

URG analysis of the extended Kondo model with interactions in various angular momentum channels

Abhirup Mukherjee, Siddhartha Lal

I. HAMILTONIAN

We consider an impurity spin \vec{S}_d interacting with a two-dimensional tight-binding conduction bath through a general interaction of the form

$$\sum_{\vec{k}_1, \vec{k}_2, \sigma_1, \sigma_2} J_{\vec{k}_1, \vec{k}_2} \vec{S}_d \cdot \frac{1}{2} \vec{\tau}_{\sigma_1, \sigma_2} c_{\vec{k}_1, \sigma_1}^\dagger c_{\vec{k}_2, \sigma_2} \quad (1)$$

where $\vec{\tau}$ is the vector of sigma matrices and \vec{k}_1, \vec{k}_2 are momentum states of the conduction bath. The precise form of $J_{\vec{k}_1, \vec{k}_2}$ depends on the symmetry of the symmetry of the impurity-bath interaction. We consider the following three cases:

- a d-wave interaction, where the impurity couples with a coherent d-wave combination f_σ of the bath sites closest to it: $f_\sigma \equiv \frac{1}{2} (c_{L, \sigma}^\dagger + c_{R, \sigma}^\dagger - c_{U, \sigma}^\dagger - c_{D, \sigma}^\dagger)$, where L, R, U and D indicate electrons at the positions $(x, y) = (-a, 0), (a, 0), (0, a)$ and $(0, -a)$ respectively, a being the lattice spacing of the conduction bath lattice. The corresponding interaction (in real space) is of the form $\vec{S}_d \cdot \sum_{\sigma_1, \sigma_2} \frac{1}{2} \vec{\tau}_{\sigma_1, \sigma_2} f_{\sigma_1}^\dagger f_{\sigma_2}$. When fourier-transformed to momentum space, it gives rise to the momentum-dependent Kondo coupling

$$J_{\vec{k}_1, \vec{k}_2} = J \prod_{i=1,2} [\cos(ak_i^x) - \cos(ak_i^y)] \quad (2)$$

For reference, we define the Fourier transforms as $c_{L(R), \sigma}^\dagger = \sum_{\vec{k}} c_{\vec{k}, \sigma}^\dagger e^{- (+) ik^x a}$, $c_{U(D), \sigma}^\dagger = \sum_{\vec{k}} c_{\vec{k}, \sigma}^\dagger e^{- (+) ik^y a}$.

- a p-wave interaction, where the impurity couples with the p-wave electron $p_\sigma \equiv \frac{1}{2} (c_{L, \sigma}^\dagger + c_{R, \sigma}^\dagger + c_{U, \sigma}^\dagger + c_{D, \sigma}^\dagger)$. The momentum-dependent Kondo coupling in this case is

$$J_{\vec{k}_1, \vec{k}_2} = J \prod_{i=1,2} [\cos(ak_i^x) + \cos(ak_i^y)] \quad (3)$$

Since we are considering a 2-dimensional conduction bath in the tight-binding limit, such a Kondo coupling vanishes close to the Fermi surface. As a result, this case is not interesting for our purpose.

- a p-wave interaction, but without the off-site terms in the bath. This amounts to considering the Kondo interaction term $J \vec{S}_d \cdot \sum_{\sigma_1, \sigma_2} \frac{1}{2} \vec{\tau}_{\sigma_1, \sigma_2} \frac{1}{4} \sum_{i=L, R, U, D} c_{i, \sigma_1}^\dagger c_{i, \sigma_2}$. The momentum-dependent Kondo coupling in this case is

$$J_{\vec{k}_1, \vec{k}_2} = J_{\vec{k}_1 - \vec{k}_2} \equiv \frac{1}{2} J \cos[a(k_1^x - k_2^x) + x \rightarrow y] \quad (4)$$

This does not vanish identically on the Fermi surface, and is therefore of potential interest to us.

We also consider correlation terms on the bath sites L, R, U and D . In momentum space, it is of the general form

$$-\frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4, \sigma, \sigma'} W_{\{\vec{k}_i\}} \sigma \sigma' c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{\vec{k}_3, \sigma'}^\dagger c_{\vec{k}_4, \sigma'} \quad (5)$$

where the form of $W_{\{\vec{k}_i\}}$ is again determined by the orbitals participating in the interaction. We ignore the p-wave interaction (for the same reason as above) and consider just the d-wave interaction and a p-wave interaction without off-site terms. These two cases lead to the following Hamiltonian structures:

- a d-wave interaction, of the form $-\frac{W}{2} \left(f_{\uparrow}^{\dagger} f_{\uparrow} - f_{\downarrow}^{\dagger} f_{\downarrow} \right)^2$, leading to the momentum-dependence

$$W_{\{\vec{k}_i\}} = W \prod_{i=1,2,3,4} [\cos(ak_i^x) - \cos(ak_i^y)] \quad (6)$$

- a p-wave interaction without off-site terms, $-\frac{1}{2}W\frac{1}{4}\sum_{i=L,R,U,D}\left(c_{i,\uparrow}^{\dagger}c_{i,\uparrow}-c_{i,\downarrow}^{\dagger}c_{i,\downarrow}\right)^2$, leading to the following form in momentum space:

$$W_{\{\vec{k}_i\}} = W_{\vec{k}_1-\vec{k}_2,\vec{k}_3-\vec{k}_4} = \frac{1}{2}W[\cos(a(k_1^x-k_2^x+k_3^x-k_4^x))+x\rightarrow y] \quad (7)$$

Owing to hermiticity of the term, we must have $W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}^* = W_{\vec{k}_4,\vec{k}_3,\vec{k}_2,\vec{k}_1}$. We will also find it convenient to separate the bath interaction into parallel and anti-parallel parts:

$$\sum_{\{\vec{k}_i\},\sigma,\sigma'} W_{\{\vec{k}_i\}} \sigma \sigma' c_{\vec{k}_1,\sigma}^{\dagger} c_{\vec{k}_2,\sigma} c_{\vec{k}_3,\sigma'}^{\dagger} c_{\vec{k}_4,\sigma'} = \sum_{\{\vec{k}_i\},\sigma} \left[W_{\{\vec{k}_i\}}^S c_{\vec{k}_1,\sigma}^{\dagger} c_{\vec{k}_2,\sigma} c_{\vec{k}_3,\sigma}^{\dagger} c_{\vec{k}_4,\sigma} - W_{\{\vec{k}_i\}}^A c_{\vec{k}_1,\sigma}^{\dagger} c_{\vec{k}_2,\sigma} c_{\vec{k}_3,\bar{\sigma}}^{\dagger} c_{\vec{k}_4,\bar{\sigma}} \right] \quad (8)$$

To summarise, the total Hamiltonian we consider is of the form

$$H = -2t \sum_{kx,ky} [\cos(ak_x) + \cos(ak_y)] c_{\vec{k},\sigma}^{\dagger} c_{\vec{k},\sigma} + \sum_{\vec{k}_1,\vec{k}_2,\sigma_1,\sigma_2} J_{\vec{k}_1,\vec{k}_2} \vec{S}_d \cdot \frac{1}{2} \vec{\tau}_{\sigma_1,\sigma_2} c_{\vec{k}_1,\sigma_1}^{\dagger} c_{\vec{k}_2,\sigma_2} \\ - \frac{1}{2} \sum_{\{\vec{k}_i\},\sigma} \left[W_{\{\vec{k}_i\}}^S c_{\vec{k}_1,\sigma}^{\dagger} c_{\vec{k}_2,\sigma} c_{\vec{k}_3,\sigma}^{\dagger} c_{\vec{k}_4,\sigma} - W_{\{\vec{k}_i\}}^A c_{\vec{k}_1,\sigma}^{\dagger} c_{\vec{k}_2,\sigma} c_{\vec{k}_3,\bar{\sigma}}^{\dagger} c_{\vec{k}_4,\bar{\sigma}} \right], \quad (9)$$

where $J_{\{\vec{k}_i\}}$ takes one of the two forms in eqs. 2 and 4, and $W_{\{\vec{k}_i\}}$ can similarly take either of the two forms in eqs. 6 and 7.

II. RG SCHEME

At any given step j of the RG procedure, we decouple the states $\{\vec{q}\}$ on the isoenergetic surface of energy ε_j . The diagonal Hamiltonian H_D for this step consists of all terms that do not change the occupancy of the states $\{\vec{q}\}$:

$$H_D^{(j)} = \varepsilon_j \sum_{q,\sigma} \tau_{q,\sigma} + \frac{1}{2} \sum_{\vec{q}} J_{\vec{q},\vec{q}} S_d^z (\hat{n}_{\vec{q},\uparrow} - \hat{n}_{\vec{q},\downarrow}) - \frac{1}{2} \sum_{\vec{q}} [W_{\vec{q}}^S (\hat{n}_{\vec{q},\uparrow} + \hat{n}_{\vec{q},\downarrow}) - 2W_{\vec{q}}^A \hat{n}_{\vec{q},\uparrow} \hat{n}_{\vec{q},\downarrow}] . \quad (10)$$

where $\tau = \hat{n} - 1/2$ and $W_{\vec{q}}$ is a shorthand for $W_{\vec{q},\vec{q},\vec{q},\vec{q}}$. The three terms, respectively, are the kinetic energy of the momentum states on the isoenergetic shell that we are decoupling, the Ising interaction energy between the impurity spin and the spins formed by these momentum states and, finally, the local correlation energy associated with these states arising from the W term.

The off-diagonal part of the Hamiltonian on the other hand leads to scattering in the states $\{\vec{q}\}$:

$$\begin{aligned}
H_X^{(j)} = & \underbrace{\sum_{\vec{k}, \vec{q}, \sigma, \sigma'} J_{\vec{k}, \vec{q}} \vec{S}_d \cdot \vec{\tau}_{\sigma, \sigma'} \left[c_{\vec{q}\sigma}^\dagger c_{\vec{k}, \sigma'} + \text{h.c.} \right]}_{T_1^\dagger + T_1} \\
& - \frac{1}{2} \underbrace{\sum_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{k}_4, \sigma, \sigma'} W_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{k}_4} \sigma \sigma' \left[c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{\vec{k}_3, \sigma'}^\dagger c_{\vec{k}_4, \sigma'} + \text{h.c.} \right]}_{T_2^\dagger + T_2} \\
& - \frac{1}{2} \underbrace{\sum_{\vec{q}, \vec{k}_2, \vec{q}', \vec{k}_4, \sigma, \sigma'} W_{\vec{q}, \vec{k}_2, \vec{q}', \vec{k}_4} \sigma \sigma' \left[c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_4, \sigma'} + \text{h.c.} \right]}_{T_3^\dagger + T_3} \\
& - \frac{1}{2} \underbrace{\sum_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{q}', \sigma, \sigma'} W_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{q}'} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{\vec{k}_3, \sigma'}^\dagger c_{\vec{q}', \sigma'}}_{T_4} \\
& - \frac{1}{2} \underbrace{\sum_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{q}', \sigma, \sigma'} W_{\vec{q}, \vec{k}_2, \vec{k}_3, \vec{q}'} \sigma \sigma' c_{\vec{k}_3, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_2, \sigma}}_{T_5} \\
& - \frac{1}{2} \underbrace{\sum_{\vec{q}, \vec{k}_2, \vec{q}', \vec{q}_3, \sigma, \sigma'} W_{\vec{q}, \vec{k}_2, \vec{q}', \vec{q}_3} \sigma \sigma' \left[c_{\vec{q}', \sigma'}^\dagger c_{\vec{q}_3, \sigma'} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_2, \sigma} + \text{h.c.} \right]}_{T_6^\dagger + T_6}, \\
& + \underbrace{\sum_{\vec{q}, \vec{q}', \sigma, \sigma'} J_{\vec{k}, \vec{q}} \vec{S}_d \cdot \vec{\tau}_{\sigma, \sigma'} c_{\vec{q}\sigma}^\dagger c_{\vec{q}', \sigma'}}_{T_7}
\end{aligned} \tag{11}$$

The first term T_1 is an impurity-mediated scattering between the states \vec{q} at energy ε_j and the states \vec{k} at energies below ε_j . Terms T_2 through T_6 involve two-particle scattering between these momentum states involving an increasing number of participating states from the isoenergetic shell ε_j , through the Hubbard-like local term W . The renormalisation of the Hamiltonian is constructed from the general expression

$$\Delta H^{(j)} = H_X \frac{1}{\omega - H_D} H_X. \tag{12}$$

III. RENORMALISATION OF THE BATH CORRELATION TERM W

In order to lead to a renormalisation of the W -term, there must be a total of four uncontracted momentum indices k_i and two contracted indices q_1, q_2 . The following combinations of scattering processes are compatible: (i) $T_2^\dagger GT_6 + T_6^\dagger GT_2$, (ii) $T_3^\dagger GT_3 + T_3 GT_3^\dagger$, (iii) $T_4 GT_4$, (iv) $T_5 GT_5$ and (v) $T_4 GT_5 + T_5 GT_4$.

A. Correlated scattering involve one electron on the shell ε_j

The first term is of the form

$$\begin{aligned}
T_2 GT_6^\dagger = & \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} \sum_{\vec{q}, \vec{q}'} \sigma \sigma' W_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{q}} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \frac{1}{\omega - H_D} \left(W_{\vec{q}', \vec{q}', \vec{q}, \vec{k}_4} \hat{n}_{\vec{q}', \sigma} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} - W_{\vec{q}', \vec{q}', \vec{q}, \vec{k}_4} \hat{n}_{\vec{q}', \sigma} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} \right. \\
& \left. - W_{\vec{q}, \vec{q}', \vec{q}', \vec{k}_4} c_{\vec{q}, \sigma}^\dagger \left(1 - \hat{n}_{\vec{q}', \sigma} \right) c_{\vec{k}_4, \sigma} \right). \tag{13}
\end{aligned}$$

where \vec{q} and \vec{q}' are electronic states on the isoenergetic shells of energy $\pm\varepsilon_j$. The change in occupancy of the state $\vec{q}\sigma$ from 0 to 1 leads to an excited state energy $H_D = \varepsilon_{\vec{q}}\tau_{q\sigma} - \frac{1}{2}W_{\vec{q}}(\hat{n}_{\vec{q},\uparrow} - \hat{n}_{\vec{q},\downarrow})^2 = \frac{1}{2}\varepsilon_{\vec{q}} - \frac{1}{2}W_{\vec{q}}$, where $W_{\vec{q}}$ is a shorthand for $W_{\vec{q},\vec{q},\vec{q},\vec{q}}$. We consider the first two terms on the right for the time being. The number operators $\hat{n}_{\vec{q}',\sigma}, \hat{n}_{\vec{q}',\bar{\sigma}}$ project the initial state to that in which \vec{q}' is occupied, henceforth referred to as the particle sector (PS). The operator $c_{\vec{q},\sigma}^\dagger$ can be combined with its Hermitian conjugate on the other side to produce a hole operator, leading to another projection onto the set of initial states in which the momentum state \vec{q} is unoccupied, henceforth referred to as the hole sector (HS). Since the two terms are otherwise identical, their opposite signs lead to them cancelling each other. The remaining term involves the hole projection operators $1 - \hat{n}_{\vec{q}',\sigma}$ and $1 - \hat{n}_{\vec{q},\sigma}$. Evaluating this term in the same way leads to

$$T_2GT_6^\dagger = - \sum_{\{\vec{k}_i\},\sigma,\sigma'} \sigma\sigma' c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{k}_4,\sigma} \sum_{\vec{q},\vec{q}' \in \text{HS}} \frac{W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{q}} W_{\vec{q},\vec{q}',\vec{q}',\vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} . \quad (14)$$

The particle-hole transformed term $T_6^\dagger GT_2$ can be evaluated in the same way:

$$T_6^\dagger GT_2 = \sum_{\{\vec{k}_i\}} \sum_{\sigma,\sigma'} \sum_{\vec{q},\vec{q}'} \left(W_{\vec{q}',\vec{q}',\vec{q},\vec{k}_4} \hat{n}_{\vec{q}',\bar{\sigma}} c_{\vec{q},\sigma}^\dagger c_{\vec{k}_4,\sigma} - W_{\vec{q}',\vec{q}',\vec{q},\vec{k}_4} \hat{n}_{\vec{q}',\sigma} c_{\vec{q},\sigma}^\dagger c_{\vec{k}_4,\sigma} - W_{\vec{q},\vec{q}',\vec{q}',\vec{k}_4} c_{\vec{q},\sigma}^\dagger (1 - \hat{n}_{\vec{q}',\sigma}) c_{\vec{k}_4,\sigma} \right) \frac{1}{\omega - H_D} \times \\ \sigma\sigma' W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{q}} c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{q},\sigma} . \quad (15)$$

For such a scattering process, the excited energy is given by $H_D = \varepsilon_{\vec{q}}\tau_{q\sigma} - \frac{1}{2}W_{\vec{q}}(\hat{n}_{\vec{q},\uparrow} - \hat{n}_{\vec{q},\downarrow})^2 = -\frac{1}{2}\varepsilon_{\vec{q}} - \frac{1}{2}W_{\vec{q}}$. The change of the sign in front of $\varepsilon_{\vec{q}}$ arises from the fact that in this process, the state \vec{q} is occupied in the intermediate excited state, owing to the $c_{\vec{q},\sigma}$ operator to the right of the Greens function. Cancelling the first two terms in eq. 15 (just as in the previous process) and evaluating the last term gives

$$T_6^\dagger GT_2 = \sum_{\{\vec{k}_i\},\sigma\sigma'} \sigma\sigma' c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{k}_4,\sigma} \sum_{\substack{\vec{q} \in \text{PS} \\ \vec{q}' \in \text{HS}}} \frac{W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{q}} W_{\vec{q},\vec{q}',\vec{q}',\vec{k}_4}}{\omega + \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \\ = \sum_{\{\vec{k}_i\},\sigma\sigma'} \sigma\sigma' c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{k}_4,\sigma} \sum_{\vec{q},\vec{q}' \in \text{HS}} \frac{W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{q}_t} W_{\vec{q}_t,\vec{q}',\vec{q}',\vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} . \quad (16)$$

At the last step, we exchanged the sum over the PS with a sum over the HS, leading to the transformation $\vec{q} \rightarrow \vec{q}_t$, where $\vec{q}_t = (\pi, \pi) - \vec{q}$ is the particle-hole transformed partner of the state at \vec{q} , and is obtained by reflecting the state \vec{q} about the nearest nodal point in the Brillouin zone. These states are on isoenergetic contours that are at equal distance from but on opposite sides of the Fermi surface: $\varepsilon_{\vec{q}} = -\varepsilon_{\vec{q}_t}$.

Another pair of terms is obtained by taking the hermitian conjugate of the scattering terms, $T_6GT_2^\dagger$ and $T_2^\dagger GT_6$. These are simply Hermitian conjugates of the two terms considered above:

$$T_2^\dagger GT_6 = - \sum_{\{\vec{k}_i\},\sigma\sigma'} \sigma\sigma' c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{k}_4,\sigma} \sum_{\vec{q},\vec{q}' \in \text{HS}} \frac{W_{\vec{q}_t,\vec{k}_4,\vec{k}_1,\vec{k}_2} W_{\vec{k}_3,\vec{q}',\vec{q}',\vec{q}_t}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} \\ T_6GT_2^\dagger = \sum_{\{\vec{k}_i\},\sigma\sigma'} \sigma\sigma' c_{\vec{k}_1,\sigma'}^\dagger c_{\vec{k}_2,\sigma'} c_{\vec{k}_3,\sigma}^\dagger c_{\vec{k}_4,\sigma} \sum_{\vec{q},\vec{q}' \in \text{HS}} \frac{W_{\vec{q},\vec{k}_4,\vec{k}_1,\vec{k}_2} W_{\vec{k}_3,\vec{q}',\vec{q}',\vec{q}}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} . \quad (17)$$

B. Scattering from the infrared subspace into the ultraviolet subspace

We now consider the second term $T_3^\dagger GT_3$:

$$\begin{aligned}
T_3^\dagger GT_3 &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} \frac{1}{\omega - H_D} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}} \sigma \sigma' c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_4, \sigma} c_{\vec{k}_2, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_3, \sigma}^\dagger \sum_{\vec{q}, \vec{q}'} \hat{n}_{\vec{q}, \sigma} \hat{n}_{\vec{q}', \sigma'} \frac{W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega + \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{PS}} \frac{W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega + \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}}, \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}_t, \vec{k}_4, \vec{q}_t', \vec{k}_2} W_{\vec{k}_1, \vec{q}_t', \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}_t}},
\end{aligned} \tag{18}$$

where \vec{q}, \vec{q}' are summed over all momentum states in the isoenergetic shell and in the particle sector (PS) (states that are occupied in the ground state). At the last step, we again replaced the sum over the particle sector with one over the hole sector by transforming $\vec{q}, \vec{q}' \rightarrow \vec{q}_t, \vec{q}_t'$ and using $\varepsilon_{\vec{q}_t} = -\varepsilon_{\vec{q}}$ in the denominator.

The particle-hole transformed term is $T_3 GT_3^\dagger$:

$$\begin{aligned}
T_3 GT_3^\dagger &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}} \sigma \sigma' c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \frac{1}{\omega - H_D} W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}}.
\end{aligned} \tag{19}$$

We can obtain two additional terms by switching the sequence of operators on the right hand side of the propagator:

$$\begin{aligned}
T_3^\dagger G \overline{T}_3 &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} \frac{1}{\omega - H_D} W_{\vec{k}_3, \vec{q}, \vec{k}_1, \vec{q}'} \sigma \sigma' c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}_t, \vec{k}_4, \vec{q}_t', \vec{k}_2} W_{\vec{k}_3, \vec{q}_t, \vec{k}_1, \vec{q}_t'}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}_t}},
\end{aligned} \tag{20}$$

$$\begin{aligned}
T_3 G \overline{T}_3^\dagger &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}} \sigma \sigma' c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \frac{1}{\omega - H_D} W_{\vec{q}', \vec{k}_2, \vec{q}, \vec{k}_4} \sigma \sigma' c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}', \vec{k}_2, \vec{q}, \vec{k}_4} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}}.
\end{aligned} \tag{21}$$

C. Coherent simultaneous scattering within the infrared and ultraviolet subspaces

The remaining sets of terms that we need to consider are:

$$\begin{aligned}
T_4 GT_4^\dagger &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}'} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} \frac{1}{\omega - H_D} W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}} \sigma \sigma' c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} \hat{n}_{\vec{q}, \sigma} (1 - \hat{n}_{\vec{q}', \sigma'}) c_{\vec{k}_4, \sigma} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}'} W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}}}{\omega + \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{q}_t'} W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}_t}}.
\end{aligned} \tag{22}$$

$$\begin{aligned}
T_5^\dagger G T_5^\dagger &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4} \sigma \sigma' c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} \frac{1}{\omega - H_D} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2} \sigma \sigma' c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} \\
&= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} \hat{n}_{\vec{q}, \sigma} (1 - \hat{n}_{\vec{q}', \sigma'}) c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_2, \sigma'} \frac{W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2}}{\omega + \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}}.
\end{aligned} \tag{23}$$

$$\begin{aligned}
T_5^\dagger G T_4 &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2} \sigma \sigma' c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} \frac{1}{\omega - H_D} W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}'} \sigma \sigma' c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} \hat{n}_{\vec{q}', \sigma'} (1 - \hat{n}_{\vec{q}, \sigma}) c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_4, \sigma} c_{\vec{k}_1, \sigma'}^\dagger \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}'} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}'} W_{\vec{k}_3, \vec{q}, \vec{q}', \vec{k}_2}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}}.
\end{aligned} \tag{24}$$

$$\begin{aligned}
T_4^\dagger G T_5 &= \frac{1}{4} \sum_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}} \sigma \sigma' c_{\vec{q}', \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{q}, \sigma} \frac{1}{\omega - H_D} W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4} \sigma \sigma' c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{q}', \sigma'} c_{\vec{q}, \sigma}^\dagger c_{\vec{k}_4, \sigma} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\vec{q}, \vec{q}'} \sum_{\sigma, \sigma'} \hat{n}_{\vec{q}', \sigma'} (1 - \hat{n}_{\vec{q}, \sigma}) c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_4, \sigma} \frac{W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}} W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \\
&= -\frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \frac{W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}} W_{\vec{k}_1, \vec{q}', \vec{q}, \vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}}.
\end{aligned} \tag{25}$$

D. Net renormalisation for the bath correlation term

Adding contributions from all these terms, the total renormalisation in the Hamiltonian in the context of W comes out to be

$$\begin{aligned}
\Delta H \Big|_W &= \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \left[-\frac{W_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{q}} W_{\vec{q}, \vec{q}', \vec{q}', \vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} + \frac{W_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{q}_t} W_{\vec{q}_t, \vec{q}', \vec{q}', \vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} \right. \\
&\quad - \frac{W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{k}_2} W_{\vec{k}_3, \vec{q}', \vec{q}', \vec{q}_t}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} + \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{k}_2} W_{\vec{k}_3, \vec{q}', \vec{q}', \vec{q}}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} + \frac{W_{\vec{q}_t, \vec{k}_4, \vec{q}_t, \vec{k}_2} W_{\vec{k}_1, \vec{q}_t, \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} + \frac{W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \\
&\quad + \frac{W_{\vec{q}_t, \vec{k}_4, \vec{q}_t, \vec{k}_2} W_{\vec{k}_3, \vec{q}_t, \vec{k}_1, \vec{q}_t}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} + \frac{W_{\vec{q}', \vec{k}_2, \vec{q}, \vec{k}_4} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} - \frac{W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{q}} W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} - \frac{W_{\vec{k}_1, \vec{q}', \vec{q}_t, \vec{k}_4} W_{\vec{k}_3, \vec{q}_t, \vec{q}', \vec{k}_2}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}_t}} \\
&\quad \left. - \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}_t} W_{\vec{k}_3, \vec{q}, \vec{q}_t, \vec{k}_2}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} - \frac{W_{\vec{q}_t, \vec{k}_2, \vec{k}_3, \vec{q}} W_{\vec{k}_1, \vec{q}_t, \vec{q}, \vec{k}_4}}{\omega - \frac{1}{2}\varepsilon_{\vec{q}} + \frac{1}{2}W_{\vec{q}}} \right].
\end{aligned} \tag{26}$$

For both the forms of $W_{\{\vec{k}_i\}}$ that we are considering here (and mentioned below eq. 9), the couplings $W_{\vec{q}}$ and $W_{\vec{q}_t}$ are equal, where $\vec{q}_t = \vec{\pi} - \vec{q}$. Moreover, we have the following relations between the scattering vertex strengths:

$$W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{q}'} = W_{\vec{k}_1, \vec{q}', \vec{q}_t, \vec{k}_4}, \quad W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}_t} = W_{\vec{k}_3, \vec{q}_t, \vec{q}', \vec{k}_2}, \quad W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} = W_{\vec{q}', \vec{k}_2, \vec{q}, \vec{k}_4}, \quad W_{\vec{k}_1, \vec{q}_t, \vec{k}_3, \vec{q}_t} = W_{\vec{k}_3, \vec{q}_t, \vec{k}_1, \vec{q}_t} \tag{27}$$

leading to the simplified expression

$$\begin{aligned} \Delta H \Big|_W = & \frac{1}{4} \sum_{\{\vec{k}_i\}} \sum_{\sigma, \sigma'} c_{\vec{k}_1, \sigma'}^\dagger c_{\vec{k}_2, \sigma'} c_{\vec{k}_3, \sigma}^\dagger c_{\vec{k}_4, \sigma} \sum_{\vec{q}, \vec{q}' \in \text{HS}} \left[-\frac{W_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{q}} W_{\vec{q}, \vec{q}', \vec{q}', \vec{k}_4}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} + \frac{W_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{q}_t} W_{\vec{q}_t, \vec{q}', \vec{q}', \vec{k}_4}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} \right. \\ & - \frac{W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{k}_2} W_{\vec{k}_3, \vec{q}', \vec{q}', \vec{q}_t}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} + \frac{W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{k}_2} W_{\vec{k}_3, \vec{q}', \vec{q}', \vec{q}}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} + \frac{2W_{\vec{q}_t, \vec{k}_4, \vec{q}_t, \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} + \frac{2W_{\vec{q}, \vec{k}_4, \vec{q}', \vec{k}_2} W_{\vec{k}_1, \vec{q}', \vec{k}_3, \vec{q}}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} \\ & \left. - \frac{2W_{\vec{q}_t, \vec{k}_4, \vec{k}_1, \vec{q}} W_{\vec{q}', \vec{k}_2, \vec{k}_3, \vec{q}_t}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} - \frac{2W_{\vec{q}, \vec{k}_4, \vec{k}_1, \vec{q}_t} W_{\vec{k}_3, \vec{q}, \vec{q}_t, \vec{k}_2}}{\omega - \frac{1}{2} \varepsilon_{\vec{q}} + \frac{1}{2} W_{\vec{q}}} \right]. \end{aligned} \quad (28)$$

IV. RENORMALISATION OF THE KONDO SCATTERING TERM J

We take a closer look at the Kondo scattering terms T_1 and T_7 in H_X :

$$\begin{aligned} T_1^\dagger + T_7 = & \frac{1}{2} \underbrace{\sum_{\vec{k}, \vec{q}, \sigma} J_{\vec{k}, \vec{q}} S_d^z \sigma c_{\vec{q}, \sigma}^\dagger c_{\vec{k}, \sigma}}_{T_{1,z}^\dagger} + \frac{1}{2} \underbrace{\sum_{\vec{k}, \vec{q}} J_{\vec{k}, \vec{q}} S_d^+ c_{\vec{q}, \downarrow}^\dagger c_{\vec{k}, \uparrow}}_{T_{1,+}^\dagger} + \frac{1}{2} \underbrace{\sum_{\vec{k}, \vec{q}} S_d^- c_{\vec{q}, \uparrow}^\dagger c_{\vec{k}, \downarrow}}_{T_{1,-}^\dagger} \\ & \frac{1}{2} \underbrace{\sum_{\vec{q}', \vec{q}, \sigma} J_{\vec{q}', \vec{q}} S_d^z \sigma c_{\vec{q}, \sigma}^\dagger c_{\vec{q}', \sigma}}_{T_{7,z}^\dagger} + \frac{1}{2} \underbrace{\sum_{\vec{q}', \vec{q}} J_{\vec{q}', \vec{q}} S_d^+ c_{\vec{q}, \downarrow}^\dagger c_{\vec{q}', \uparrow}}_{T_{7,+}^\dagger} + \frac{1}{2} \underbrace{\sum_{\vec{q}', \vec{q}} S_d^- c_{\vec{q}, \uparrow}^\dagger c_{\vec{q}', \downarrow}}_{T_{7,-}^\dagger} \end{aligned} \quad (29)$$

We note that scattering processes involving the pairs $(T_{1,\pm\mp}^\dagger, T_{1,\pm\mp})$ and $(T_{7,z}, T_6)$ will renormalise the S_d^z term, while those involving the pairs $(T_{1,z}, T_{1,\pm\mp})$ and $(T_{7,\pm\mp}, T_6)$ will renormalise the S_d^\pm terms.

A. Impurity-mediated spin-flip scattering purely through Kondo-like processes

We first consider the renormalisation to the S_d^z term, arising purely from the Kondo terms:

$$\sum_{\sigma=\pm} T_{1,\sigma\bar{\sigma}}^\dagger G T_{1,\sigma\bar{\sigma}} = \sum_{\sigma=\pm} \frac{1}{4} \sum_{\vec{k}_2, \vec{q}} J_{\vec{k}_2, \vec{q}} S_d^\sigma c_{\vec{q}, \bar{\sigma}}^\dagger c_{\vec{k}_2, \sigma} \frac{1}{\omega - H_D} \sum_{\vec{k}_1, \vec{q}} J_{\vec{k}_1, \vec{q}} S_d^{\bar{\sigma}} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{q}, \bar{\sigma}}, \quad (30)$$

where $c_{k,+(-)} \equiv c_{k,\uparrow(\downarrow)}$. The excitation energy for such processes is given by $H_D = |\varepsilon_j| - J_{\vec{q}}/4 - W_{\vec{q}}/2$, due to the fact that the impurity spin flip and the spin flip of the conduction bath state \vec{q} occurs in an anti-parallel fashion. Substituting this, performing the usual contraction and projection of the state \vec{q} and carrying out the spin manipulation $S_d^\sigma S_d^{\bar{\sigma}} = \frac{1}{2} + \sigma S_d^z$ results in the expression

$$\begin{aligned} \sum_{\sigma=\pm} T_{1,\sigma\bar{\sigma}}^\dagger G T_{1,\sigma\bar{\sigma}} = & \sum_{\sigma=\pm} \frac{1}{4} \sum_{\vec{k}_2, \vec{k}_1} \left(\frac{1}{2} + \sigma S_d^z \right) c_{\vec{k}_2, \sigma} c_{\vec{k}_1, \sigma}^\dagger \sum_{\vec{q}} \hat{n}_{\vec{q}, \bar{\sigma}} \frac{J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} \\ & = -\frac{1}{2} \sum_{\vec{k}_2, \vec{k}_1} S_d^z \sigma \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{PS}} \frac{J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} + \left[\text{pot. scatt. terms} \right]. \end{aligned} \quad (31)$$

The particle-hole exchanged partner is

$$\begin{aligned}
\sum_{\sigma=\pm} T_{1,\sigma\bar{\sigma}} G T_{1,\sigma\bar{\sigma}}^\dagger &= \sum_{\sigma=\pm} \frac{1}{4} \sum_{\vec{k}_1, \vec{q}} J_{\vec{k}_1, \vec{q}} S_d^{\bar{\sigma}} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{q}, \bar{\sigma}} \frac{1}{\omega - H_D} \sum_{\vec{k}_2, \vec{q}} J_{\vec{k}_2, \vec{q}} S_d^\sigma c_{\vec{q}, \bar{\sigma}}^\dagger c_{\vec{k}_2, \sigma} \\
&= \sum_{\sigma=\pm} \frac{1}{4} \sum_{\vec{k}_2, \vec{k}_1} \left(\frac{1}{2} + \bar{\sigma} S_d^z \right) c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q}} (1 - \hat{n}_{\vec{q}, \bar{\sigma}}) \frac{J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} \\
&= -\frac{1}{2} \sum_{\vec{k}_2, \vec{k}_1, \sigma} S_d^z \sigma \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{HS}} \frac{J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} + \left[\text{pot. scatt. terms} \right] \\
&= -\frac{1}{2} \sum_{\vec{k}_2, \vec{k}_1, \sigma} S_d^z \sigma \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{PS}} \frac{J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} + \left[\text{pot. scatt. terms} \right].
\end{aligned} \tag{32}$$

At the last step, we converted the sum over the hole sector into one over the particle sector. As argued elsewhere, transforming from the particle to the hole sector results in the inversion of the sign of the factor $[\cos(aq_1^x) - \cos(aq_1^y)]$, leaving the product $J_{\vec{k}_2, \vec{q}} J_{\vec{k}_1, \vec{q}}$ unchanged. The couplings in the denominators involve the product of four such factors, so they also remain unchanged.

B. Scattering processes involving the Kondo interaction as well as the bath interaction

Next, we consider scattering processes involving T_7, T_6 :

$$\begin{aligned}
T_{7,z} G T_6 &= \frac{1}{4} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}, \sigma} \sigma J_{-\vec{q}, \vec{q}} S_d^z c_{\vec{q}, \sigma}^\dagger c_{-\vec{q}, \sigma} \frac{1}{\omega - H_D} \left(-W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2} \right) \left(2c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{-\vec{q}, \sigma}^\dagger c_{\vec{q}, \sigma} - 2c_{\vec{k}_1, \bar{\sigma}}^\dagger c_{\vec{k}_2, \bar{\sigma}} c_{-\vec{q}, \sigma}^\dagger c_{\vec{q}, \sigma} \right) \\
&= -\frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}, \sigma} \sigma S_d^z \left(c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} - c_{\vec{k}_1, \bar{\sigma}}^\dagger c_{\vec{k}_2, \bar{\sigma}} \right) \sum_{\vec{q} \in \text{PS}} \frac{J_{-\vec{q}, \vec{q}} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} \\
&= -2 \sum_{\vec{k}_1, \vec{k}_2, \sigma} \sigma S_d^z \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{PS}} \frac{J_{-\vec{q}, \vec{q}} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2}
\end{aligned} \tag{33}$$

Another scattering process is obtained by switching the operators T_7 and T_6 :

$$\begin{aligned}
T_6^\dagger G T_{7,z} &= \frac{1}{4} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}, \sigma} \left(-W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2} \right) \left(2c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} c_{-\vec{q}, \sigma}^\dagger c_{\vec{q}, \sigma} - 2c_{\vec{k}_1, \bar{\sigma}}^\dagger c_{\vec{k}_2, \bar{\sigma}} c_{-\vec{q}, \sigma}^\dagger c_{\vec{q}, \sigma} \right) \frac{1}{\omega - H_D} \sigma J_{-\vec{q}, \vec{q}} S_d^z c_{\vec{q}, \sigma}^\dagger c_{-\vec{q}, \sigma} \\
&= -\frac{1}{2} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}, \sigma} \sigma S_d^z \left(c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} - c_{\vec{k}_1, \bar{\sigma}}^\dagger c_{\vec{k}_2, \bar{\sigma}} \right) \sum_{\vec{q} \in \text{HS}} \frac{J_{-\vec{q}, \vec{q}} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} \\
&= -2 \sum_{\vec{k}_1, \vec{k}_2, \sigma} \sigma S_d^z \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{HS}} \frac{J_{-\vec{q}, \vec{q}} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2} \\
&= -2 \sum_{\vec{k}_1, \vec{k}_2, \sigma} \sigma S_d^z \frac{1}{2} c_{\vec{k}_1, \sigma}^\dagger c_{\vec{k}_2, \sigma} \sum_{\vec{q} \in \text{PS}} \frac{J_{-\vec{q}, \vec{q}} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}}{\omega - |\varepsilon_j| + J_{\vec{q}}/4 + W_{\vec{q}}/2}
\end{aligned} \tag{34}$$

At the last step, we again transformed from the particle sector to the hole sector using the arguments mentioned just above.

C. Net renormalisation to the Kondo interaction

Owing to spin-rotation symmetry of the Kondo interaction, it suffices to calculate the renormalisation for the Ising-like interaction term, since that of the spin-flip terms will be equal to it. Upon adding the Hamiltonian renormalisation

from the four classes eqs. 31, 32, 33 and 34, the total renormalisation in the Ising part of the Kondo interaction comes out to be

$$\Delta J_{\vec{k}_1, \vec{k}_2}^{(j)} = - \sum_{\vec{q} \in \text{PS}} \frac{J_{\vec{k}_2, \vec{q}}^{(j)} J_{\vec{k}_1, \vec{q}}^{(j)} + 4 J_{-\vec{q}, \vec{q}}^{(j)} W_{\vec{q}, -\vec{q}, \vec{k}_1, \vec{k}_2}^{(j)}}{\omega - |\varepsilon_j| + J_{\vec{q}}^{(j)}/4 + W_{\vec{q}}^{(j)}/2} \quad (35)$$