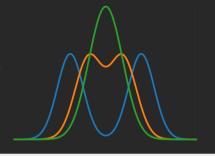
Unitary Renormalization Group Solution of the Single-Impurity Anderson model



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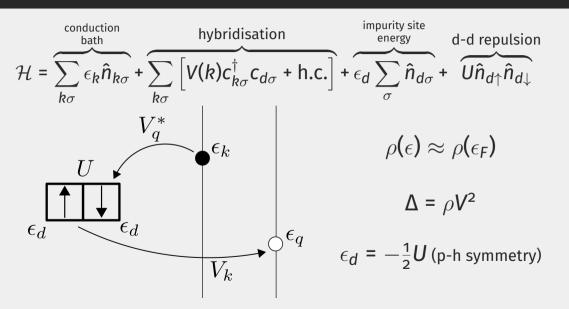
JULY 11, 2021





THE SINGLE-IMPURITY ANDERSON MODEL

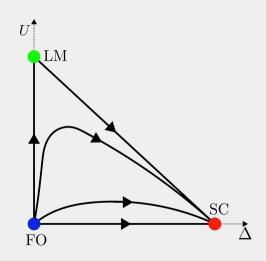
THE SINGLE-IMPURITY ANDERSON MODEL



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.



Krishna-murthy, Wilson, and Wilkins 1975.

■ Is it possible to get **non-perturbative scaling equations** for the whole journey?

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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?

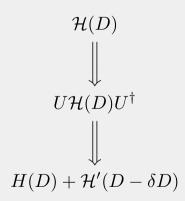


THE UNITARY RENORMALIZATION GROUP

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.

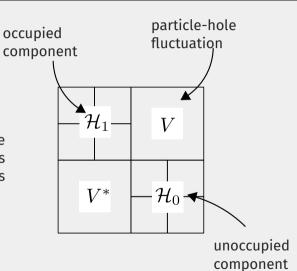


Mukherjee and Lal 2020.

URG: FORMALISM

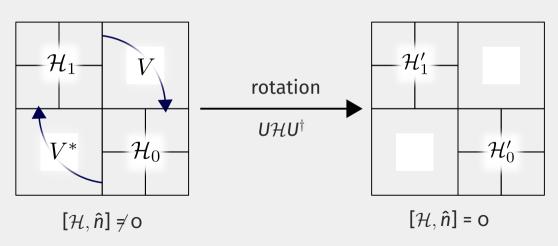
Step 1:

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

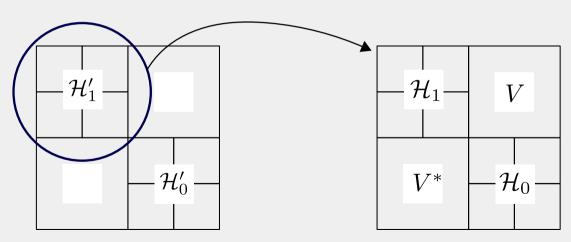


URG: FORMALISM

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



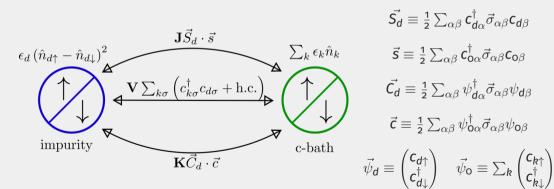
Step 3: Repeat the process with the new blocks.



GENERALIZED SIAM

MODEL: GENERALIZED SIAM

$$H = H_{SIAM} + J\vec{S_d} \cdot \vec{S} + K\vec{C_d} \cdot \vec{C}$$



$$ec{S_d} \equiv rac{1}{2} \sum_{lphaeta} c_{dlpha}^{\dagger} \vec{\sigma}_{lphaeta} c_{deta}$$
 $ec{S} \equiv rac{1}{2} \sum_{lphaeta} c_{olpha}^{\dagger} \vec{\sigma}_{lphaeta} c_{oeta}$
 $ec{C_d} \equiv rac{1}{2} \sum_{lphaeta} \psi_{dlpha}^{\dagger} \vec{\sigma}_{lphaeta} \psi_{deta}$
 $ec{c} \equiv rac{1}{2} \sum_{lphaeta} \psi_{olpha}^{\dagger} \vec{\sigma}_{lphaeta} \psi_{oeta}$

Schrieffer and Wolff 1966.

RG EQUATIONS, THEIR FEATURES AND FIXED POINTS

RG EQUATIONS

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

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

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

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

PASSAGE TO POOR MAN'S SCALING RESULTS

Symmetric SIAM

■
$$J = 0, K = 0$$

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

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

PASSAGE TO POOR MAN'S SCALING RESULTS

Asymmetric SIAM

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

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

$$\blacksquare$$
 $U \gg D \gg \epsilon_d$

$$\longrightarrow$$

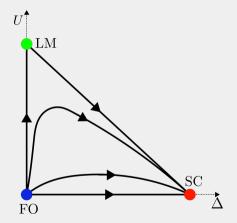
$$\delta U = \delta V = 0$$

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

FIXED POINTS

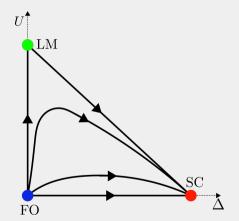
$$\blacksquare J = K = O \longrightarrow \Delta V = O$$

- \blacksquare $J, K, V = O^+ \longrightarrow (V^*, J^*, K^*) = large, U^* = O$
 - ► strong-coupling fixed point

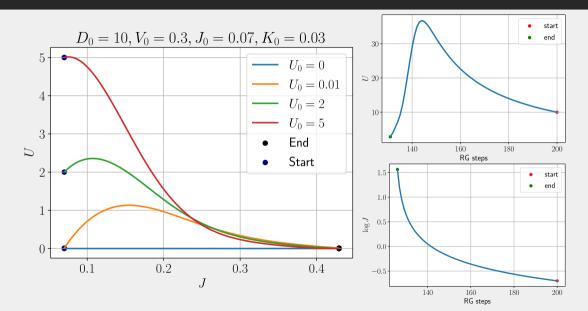


FIXED POINTS

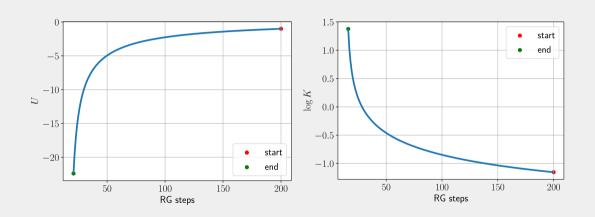
- $J = K = V = o \longrightarrow all couplings marginal$
 - ► line of fixed points on y-axis
- $U = O^+ \longrightarrow local moment fixed point$
 - ground-state is a decoupled impurity spin



RESULTS: $U > 0, \overline{J} > K$



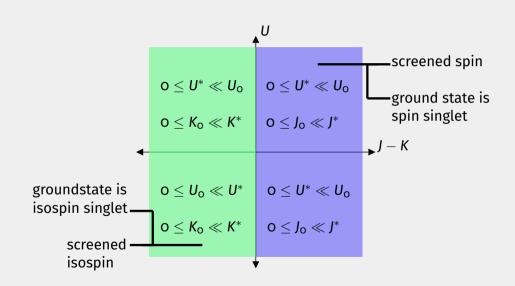
RESULTS: U < o, J < K



LOW ENERGY EFFECTIVE THEORY AND GROUND

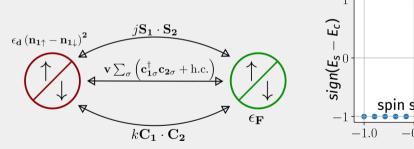
STATE WAVEFUNCTIONS

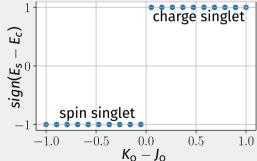
RESULTS: PHASE DIAGRAM



RESULTS: EFFECTIVE ZERO-MODE HAMILTONIAN

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





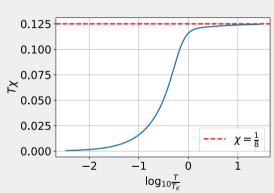
Wilson 1975; Krishna-murthy, Wilson, and Wilkins 1975; Taraphder and Coleman 1991.

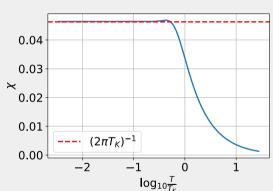
IMPURITY SUSCEPTIBILITIES AND IMPURITY

SPECTRAL FUNCTION

RESULTS: SPIN SUSCEPTIBILITY

$$\chi_{s} = \lim_{B \to o} \frac{\partial m}{\partial B}$$





$$\chi (T \to 0) = (2i)^{-1}$$

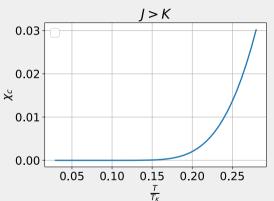
$$T_K \equiv \frac{2N^*}{\pi} (D^* - 2\omega)$$

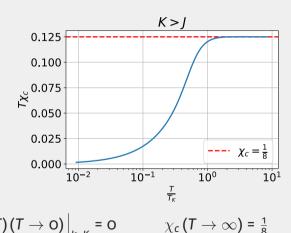
$$(\chi \times T)(T \to \infty) = \frac{1}{9}$$

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

RESULTS: CHARGE SUSCEPTIBILITY

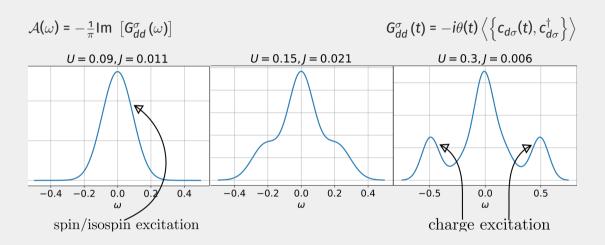
$$\chi_{c} = \lim_{\mu \to 0} \frac{\partial N}{\partial \mu}$$





$$(\chi_c \times T)(T \to 0)\Big|_{K>J} = \frac{1}{2k}$$
 $(\chi_c \times T)(T \to 0)\Big|_{J>K} = 0$
Taraphder and Coleman 1991; Zitko and Bonca 2006.

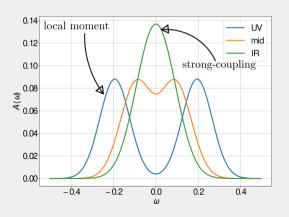
RESULTS: IMPURITY SPECTRAL FUNCTION



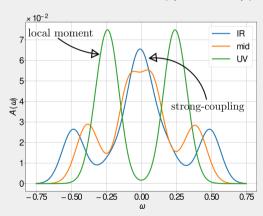
Hewson 1993; Bulla, Costi, and Pruschke 2008.

RESULTS: SPECTRAL FUNCTION RENORMALIZATION

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



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



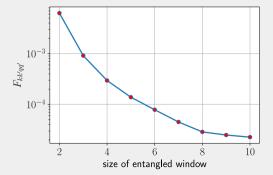
ENTANGLEMENT MEASURES AND TOPOLOGICAL

FEATURES OF LOW ENERGY THEORY

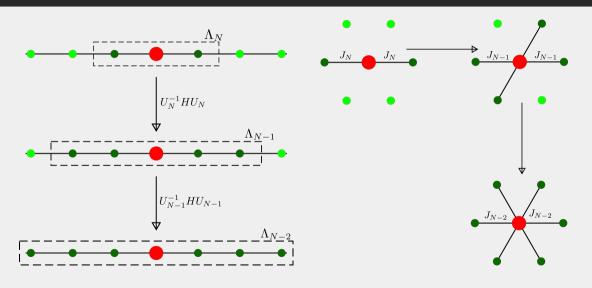
RESULTS: KONDO CLOUD HAMILTONIAN

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

 $H_{\text{cloud}}^* = \overbrace{H_{\text{o}}^*}^{\text{kinetic energy}} + \underbrace{\sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'}}_{\text{k} + \sigma\sigma'} + \underbrace{\sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^{\dagger} c_{k\uparrow}^{\dagger} c_{q\uparrow} c_{q'\downarrow}}_{\text{k} + \sigma\sigma'}$

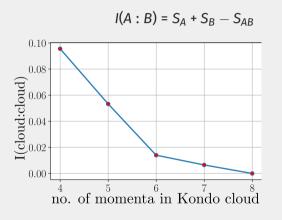


RESULTS: REVERSE RG: OVERVIEW

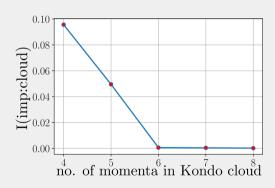


Mukherjee 2020.

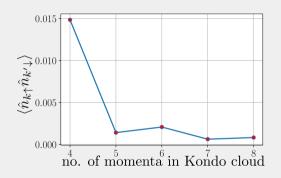
RESULTS: REVERSE RG: MUTUAL INFORMATION

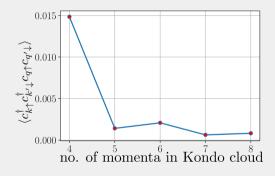


$$S_A = -\text{Tr} \left[\rho_A \ln \rho_A \right]$$



RESULTS: REVERSE RG: CORRELATIONS





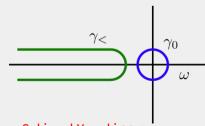
RESULTS: LUTTINGER'S THEOREM

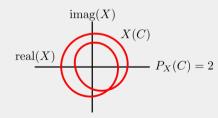
total no. of poles of imp. Greens func.

N =
$$P_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2}P_{\text{Det } G_d}(\Gamma_{\text{O}}) + \frac{1}{V_L}$$

no. of poles of cbath Greens func

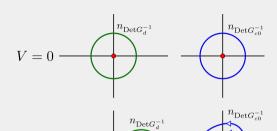
$$P_X(C) \equiv \frac{1}{2\pi i} \oint_C dz \frac{\partial \ln X}{\partial z} = \text{no. of poles of } X \text{ enclosed by curve } C$$
$$= \frac{1}{2\pi i} \oint_{X(C)} \frac{dX}{X} = \text{winding number of } X(C) \text{ around the origin}$$





Seki and Yunoki 2017.

RESULTS: LUTTINGER'S THEOREM



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

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

$$V_L = V_L^{\circ} + 1$$

 $V \neq 0$

RESULTS: LOCAL FERMI LIQUID

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

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

$$E_1^{(4)} = -\frac{16t^4}{2l^{*3}}, E_2^{(4)} = -\frac{16t^4}{9l^{*3}}$$

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

Nozières 1974.

RESULTS: WILSON RATIO (T = 0)

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

$$\epsilon_{k\sigma}$$
 = $\epsilon_{k}^{\mathrm{o}}$ + $\sum_{q} f_{kq} \left\langle n_{q\overline{\sigma}} \right\rangle$

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

$$\chi_c(T \to 0) = 0$$

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

$$\blacksquare$$
 $\chi_{\rm s}({\it T}
ightarrow {\rm o})$ = 2 $ho_{\rm imp}$

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

Hewson 1994.

Results: Relation between R and ΔV_L

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

$$\longrightarrow$$

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

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- particle-hole symmetry
- strong-coupling fixed-point

$$\blacksquare$$
 $T = 0$

- Friedel's sum rule
- scattering theory arguments

$$\longrightarrow$$

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

$$\longrightarrow$$

$$\frac{1}{\pi}\delta(o) = \tilde{N} = \Delta V_L$$

RESULTS: RELATION BETWEEN R AND ΔV_L

- particle-hole symmetry
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- Friedel's sum rule
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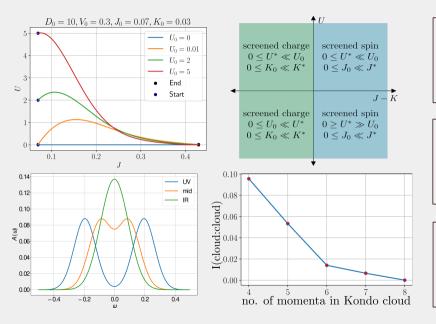
$$\longrightarrow$$
 R = 1+sin² δ (o)

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

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

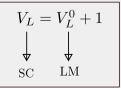
 $\Delta V_L = 1 \longrightarrow R = 2$

SUMMARY OF RESULTS



$$\begin{aligned} H_{cloud} &= H_0 \\ &+ H_{FL} \\ &+ H_{NFL} \end{aligned}$$

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



FUTURE DIRECTIONS

■ Analytical expression for temperature-dependent Wilson ratio

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- Separating the contributions of various parts of the Kondo cloud to the spectral function

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- 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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Anderson, P W (1970). "A poor man's derivation of scaling laws for the Kondo problem". In: Journal of Physics C: Solid State Physics 3.12, pp. 2436-2441. DOI:
     10.1088/0022-3719/3/12/008.URL: https://doi.org/10.1088/0022-3719/3/12/008.
```

Bulla, Ralf, Theo A. Costi, and Thomas Pruschke (2008). "Numerical renormalization group method for quantum impurity systems". In: Rev. Mod. Phys. 80

(2), pp. 395-450, poi: 10.1103/RevModPhys.80.395, uRL: https://link.aps.org/doi/10.1103/RevModPhys.80.395.

Głazek, Stanisław D. and Kenneth G. Wilson (1993), "Renormalization of Hamiltonians", In: Phys. Rev. D 48 (12), pp. 5863-5872, por:

10.1103/PhysRevD.48.5863. URL: https://link.aps.org/doi/10.1103/PhysRevD.48.5863. Haldane, F. D. M. (1978), "Scaling Theory of the Asymmetric Anderson Model", In: Phys. Rev. Lett. 40 (6), pp. 416-419, poi:

10.1103/PhysRevLett.40.416. URL: https://link.aps.org/doi/10.1103/PhysRevLett.40.416.

Hewson, A. C. (1993). The Kondo Problem to Heavy Fermions. Cambridge University Press.

(1994). "Renormalization group and Fermi liquid theory". In: Advances in Physics 43.

lefferson, I H (1977). "A renormalisation group approach to the mixed valence problem". In: Journal of Physics C: Solid State Physics 10.18, pp. 3589-3599. DOI: 10.1088/0022-3719/10/18/023. URL: https://doi.org/10.1088/0022-3719/10/18/023.

Krishna-murthy, H. R., K. G. Wilson, and I. W. Wilkins (1975), "Temperature-Dependent Susceptibility of the Symmetric Anderson Model: Connection to the

Kondo Model", In: Phys. Rev. Lett. 35 (16), pp. 1101-1104, DOI: 10.1103/PhysRevLett. 35.1101, URL: https://link.aps.org/doi/10.1103/PhysRevLett.35.1101.

Martin, Richard M (1982). "Fermi-surface sum rule and its consequences for periodic kondo and mixed-valence systems". In: Physical Review Letters 48.5, p. 362. Mukheriee, Anirban (2020). "Unitary renormalization group for correlated electrons", PhD thesis, Indian Institute of Science Education and Research

Kolkata.

Mukheriee, Anirban and Siddhartha Lal (2020), "Holographic unitary renormalization group for correlated electrons - I: A tensor network approach", In:

Nuclear Physics B 960. DOI: https://doi.org/10.1016/j.nuclphysb.2020.115170. URL: http://www.sciencedirect.com/science/article/pii/S055032132030256X.

Nozières, P. (1974). "A Fermi-Liquid Description of the Kondo Problem at Low Temperatures". In: Journal of Low Temperature Physics 17.

Schrieffer, I. R. and P. A. Wolff (1966), "Relation between the Anderson and Kondo Hamiltonians", In: Phys. Rev. 149 (2), pp. 491–492, pol:

10.1103/PhysRev.149.491.URL: https://link.aps.org/doi/10.1103/PhysRev.149.491.

Seki, Kazuhiro and Sejii Yunoki (2017), "Topological interpretation of the Luttinger theorem", In: Physical Review B 96, pol:

10.1103/physrevb.96.085124.URL: http://dx.doi.org/10.1103/PhysRevB.96.085124.

Taraphder, A. and P. Coleman (May 1991), "Heavy-fermion behavior in a negative-U Anderson model", In: Phys. Rev. Lett. 66 (21), pp. 2814–2817, DOI: 10.1103/PhysRevLett.66.2814.uru: https://link.aps.org/doi/10.1103/PhysRevLett.66.2814.

Wegner, Franz (1994), "Flow-equations for Hamiltonians". In: Annalen der Physik 506.2, pp. 77-91, DOI: https://doi.org/10.1002/andp.19945060203.eprint:

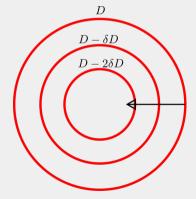
https://onlinelibrary.wilev.com/doi/pdf/10.1002/andp.19945060203.URL:

https://onlinelibrary.wiley.com/doi/abs/10.1002/andp.19945060203. Wilson, K. G. (1975). "The Renormalization group: Critical phenomena and the Kondo Problem". In: Reviews of Modern Physics 47.

Zitko, Rok and Janez Bonca (2006). "Spin-charge separation and simultaneous spin and charge Kondo effect". In: Phys. Rev. B 74 (22), p. 224411. DOI: 10.1103/PhysRevB.74.224411. URL: https://link.aps.org/doi/10.1103/PhysRevB.74.224411.

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

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

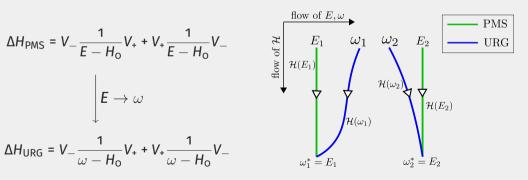
E = exact eigenvalue

 ω = URG quantum fluctuation scale

$$\Delta H_{PMS} = V_{-} \frac{1}{E - H_{0}} V_{+} + V_{+} \frac{1}{E - H_{0}} V_{-}$$

$$\downarrow E \rightarrow \omega$$

$$\Delta H_{URG} = V_{-} \frac{1}{\omega - H_{0}} V_{+} + V_{+} \frac{1}{\omega - H_{0}} V_{-}$$



URG: RELATION TO CONTINUOUS UNITARY TRANSFORMATION RG

diagonal part off-diagonal part
$$H = \widehat{H_d} + \widehat{H_X}$$

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

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

- 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

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

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

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

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