Unitary Renormalization Group Approach to Single-Impurity Anderson Model

Abhirup Mukherjee

Supervisor: Dr. Siddhartha Lal

Department of Physics, IISER Kolkata

January 14, 2021

Contents

1 Star Graph URG

The star graph problem consists of N spin-like degrees of freedom (lablled 1 through N) individually talking to a spin at the center (labelled 0). Each spin i ($\in [0, N]$) has an on-site energy ϵ_i. The coupling strength between 0 and i ($\in [1, N]$) is J_i. We choose the on-site energies such that $\epsilon_{i+1} > \epsilon_i, i \in [N-1, 1]$. In this way, ϵ_1 is the infrared limit and ϵ_N is the ultraviolet limit.

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \vec{S}_0 \cdot \vec{S}_i \tag{1.1}$$

By converting the last term into S^z and $S^\pm$, we can write the Hamiltonian as

$$\mathcal{H} = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i \left[S_0^z S_i^z + \frac{1}{2} \left(S_0^+ S_i^- + S_0^- S_i^+ \right) \right] \tag{1.2}$$

The diagonal terms are the ones that preserve the number or (in this case) spin.

$$\mathcal{H}^D = \sum_{i=0}^{N} \epsilon_i S_i^z + \sum_{i=1}^{N} J_i S_0^z S_i^z \tag{1.3}$$

This is the piece that comes in the denominator. The off-diagonal terms are the ones that change the number or spin. For this problem, they are the last two terms, $S_0^+ S_i^-$ and $S_0^- S_i^+$.

The RG involves decoupling the nodes N through 1, and looking at the resultant renormalization in ϵ_i and J_i. As a simplification, we will ignore the lower nodes in the denominator and keep only the node currently being decoupled, ie node N. Since node 0 is connected to node N, we will keep node 0 in the denominator as well. Making this simplification gives

$$\mathcal{H}^D = \epsilon_0 S_0^z + \epsilon_N S_N^z + J_N S_0^z S_N^z \tag{1.4}$$

1.1 Particle sector

This sector consists of the renormalization caused due to particle excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, N, is upwards in the excited state.

$$\Delta^+ \mathcal{H} = \frac{1}{2} J_N S_0^+ S_N^- \frac{1}{\hat{\omega} - \mathcal{H}^D} \frac{1}{2} J_N S_0^- S_N^+ \tag{1.5}$$

Note that we have chosen those particle scattering term because the S_N^+ on the right will create an up spin in the intermediate state, hence justifying the particle sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an

$S_0^- S_N^+$ in front, we can substitute $S_0^z = -\frac{1}{2}$ and $S_N^z = \frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front ($S^+ \left|\frac{1}{2}\right\rangle = S^- \left|-\frac{1}{2}\right\rangle = 0$). Therefore, from eq. 1.4.

$$\mathcal{H}^D = -\frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N - \frac{1}{4}J_N \tag{1.6}$$

Substituting this in $\Delta^+\mathcal{H}$ gives

$$\Delta^+\mathcal{H} = \frac{1}{2}J_N S_0^+ S_N^- \frac{1}{\hat{\omega} + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2}J_N S_0^- S_N^+ \tag{1.7}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue ω^+. The $+$ in the superscript indicates that it is from hte particle sector.

$$\begin{aligned}
\Delta^+\mathcal{H} &= \frac{1}{2}J_N S_0^+ S_N^- \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \frac{1}{2}J_N S_0^- S_N^+ \\
&= \frac{1}{4}J_N^2 S_0^+ S_N^- S_0^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
&= \frac{1}{4}J_N^2 S_0^+ S_0^- S_N^- S_N^+ \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{1.8}$$

Here we used the fact that the spins commute. We can now use the identities $S^+S^- = \left(\frac{1}{2} + S^z\right)$ and $S^-S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right)\left(\frac{1}{2} - S_N^z\right) \tag{1.9}$$

Since we want a particle in the intermediate state, we must have a hole in the initial state. Hence, we can substitute $S_N^z = -\frac{1}{2}$ in the last equation:

$$S_0^+ S_0^- S_N^- S_N^+ = \left(\frac{1}{2} + S_0^z\right) \tag{1.10}$$

This gives

$$\Delta^+\mathcal{H} = \frac{1}{4}J_N^2 \left(\frac{1}{2} + S_0^z\right) \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.11}$$

This is the final form and we can now read off the renormalizations. The term with S_0^z will renormalize the term in the Hamiltonian that comes with S_0^z, which is the term with ϵ_0.

$$\Delta^+\epsilon_0 = \frac{1}{4}J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.12}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is N:

$$\Delta^+\epsilon_N = \frac{1}{8}J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.13}$$

1.2 Hole sector

This sector consists of the renormalization caused due to hole excitations in the intermediate state. In the spin language, this translates to looking at those terms where the node that is being decoupled, N, is downwards in the excited state.

$$\Delta^{-}\mathcal{H} = \frac{1}{2}J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \mathcal{H}^D}\frac{1}{2}J_N S_0^+ S_N^- \tag{1.14}$$

Note that we have chosen those particle scattering term because the S_N^- on the right will create a down spin in the intermediate state, hence justifying the hole sector. The next order of business is to evaluate the $\mathcal{H}^D$ in the propagator. Since the propagator has an $S_0^+ S_N^-$ in front, we can substitute $S_0^z = \frac{1}{2}$ and $S_N^z = -\frac{1}{2}$ in $\mathcal{H}^D$. Any other value would be annihilated by the operator at the front ($S^+ |\frac{1}{2}\rangle = S^- |{-\frac{1}{2}}\rangle = 0$). Therefore, from eq. 1.4.

$$\mathcal{H}^D = \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N - \frac{1}{4}J_N \tag{1.15}$$

Substituting this in $\Delta^{-}\mathcal{H}$ gives

$$\Delta^{-}\mathcal{H} = \frac{1}{2}J_N S_0^- S_N^+ \frac{1}{\hat{\omega} - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}\frac{1}{2}J_N S_0^+ S_N^- \tag{1.16}$$

At this point we make another simplification, we replace $\hat{\omega}$ by its eigenvalue ω^-.

$$\begin{aligned}
\Delta^{-}\mathcal{H} &= \frac{1}{2}J_N S_0^- S_N^+ \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}\frac{1}{2}J_N S_0^+ S_N^- \\
&= \frac{1}{4}J_N^2 S_0^- S_N^+ S_0^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \\
&= \frac{1}{4}J_N^2 S_0^- S_0^+ S_N^+ S_N^- \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N}
\end{aligned} \tag{1.17}$$

Here we used the fact that the spins commute. We can now use the identities $S^+S^- = \left(\frac{1}{2} + S^z\right)$ and $S^-S^+ = \left(\frac{1}{2} - S^z\right)$ to write

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right)\left(\frac{1}{2} + S_N^z\right) \tag{1.18}$$

Since we want a hole in the intermediate state, we must have a particle in the initial state. Hence, we can substitute $S_N^z = \frac{1}{2}$ in the last equation:

$$S_0^- S_0^+ S_N^+ S_N^- = \left(\frac{1}{2} - S_0^z\right) \tag{1.19}$$

This gives

$$\Delta^{-}\mathcal{H} = \frac{1}{4}J_N^2 \left(\frac{1}{2} - S_0^z\right)\frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4}J_N} \tag{1.20}$$

This is the final form and we can now read off the renormalizations. The term with S_0^z will renormalize the term in the Hamiltonian that comes with S_0^z, which is the term with ϵ_0.

$$\Delta^- \epsilon_0 = -\frac{1}{4} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \tag{1.21}$$

The remaining part is operator less and will hence renormalize the on-site energy of the term that was just decoupled, that is N:

$$\Delta^- \epsilon_N = \frac{1}{8} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \tag{1.22}$$

1.3 Summary

These are the scaling equations for the couplings ϵ_0 and ϵ_N on decoupling the N^{th} node. Further calculations will involve checking where the couplings are relevant, what fixed point conditions exist and form of the effective Hamiltonians at the fixed points. If we consider the RG equations for ϵ_0 for the time being,

$$\begin{aligned} \Delta^+ \epsilon_0 &= \frac{1}{4} J_N^2 \frac{1}{\omega^+ + \frac{1}{2}\epsilon_0 - \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \\ \Delta^- \epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega^- - \frac{1}{2}\epsilon_0 + \frac{1}{2}\epsilon_N + \frac{1}{4} J_N} \end{aligned} \tag{1.23}$$

Since J_N does not renormalize and ϵ_N is the unrenormalized guy, we can abosrb them into the ω to make matters simpler: $\omega_N^+ = \omega^+ + \frac{1}{4} J_N - \frac{1}{2}\epsilon_N$, $\omega_N^- = \omega^- + \frac{1}{4} J_N + \frac{1}{2}\epsilon_N$.

$$\begin{aligned} \Delta^+ \epsilon_0 &= \frac{1}{4} J_N^2 \frac{1}{\omega_N^+ + \frac{1}{2}\epsilon_0} \\ \Delta^- \epsilon_0 &= -\frac{1}{4} J_N^2 \frac{1}{\omega_N^- - \frac{1}{2}\epsilon_0} \end{aligned} \tag{1.24}$$

$\omega^\pm$ are numbers that remain fixed during renormalization. In general they also renormalize, but we haven't kept track of that in this simplified calculation. Note the property of ω_N^+ that it grows as we go on decoupling the nodes, because $\epsilon_N > \epsilon_{N-1}$. In contrast, ω_N^- shrinks as we go on decoupling nodes, for the same reason.

We can now look for nature of flow ((ir)relevance) and fixed points. From the URG prescription, we know that a fixed point is reached when the denominator vanishes.

For the hole sector, $\Delta^- \epsilon_0$ is positive when $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$ and negative otherwise.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 > 0$, ϵ_0 is irrelevant. This will again lead to a runaway denominator, where ϵ_0 goes on decreasing and ω_N^- goes on increasing such that the denominator goes on increasing and there is no way of making it 0.

- For $\omega_N^- - \frac{1}{2}\epsilon_0 < 0$, ϵ_0 is relevant, so ϵ_0 will increase and ω_N^- will decrease, so the denominator will never be zero.

For the particle sector, $\Delta^+\epsilon_0$ is positive when $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$ and negative otherwise. Hence, ϵ_0 will grow in the former regime and shrink in the latter.Lets consider the two cases separately:

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 > 0$, ϵ_0 will grow. Since ω_N^+ also grows, the expression $\omega_N^+ + \frac{1}{2}\epsilon_0$ will become more and more positive as the RG progresses and there is no possibility of the denominator becoming zero. We cannot reach a fixed point in this regime, so ignore this regime.

- When $\omega_N^+ + \frac{1}{2}\epsilon_0 < 0$, ϵ_0 will shrink. Here it is possible to reach a fixed point, but in this case, both ϵ_i as well as ϵ_0 are decreasing, so this is like an overall scaling of the Hamiltonian. It is unlikely that it contains interesting physics, so we ignore this case as well and move on to the hole sector.