URG analysis of the extended Kondo model with d-wave interaction

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I. HAMILTONIAN

We consider an impurity spin $\vec{S}_d$ interacting with a two-dimensional tight-binding conduction bath through the d-wave channel :

$$J\vec{S}_d \cdot \vec{S}_f, \quad \vec{S}_f = \frac{1}{2}\sum_{\sigma,\sigma'} \vec{\tau}_{\sigma,\sigma'} f^\dagger_\sigma f_{\sigma'} . \tag{1}$$

where $\vec{\tau}$ is the vector of sigma matrices. The spin $\vec{S}_f$ is constructed in terms of the d-wave electron $f_\sigma = \frac{1}{2}\left(c^\dagger_{L,\sigma} + c^\dagger_{R,\sigma} - c^\dagger_{U\sigma} - c^\dagger_{D\sigma}\right)$, 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. We also consider local bath correlations in the $d-$wave channel:

$$-\frac{W}{2}\left(f^\dagger_\uparrow f_\uparrow - f^\dagger_\downarrow f_\downarrow\right)^2 . \tag{2}$$

In order to facilitate a momentum-space decoupling RG scheme, we Fourier transform the $d-$wave operator to momentum space:

$$f_\sigma = \frac{1}{2}\left(c^\dagger_{L,\sigma} + c^\dagger_{R,\sigma} - c^\dagger_{U\sigma} - c^\dagger_{D\sigma}\right) = \frac{1}{2}\sum_{\vec{k}} c^\dagger_{\vec{k},\sigma}\left[e^{-ik^x a} + e^{ik^x a} - e^{-ik^y a} - e^{ik^y a}\right] = \sum_{\vec{k}} \left[\cos\left(ak^x\right) - \cos\left(ak^y\right)\right] c^\dagger_{\vec{k},\sigma} . \tag{3}$$

The Kondo interaction term takes the following form in momentum space:

$$J\vec{S}_d \cdot \vec{S}_f = \frac{1}{2}J \sum_{\vec{k}_1,\vec{k}_2,\sigma,\sigma'} \vec{S}_d \cdot \vec{\tau}_{\sigma,\sigma'} c^\dagger_{\vec{k}_1\sigma} c_{\vec{k}_2,\sigma'} \prod_{i=1,2}\left[\cos\left(ak^x_i\right) - \cos\left(ak^y_i\right)\right] . \tag{4}$$

The local correlation term can be similarly written in momentum space:

$$-\frac{W}{2}\left(f^\dagger_\uparrow f_\uparrow - f^\dagger_\downarrow f_\downarrow\right)^2 = -\frac{W}{2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4,\sigma}\left(c^\dagger_{\vec{k}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{k}_3,\sigma} c_{\vec{k}_4,\sigma} - c^\dagger_{\vec{k}_1\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{k}_3\bar{\sigma}} c_{\vec{k}_4,\bar{\sigma}}\right) \prod_{i=1,2,3,4}\left[\cos\left(ak^x_i\right) - \cos\left(ak^y_i\right)\right] . \tag{5}$$

Combining all the terms, the Hamiltonian can be formally written as

$$H = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{2}\sum_{\vec{k}_1,\vec{k}_2,\sigma,\sigma'} J_{\vec{k}_1,\vec{k}_2} \vec{S}_d \cdot \vec{\tau}_{\sigma,\sigma'} c^\dagger_{\vec{k}_1\sigma} c_{\vec{k}_2,\sigma'} - \frac{1}{2}\sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4,\sigma,\sigma'} W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} \sigma\sigma' c^\dagger_{\vec{k}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{k}_3,\sigma'} c_{\vec{k}_4,\sigma'} . \tag{6}$$

with

$$\begin{aligned} \varepsilon_{\vec{k}} &= -2t\left[\cos\left(ak^x\right) + \cos\left(ak^y\right)\right] , \\ J_{\vec{k}_1,\vec{k}_2} &= J\prod_{i=1,2}\left[\cos\left(ak^x_i\right) - \cos\left(ak^y_i\right)\right] , \\ W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} &= W\prod_{i=1,2,3,4}\left[\cos\left(ak^x_i\right) - \cos\left(ak^y_i\right)\right] . \end{aligned} \tag{7}$$

The coupling $W_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4}$ has certain symmetries. It is independent of the sequence of momentum indices. It remains invariant if any number of the momenta undergo rotation by an integer multiple of $\pi/2$. It also remains invariant if an even number of momenta are reflected about the nodal point in the corresponding quadrant.

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 $\{\vec{q}\}$:

$$H_D^{(j)} = \varepsilon_j \sum_{q,\sigma} \tau_{q,\sigma} + \sum_{\vec{q}} J_{\vec{q},\vec{q}} S_d^z \left(\hat{n}_{\vec{q},\uparrow} - \hat{n}_{\vec{q},\downarrow}\right) - \frac{1}{2} \sum_{\vec{q}_1,\vec{q}_2} W_{\vec{q}_1,\vec{q}_1,\vec{q}_2,\vec{q}_2} \left(\hat{n}_{\vec{q}_1,\uparrow} - \hat{n}_{\vec{q}_1,\downarrow}\right)\left(\hat{n}_{\vec{q}_2,\uparrow} - \hat{n}_{\vec{q}_2,\downarrow}\right) \ . \tag{8}$$

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 $\{\vec{q}\}$:

$$\begin{aligned} H_X^{(j)} = & \underbrace{\sum_{\vec{k},\vec{q},\sigma,\sigma'} J_{\vec{k},\vec{q}} \vec{S}_d \cdot \vec{\tau}_{\sigma,\sigma'} \left[c^\dagger_{\vec{q}\sigma} c_{\vec{k},\sigma} + \text{h.c.}\right]}_{T_1^\dagger + T_1} \\ & \underbrace{-\frac{1}{2} \sum_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4,\sigma,\sigma'} W_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} \sigma\sigma' \left[c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{k}_3,\sigma'} c_{\vec{k}_4,\sigma'} + \text{h.c.}\right]}_{T_2^\dagger + T_2} \\ & \underbrace{-\frac{1}{2} \sum_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4,\sigma,\sigma'} W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} \sigma\sigma' \left[c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{q}_2,\sigma'} c_{\vec{k}_4,\sigma'} + \text{h.c.}\right]}_{T_3^\dagger + T_3} \\ & \underbrace{-\frac{1}{2} \sum_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{q}_2,\sigma,\sigma'} W_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{q}_2} \sigma\sigma' \left(c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{k}_3,\sigma'} c_{\vec{q}_2,\sigma'} + c^\dagger_{\vec{k}_3,\sigma'} c_{\vec{q}_2,\sigma'} c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma}\right)}_{T_4 + T_5^\dagger} \\ & \underbrace{-\frac{1}{2} \sum_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{q}_3,\sigma,\sigma'} W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{q}_3} \sigma\sigma' \left[c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{q}_2,\sigma'} c_{\vec{q}_3,\sigma'} + \text{h.c.}\right]}_{T_6 + T_6^\dagger} \ . \end{aligned} \tag{9}$$

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 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

$$\Delta H^{(j)} = H_X \frac{1}{\omega - H_D} H_X \ . \tag{10}$$

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) $T_2^\dagger G T_6 + T_6^\dagger G T_2$, (ii) $T_3^\dagger G T_3 + T_3 G T_3^\dagger$ and (iii) $T_4^\dagger G T_4 + T_5^\dagger G T_5$.

The first term is of the form

$$T_2^\dagger G T_6 = \sum \sigma_1 \sigma_1' W_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} c^\dagger_{\vec{q}_1,\sigma_1} c_{\vec{k}_2,\sigma_1} c^\dagger_{\vec{k}_3,\sigma_1'} c_{\vec{k}_4,\sigma_1'} \frac{1}{\omega - H_D} \sigma_1 \sigma_2' W_{\vec{q}_1,\vec{q}_2,\vec{q}_2,\vec{k}_2'} \hat{n}_{\vec{q}_2,\sigma_2'} c^\dagger_{\vec{k}_2',\sigma_1} c_{\vec{q}_1,\sigma_1} \ . \tag{11}$$

The change in occupancy of the state $\vec{q}_1\sigma_1$ from 1 to 0 leads to an excited state energy $H_D = \varepsilon(q_1)\tau_{q_1\sigma_1} - \frac{1}{2} W\left(\vec{q}_1\right)\left(\hat{n}_{\vec{q}_1,\uparrow} - \hat{n}_{\vec{q}_1,\uparrow}\right)^2 = -\frac{1}{2}\varepsilon(q_1) - \frac{1}{2} W\left(\vec{q}_1\right)$, where $W\left(\vec{q}_1\right)$ is a shorthand for $W\left(\vec{q}_1, \vec{q}_1, \vec{q}_1, \vec{q}_1\right)$. The number operator $\hat{n}_{\vec{q}_2,\sigma_2'}$ projects the initial state to that in which $\vec{q}_2$ is occupied. The operator $c_{\vec{q}_1,\sigma_1}$ can be combined with its hermitian conjugate on the other side to give another number operator, leading to another projection. Both the number operators reduce to unity upon acting on the projected states:

$$T_2^\dagger G T_6 = \sum \sigma_1^2 \sigma_1' W_{\vec{q}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} W_{\vec{q}_1,\vec{q}_2,\vec{q}_2,\vec{k}_2'} c_{\vec{k}_2,\sigma_1} c^\dagger_{\vec{k}_3,\sigma_1'} c_{\vec{k}_4,\sigma_1'} c^\dagger_{\vec{k}_2',\sigma_1} \frac{1}{\omega + \frac{1}{2}\varepsilon(q_1) + \frac{1}{2}W\left(\vec{q}_1\right)} \sum_{\sigma_2'} \sigma_2' \,. \tag{12}$$

Since there is a sum over the spin factor $\sigma_2' = \pm 1$, this term vanishes identically. The particle-hole transformed term $T_6^\dagger G T_2$ vanishes for the same reason.

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

$$\begin{aligned} T_3^\dagger G T_3 &= \frac{1}{4} \sum W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} \sigma\sigma' c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{q}_2,\sigma'} c_{\vec{k}_4,\sigma'} \frac{1}{\omega - H_D} W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'} \sigma\sigma' c^\dagger_{\vec{k}_4',\sigma'} c_{\vec{q}_2,\sigma'} c^\dagger_{\vec{k}_2',\sigma} c_{\vec{q}_1,\sigma} \\ &= \frac{1}{4} \sum \hat{n}_{\vec{q}_1,\sigma} \hat{n}_{\vec{q}_2,\sigma'} c_{\vec{k}_2,\sigma} c_{\vec{k}_4,\sigma'} c^\dagger_{\vec{k}_4',\sigma'} c^\dagger_{\vec{k}_2',\sigma} \frac{W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'}}{\omega + \frac{1}{2}\left[\varepsilon(q_1) + \varepsilon(q_2)\right] + \frac{1}{2}\left[\sqrt{W\left(\vec{q}_1\right)} + \sigma\sigma' \sqrt{W\left(\vec{q}_2\right)}\right]^2} \\ &= \frac{1}{4} \sum c^\dagger_{\vec{k}_4',\sigma'} c_{\vec{k}_4,\sigma'} c^\dagger_{\vec{k}_2',\sigma} c_{\vec{k}_2,\sigma} \sum_{\vec{q}_1,\vec{q}_2} \frac{W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'}}{\omega + \frac{1}{2}\left[\varepsilon(q_1) + \varepsilon(q_2)\right] + \frac{1}{2}\left[\sqrt{W\left(\vec{q}_1\right)} + \sigma\sigma' \sqrt{W\left(\vec{q}_2\right)}\right]^2} \,, \end{aligned} \tag{13}$$

where the final sum over $\vec{q}_1, \vec{q}_2$ is over all the states that are occupied.

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

$$\begin{aligned} T_3 G T_3^\dagger &= \frac{1}{4} \sum W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'} \sigma\sigma' c^\dagger_{\vec{k}_4',\sigma'} c_{\vec{q}_2,\sigma'} c^\dagger_{\vec{k}_2',\sigma} c_{\vec{q}_1,\sigma} \frac{1}{\omega - H_D} W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} \sigma\sigma' c^\dagger_{\vec{q}_1,\sigma} c_{\vec{k}_2,\sigma} c^\dagger_{\vec{q}_2,\sigma'} c_{\vec{k}_4,\sigma'} \\ &= \frac{1}{4} \sum \left(1 - \hat{n}_{\vec{q}_1,\sigma}\right)\left(1 - \hat{n}_{\vec{q}_2,\sigma'}\right) c^\dagger_{\vec{k}_4',\sigma'} c^\dagger_{\vec{k}_2',\sigma} c_{\vec{k}_2,\sigma} c_{\vec{k}_4,\sigma'} \frac{W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'}}{\omega + \frac{1}{2}\left[\varepsilon(q_1) + \varepsilon(q_2)\right] + \frac{1}{2}\left[\sqrt{W\left(\vec{q}_1\right)} + \sigma\sigma' \sqrt{W\left(\vec{q}_2\right)}\right]^2} \\ &= \frac{1}{4} \sum c_{\vec{k}_2,\sigma} c_{\vec{k}_4,\sigma'} c^\dagger_{\vec{k}_4',\sigma'} c^\dagger_{\vec{k}_2',\sigma} \sum_{\vec{q}_1,\vec{q}_2} \frac{W_{\vec{q}_1,\vec{k}_2,\vec{q}_2,\vec{k}_4} W_{\vec{q}_1,\vec{k}_2',\vec{q}_2,\vec{k}_4'}}{\omega + \frac{1}{2}\left[\varepsilon(q_1) + \varepsilon(q_2)\right] + \frac{1}{2}\left[\sqrt{W\left(\vec{q}_1\right)} + \sigma\sigma' \sqrt{W\left(\vec{q}_2\right)}\right]^2} \,, \end{aligned} \tag{14}$$