Unitary Renormalization Group Approach to the Single-Impurity Anderson model

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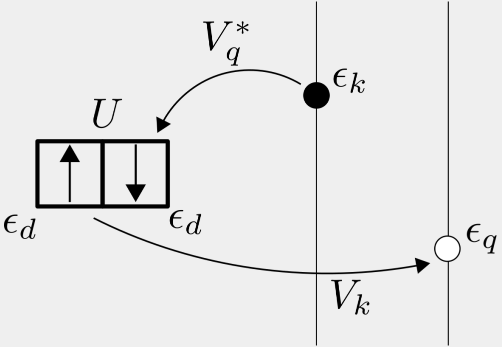
$$\mathcal{H} = \overbrace{\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma}}^{\text{conduction bath}} + \overbrace{\sum_{k\sigma} \left[V(k) c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right]}^{\text{hybridisation}} + \overbrace{\epsilon_d \sum_{\sigma} \hat{n}_{d\sigma}}^{\text{impurity site energy}}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



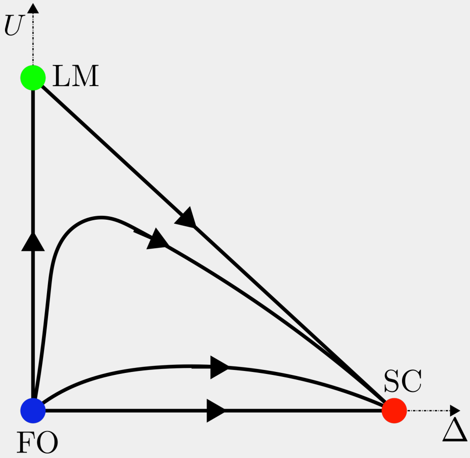
$$\rho(\epsilon) \approx \rho(\epsilon_F)$$

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

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

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.



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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?

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

$$\Downarrow$$

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

$$\Downarrow$$

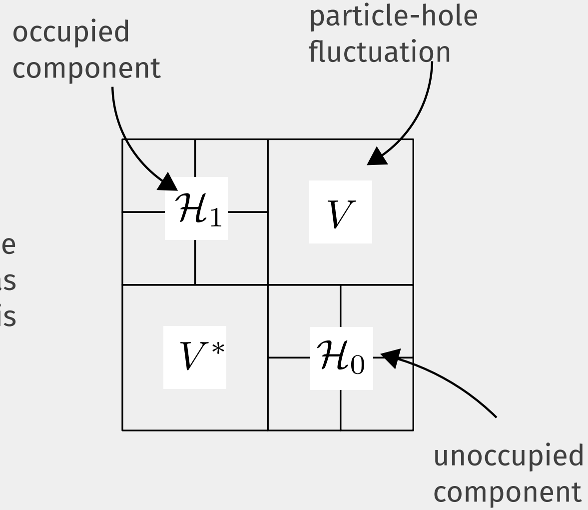
$$H(D) + \mathcal{H}'(D - \delta D)$$

The Short Version

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

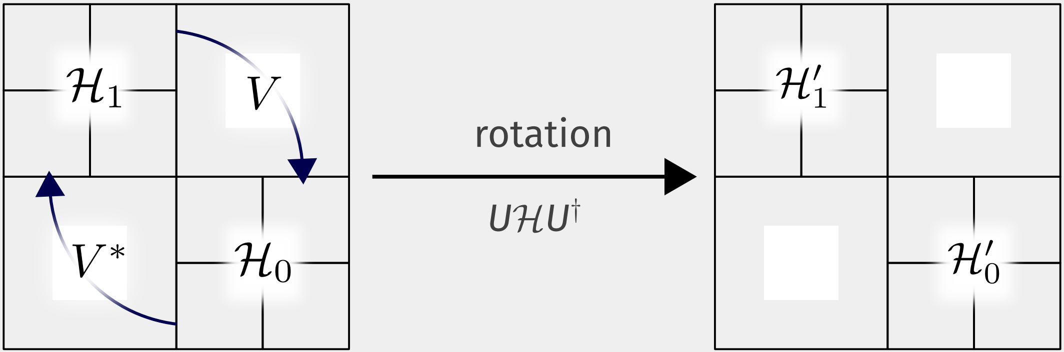
Step 1:

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



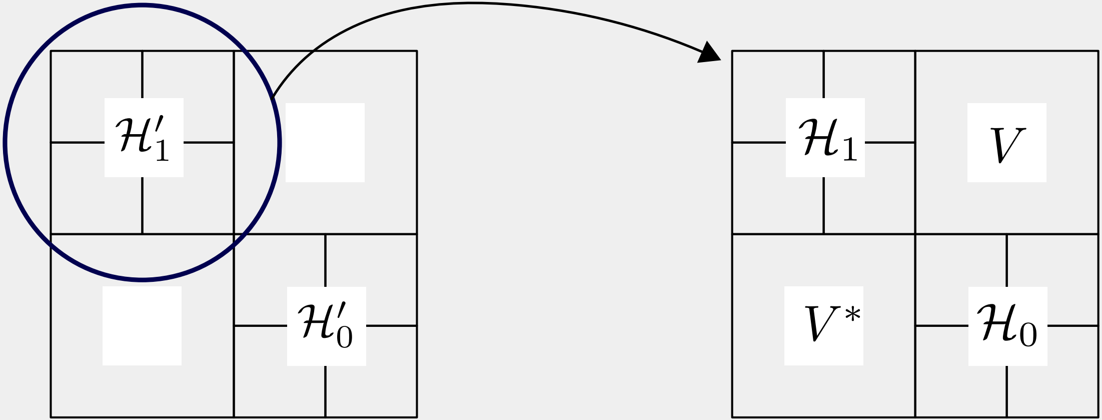
Unitary Renormalization Group Formalism

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.



Results: RG Equations

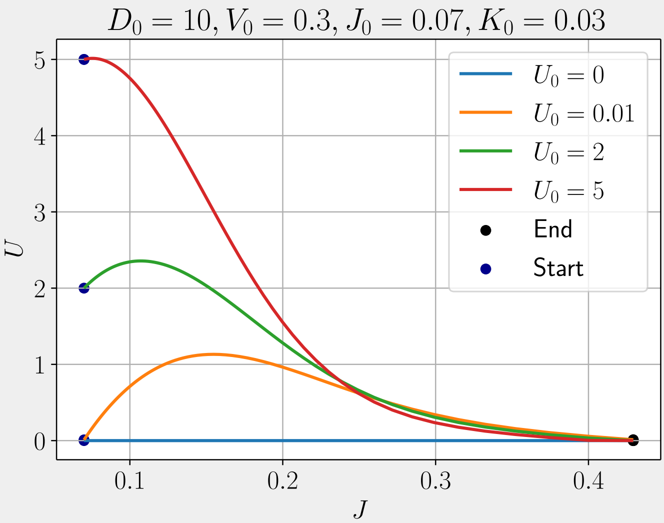
$$\Delta U = 4|V|^2 \left[\frac{1}{\omega - \frac{1}{2}D + \frac{U}{2} + \frac{1}{2}J} - \frac{1}{\omega - \frac{1}{2}D - \frac{U}{2} + \frac{1}{2}K}\right] + \sum_{k<\Lambda_j} \frac{3}{4}\frac{K^2 - J^2}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}$$

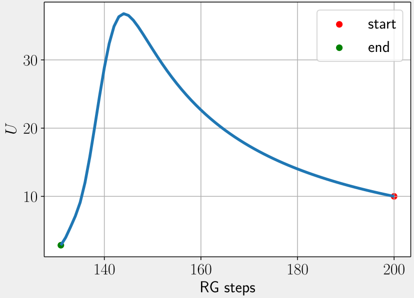
$$\Delta V = \frac{VK}{16}\left(\frac{1}{\omega - \frac{1}{2}D - \frac{U}{2} + \frac{1}{2}K} + \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}\right) - \frac{3VJ}{4}\left(\frac{1}{\omega - \frac{1}{2}D + \frac{U}{2} + \frac{1}{2}J} + \frac{1}{\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K}\right)$$

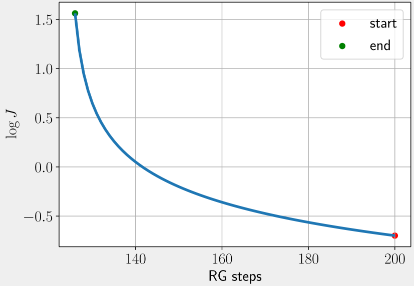
$$\Delta J = -J^2\left(\omega - \frac{1}{2}D + \frac{1}{4}J + \frac{1}{4}K\right)^{-1}$$

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

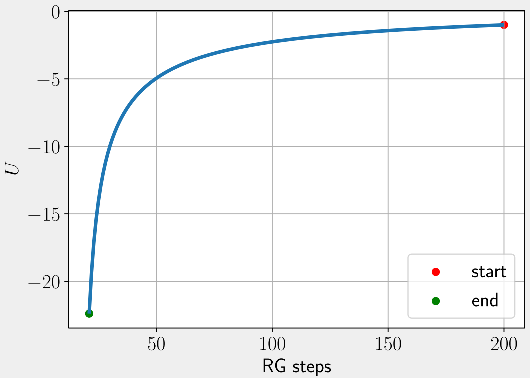
Results: $U > 0, J > K$

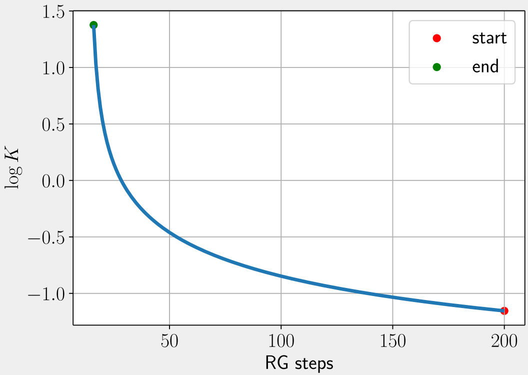


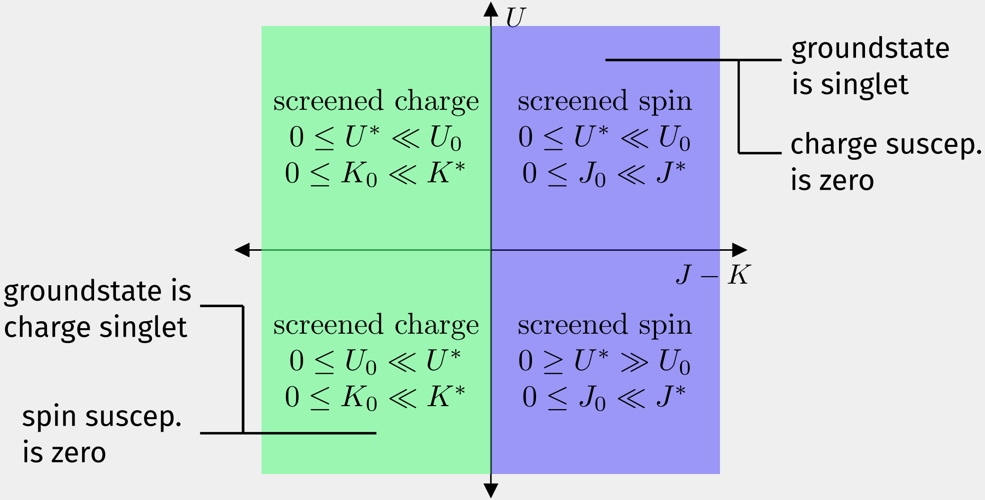




Results: $U < 0, J < K$

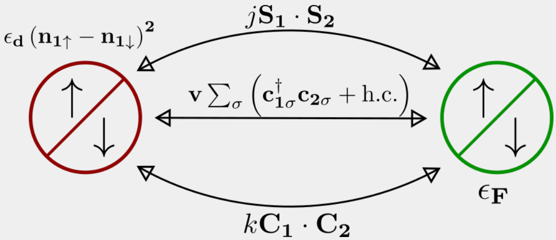


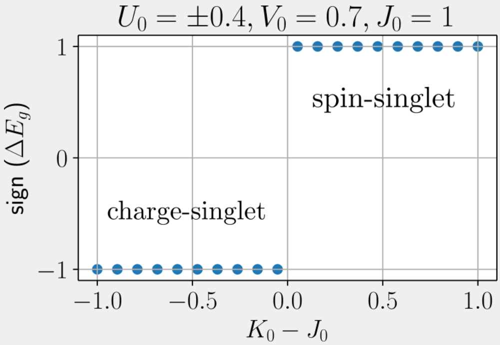



U
J − K
screened charge
0 ≤ U* ≪ U0
0 ≤ K0 ≪ K*
screened spin
0 ≤ U* ≪ U0
0 ≤ J0 ≪ J*
screened charge
0 ≤ U0 ≪ U*
0 ≤ K0 ≪ K*
screened spin
0 ≥ U* ≫ U0
0 ≤ J0 ≪ J*
groundstate
is singlet
charge suscep.
is zero
groundstate is
charge singlet
spin suscep.
is zero

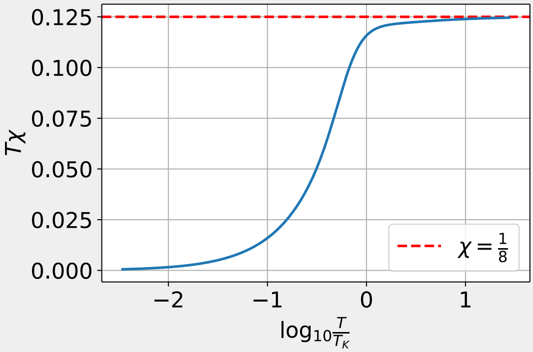
Results: Effective Zero-mode Hamiltonian

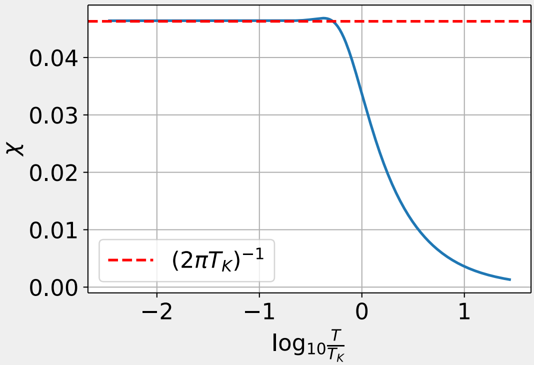
$$H_{IR} = \epsilon_d^* \left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow}\right)^2 + V^* \sqrt{N^*} \sum_\sigma \left(c^\dagger_{1\sigma} c_{2\sigma} + \text{h.c.}\right) + J^* N^* \vec{S}_1 \cdot \vec{S}_2 + K^* N^* \vec{C}_1 \cdot \vec{C}_2$$





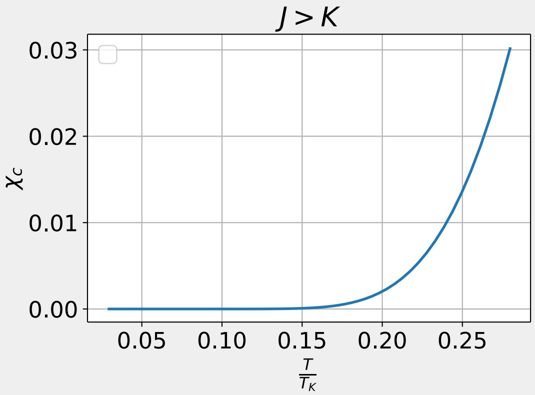
Results: Spin Susceptibility

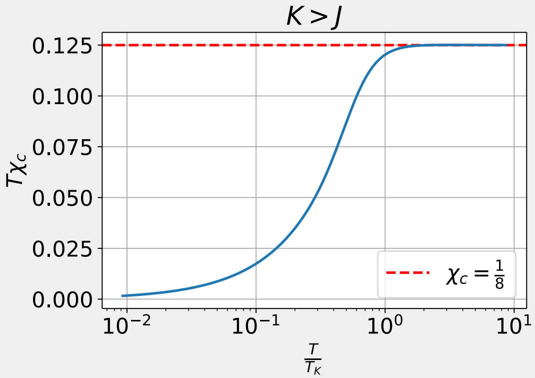




$(\chi \times T)(T \to 0) = \frac{1}{2j}$ $\quad T_K \equiv \frac{2N^*}{\pi}(D^* - 2\omega) \quad$ $\chi(T \to \infty) = \frac{1}{8}$

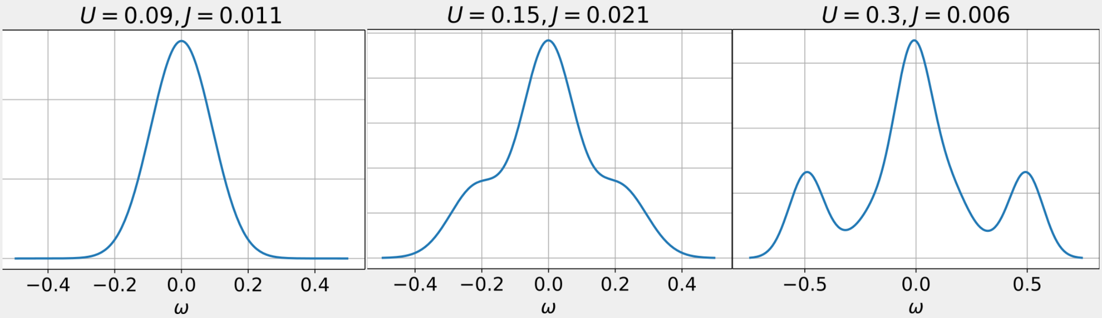
Results: Charge Susceptibility





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

Results: Spectral Function



Conclusions

- No renormalization in U unless J or Δ is nonzero.
- The spin-spin interaction is the main interaction
- U remains non-zero at strong-coupling

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!