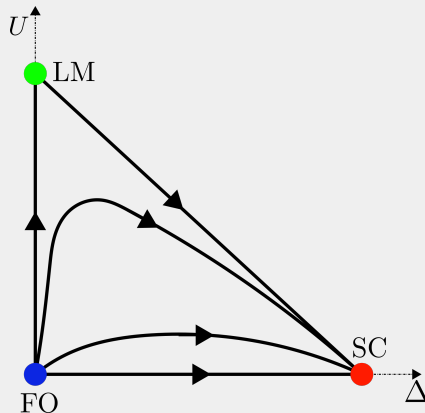
■  $J = K = 0 \longrightarrow \Delta V = 0$

■  $J, K, V = 0^+ \longrightarrow (V^*, J^*, K^*) = \text{large}, U^* = 0$   
► **strong-coupling fixed point**



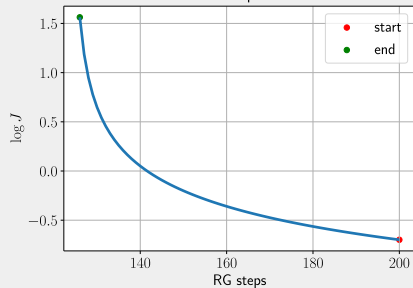
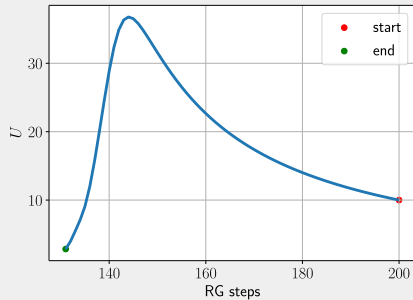
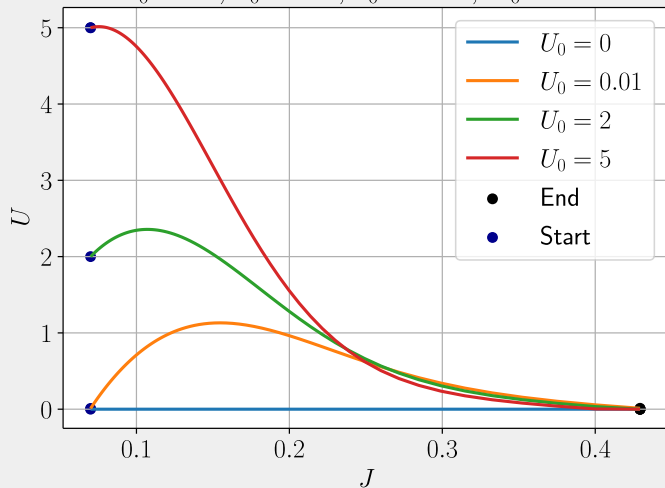
# FIXED POINTS

- $J = K = V = 0 \longrightarrow$  all couplings marginal
  - ▶ line of fixed points on y-axis
- $U = 0^+ \longrightarrow$  **local moment fixed point**
  - ▶ ground-state is a decoupled impurity spin



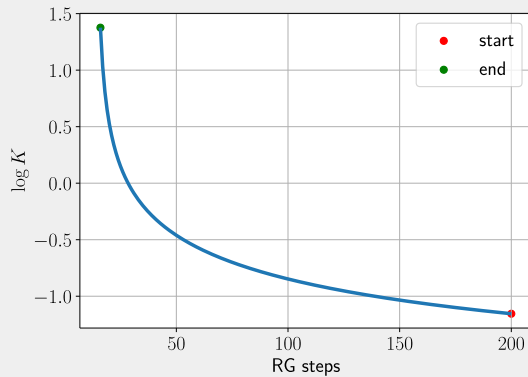
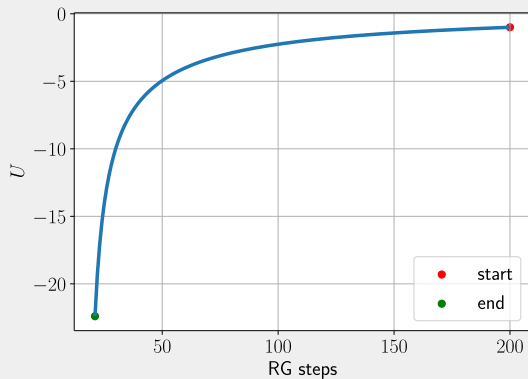
# RESULTS: $U > 0, J > K$

$$D_0 = 10, V_0 = 0.3, J_0 = 0.07, K_0 = 0.03$$



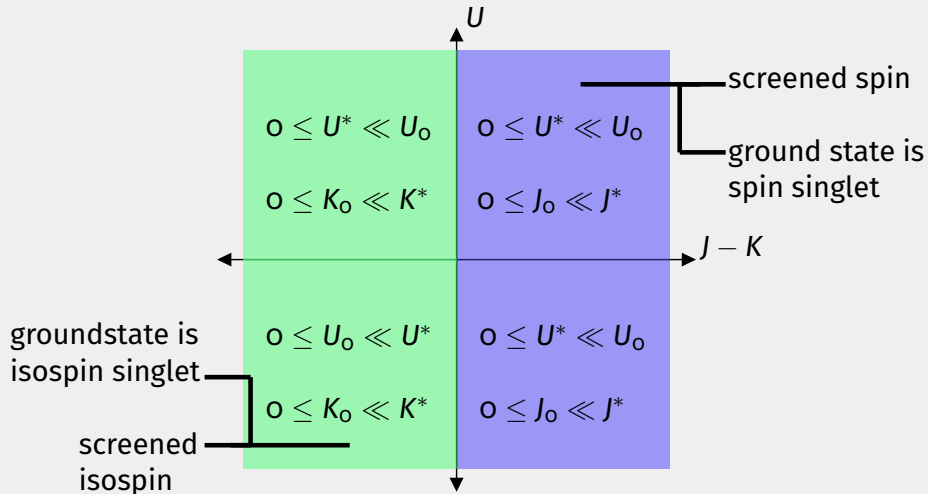


RESULTS:  $U < 0, J < K$



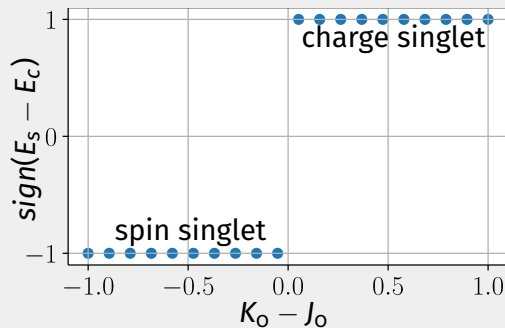
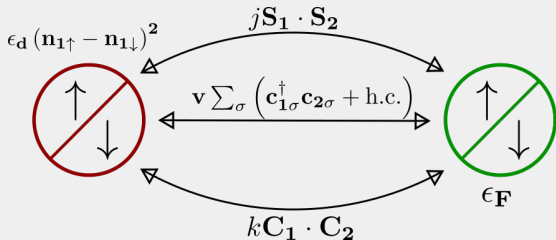
# **LOW ENERGY EFFECTIVE THEORY AND GROUND STATE WAVEFUNCTIONS**

# RESULTS: PHASE DIAGRAM



# RESULTS: EFFECTIVE ZERO-MODE HAMILTONIAN

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

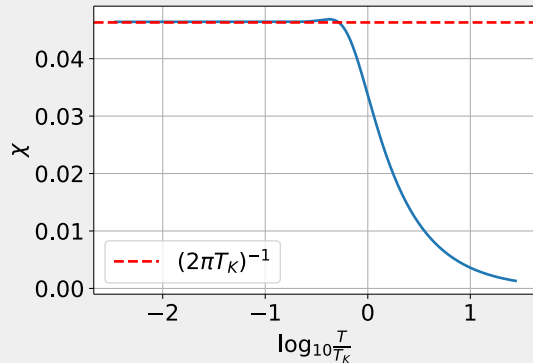
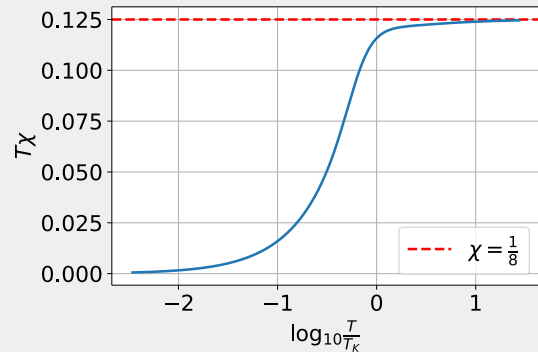


Wilson 1975; Krishna-murthy, Wilson, and Wilkins 1975; Taraphder and Coleman 1991.

# **IMPURITY SUSCEPTIBILITIES AND IMPURITY SPECTRAL FUNCTION**

# RESULTS: SPIN SUSCEPTIBILITY

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



$$\chi(T \rightarrow 0) = (2j)^{-1}$$

$$T_K \equiv \frac{2N^*}{\pi} (D^* - 2\omega)$$

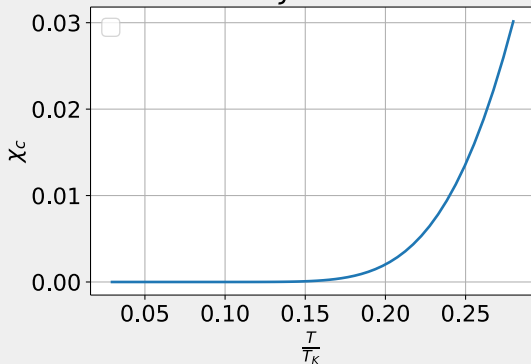
$$(\chi \times T)(T \rightarrow \infty) = \frac{1}{8}$$

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

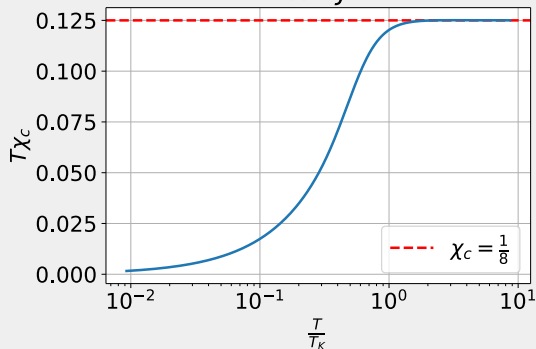
# RESULTS: CHARGE SUSCEPTIBILITY

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

$J > K$



$K > J$



$$(\chi_c \times T)(T \rightarrow 0) \Big|_{K > J} = \frac{1}{2k}$$

$$(\chi_c \times T)(T \rightarrow 0) \Big|_{J > K} = 0$$

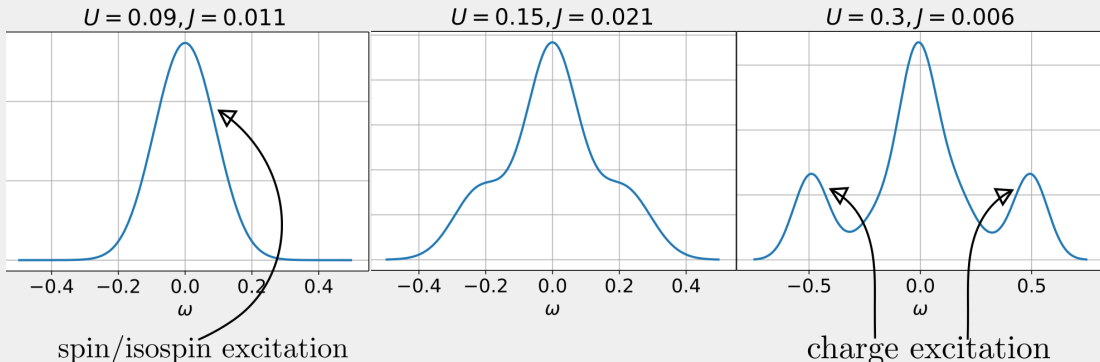
$$\chi_c(T \rightarrow \infty) = \frac{1}{8}$$

Taraphder and Coleman 1991; Zitko and Bonca 2006.

# RESULTS: IMPURITY SPECTRAL FUNCTION

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} [G_{dd}^{\sigma}(\omega)]$$

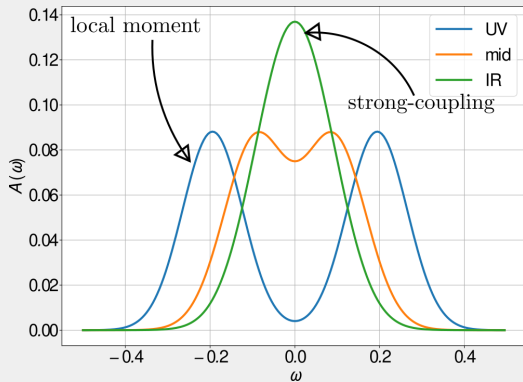
$$G_{dd}^{\sigma}(t) = -i\theta(t) \langle \{c_{d\sigma}(t), c_{d\sigma}^{\dagger}\} \rangle$$



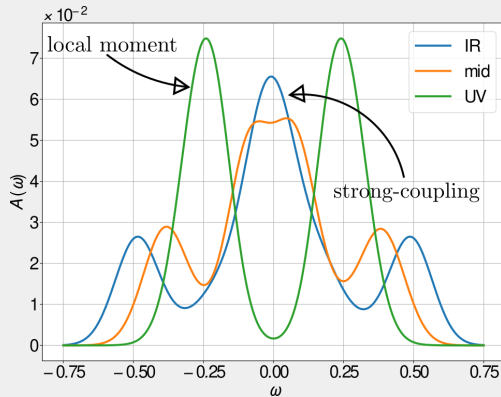


# RESULTS: SPECTRAL FUNCTION RENORMALIZATION

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} [G_{dd}^{\sigma}(\omega)]$$



$$G_{dd}^{\sigma}(t) = -i\theta(t) \langle \{c_{d\sigma}(t), c_{d\sigma}^{\dagger}\} \rangle$$

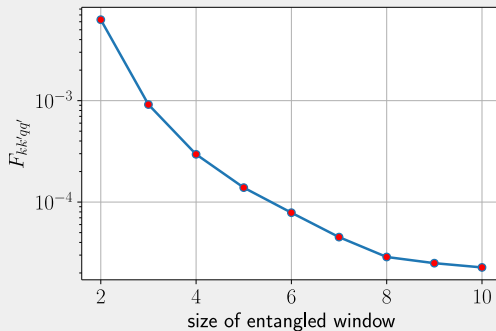


# **ENTANGLEMENT MEASURES AND TOPOLOGICAL FEATURES OF LOW ENERGY THEORY**

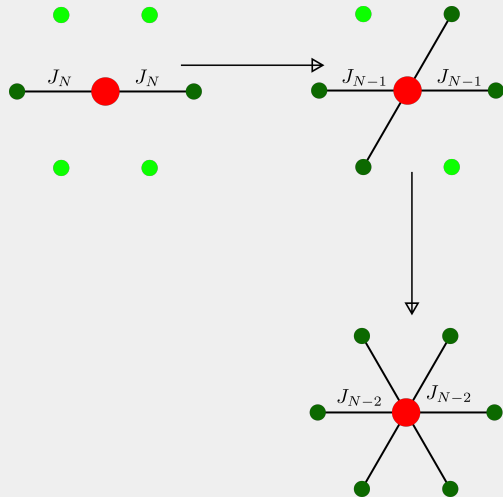
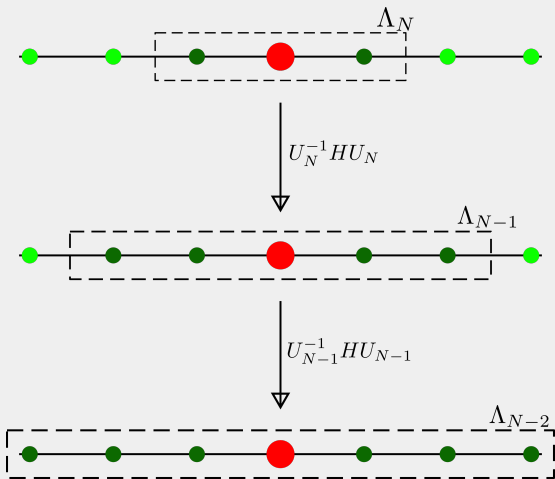
# RESULTS: KONDO CLOUD HAMILTONIAN

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

$$H_{\text{cloud}}^* = \underbrace{H_{\text{O}}^*}_{\text{kinetic energy}} + \underbrace{\sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'}}_{\text{Fermi liquid-type interaction}} + \underbrace{\sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger c_{q\uparrow} c_{q'\downarrow}}_{\text{non-Fermi liquid-type interaction}}$$

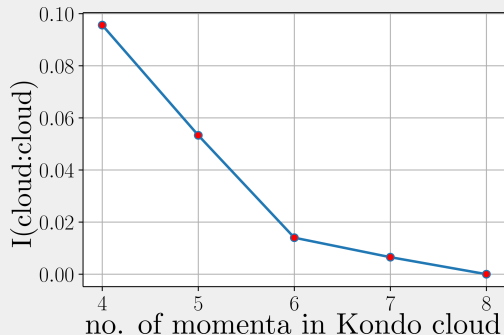


# RESULTS: REVERSE RG: OVERVIEW

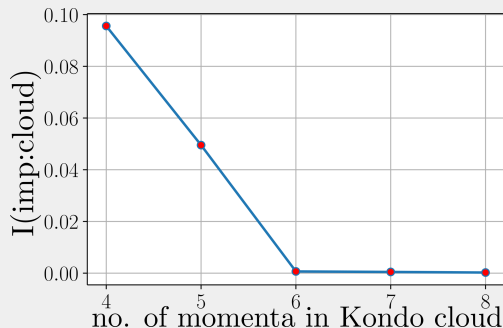


# RESULTS: REVERSE RG: MUTUAL INFORMATION

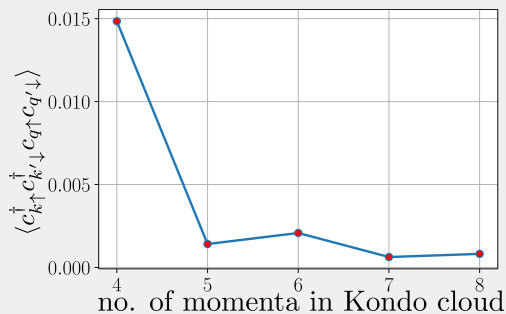
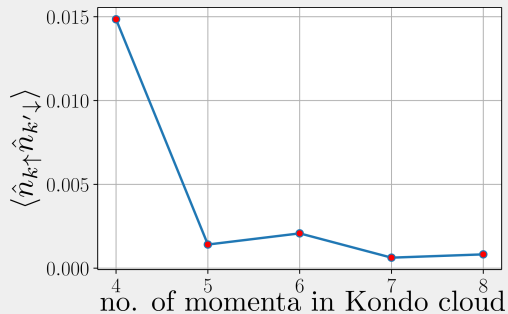
$$I(A : B) = S_A + S_B - S_{AB}$$



$$S_A = -\text{Tr} [\rho_A \ln \rho_A]$$



# RESULTS: REVERSE RG: CORRELATIONS

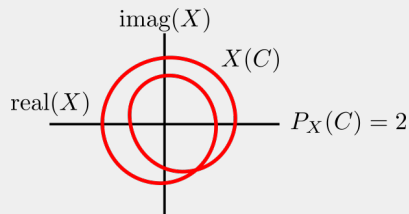
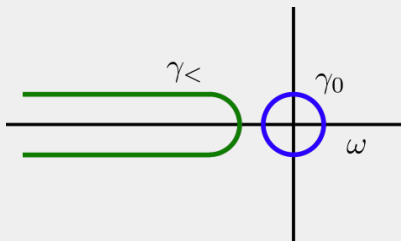


# RESULTS: LUTTINGER'S THEOREM

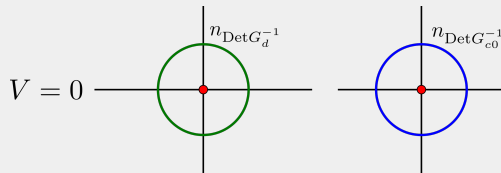
$$\overbrace{N}^{\text{total no. of particles}} = \overbrace{P_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2}P_{\text{Det } G_d}(\Gamma_0)}^{\text{no. of poles of imp. Greens func.}} + \overbrace{V_L}^{\text{no. of poles of cbath Greens func.}}$$

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

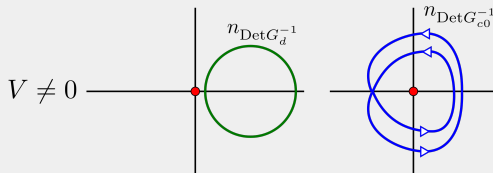
$$= \frac{1}{2\pi i} \oint_{X(C)} \frac{dX}{X} = \text{winding number of } X(C) \text{ around the origin}$$



# RESULTS: LUTTINGER'S THEOREM



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



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

$$V_L = V_L^O + 1$$



# RESULTS: LOCAL FERMI LIQUID

$$H^* = \overbrace{J^* \vec{S}_d \cdot \vec{S} + K^* \vec{C}_d \cdot \vec{C} + V^* (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.})}^{\text{solve exactly}} + \overbrace{t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma}}^{\text{treat as perturbation}}$$

$\downarrow$  4<sup>th</sup> fourth order pert.

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

$$H^* \sim J^* \vec{S}_d \cdot \vec{S} + K^* \vec{C}_d \cdot \vec{C} + V^* (c_{d\sigma}^\dagger c_{0\sigma} + \text{h.c.}) + \overbrace{\frac{t^4}{J^{*3}} \hat{n}_{1\uparrow} \hat{n}_{1\downarrow}}^{\text{local Fermi liquid}}$$

## RESULTS: WILSON RATIO ( $T = 0$ )

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

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

$$\blacksquare f_{\uparrow\uparrow} = 0$$

$$\blacksquare \chi_c(T \rightarrow 0) = 0$$



$$\blacksquare C_v(T \rightarrow 0) = \rho_{\text{imp}} T$$

$$\blacksquare \chi_s(T \rightarrow 0) = 2\rho_{\text{imp}}$$

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

## RESULTS: RELATION BETWEEN $R$ AND $\Delta V_L$

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



$$\frac{\chi_s}{C_V/T} = 1 + U\rho_{\text{imp}}(0)$$

$$\rho_{\text{imp}}(0) = (\pi\Delta)^{-1} \sin^2 \delta(0)$$

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

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- scattering theory results



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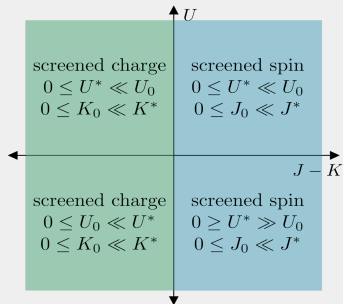
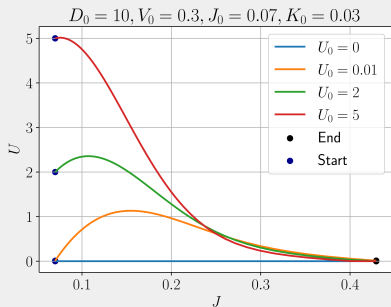
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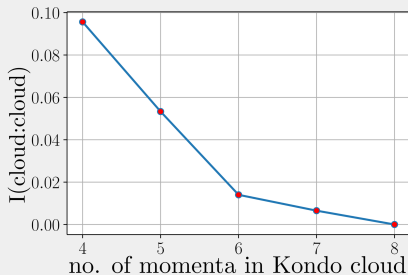
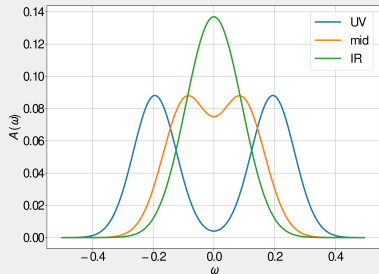
$$R = 1 + \sin^2 \left( \frac{\pi}{2} \Delta V_L \right)$$

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

## **SUMMARY OF RESULTS**



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



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

$$V_L = V_L^0 + 1$$

$\downarrow$  SC       $\downarrow$  LM

## **FUTURE DIRECTIONS**



## WHAT'S NEXT?

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- We can also check how using more feature-full baths (with non-trivial self-energy) can change the phase diagram.

## 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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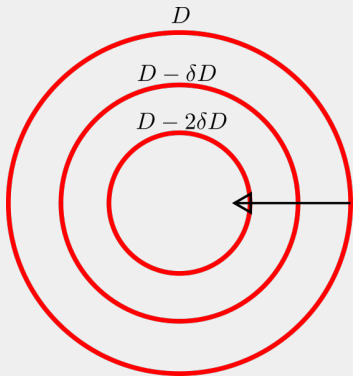


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# URG: RELATION TO POOR MAN'S SCALING

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



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

# URG: RELATION TO POOR MAN'S SCALING

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

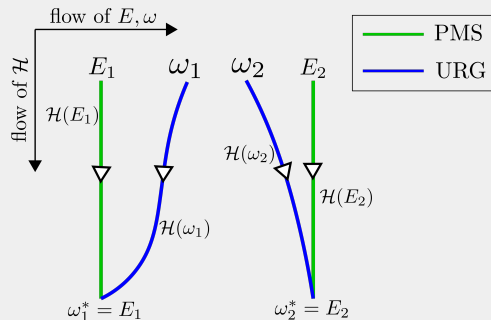
$E$  = exact eigenvalue

$\omega$  = URG quantum fluctuation scale

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

$E \rightarrow \omega$

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



# URG: RELATION TO CONTINUOUS UNITARY TRANSFORMATION RG

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

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

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

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

# URG: RELATION TO CONTINUOUS UNITARY TRANSFORMATION RG

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

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

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

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