Notes for discussion

1. What I get:

$$\mathcal{H}^D = \epsilon_q \hat{n}_{q\beta} + \frac{J}{2} S^z \sigma^z_{\beta\beta} \hat{n}_{q\beta} \quad \text{[dropping the terms on lower shell]}$$

$$\eta_{q\beta} = \frac{J}{2} \sum_{k\alpha} \vec{S} \cdot \vec{\sigma}_{\alpha\beta} c^\dagger_{k\alpha} c_{q\beta} \frac{1}{\hat{\omega} - \epsilon_q \hat{n}_{q\beta} - \frac{J}{2} S^z \sigma^z_{\beta\beta} \hat{n}_{q\beta}}$$

$$\Delta\mathcal{H} = \left(\frac{J}{2}\right)^2 \sum_{q\beta} \tau_{q\beta} \sum_{\substack{k,k' \\ \alpha\gamma}} \left\{ \vec{S} \cdot \vec{\sigma}_{\beta\gamma} c^\dagger_{q\beta} c_{k',\gamma}, \vec{S} \cdot \vec{\sigma}_{\alpha\beta} c^\dagger_{k\alpha} c_{q,\beta} \frac{1}{\hat{\omega} - \epsilon_q \hat{n}_{q\beta} - \frac{J}{2} S^z \sigma^z_{\beta\beta} \hat{n}_{q\beta}} \right\}$$

What you have is

$$\begin{aligned} \Delta\hat{H}_{(j)} &= \sum_{\substack{m=1, \\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2 \tau_{j,\hat{s}_m,\beta}}{2(2\omega\tau_{j,\hat{s}_m,\beta} - \epsilon_{j,l}\tau_{j,\hat{s}_m,\beta} - J^{(j)} S^z s^z_{j,\hat{s}_m})} \times \Big[S^a S^b \sigma^a_{\alpha\beta} \sigma^b_{\beta\gamma} \sum_{\substack{(j_1, j_2 < j), \\ n,o}} c^\dagger_{j_1,\hat{s}_n,\alpha} c_{j_2,\hat{s}_o,\gamma} (1 - \hat{n}_{j,\hat{s}_m,\beta}) + S^b S^a \sigma^b_{\beta\gamma} \\ &+ \sum_{\substack{m=1, \\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2}{2(2\omega\tau_{j,\hat{s}_m,\beta} - \epsilon_{j,l}\tau_{j,\hat{s}_m,\beta} - J^{(j)} S^z s^z_{j,\hat{s}_m})} \Big[S^x S^y \sigma^x_{\alpha\beta} \sigma^y_{\beta\alpha} c^\dagger_{j,\hat{s}_m,\alpha} c_{j,\hat{s}_m,\beta} c^\dagger_{j,\hat{s}_m,\beta} c_{j,\hat{s}_m,\alpha} + S^y S^x \sigma^x_{\alpha\beta} \sigma^y_{\beta\alpha} c^\dagger_{j,\hat{s}_m,\beta} c_{j} \end{aligned}$$

- How do you bring the $\frac{1}{\omega\ldots}$ factor to the front?
- How do you get the third and fourth lines? The $\left(\vec{S} \cdot \vec{\sigma_{\alpha\beta}}\right) \left(\vec{S} \cdot \vec{\sigma}_{\beta\gamma}\right)$ type term should give just the $S^a S^b$ term which you have in the first and second lines?
- How does the $\epsilon_q \hat{n}_{q\beta}$ change to $\epsilon_q \tau_{q\beta}$? Similarly, how does the $JS^z \frac{\sigma^z_{\beta\beta}}{2} \hat{n}_{q\beta}$ change to $JS^z s^z_q$, when there is no summation inside the denominator?
- You mentioned in the docs that interchanging $\sigma^a_{\alpha\beta}$ with $\sigma^b_{\beta\gamma}$ will give a minus sign. But these are matrix elements (c-numbers) and hence should just commute.
- You mentioned that the $\tau_{q\beta}$ in the numerator of the first line of your expression should not be there. But then, what happens to the $\tau_{q\beta}$ I have at the front of my $\Delta\mathcal{H}$?
- How do I convert $\sigma^a_{\alpha\beta} \sigma^b_{\beta\gamma}$ to $\epsilon^{abd} \sigma^d_{\alpha\gamma}$? There is no such identity for **matrix elements**?

2. The **only change** in the Kondo cloud effective Hamiltonian is interchanging the s^+ and s^-. That should give

$$H_{\text{eff}} = \frac{J^*}{2} s_z + J^* s^- s^+ = \frac{J^*}{2} s^z + J^* \left(\frac{1}{2} - s^z \right) = +\frac{3}{4} J^* \tag{0.2}$$

after putting $s^z = -\frac{1}{2}$. This is different from the $-\frac{3}{4}J^*$ you mentioned in the docs. You said "The resulting expression will have one sign change". But I can't see such a sign change.

The equations are

$$\begin{aligned}
a_1 \left(H_0^* - \frac{J^*}{2} s^z \right) |\phi_1\rangle + a_0 \frac{J^*}{2} s^+ |\phi_0\rangle &= a_1 E |\phi_1\rangle \\
a_0 \left(H_0^* + \frac{J^*}{2} s^z \right) |\phi_0\rangle + a_1 \frac{J^*}{2} s^- |\phi_1\rangle &= a_0 E |\phi_0\rangle
\end{aligned} \tag{0.3}$$

From the first equation,

$$|\phi_1\rangle = \frac{a_0}{a_1} \frac{J^*}{2} \left[E - H_0^* + \frac{J^*}{2} s^z \right]^{-1} s^+ |\phi_0\rangle \tag{0.4}$$

Substituting this into the second equation,

$$a_0 \left(H_0^* + \frac{J^*}{2} s^z \right) |\phi_0\rangle + a_0 \left(\frac{J^*}{2} \right)^2 s^- \left[E - H_0^* + \frac{J^*}{2} s^z \right]^{-1} s^+ |\phi_0\rangle = a_0 E |\phi_0\rangle \tag{0.5}$$

$$\implies (E - H_0^*) |\phi_0\rangle = \frac{J^*}{2} s^z |\phi_0\rangle + \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{E - H_0^* + \frac{J^*}{2} s^z} s^+ |\phi_0\rangle \tag{0.6}$$

The effective Hamiltonian can be read off:

$$\begin{aligned}
H_{\text{eff}} &= \frac{J^*}{2} s^z + \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{E - H_0^* + \frac{J^*}{2} s^z} s^+ \\
&\sim \frac{J^*}{2} s^z + \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{E + \frac{J^*}{2} s^z} s^+ \\
&\sim \frac{J^*}{2} s^z + \left(\frac{J^*}{2} \right)^2 s^- \frac{1}{\frac{J^*}{2} s^z} s^+ && [E = 0] \\
&\sim \frac{J^*}{2} s^z + \frac{J^*}{2} s^- s^+ \times 2 && \left[\frac{1}{s^z} s^+ = 2 s^+ \right] \\
&\sim \frac{J^*}{2} s^z + J^* \left(\frac{1}{2} - s^z \right)
\end{aligned} \tag{0.7}$$