Unitary Renormalization Group Approach to the Single-Impurity Anderson model

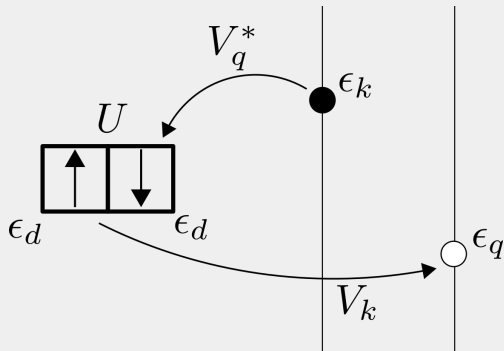Abhirup Mukherjee (18IP014)

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- About the model

- Some outstanding questions

- Unitary Renormalization Group (URG) formalism

- A few results

- Discussion and Future Goals

$$\mathcal{H}_{\mathsf{siam}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left[V(k) c^{\dagger}_{k\sigma} c_{d\sigma} + \mathsf{h.c.} \right] + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$
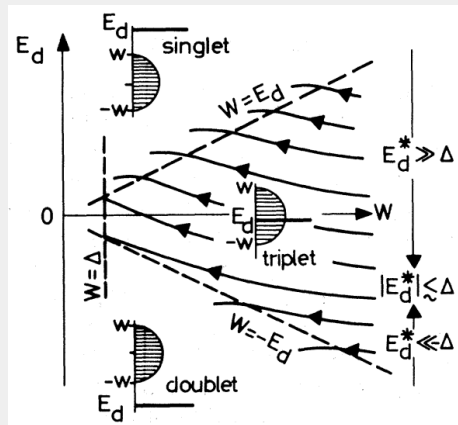
Poor Man's Scaling Results

For large U, Haldane and Jefferson find[1] three low energy theories:

- the **frozen impururity fixed point** ($\langle n_d \rangle$ = 0)
- the **local moment fixed point** ($\langle n_d \rangle$ = 1), and
- the **valence fluctuation fixed point** ($\langle n_d \rangle \sim \frac{1}{2}$).
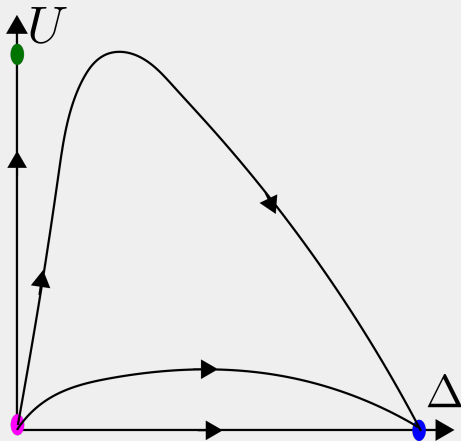

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[1] Haldane-1978, Jefferson-1977, Hewson, A. C.-1993-The Kondo Problem to Heavy Fermions

NRG Results - Symmetric Model

For the symmetric Anderson model[1]:

- 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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[1]Krishna-murthy et al, 1980

NRG Results - Asymmetric Model

Two more fixed points exist -

- the **valence fluctuation** fixed point ($\epsilon_d = V = 0, U = \infty$)

- the **frozen impurity** fixed point ($U = V = 0, \epsilon_d = \infty$)

Some Outstanding Questions

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- How does NRG obtain the local moment in the **absence of hybridisation**?

- 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.

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

$$\Downarrow$$

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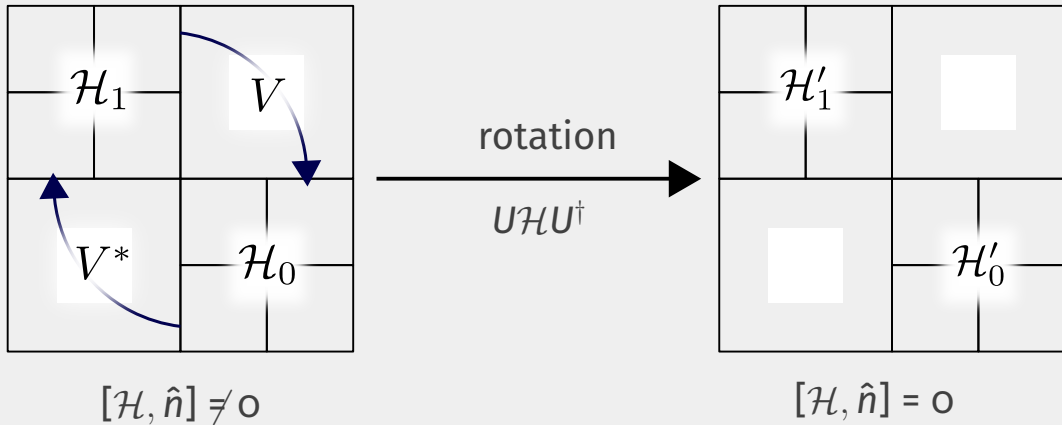
$$\Downarrow$$

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

Step 1:

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

occupied component

particle-hole fluctuation

$\mathcal{H}_1$

V

V^*

$\mathcal{H}_0$

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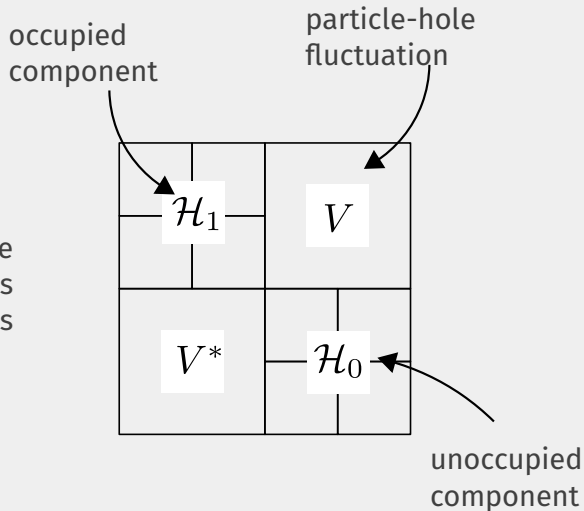
Step 2:
Rotate the Hamiltonian to kill the off-diagonal blocks.

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

rotation

$U\mathcal{H}U^\dagger$

Step 3:
Repeat the process with the new blocks.
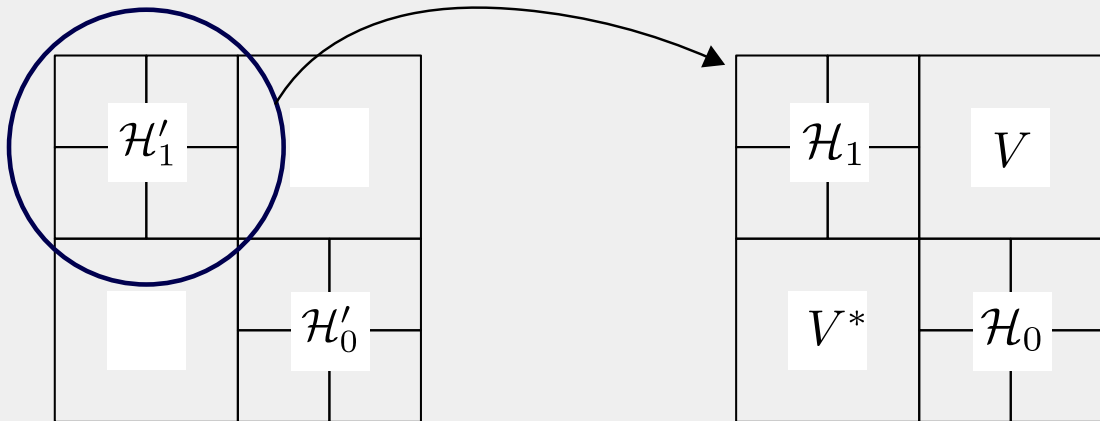
Some Characteristic features of the URG

- Presence of the quantum fluctuation energy scale ω

- Presence of finite-valued fixed points

- Spectrum-preserving transformations

- Tractable low-energy effective Hamiltonians

Results

$$\mathcal{H} = \overbrace{\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left[V(k) c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right] + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}^{\text{SIAM}} + J \vec{S}_d \cdot \underbrace{\sum_{kq\alpha\beta} \vec{\sigma}_{\alpha,\beta} c_{k\alpha}^\dagger c_{q\beta}}_{\text{spin-spin interaction}}$$
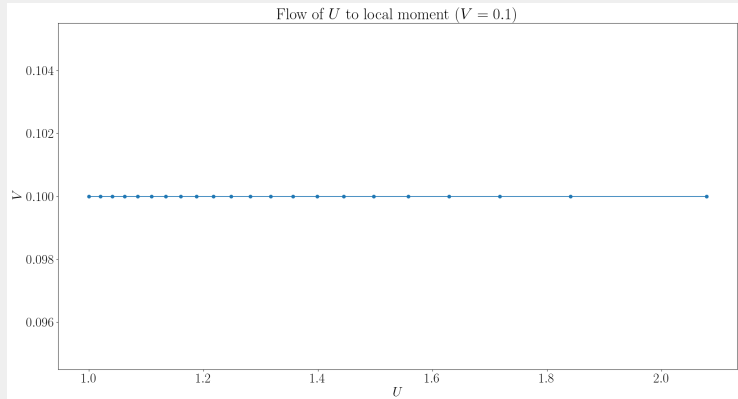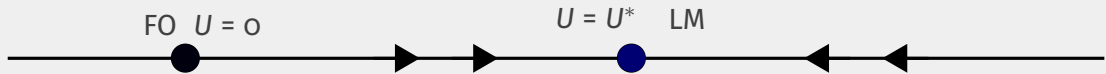
RG Equations

$$\Delta U = \left(U + \frac{1}{2}J \right) \sum_{|q|=\Lambda_n} \frac{|V(q)|^2}{(\omega - \epsilon_q - \frac{1}{2}U - \frac{1}{4}J)(\omega - \epsilon_q)}$$
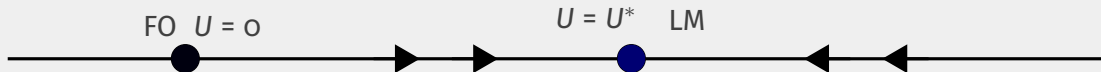
$$\Delta V(q) = -\frac{3}{4}J \sum_{|q|=\Lambda_n} \frac{V(q)}{\omega - \epsilon_q - \frac{1}{2}U - \frac{1}{4}J}$$

$$\Delta J = -\frac{1}{4}J^2 \sum_{\substack{|q|=\Lambda_n \\ k<\Lambda_n}} \frac{1}{\omega - \epsilon_q - \frac{1}{2}U - \frac{1}{4}J}$$
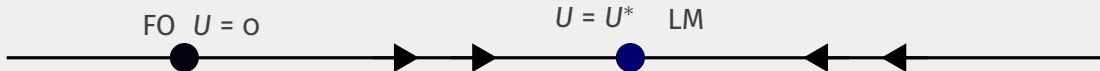
FO $U = 0$ $U = U^*$ LM

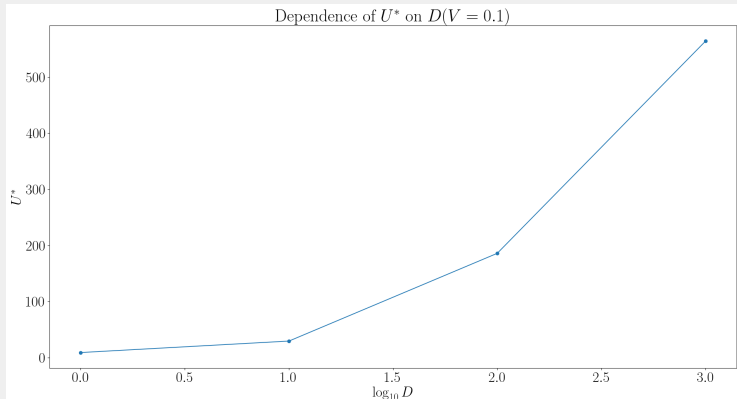Flow of U to local moment ($V = 0.1$)

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■ **No separatrix** for the
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FO $U = 0$ $U = U^*$ LM

- **No separatrix** for the flows to the local moment

- Local moment forms at **finite** U.

Dependence of U^* on $D(V = 0.1)$
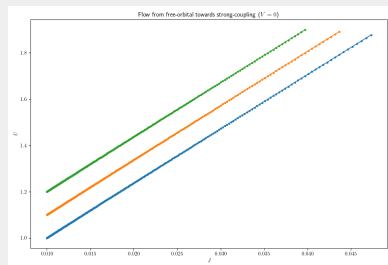
- J now drives the flow towards strong-coupling fixed point.

- This is in contrast to the NRG flow diagram where $\Delta \sim \frac{V^2}{U}$ was the driver of the flow.
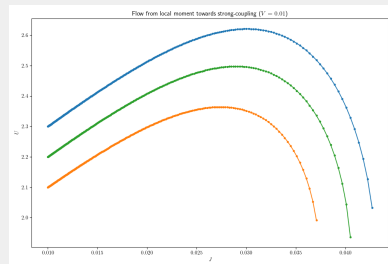
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Flow from local moment towards strong-coupling ($V = 0.01$)

Flow from free-orbital towards strong-coupling ($V = 0$)

Conclusions
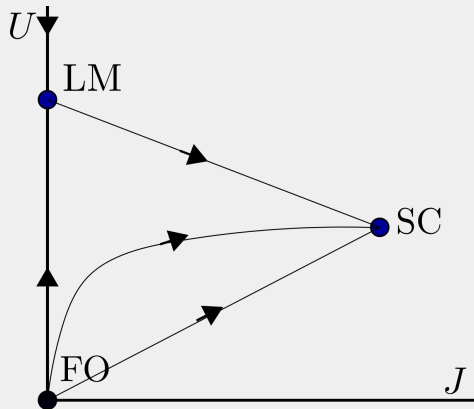
- Our analysis suggests that indeed there cannot be any renormalization in *U* unless at least one of *J* and Δ are nonzero.

- We also find that the main interaction that drives the flow to the strong-coupling regime is the spin-spin interaction.

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!