

Multi-channel Kondo model URG

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I. INTRODUCTION

The multi-channel Kondo model is described by the Hamiltonian

$$H = \sum_{k,\alpha,\gamma} \epsilon_k^\gamma \hat{n}_{k\alpha}^\gamma + J \sum_{kk',\gamma} \vec{S}_d \cdot \vec{s}_{\alpha\alpha'} c_{k\alpha}^\gamma c_{k'\alpha'}^\gamma. \quad (\text{I.1})$$

It is mostly identical to the single-channel Kondo model: k, k' sum over the momentum states, α, α' sum over the spin indices and γ sums over the various channels. \vec{S}_d, \vec{s} are the impurity and conduction bath spin vectors. The renormalization at step j is given by

$$\Delta H_j = \{c^\dagger T, \eta\} = \left(c^\dagger T \frac{1}{\hat{\omega} - H_D} T^\dagger c + T^\dagger c \frac{1}{\hat{\omega} - H_D} c^\dagger T \right) \quad (\text{I.2})$$

$$c^\dagger T = J \sum_{k < \Lambda_j, \alpha} \vec{S}_d \cdot \vec{s}_{\beta\alpha} c_{q\beta}^\dagger c_{k\alpha}, \quad H_D = \epsilon_q \tau_{q\beta} + J S_d^z s_q^z \quad (\text{I.3})$$

Usually we treat the $\hat{\omega}$ as number(s) and study the renormalization in the couplings as functions of the quantum fluctuation scales. Each value of the fluctuation scale defines an eigendirection of $\hat{\omega}$. We have then essentially traded off the complexity in the non-commutation of the diagonal and off-diagonal terms for all the directions in the manifold of $\hat{\omega}$.

Here we will do something different. We will redefine the $\hat{\omega}$ by pulling out the off-diagonal term from it: $\hat{\omega} \rightarrow \hat{\omega} - H_X$, and then study the renormalization at various orders by expanding the denominator in powers of H_X . Such a redefinition essentially amounts to a rotation of the eigendirections of $\hat{\omega}$. This is done in order to extract some information out of $\hat{\omega}$, specifically the dependence of the RG equations on the channel number $K = \sum_\gamma$. This dependence is in principle present even if we do not do such a redefinition and expansion, in the various directions and values of ω , because those values encode the non-perturbative information regarding scattering at all loops. However, it is difficult to read off this information directly. This step of redefinition followed by expansion is being done with the sole aim of exposing such information.

The expansion we are talking about is

$$\eta = \frac{1}{\hat{\omega} - H_D} T^\dagger c = \frac{1}{\omega' - H_D - H_X} T^\dagger c \simeq \frac{1}{\omega' - H_D} T^\dagger c + \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c \quad (\text{I.4})$$

where $H_X = J \sum_{k,k' < \Lambda_j, \alpha, \alpha'} \vec{S}_d \cdot \vec{s}_{\alpha\alpha'} c_{k\alpha}^\dagger c_{k'\alpha'}$ is scattering between the entangled electrons. With this change, the second and third order renormalizations will take the form

$$\Delta H_j^{(2)} = c^\dagger T \frac{1}{\omega' - H_D} T^\dagger c + T^\dagger c \frac{1}{\omega - H_D} c^\dagger T \quad (\text{I.5})$$

$$\Delta H_j^{(3)} = c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c + T^\dagger c \frac{1}{\omega - H_D} H_X \frac{1}{\omega - H_D} c^\dagger T \quad (\text{I.6})$$

II. LEADING ORDER RENORMALIZATION

$$\Delta H_j^{(2)} = \underbrace{c^\dagger T \frac{1}{\omega' - H_D} T^\dagger c}_{\text{first term}} - \underbrace{T^\dagger c \frac{1}{\omega - H_D} c^\dagger T}_{\text{second term}} \quad (\text{II.1})$$

A. Second term

$$T^\dagger c \frac{1}{\hat{\omega} - H_D} c^\dagger T = J^2 \sum_{q\beta k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{q\beta} \vec{S}_d \cdot \vec{s}_{\alpha' \beta} \frac{1}{\omega - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} c_{q\beta}^\dagger c_{k\alpha} \vec{S}_d \cdot \vec{s}_{\beta \alpha} \quad (\text{II.2})$$

In the denominator, the state $q\beta$ is occupied, so we will substitute $\tau = +\frac{1}{2}$ and $s_q^z = \beta$. We will also substitute $\epsilon_q = +D$, because the state was initially unoccupied.

$$T^\dagger c \frac{1}{\hat{\omega} - H_D} c^\dagger T = J^2 \sum_{q\beta k k' \alpha \alpha', a, b} c_{k' \alpha'}^\dagger c_{q\beta} S_d^a s_{\alpha' \beta}^a \frac{1}{\omega - \frac{1}{2}D - J \frac{\beta}{2} S_d^z} c_{q\beta}^\dagger c_{k\alpha} S_d^b s_{\beta \alpha}^b \quad (\text{II.3})$$

$$= J^2 \sum_{q\beta k k' \alpha \alpha', a, b} c_{k' \alpha'}^\dagger c_{q\beta} S_d^a s_{\alpha' \beta}^a \frac{\omega - \frac{1}{2}D + J \frac{\beta}{2} S_d^z}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} c_{q\beta}^\dagger c_{k\alpha} S_d^b s_{\beta \alpha}^b \quad (\text{II.4})$$

$$= J^2 \sum_{q\beta k k' \alpha \alpha', a, b} c_{k' \alpha'}^\dagger c_{k\alpha} S_d^a s_{\alpha' \beta}^a \frac{\omega - \frac{1}{2}D + J S_d^z \frac{\beta}{2}}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} S_d^b s_{\beta \alpha}^b (1 - \hat{n}_{q\beta}) \quad (\text{II.5})$$

We can perform the sum over the states being decoupled: $\sum_q \hat{n}_{q\beta} = \sum_{\epsilon_q = D - |\delta D|}^D = n_j$.

$$T^\dagger c \frac{1}{\hat{\omega} - H_D} c^\dagger T = J^2 n_j \sum_{k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{k\alpha} \sum_{\beta, a, b} S_d^a s_{\alpha' \beta}^a s_{\beta \alpha}^b \frac{(\omega - \frac{1}{2}D) + J S_d^z \frac{\beta}{2}}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} S_d^b \quad (\text{II.6})$$

We will now simplify the terms individually. The first term is simpler:

$$\text{term 3} = \frac{J^2 n_j (\omega - \frac{1}{2}D)}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{k\alpha} \sum_{\beta, a, b} S_d^a S_d^b s_{\alpha' \beta}^a s_{\beta \alpha}^b \quad (\text{II.7})$$

The final sum can be performed using the following trick. In order to renormalize the Hamiltonian, the two impurity spin operators S_d^a and S_d^b have to multiply to produce another spin operator S_d^c and that will happen only for $a \neq b$. For $a \neq b$, we have the relation $S_d^a S_d^b = \frac{i}{2} \sum_c \epsilon^{abc} S_d^c$.

$$\sum_{a, b, \beta} S_d^a S_d^b s_{\alpha' \beta}^a s_{\beta \alpha}^b = \sum_{a, b} S_d^a S_d^b (s^a s^b)_{\alpha' \alpha} = -\frac{1}{4} \sum_{a, b, c_1, c_2} \epsilon^{abc_1} \epsilon^{abc_2} S_d^{c_1} (s^{c_2})_{\alpha' \alpha} \quad (\text{II.8})$$

The double ϵ can be evaluated easily: $\sum_{ab} \epsilon^{abc_1} \epsilon^{abc_2} = \sum_b (\delta_{c_1 c_2} - \delta_{bc_2} \delta_{bc_1}) = 2\delta_{c_1 c_2}$. Substituting this gives

$$\text{term 3} = \frac{J^2 n_j (\omega - \frac{1}{2}D)}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{k\alpha} \sum_c \left(-\frac{1}{2}\right) S_d^c s_{\alpha' \alpha}^c = \left(-\frac{1}{2}\right) \frac{J^2 n_j (\omega - \frac{1}{2}D)}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{k\alpha} \vec{S}_d \cdot \vec{s}_{\alpha' \alpha} \quad (\text{II.9})$$

The second term takes a bit more work:

$$\text{term 4} = \frac{1}{2} \frac{J^3 n_j}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha'} c_{k' \alpha'}^\dagger c_{k\alpha} \sum_{\beta, a, b} \beta S_d^a S_d^z S_d^b s_{\alpha' \beta}^a s_{\beta \alpha}^b \quad (\text{II.10})$$

Here we will use the identity:

$$S_d^a S_d^z S_d^b = \left(\frac{1}{4} \delta^{az} + \frac{i}{2} \sum_c \epsilon^{azc} S_d^c\right) S_d^b = \left(\frac{1}{4} \delta^{az} S_d^b + \frac{i}{8} \epsilon^{azb} - \frac{1}{4} \sum_{c_1, c} \epsilon^{azc_1} \epsilon^{c_1 bc} S_d^c\right) = \frac{1}{4} (\delta^{az} S_d^b - \delta^{ab} S_d^z + \delta^{bz} S_d^a) + \frac{i}{8} \epsilon^{azb} \quad (\text{II.11})$$

We will drop the last numerical term because such a term cannot renormalize the Hamiltonian. Substituting this gives

$$\text{term 4} = \frac{J^3 n_j}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \frac{1}{4} \sum_{k k' \alpha \alpha', c} c_{k' \alpha'}^\dagger c_{k\alpha} \left(\vec{S}_d \cdot \vec{s}_{\alpha' \alpha} - S_d^z \sum_{\beta} \beta s_{\alpha' \beta}^a s_{\beta \alpha}^a \right) \quad (\text{II.12})$$

B. First term

$$c^\dagger T \frac{1}{\hat{\omega} - H_D} T^\dagger c = J^2 \sum_{q\beta k k' \alpha \alpha'} c_{q\beta}^\dagger c_{k\alpha} \vec{S}_d \cdot \vec{s}_{\beta\alpha} \frac{1}{\omega' - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} c_{k'\alpha'}^\dagger c_{q\beta} \vec{S}_d \cdot \vec{s}_{\alpha'\beta} \quad (\text{II.13})$$

Here the intermediate state is unoccupied, so we put $\tau = -\frac{1}{2}$, $s_q^z = -\frac{\beta}{2}$ and since the initial state was occupied, we put $\epsilon_q = D$.

$$c^\dagger T \frac{1}{\hat{\omega} - H_D} T^\dagger c = \sum_{q\beta k k' \alpha \alpha' ab} c_{q\beta}^\dagger c_{k\alpha} S_d^a s_{\beta\alpha}^a \frac{J^2}{\omega' - \frac{1}{2}D + J \frac{\beta}{2} S_d^z} c_{k'\alpha'}^\dagger c_{q\beta} S_d^b s_{\alpha'\beta}^b \quad (\text{II.14})$$

$$= J^2 \sum_{q\beta k k' \alpha \alpha' ab} c_{q\beta}^\dagger c_{k\alpha} S_d^a s_{\beta\alpha}^a \frac{(\omega' - \frac{1}{2}D) - J \frac{\beta}{2} S_d^z}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} c_{k'\alpha'}^\dagger c_{q\beta} S_d^b s_{\alpha'\beta}^b \quad (\text{II.15})$$

$$= J^2 \sum_{q\beta k k' \alpha \alpha' ab} c_{q\beta}^\dagger c_{k'\alpha'}^\dagger c_{k\alpha} S_d^a s_{\beta\alpha}^a \frac{-(\omega' - \frac{1}{2}D) + J \frac{\beta}{2} S_d^z}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} c_{q\beta} S_d^b s_{\alpha'\beta}^b \quad \left[c_k c_{k'}^\dagger \sim -c_{k'}^\dagger c_k \right] \quad (\text{II.16})$$

$$= J^2 \sum_{q\beta k k' \alpha \alpha' ab} c_{k'\alpha'}^\dagger c_{k\alpha} S_d^a s_{\beta\alpha}^a \frac{-(\omega' - \frac{1}{2}D) + J \frac{\beta}{2} S_d^z}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} S_d^b s_{\alpha'\beta}^b \hat{n}_{q\beta} \quad (\text{II.17})$$

$$= J^2 n_j \sum_{\beta k k' \alpha \alpha' ab} c_{k'\alpha'}^\dagger c_{k\alpha} S_d^a s_{\beta\alpha}^a \frac{-(\omega' - \frac{1}{2}D) + J S_d^z \frac{1}{2} \beta}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} S_d^b s_{\alpha'\beta}^b \quad (\text{II.18})$$

We again simplify the terms individually, calling them term 1 and term 2. Term 1 can be made identical in form to term 1 using the relation: $s^b s^a = -s^b s^a$ for $a \neq b$. With this change, term 3 becomes

$$\text{term 1} = \frac{J^2 n_j (\omega' - \frac{1}{2}D)}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha' ab} c_{k'\alpha'}^\dagger c_{k\alpha} S_d^a S_d^b (s^a s^b)_{\alpha'\alpha} = \frac{1}{2} \frac{J^2 n_j (\omega' - \frac{1}{2}D)}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha', c} c_{k'\alpha'}^\dagger c_{k\alpha} \vec{S}_d \cdot \vec{s}_{\alpha'\alpha} \quad (\text{II.19})$$

For term 2, we will use eq. II.11 to get

$$\text{term 2} = \frac{J^3 n_j}{(\omega' - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \frac{1}{4} \sum_{k k' \alpha \alpha', c} c_{k'\alpha'}^\dagger c_{k\alpha} \left(\vec{S}_d \cdot \vec{s}_{\alpha'\alpha} - S_d^z \sum_{\beta} \beta s_{\alpha'\beta}^a s_{\beta\alpha}^a \right) \quad (\text{II.20})$$

C. Total renormalization $\Delta H^{(2)}$

From the formula for the renormalization $\Delta H^{(2)}$, we write

$$\Delta H^{(2)} = \text{term 1} + \text{term 2} + \text{term 3} + \text{term 4} \quad (\text{II.21})$$

These four terms are given by eqs. II.9, II.12, II.19 and II.20. From the constraints of URG and particle-hole symmetry, we have the constraint $\omega + \omega' = H_d^0 + H_d^1$. H_d^0 is the diagonal part when the current node is unoccupied and H_d^1 is when its occupied. For our case, $H_d^0 + H_d^1 = \sum \epsilon_q \tau_q = D$, because both the hole and particle states have energy of $\frac{D}{2}$ (ϵ_q and τ flip sign together). We therefore have $(\omega - D/2) = -(\omega' - D/2)$. With this relation, we have term 2 = term 4 and term 3 = -term 1. The total renormalization at second order is therefore

$$\Delta H^{(2)} = -2 \times \text{term 3} = -\frac{J^2 n_j (\omega - \frac{1}{2}D)}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \sum_{k k' \alpha \alpha', c} c_{k'\alpha'}^\dagger c_{k\alpha} \vec{S}_d \cdot \vec{s}_{\alpha'\alpha} \quad (\text{II.22})$$

which gives

$$\Delta J^{(2)} = -\frac{J^2 n_j (\omega - \frac{1}{2}D)}{(\omega - \frac{1}{2}D)^2 - \frac{1}{16}J^2} \quad (\text{II.23})$$

For $\omega < D/2$, we get the flow towards the strong-coupling fixed point. That is, there is an attractive stable fixed point at $J^* = 4|\omega - D/2|$ for all bare $J > 0$. We also get a decay towards the local moment fixed point $J^* = 0$ for $J < 0$. For $\omega = -D/2$ and $J \ll D$, we get the one-loop PMS form.

$$\Delta J^{(2)} = \frac{J^2 n_j D}{D^2 - \frac{1}{16} J^2} \simeq \frac{J^2 n_j}{D} \quad (\text{II.24})$$

III. NEXT-TO-LEADING ORDER RENORMALIZATION

$$\Delta H_j^{(3)} = \underbrace{c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c}_{\text{first term}} + \underbrace{T^\dagger c \frac{1}{\omega - H_D} H_X \frac{1}{\omega - H_D} c^\dagger T}_{\text{second term}} \quad (\text{III.1})$$

A. First term

$$\begin{aligned} & c^\dagger T \frac{1}{\omega' - H_D} H_X \frac{1}{\omega' - H_D} T^\dagger c \\ &= \sum_{\substack{q, k, k', k_1, k_2, \\ \beta, \alpha, \alpha', \alpha_1, \alpha_2, \\ l_1, l_2, a, b, c}} c_{q\beta, l_1}^\dagger c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a \frac{J^2}{\omega' - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} S_d^b s_{\alpha_1 \alpha_2}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \frac{J}{\omega' - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} c_{k' \alpha', l_1}^\dagger c_{q\beta, l_1} S_d^c s_{\alpha' \beta}^c \end{aligned} \quad (\text{III.2})$$

q sums over the momenta being decoupled. k, k', k_1, k_2 sum over the momenta not being decoupled. $\beta, \alpha, \alpha', \alpha_1, \alpha_2$ sum over the spin indices. l_1, l_2 sum over the channels. We substitute $s_q^z = -\frac{\beta}{2}$ and $\epsilon_q \tau_{q\beta} = \frac{D}{2}$. The term inside the summation becomes

$$\begin{aligned} & J^3 c_{q\beta, l_1}^\dagger c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a \frac{1}{\omega' - \frac{D}{2} + J \frac{\beta}{2} S_d^z} S_d^b s_{\alpha_1 \alpha_2}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \frac{1}{\omega' - \frac{D}{2} + J \frac{\beta}{2} S_d^z} c_{k' \alpha', l_1}^\dagger c_{q\beta, l_1} S_d^c s_{\alpha' \beta}^c \\ &= \frac{J^3 c_{q\beta, l_1}^\dagger c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b s_{\alpha_1 \alpha_2}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) c_{k' \alpha', l_1}^\dagger c_{q\beta, l_1} S_d^c s_{\alpha' \beta}^c}{\left[\left(\omega' - \frac{D}{2} \right)^2 - \frac{1}{16} J^2 \right]^2} \end{aligned} \quad (\text{III.3})$$

We will start simplifying this equation by summing over q . $c_{q\beta}^\dagger$ and $c_{q\beta}$ can be easily combined to form $\hat{n}_{q\beta}$, because they anti-commute with the other momenta. The sum gives $\sum_q \hat{n}_{q\beta l_1} = n_j$. This gives (without writing the summations explicitly)

$$\frac{J^3 n_j c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b s_{\alpha_1 \alpha_2}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) c_{k' \alpha', l_1}^\dagger S_d^c s_{\alpha' \beta}^c}{\left[\left(\omega' - \frac{D}{2} \right)^2 - \frac{1}{16} J^2 \right]^2} \quad (\text{III.4})$$

The next simplification involves identifying how to contract the operators. The contractions have to be done so as to reproduce the original $\vec{S}_d \cdot \vec{s} c^\dagger c$ form so that we can read off the renormalization. Currently, there are four distinct electron labels, k, k', k_1, k_2 . There are two ways to contract them. The first is by choosing $k_1 \alpha_1 = k_2 \alpha_2$. However, this term vanishes:

$$\begin{aligned} \sum_{k_1 \alpha_1, b} S_d^b s_{\alpha_1 \alpha_1}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_1 \alpha_1, l_2} &= \sum_{b, k_1 \alpha_1} S_d^b s_{\alpha_1 \alpha_1}^b \hat{n}_{k_1 \alpha_1, l_2} = \sum_b S_d^b \left(\sum_{\alpha_1} s_{\alpha_1 \alpha_1}^b \right) \int_{-D+|\delta D|}^0 d\epsilon \rho(\epsilon) \\ &= \sum_b S_d^b \text{Trace}(s^b) \int_{-D+|\delta D|}^0 d\epsilon \rho(\epsilon) = 0 \end{aligned} \quad (\text{III.5})$$

The other way to contract the indices is by selecting $k\alpha = k'\alpha'$. Those two operators can again be brought together without any change of sign because there will be an even number of flips. Summing over $k = k'$ and the channel

index l_1 then gives $\sum_{l_1} \sum_k (1 - \hat{n}_{k\alpha}) = \sum_{l_1} \int_{-D+|\delta D|}^0 n_j = \frac{1}{2} K n_j N_j$, where $n_j = \rho|\delta D|$ and $N_j = \rho D$. $K = \sum_{l_1}$ is the total number of conduction bath channels. The factor of half is inserted to model the probability of transition appropriately; not all values of ϵ_k will contribute equally to the renormalization. The entire expression is now

$$\begin{aligned} & \sum_{\substack{k_1, k_2, \beta, \alpha, \\ \alpha', \alpha_1, \alpha_2, \\ l_2, a, b, c}} \frac{J^3 K N_j n_j S_d^a s_{\beta\alpha}^a \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b s_{\alpha_1 \alpha_2}^b c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^c s_{\alpha' \beta}^c}{2 \left[\left(\omega' - \frac{D}{2} \right)^2 - \frac{1}{16} J^2 \right]^2} \\ &= \frac{J^3 K N_j n_j}{2 \left[\left(\omega' - \frac{D}{2} \right)^2 - \frac{1}{16} J^2 \right]^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1 \alpha_1, l_2}^\dagger c_{k_2 \alpha_2, l_2} \sum_{\substack{\beta, \alpha, \\ a, b, c}} S_d^a s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^b s_{\alpha\beta}^c \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^c \end{aligned} \quad (\text{III.6})$$

We now need to simplify the final summation.

$$\sum_{\substack{\beta, \alpha, \\ a, b, c}} s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^b s_{\alpha\beta}^c S_d^a \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^c \quad (\text{III.7})$$

The internal product can be evaluated as follows:

$$\left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) S_d^b \left(\omega' - \frac{D}{2} - J \frac{\beta}{2} S_d^z \right) = \left(\omega' - \frac{D}{2} \right)^2 S_d^b - \frac{\beta J}{2} \left(\omega' - \frac{D}{2} \right) \{S_d^z, S_d^b\} + \frac{J^2}{4} S_d^z S_d^b S_d^z \quad (\text{III.8})$$

The anticommutator is $\{S_d^z, S_d^b\} = \frac{\delta^{bz}}{2}$. The triple operator product is given by eq. II.11: $S_d^z S_d^b S_d^z = \frac{1}{4} S_d^b (2\delta^{bz} - 1)$. The right-hand side of eq. III.8 becomes

$$\left[\left(\omega' - \frac{D}{2} \right)^2 + \frac{J^2}{16} (2\delta^{bz} - 1) \right] S_d^b - \frac{\beta J}{4} \delta^{bz} \left(\omega' - \frac{D}{2} \right) \equiv C_1^b S_d^b + C_2^b \quad (\text{III.9})$$

Eq. III.7 takes the form

$$\sum_{\substack{\beta, \alpha, \\ a, b, c}} s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^b s_{\alpha\beta}^c (C_1^b S_d^a S_d^b S_d^c + C_2^b S_d^a S_d^c) \quad (\text{III.10})$$

These spin products can again be evaluated using standard identities:

$$S_d^a S_d^c = \frac{i}{2} \sum_e \epsilon^{ace} S_d^e, \quad S_d^a S_d^b S_d^c = \frac{1}{4} (\delta^{ab} S_d^c - \delta^{ac} S_d^b + \delta^{bc} S_d^a) \quad (\text{III.11})$$

We have dropped constant terms in both equations because such terms cannot renormalize the Hamiltonian. This gives, for eq. III.7,

$$\sum_{\substack{\beta, \alpha, \\ a, b, c}} s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^b s_{\alpha\beta}^c \left[\frac{1}{4} C_1^b (\delta^{ab} S_d^c - \delta^{ac} S_d^b + \delta^{bc} S_d^a) + C_2^b \frac{i}{2} \sum_e \epsilon^{ace} S_d^e \right] \quad (\text{III.12})$$

We take the first term. Define $C_1^b = C_{11} + C_{12} \delta^{bz}$. Also note that the indices α, β can be easily summed over: $\sum_{\alpha\beta} s_{\beta\alpha}^a c_{\alpha\beta}^c = \text{Trace}(s^a s^c) = \frac{1}{2} \delta^{ac}$. The term in product with C_1^b becomes

$$\frac{1}{2} \sum_{a,b} s_{\alpha_1 \alpha_2}^b \frac{1}{4} (C_{11} + C_{12} \delta^{bz}) (2\delta^{ab} S_d^a - S_d^b) = -\frac{1}{8} \sum_b s_{\alpha_1 \alpha_2}^b (C_{11} + C_{12} \delta^{bz}) S_d^b = -\frac{1}{8} (C_{11} \vec{S}_d \cdot \vec{s}_{\alpha_1 \alpha_2} + C_{12} s_{\alpha_1 \alpha_2}^z S_d^z) \quad (\text{III.13})$$

The term in product with C_2^b can be written as

$$\begin{aligned} & -\frac{iJ \left(\omega' - \frac{D}{2} \right)}{8} \sum_{\substack{\beta, \alpha, \\ a, b, c}} \delta^{bz} \beta s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^b s_{\alpha\beta}^c \sum_e \epsilon^{ace} S_d^e = -\frac{iJ \left(\omega' - \frac{D}{2} \right)}{8} \sum_{\substack{\beta, \alpha, \\ a, c}} \beta s_{\beta\alpha}^a s_{\alpha_1 \alpha_2}^z s_{\alpha\beta}^c \sum_e \epsilon^{ace} S_d^e \\ &= \frac{-iJ \left(\omega' - \frac{D}{2} \right)}{8} \sum_{\beta, a, c, e} \beta (s^c s^a)_{\beta\beta} s_{\alpha_1 \alpha_2}^z \epsilon^{ace} S_d^e \end{aligned} \quad (\text{III.14})$$

Since $a \neq c$ ($a = c$ would make $\epsilon^{ace} = 0$), we can use $(s^c s^a)_{\beta\beta} = \frac{i}{2} \sum_f \epsilon^{caf} s_{\beta\beta}^f = \frac{i\beta}{4} \epsilon^{caz}$. Substituting this gives

$$\frac{J(\omega' - \frac{D}{2})}{32} \sum_{a,c,e} s_{\alpha_1\alpha_2}^z \epsilon^{ace} \epsilon^{caz} S_d^e = \frac{J(\omega' - \frac{D}{2})}{16} s_{\alpha_1\alpha_2}^z S_d^z \quad (\text{III.15})$$

Once we note that $\mathcal{C}_{11} = (\omega' - \frac{D}{2})^2 - \frac{1}{16}J^2$ and $\omega' - D/2 - 2\mathcal{C}_{12}/J = \omega' - D/2 - J/4$ and when we substitute eqs. III.13 and III.15 into eq. III.6, we get

$$- \frac{1}{16} \frac{J^3 K N_j n_j}{(\omega' - \frac{D}{2})^2 - \frac{1}{16}J^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \vec{S}_d \cdot \vec{s}_{\alpha_1\alpha_2} + \frac{J^4 K N_j n_j (\omega' - D/2 - J/4)}{32 \left[(\omega' - \frac{D}{2})^2 - \frac{1}{16}J^2 \right]^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} S_d^z s_{\alpha_1\alpha_2}^z \quad (\text{III.16})$$

B. Second term

$$\begin{aligned} & T^\dagger c \frac{1}{\omega - H_D} H_X \frac{1}{\omega - H_D} c^\dagger T \\ &= \sum_{\substack{q, k, k', k_1, k_2, \\ \beta, \alpha, \alpha', \alpha_1, \alpha_2, \\ l_1, l_2, a, b, c}} c_{k'\alpha', l_1}^\dagger c_{q\beta, l_1} S_d^c s_{\alpha'\beta}^c \frac{J^2}{\omega - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} S_d^b s_{\alpha_1\alpha_2}^b c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \frac{J}{\omega - \epsilon_q \tau_{q\beta} - J S_d^z s_q^z} c_{q\beta, l_1}^\dagger c_{k\alpha, l_1} S_d^a s_{\beta\alpha}^a \end{aligned} \quad (\text{III.17})$$

We take similar steps as before: 1. $\epsilon_q \tau_{q\beta} = \frac{D}{2}$ 2. $s_q^z = \frac{\beta}{2}$ 3. Sum over q to get n_j 4. Contract $k\alpha, k'\alpha'$ to get $K N_j n_j$ 5. Compute the internal product to obtain $\mathcal{C}_1^b S_d^b - \mathcal{C}_2^b$. The expression at this point is

$$\frac{J^3 K N_j n_j}{2 \left[(\omega - \frac{D}{2})^2 - \frac{1}{16}J^2 \right]^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \sum_{\substack{\beta, \alpha, \\ a, b, c}} s_{\beta\alpha}^a s_{\alpha_1\alpha_2}^b s_{\alpha\beta}^c S_d^c (\mathcal{C}_1^b S_d^b - \mathcal{C}_2^b) S_d^a \quad (\text{III.18})$$

\mathcal{C}_1^b is exactly the same as before, the only difference being ω replaces ω' . The sign of \mathcal{C}_2^b has also flipped, because $\beta \rightarrow -\beta$. The other difference is that S_d^a and S_d^c have switched places. Eq. III.12 is replaced by

$$\sum_{\substack{\beta, \alpha, \\ a, b, c}} s_{\beta\alpha}^a s_{\alpha_1\alpha_2}^b s_{\alpha\beta}^c \left[\frac{1}{4} \mathcal{C}_1^b (\delta^{ab} S_d^c - \delta^{ac} S_d^b + \delta^{bc} S_d^a) + \mathcal{C}_2^b \frac{i}{2} \sum_e \epsilon^{ace} S_d^e \right] \quad (\text{III.19})$$

Note that even though \mathcal{C}_2^b came with a minus sign in eq. III.18, that minus sign has been canceled by a second minus sign that arises from the exchange of $a \leftrightarrow c$ in ϵ^{ace} . Since eq. III.19 is identical to eq. III.12, we can directly write down the renormalization in this case:

$$- \frac{1}{16} \frac{J^3 K N_j n_j}{(\omega - \frac{D}{2})^2 - \frac{1}{16}J^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \vec{S}_d \cdot \vec{s}_{\alpha_1\alpha_2} + \frac{J^4 K N_j n_j (\omega - D/2 - J/4)}{32 \left[(\omega - \frac{D}{2})^2 - \frac{1}{16}J^2 \right]^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} S_d^z s_{\alpha_1\alpha_2}^z \quad (\text{III.20})$$

C. Total renormalization $\Delta H^{(3)}$

We will again use the relation $\omega - D/2 = -(\omega' - D/2)$. The total renormalization at this order is obtained by adding eqs. III.16 and III.20.

$$\Delta H^{(3)} = - \frac{J^3 K N_j n_j / 8}{(\omega - \frac{D}{2})^2 - \frac{1}{16}J^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} \vec{S}_d \cdot \vec{s}_{\alpha_1\alpha_2} - \frac{J^5 K N_j n_j / 64}{\left[(\omega - \frac{D}{2})^2 - \frac{1}{16}J^2 \right]^2} \sum_{\substack{k_1, k_2, \\ \alpha_1, \alpha_2, l_2}} c_{k_1\alpha_1, l_2}^\dagger c_{k_2\alpha_2, l_2} S_d^z s_{\alpha_1\alpha_2}^z \quad (\text{III.21})$$