

Notes for discussion

1. What I get:

$$\begin{aligned}\mathcal{H}^D &= \epsilon_q \hat{n}_{q\beta} + \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta} \quad [\text{dropping the terms on lower shell}] \\ \eta_{q\beta} &= \frac{J}{2} \sum_{k\alpha} \vec{S} \cdot \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{q\beta} \frac{1}{\hat{\omega} - \epsilon_q \hat{n}_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \\ \Delta\mathcal{H} &= \left(\frac{J}{2}\right)^2 \sum_{q\beta} \tau_{q\beta} \sum_{\substack{k,k' \\ \alpha\gamma}} \left\{ \vec{S} \cdot \vec{\sigma}_{\beta\gamma} c_{q\beta}^\dagger c_{k'\gamma}, \vec{S} \cdot \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{q,\beta} \frac{1}{\hat{\omega} - \epsilon_q \hat{n}_{q\beta} - \frac{J}{2} S^z \sigma_{\beta\beta}^z \hat{n}_{q\beta}} \right\}\end{aligned}$$

What you have is

$$\begin{aligned}\Delta\hat{H}_{(j)} &= \sum_{\substack{m=1, \\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2 \tau_{j,\hat{s}_m,\beta}}{2(2\omega\tau_{j,\hat{s}_m,\beta} - \epsilon_{j,l}\tau_{j,\hat{s}_m,\beta} - J^{(j)}S^z s_{j,\hat{s}_m}^z)} \times \left[S^a S^b \sigma_{\alpha\beta}^a \sigma_{\beta\gamma}^b \sum_{\substack{(j_1,j_2 \leq j), \\ n,o}} c_{j_1,\hat{s}_n,\alpha}^\dagger c_{j_2,\hat{s}_o,\gamma} (1 - \hat{n}_{j,\hat{s}_m,\beta}) + S^b S^a \sigma_{\beta\gamma}^b \right. \\ &+ \sum_{\substack{m=1, \\ \beta=\uparrow/\downarrow}}^{n_j} \frac{(J^{(j)})^2}{2(2\omega\tau_{j,\hat{s}_m,\beta} - \epsilon_{j,l}\tau_{j,\hat{s}_m,\beta} - J^{(j)}S^z s_{j,\hat{s}_m}^z)} \left[S^x S^y \sigma_{\alpha\beta}^x \sigma_{\beta\alpha}^y c_{j,\hat{s}_m,\alpha}^\dagger c_{j,\hat{s}_m,\beta} c_{j,\hat{s}_m,\beta}^\dagger c_{j,\hat{s}_m,\alpha} + S^y S^x \sigma_{\alpha\beta}^x \sigma_{\beta\alpha}^y c_{j,\hat{s}_m,\beta}^\dagger c_{j,\hat{s}_m,\alpha} \right] \end{aligned}$$

- How do you bring the $\frac{1}{\omega \dots}$ factor to the front?
- How do you get the third and fourth lines? The $\left(\vec{S} \cdot \vec{\sigma}_{\alpha\beta}^{\rightarrow}\right) \left(\vec{S} \cdot \vec{\sigma}_{\beta\gamma}^{\rightarrow}\right)$ 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 $J S^z \frac{\sigma_{\beta\beta}^z}{2} \hat{n}_{q\beta}$ change to $J S^z s_q^z$, when there is no summation inside the denominator?
- You mentioned in the docs that interchanging $\sigma_{\alpha\beta}^a$ with $\sigma_{\beta\gamma}^b$ 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 $\sigma_{\alpha\beta}^a \sigma_{\beta\gamma}^b$ to $\epsilon^{abd} \sigma_{\alpha\gamma}^d$? 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

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

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

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

From the first equation,

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

Substituting this into the second equation,

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

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

The effective Hamiltonian can be read off:

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