Unitary Renormalization Group Approach to the Single-Impurity Anderson model

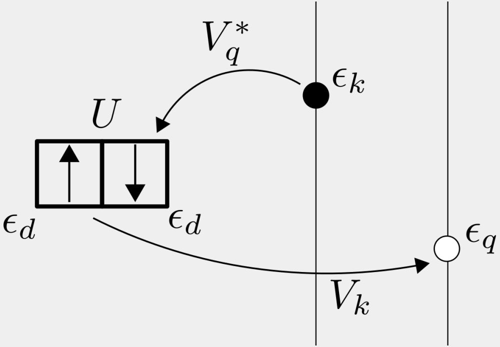
Abhirup Mukherjee (18IP014)

Supervisor: Dr. Siddhartha Lal

IISER Kolkata

January 8, 2021

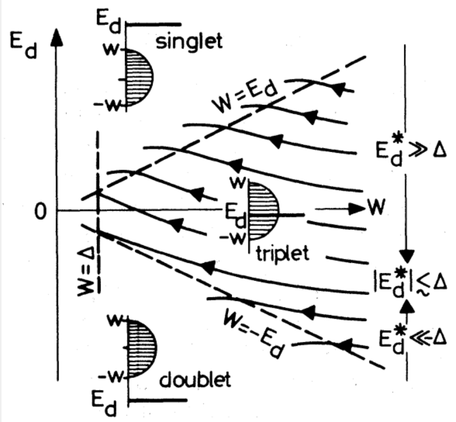
$$\mathcal{H}_{\text{siam}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left[V(k) c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.} \right] + \epsilon_d \sum_\sigma \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$$



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** ($\langle n_d \rangle \sim \frac{1}{2}$).

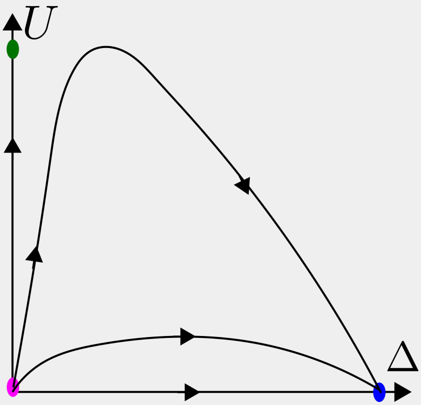


[1]Haldane-1978, Jefferson-1977, Hewson, A. C.-1993-The Kondo Problem to Heavy Fermions

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.



[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

- Is it possible to get **nonperturbative scaling equations** for the whole journey?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?
- What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?
- What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?
- Can we get **better estimates of dynamic quantities** in the crossover region?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?
- What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?
- Can we get **better estimates of dynamic quantities** in the crossover region?
- Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the bath spectral function or the many-particle entanglement?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?
- What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?
- Can we get **better estimates of dynamic quantities** in the crossover region?
- Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the bath spectral function or the many-particle entanglement?
- How does NRG obtain the local moment in the **absence of hybridisation**?

Some Outstanding Questions

- Is it possible to get **nonperturbative scaling equations** for the whole journey?
- Can we get Hamiltonians and wavefunctions in the **crossover region** ($T \sim T_K$)?
- What is the nature of the strong-coupling fixed point for a **finite system** ($J \neq \infty$)? Will the results change if we introduce a **non-uniform density of states**?
- Can we get **better estimates of dynamic quantities** in the crossover region?
- Is it possible to show the **transfer of spectral weight** along the flow, possibly by tracking the bath spectral function or the many-particle entanglement?
- 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.

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

$$\Downarrow$$

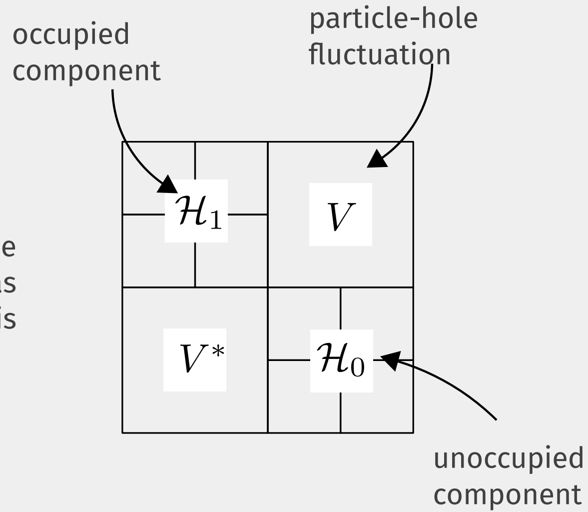
$$U\mathcal{H}(D)U^\dagger$$

$$\Downarrow$$

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

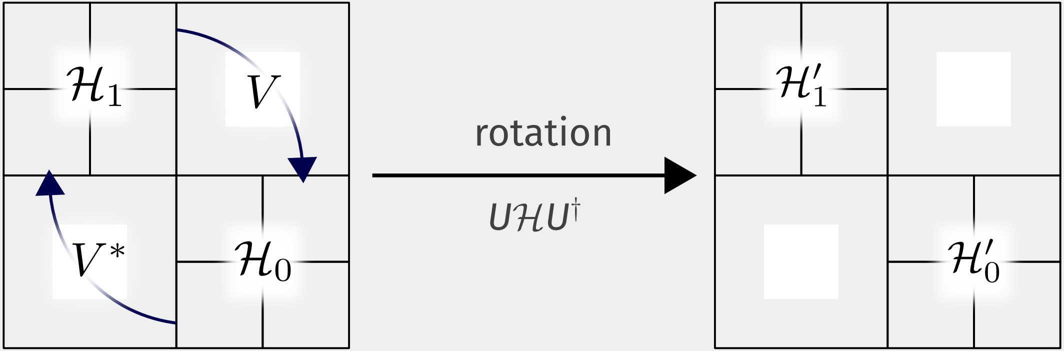
Step 1:

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



Step 2:

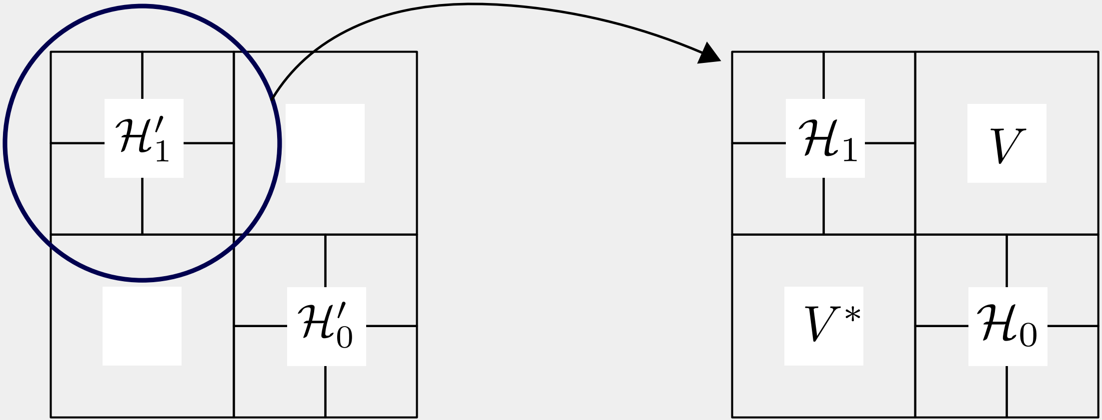
Rotate the Hamiltonian to kill the off-diagonal blocks.



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

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

Step 3:
Repeat the process with the new blocks.



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

$$\mathcal{H} = \overbrace{\sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \sum_{k\sigma} \left[V(k) c^\dagger_{k\sigma} c_{d\sigma} + \text{h.c.}\right] + \epsilon_d \sum_{\sigma} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}}^{SIAM}$$

$$+ \underbrace{J\vec{S_d} \cdot \sum_{kq\alpha\beta} \vec{\sigma}_{\alpha,\beta} c^\dagger_{k\alpha} c_{q\beta}}_{\text{spin-exchange}} + \underbrace{J\vec{C_d} \cdot \sum_{kq\alpha\beta} \vec{\sigma}_{\alpha,\beta} \psi^\dagger_{k\alpha} \psi_{q\beta}}_{\text{isospin-exchange}}$$

RG Equations

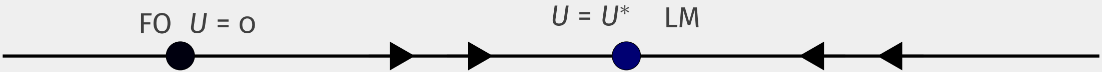
$$\Delta U = \left(U + \frac{1}{2}J\right) \sum_{|q|=\Lambda_n} \frac{|V(q)|^2}{(\omega - \epsilon_q - \frac{1}{2}U - \frac{1}{4}J)(\omega - \epsilon_q)}$$

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

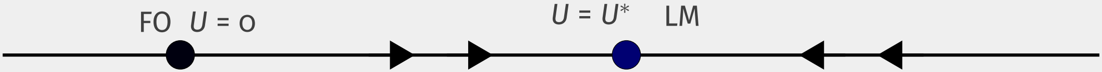
$$\Delta J = -\frac{1}{4}J^2 \sum_{\substack{|q|=\Lambda_n \\ k<\Lambda_n}} \frac{1}{\omega - \epsilon_q - \frac{1}{2}U - \frac{1}{4}J}$$

RG Equations

- Particle-hole symmetric
- Hermitian
- $SU(2)$-symmetric
- Reduce to Poor Man's scaling and Kondo 1-loop forms

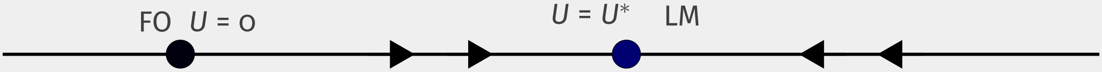


fo2lm.png



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

Results ($J = 0$)

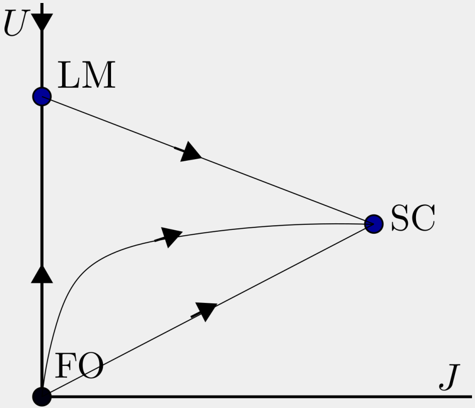


- **No separatrix** for the flows to the local moment
- Local moment forms at **finite** U.

UvsbareD.png

Results ($J > 0$)

- 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.



Results ($J > 0$)

lm2sc.png

- 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.

ng

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!