Quantum criticality in a Kondo-Mott lattice model

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I. IMPURITY MODEL

$$H_{\text{aux}}(\mathbf{r}_d) = H^{(0)} + H_f(\mathbf{r}_d) + H_c(\mathbf{r}_d) + H_{fc}(\mathbf{r}_d) \ , \tag{1}$$

$$\begin{aligned}
H^{(0)} =& -t_f \sum_{\langle i,j\rangle,\sigma} \left(f^\dagger_{i,\sigma} f_{j,\sigma} + \text{h.c.}\right) - t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}\right) - \mu \sum_{i,\sigma} \left(f^\dagger_{i,\sigma} f_{i,\sigma} + c^\dagger_{i,\sigma} c_{i,\sigma}\right) \ , \\
H_f(\mathbf{r}_d) =& V_f \sum_{Z\in\text{NN}} \sum_\sigma \left(f^\dagger_{\mathbf{r}_d,\sigma} f_{Z,\sigma} + \text{h.c.}\right) + \epsilon_f \sum_\sigma f^\dagger_{\mathbf{r}_d,\sigma} f_{\mathbf{r}_d,\sigma} + U_f f^\dagger_{\mathbf{r}_d,\uparrow} f_{\mathbf{r}_d,\uparrow} f^\dagger_{\mathbf{r}_d,\downarrow} f_{\mathbf{r}_d,\downarrow} \\
&+ J_f \sum_{Z\in\text{NN}} \sum_{\alpha,\beta} \mathbf{S}_f(\mathbf{r}_d) \cdot \boldsymbol{\sigma}_{\alpha\beta} f^\dagger_{Z,\alpha} f_{Z,\beta} - \frac{W_f}{2} \sum_{Z\in\text{NN}} \left(f^\dagger_{Z,\uparrow} f_{Z,\uparrow} - f^\dagger_{Z,\downarrow} f_{Z,\downarrow}\right)^2 \ , \\
H_c(\mathbf{r}_d) =& -\frac{W}{2} \left(c^\dagger_{\mathbf{r}_d,\uparrow} c_{\mathbf{r}_d,\uparrow} - c^\dagger_{\mathbf{r}_d,\downarrow} c_{\mathbf{r}_d,\downarrow}\right)^2 \ , \\
H_{fc}(\mathbf{r}_d) =& J \sum_{\alpha,\beta} \mathbf{S}_f(\mathbf{r}_d) \cdot \boldsymbol{\sigma}_{\alpha\beta} c^\dagger_{\mathbf{r}_d,\alpha} c_{\mathbf{r}_d,\beta} + V \left(f^\dagger_{\mathbf{r}_d,\sigma} c_{\mathbf{r}_d,\sigma} + \text{h.c.}\right) \ ,
\end{aligned} \tag{2}$$

II. TILING RECONSTRUCTION

$$\begin{aligned}
H_{\text{tiled}} =& \sum_{\mathbf{r}_d} H_{\text{aux}}(\mathbf{r}_d) - (N-1) H^{(0)} \\
=& \sum_{\langle i,j\rangle,\sigma} \left[-t_f \left(f^\dagger_{i,\sigma} f_{j,\sigma} + \text{h.c.}\right) - t \left(c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}\right)\right] + \tilde{J} \sum_{\langle i,j\rangle} \mathbf{S}_f(i) \cdot \mathbf{S}_{\mathbf{f}}(j) + J \sum_i \mathbf{S}_f(i) \cdot \mathbf{S}_c(i) - U \sum_i \left(f^\dagger_{i,\uparrow} f_{i,\uparrow} - f^\dagger_{i,\downarrow} f_{i,\downarrow}\right)^2 \\
&- \mu N
\end{aligned} \tag{3}$$

III. COUPLING RENORMALISATION GROUP FLOWS

Off-diagonal terms:

$$\begin{aligned}
H_{X,f} &= \frac{1}{2} \sum_{\mathbf{q},\mathbf{k},\sigma} J_f(\mathbf{k},\mathbf{q}) S^\sigma_f \left(f^\dagger_{\mathbf{q},-\sigma} f_{\mathbf{k},\sigma} + f^\dagger_{\mathbf{k},-\sigma} f_{\mathbf{q},\sigma}\right) + \frac{1}{2} \sum_{\mathbf{q},\mathbf{k},\sigma} J_f(\mathbf{k},\mathbf{q}) \sigma S^z_f \left(f^\dagger_{\mathbf{q},\sigma} f_{\mathbf{k},\sigma} + f^\dagger_{\mathbf{k},\sigma} f_{\mathbf{q},\sigma}\right) \ , \\
H_{X,c} &= \frac{1}{2} J \sum_{\mathbf{q},\mathbf{k},\sigma} S^\sigma_f \left(c^\dagger_{\mathbf{q},-\sigma} c_{\mathbf{k},\sigma} + c^\dagger_{\mathbf{k},-\sigma} c_{\mathbf{q},\sigma}\right) + \frac{1}{2} J \sum_{\mathbf{q},\mathbf{k},\sigma} \sigma S^z_f \left(c^\dagger_{\mathbf{q},\sigma} c_{\mathbf{k},\sigma} + c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{q},\sigma}\right) \ .
\end{aligned} \tag{4}$$

A. Intra-layer processes

$$\begin{aligned}
\Delta J^{(j)}_f(\mathbf{k}_1,\mathbf{k}_2) &= -\sum_{\mathbf{q}\in\text{PS}} \left(J^{(j)}_f(\mathbf{k}_2,\mathbf{q}) J^{(j)}_f(\mathbf{q},\mathbf{k}_1) + 4 J^{(j)}_f(\mathbf{q},\boldsymbol{\pi}+\mathbf{q}) W_{\boldsymbol{\pi}+\mathbf{q},\mathbf{k}_2,\mathbf{k}_1,\mathbf{q}}\right) G_f(\omega,\mathbf{q}) \ , \\
\Delta J^{(j)} &= -\rho(\varepsilon_j)\Delta\varepsilon \cdot \left[\left(J^{(j)}\right)^2 + 4 W J^{(j)}\right] \ G(\omega,\mathbf{q}) \ ,
\end{aligned} \tag{5}$$

where $\bar{\mathbf{q}} = \boldsymbol{\pi} + \mathbf{q}$ is the charge conjugate partner of $\mathbf{q}$, and the propagators G_f and G are defined as

$$G_f(\omega, \mathbf{q}) = \frac{1}{2}\left[\left(\omega - \frac{1}{2}\left(|\varepsilon_f(\mathbf{q})| - \mu\right) + J^{(j)}_f\left(\mathbf{q}, \mathbf{q}\right)/4 + W_f(\mathbf{q})/2 - \epsilon_f\right)^{-1} + \left(\omega - \frac{1}{2}\left(|\varepsilon_f(\mathbf{q})| + \mu\right) + J^{(j)}_f\left(\mathbf{q}, \mathbf{q}\right)/4 + W_f(\mathbf{q})/2 - \epsilon_f\right)^{-1}\right],$$
$$G(\omega, \mathbf{q}) = \frac{1}{2}\left[\left(\omega - \frac{1}{2}|\varepsilon(\mathbf{q})| + J^{(j)}/4 + W/2 + \mu/2\right)^{-1} + \left(\omega - \frac{1}{2}|\varepsilon(\mathbf{q})| + J^{(j)}/4 + W/2 - \mu/2\right)^{-1}\right]. \tag{6}$$

B. Inter-layer processes

Processes that start from configurations in which $\mathbf{q}$ is occupied:

$$P_1 = \frac{1}{8}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\sigma,\sigma'} J^{(j)}_f(\mathbf{q},\mathbf{k}) S^\sigma_f f^\dagger_{\mathbf{q},-\sigma} f_{\mathbf{k},\sigma}\ G_f(\omega,\mathbf{q},\mathbf{k})\ J^{(j)} S^z_f \sigma' c^\dagger_{\mathbf{k}_1,\sigma'} c_{\mathbf{k}_2,\sigma'}\ G_f(\omega,\mathbf{q},\mathbf{k})\ J^{(j)}_f(\mathbf{q},\mathbf{k}) S^{-\sigma}_f f^\dagger_{\mathbf{k},\sigma} f_{\mathbf{q},-\sigma}\ , \tag{7}$$

where the propagator $G_f(\omega,\mathbf{q},\mathbf{k})$ for the excitations is a generalisation of eq. 6:

$$G_f(\omega,\mathbf{q},\mathbf{k}) = \left(\omega - \frac{1}{2}|\varepsilon_f(\mathbf{q})| - \frac{1}{2}|\varepsilon_f(\mathbf{k})| + J^{(j)}_f\left(\mathbf{q},\mathbf{q}\right)/4 + J^{(j)}_f\left(\mathbf{k},\mathbf{k}\right)/4 + W_f(\mathbf{q})/2 + W_f(\mathbf{k})/2 - \epsilon_f\right)^{-1}, \tag{8}$$

Using $S^\sigma S^z = -\frac{\sigma}{2}S^\sigma$ and $S^\sigma S^{-\sigma} = \frac{1}{2} + \sigma S^z$, we get

$$\begin{aligned} P_1 &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\sigma,\sigma'} \frac{-\sigma'}{16}\left(\frac{\sigma}{2} + S^z_f\right) c^\dagger_{\mathbf{k}_1,\sigma'} c_{\mathbf{k}_2,\sigma'}\ J^{(j)} \sum_{\mathbf{q}\in\mathrm{PS},\mathbf{k}\in\mathrm{HS}} \left(J^{(j)}_f(\mathbf{q},\mathbf{k})\right)^2 G^2_f(\omega,\mathbf{q},\mathbf{k}) \\ &= -\frac{1}{8}\sum_{\mathbf{k}_1,\mathbf{k}_2,\sigma'} \sigma'\ S^z_f c^\dagger_{\mathbf{k}_1,\sigma'} c_{\mathbf{k}_2,\sigma'}\ J^{(j)} \sum_{\mathbf{q}\in\mathrm{PS},\mathbf{k}\in\mathrm{HS}} \left(J^{(j)}_f(\mathbf{q},\mathbf{k})\right)^2 G^2_f(\omega,\mathbf{q},\mathbf{k})\ . \end{aligned} \tag{9}$$

Another process can be conceived with similar starting configuration but where the loop momenta are on the $c-$plane:

$$P_2 = \frac{1}{8}\sum_{\mathbf{q},\mathbf{k},\mathbf{k}_1,\mathbf{k}_2,\sigma,\sigma'} J^{(j)} S^\sigma_f c^\dagger_{\mathbf{q},-\sigma} c_{\mathbf{k},\sigma}\ \tilde{G}(\omega,\mathbf{q},\mathbf{k})\ J^{(j)}(\mathbf{k}_1,\mathbf{k}_2) S^z_f \sigma' f^\dagger_{\mathbf{k}_1,\sigma'} f_{\mathbf{k}_2,\sigma'}\ \tilde{G}(\omega,\mathbf{q},\mathbf{k})\ J^{(j)} S^{-\sigma}_f c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{q},-\sigma}\ , \tag{10}$$

where $\tilde{G}(\omega,\mathbf{q},\mathbf{k})$ is defined as

$$\tilde{G}(\omega,\mathbf{q},\mathbf{k}) = \frac{1}{\omega - \frac{1}{2}|\varepsilon(\mathbf{q})| - \frac{1}{2}|\varepsilon(\mathbf{k})| + J^{(j)}/2 + W}\ . \tag{11}$$

Using the same properties as above, the expression simplifies to:

$$P_2 = -\frac{1}{8}\sum_{\mathbf{k}_1,\mathbf{k}_2,\sigma'} \sigma'\ S^z_f f^\dagger_{\mathbf{k}_1,\sigma'} f_{\mathbf{k}_2,\sigma'}\ J^{(j)}_f(\mathbf{k}_1,\mathbf{k}_2)\left(J^{(j)}\right)^2 \sum_{\mathbf{q}\in\mathrm{HS},\mathbf{k}\in\mathrm{PS}} \tilde{G}^2(\omega,\mathbf{q},\mathbf{k})\ . \tag{12}$$

It turns out that the processes that start from unoccupied configurations in the state $\mathbf{q}$ give almost identical contributions as the present expressions, the only difference being that $\mathbf{q}$ is now summed over the hole sector (HS) while $\mathbf{k}$ is summed over the particle sector (PS). For a particle-hole symmetric system (which we have restricted ourselves to), these two summations are equal, so both the contributions are indeed identical. The total renormalisation can therefore be read off from the final expressions of P_1 and P_2 (and the hole sector is accounted for by doubling the renormalisation from just the particle sector):

$$\begin{aligned} \Delta J^{(j)}_f(\mathbf{k}_1,\mathbf{k}_2) &= -\frac{1}{2}J^{(j)}_f(\mathbf{k}_1,\mathbf{k}_2)\left(J^{(j)}\right)^2 \sum_{\mathbf{q}\in\mathrm{PS},\mathbf{k}\in\mathrm{HS}} \tilde{G}^2(\omega,\mathbf{q},\mathbf{k}) \\ \Delta J^{(j)} &= -\frac{1}{2}J^{(j)} \sum_{\mathbf{q}\in\mathrm{PS},\mathbf{k}\in\mathrm{HS}} \left(J^{(j)}_f(\mathbf{q},\mathbf{k}) G_f(\omega,\mathbf{q},\mathbf{k})\right)^2 \end{aligned} \tag{13}$$

C. Complete coupling RG equation

$$\begin{aligned} \Delta J^{(j)}_f\left(\mathbf{k}_1,\mathbf{k}_2\right) &= -\sum_{\mathbf{q}\in\mathrm{PS}}\left[\left(J^{(j)}_f\left(\mathbf{k}_2,\mathbf{q}\right) J^{(j)}_f\left(\mathbf{q},\mathbf{k}_1\right) + 4J^{(j)}_f\left(\mathbf{q},\bar{\mathbf{q}}\right) W_{\bar{\mathbf{q}},\mathbf{k}_2,\mathbf{k}_1,\mathbf{q}}\right) G_f(\omega,\mathbf{q}) + \frac{1}{2}J^{(j)}_f(\mathbf{k}_1,\mathbf{k}_2)\left(J^{(j)}\right)^2 \sum_{\mathbf{k}\in\mathrm{HS}} \tilde{G}^2(\omega,\mathbf{q},\mathbf{k})\right], \\ \Delta J^{(j)} &= -\rho(\varepsilon_j)\Delta\varepsilon\cdot\left[\left(J^{(j)}\right)^2 + 4WJ^{(j)}\right] G(\omega,\mathbf{q}) - \frac{1}{2}J^{(j)} \sum_{\mathbf{q}\in\mathrm{PS},\mathbf{k}\in\mathrm{HS}} \left(J^{(j)}_f(\mathbf{q},\mathbf{k}) G_f(\omega,\mathbf{q},\mathbf{k})\right)^2, \end{aligned} \tag{14}$$

D. Symmetries preserved under renormalisation

By Fourier transforming the real-space forms of the Kondo coupling J_f and bath interaction W, we get their $k-$space forms:

$$\begin{aligned} J_f(\mathbf{k},\mathbf{q}) &= \frac{J_f}{2}\left[\cos(k_x-q_x)+\cos(k_y-q_y)\right] \ , \\ W(\mathbf{k},\mathbf{q},\mathbf{k}',\mathbf{q}') &= \frac{W}{2}\left[\cos(k_x-q_x+k'_x-q'_x)+\cos(k_y-q_y+k'_y-q'_y)\right] \ . \end{aligned} \tag{15}$$

These are of course the unrenormalised forms; the Kondo coupling $k-$space dependence can evolve during the RG flow. The $k-$space sensitive form of the Kondo coupling and conduction bath interactions are invariant under symmetry transformations in the Brillouin zone.

Translation by a nesting vector into opposite quadrant
Define the reciprocal lattice vectors (RLVs) $\mathbf{Q}_1 = (\pi,\pi)$ and $\mathbf{Q}_2 = (\pi,-\pi)$. The bare Kondo coupling in eq. 15 is (anti)symmetric under translation of (one)both momentum by either of the two RLVs:

$$\begin{aligned} J_f(\mathbf{k}+\mathbf{Q}_i,\mathbf{q}) = J_f(\mathbf{k},\mathbf{q}+\mathbf{Q}_i) = -J_f(\mathbf{k},\mathbf{q}) \ ; \ i=1,2 \ ; \\ J_f(\mathbf{k}+\mathbf{Q}_i,\mathbf{q}+\mathbf{Q}_j) = J_f(\mathbf{k},\mathbf{q}) \ ; \ i=1,2 \quad j=1,2 \ . \end{aligned} \tag{16}$$

These symmetries survive under the renormalisation group transformations. For the first transformation (under which the Kondo coupling is antisymmetric), note that each of the terms on the right hand side of the RG equation for J_f (eq. 14) are antisymmetric as well - the third term because it's the Kondo coupling itself which automatically has the symmetry, the second term (involving W) because W is also antisymmetric under transformation of one momentum, and the first term because only one of the two J_f in the product will transform (to obtain a minus sign). This ensures that the entirety of the renormalisation transforms antisymmetrically. A very similar argument shows that the symmetry under transformation of both momenta also survives under renormalisation.

Translation into adjacent quadrant
We will make use of another symmetry. Consider two momenta $\mathbf{k}$ and $\mathbf{q}$ in the first and second quadrant, with the same $y-$component but opposite $x-$components:

$$\mathbf{k}_y = \mathbf{q}_y, \ \mathbf{k}_x = -\mathbf{q}_x \ . \tag{17}$$

We refer to $\mathbf{q}$ as $\bar{\mathbf{k}}$ to signal the fact the above relation between the two momenta. We first consider the bare interaction, where we have the symmetry

$$\begin{aligned} J_f(\mathbf{k},\bar{\mathbf{k}}') &= J_f(\bar{\mathbf{k}},\mathbf{k}'), \\ J_f(\bar{\mathbf{k}},\bar{\mathbf{k}}') &= J_f(\mathbf{k},\mathbf{k}') \ . \end{aligned} \tag{18}$$

We now argue that these symmetries are preserved during the RG flow. Using the properties $W_{\bar{\mathbf{q}},\mathbf{k}_2,\bar{\mathbf{k}}_1,\mathbf{q}} = W_{\bar{\mathbf{q}},\bar{\mathbf{k}}_2,\mathbf{k}_1,\mathbf{q}}$ and $J_f^{(j)}(\mathbf{k}_2,\mathbf{q})\, J_f^{(j)}(\mathbf{q},\bar{\mathbf{k}}_1) = J_f^{(j)}(\bar{\mathbf{k}}_2,\bar{\mathbf{q}})\, J_f^{(j)}(\bar{\mathbf{q}},\mathbf{k}_1)$ and the fact that $\bar{\mathbf{q}}$ lies on the same isoenergy shell as $\mathbf{q}$ and is already part of the summation over PS in eq. 14, we can see that $\Delta J_f^{(j)}(\bar{\mathbf{k}}_1,\mathbf{k}_2) = \Delta J_f^{(j)}(\mathbf{k}_1,\bar{\mathbf{k}}_2)$. A similar line of argument shows that $\Delta J_f^{(j)}(\bar{\mathbf{k}}_1,\bar{\mathbf{k}}_2) = \Delta J_f^{(j)}(\mathbf{k}_1,\mathbf{k}_2)$.

IV. REDUCTION TO TRUNCATED 1D REPRESENTATION

At the renormalisation group fixed point, we have a renormalised theory for the interaction of the impurity spin S_f with the $f-$layer Fermi surface:

$$H^* = \sum_{\alpha,\beta} \mathbf{S}_f\cdot\boldsymbol{\sigma}_{\alpha,\beta}\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} f_{\mathbf{q},\beta} \ . \tag{19}$$

We will now obtain a more minimal representation of this interaction. Each momentum label is summed over all four quadrants $\mathcal{Q}_1$ through $\mathcal{Q}_4$; eq. 16 relates $\mathcal{Q}_1$ with $\mathcal{Q}_3$ and $\mathcal{Q}_2$ with $\mathcal{Q}_4$:

$$\begin{aligned} \sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} f_{\mathbf{q},\beta} &= \sum_{\mathbf{q}}\left[\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} + \sum_{\mathbf{k}\in\mathcal{Q}_3,\mathcal{Q}_4} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha}\right] f_{\mathbf{q},\beta} \\ &= \sum_{\mathbf{q}}\left[\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} + \sum_{\mathbf{k}\in\mathcal{Q}_1} J_f^*(\mathbf{k}-\mathbf{Q_1},\mathbf{q}) f^\dagger_{\mathbf{k}-\mathbf{Q_1},\alpha} + \sum_{\mathbf{k}\in\mathcal{Q}_2} J_f^*(\mathbf{k}+\mathbf{Q_2},\mathbf{q}) f^\dagger_{\mathbf{k}+\mathbf{Q_2},\alpha}\right] f_{\mathbf{q},\beta} \\ &= \sum_{\mathbf{q}}\left[\sum_{\mathbf{k}\in\mathcal{Q}_1} J_f^*(\mathbf{k},\mathbf{q})\left(f^\dagger_{\mathbf{k},\alpha} - f^\dagger_{\mathbf{k}-\mathbf{Q_1},\alpha}\right) + \sum_{\mathbf{k}\in\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q})\left(f^\dagger_{\mathbf{k},\alpha} - f^\dagger_{\mathbf{k}+\mathbf{Q_2},\alpha}\right)\right] f_{\mathbf{q},\beta} \ . \end{aligned} \tag{20}$$

For ease of notation, we define new fermionic operators $A_{\mathbf{k},\sigma}$ and $B_{\mathbf{k},\sigma}$:

$$
\begin{aligned}
A_{\mathbf{k},\sigma,\pm} &= \frac{1}{\sqrt{2}}\left(f_{\mathbf{k},\sigma} \pm f_{\mathbf{k}-\mathbf{Q_1},\sigma}\right), \mathbf{k} \in \mathcal{Q}_1 \ , \\
B_{\mathbf{k},\sigma,\pm} &= \frac{1}{\sqrt{2}}\left(f_{\mathbf{k},\sigma} \pm f_{\mathbf{k}+\mathbf{Q_2},\sigma}\right), \mathbf{k} \in \mathcal{Q}_2 \ ,
\end{aligned} \tag{21}
$$

which satisfy the appropriate algebra: $\{A_{\mathbf{k},\sigma,p}, A_{\mathbf{k}',\sigma',p'}\} = \{B_{\mathbf{k},\sigma,p}, B_{\mathbf{k}',\sigma',p'}\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}\delta p, p'$ and $\{A_{\mathbf{k},\sigma,p}, B_{\mathbf{k}',\sigma',p'}\} = 0$, with $p = \pm$ denoting the flavours of the A and B fields. Note that only the $p = -1$ flavour enters the Hamiltonian. Henceforth, we drop the label $\pm$ and it is implied that A and B refer to the $p = -1$ variants.

Decomposing the sum over $\mathbf{q}$ in a similar fashion, we get

$$
\begin{aligned}
\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} f_{\mathbf{q},\beta} = {}& 2\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} J_f^*(\mathbf{k},\mathbf{q}) A^\dagger_{\mathbf{k},\alpha} A_{\mathbf{q},\beta} + 2\sum_{\mathbf{k}\in\mathcal{Q}_2,\mathbf{q}\in\mathcal{Q}_1} J_f^*(\mathbf{k},\mathbf{q}) B^\dagger_{\mathbf{k},\alpha} A_{\mathbf{q},\beta} \\
& + 2\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) A^\dagger_{\mathbf{k},\alpha} B_{\mathbf{q},\beta} + 2\sum_{\mathbf{k}\in\mathcal{Q}_2,\mathbf{q}\in\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) B^\dagger_{\mathbf{k},\alpha} B_{\mathbf{q},\beta} \ .
\end{aligned} \tag{22}
$$

To further simplify things, We first replace the summations over $\mathcal{Q}_2$ with that over $\mathcal{Q}_1$, with the mapping $\mathbf{q} \to \bar{\mathbf{q}}$ and use eq. 18:

$$
\begin{aligned}
\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} f_{\mathbf{q},\beta} &= 2\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} \left[J_f^*(\mathbf{k},\mathbf{q}) A^\dagger_{\mathbf{k},\alpha} A_{\mathbf{q},\beta} + J_f^*(\bar{\mathbf{k}},\mathbf{q}) B^\dagger_{\bar{\mathbf{k}},\alpha} A_{\bar{\mathbf{q}},\beta} + J_f^*(\mathbf{k},\bar{\mathbf{q}}) A^\dagger_{\mathbf{k},\alpha} B_{\bar{\mathbf{q}},\beta} + J_f^*(\bar{\mathbf{k}},\bar{\mathbf{q}}) B^\dagger_{\bar{\mathbf{k}},\alpha} B_{\bar{\mathbf{q}},\beta}\right] \\
&= 2\sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} \left[J_f^*(\mathbf{k},\mathbf{q})\left(A^\dagger_{\mathbf{k},\alpha} A_{\mathbf{q},\beta} + B^\dagger_{\bar{\mathbf{k}},\alpha} B_{\bar{\mathbf{q}},\beta}\right) + J_f^*(\bar{\mathbf{k}},\mathbf{q})\left(B^\dagger_{\mathbf{k},\alpha} A_{\bar{\mathbf{q}},\beta} + A^\dagger_{\mathbf{k},\alpha} B_{\bar{\mathbf{q}},\beta}\right)\right] \ .
\end{aligned} \tag{23}
$$

To remove all explicit references to operators in $\mathcal{Q}_2$, we define a new set of operators:

$$
\begin{aligned}
\gamma_{\mathbf{k},\sigma,\pm} &= \frac{1}{\sqrt{2}}\left(A_{\mathbf{k},\sigma,-} \pm B_{\bar{\mathbf{k}},\sigma,-}\right), \mathbf{k} \in \mathcal{Q}_1 \ , \\
\phi_{\mathbf{k},\sigma,\pm} &= \frac{1}{\sqrt{2}}\left(A_{\mathbf{k},\sigma,+} \pm B_{\bar{\mathbf{k}},\sigma,+}\right), \mathbf{k} \in \mathcal{Q}_1 \ ,
\end{aligned} \tag{24}
$$

where we have restored the p-values into the A and B fields in order to define two new fermionic fields: $\left\{\gamma_{\mathbf{k},\sigma,\pm}, \gamma^\dagger_{\mathbf{k}',\sigma',\pm}\right\} = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'}$, $\left\{\gamma_{\mathbf{k},\sigma,\pm}, \gamma^\dagger_{\mathbf{k}',\sigma',\mp}\right\} = 0$. In terms of these new fields, we finally obtain a Hamiltonian which is defined purely in the first quadrant $\mathcal{Q}_1$ (this is however mostly formal because there are now twice as many modes on $\mathcal{Q}_1$ than before):

$$
\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f^\dagger_{\mathbf{k},\alpha} f_{\mathbf{q},\beta} = \sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} \left[\left[J_f^*(\mathbf{k},\mathbf{q}) + J_f^*(\bar{\mathbf{k}},\mathbf{q})\right]\gamma^\dagger_{\mathbf{k},\alpha,+}\gamma_{\mathbf{q},\alpha,+} + \left[J_f^*(\mathbf{k},\mathbf{q}) - J_f^*(\bar{\mathbf{k}},\mathbf{q})\right]\gamma^\dagger_{\mathbf{k},\alpha,-}\gamma_{\mathbf{q},\alpha,-}\right] \tag{25}
$$

V. CORRELATIONS IN TRUNCATED REPRESENTATION

In order to calculate equal-time correlations (such as $\langle S_d^+ f^\dagger_{\mathbf{k}\downarrow} f_{\mathbf{k}'\uparrow}\rangle$), we combine eqs. 21 and 24 to express the bare fields $f_{\mathbf{k},\sigma}$ in terms of the new fields $\gamma_{\mathbf{k},\sigma,\pm}$ and $\phi_{\mathbf{k},\sigma,\pm}$:

$$
\begin{aligned}
f_{\mathbf{k},\sigma} &= \frac{1}{2}\left(\phi_{\mathbf{k},\sigma,+} + \phi_{\mathbf{k},\sigma,-} + \gamma_{\mathbf{k},\sigma,+} + \gamma_{\mathbf{k},\sigma,-}\right), & f_{\bar{\mathbf{k}},\sigma} &= \frac{1}{2}\left(\phi_{\mathbf{k},\sigma,+} - \phi_{\mathbf{k},\sigma,-} + \gamma_{\mathbf{k},\sigma,+} - \gamma_{\mathbf{k},\sigma,-}\right), \\
f_{\mathbf{k}-\mathbf{Q}_1,\sigma} &= \frac{1}{2}\left(\phi_{\mathbf{k},\sigma,+} + \phi_{\mathbf{k},\sigma,-} - \gamma_{\mathbf{k},\sigma,+} - \gamma_{\mathbf{k},\sigma,-}\right), & f_{\bar{\mathbf{k}}+\mathbf{Q}_2,\sigma} &= \frac{1}{2}\left(\phi_{\mathbf{k},\sigma,+} - \phi_{\mathbf{k},\sigma,-} - \gamma_{\mathbf{k},\sigma,+} + \gamma_{\mathbf{k},\sigma,-}\right),
\end{aligned} \tag{26}
$$

where the four relations act on operators in four quadrants. Suppose that both $\mathbf{k}$ and $\mathbf{k}'$ in the correlation $\langle S_d^+ f^\dagger_{\mathbf{k}\downarrow} f_{\mathbf{k}'\uparrow}\rangle$ are from the first quadrant. Since the fields ϕ do not appear in the Hamiltonian, they will not contribute to the correlation measures in the absence of symmetry breaking and entanglement. As an example, the correlation defined above can be expressed as

$$
\langle S_d^+ f^\dagger_{\mathbf{k}\downarrow} f_{\mathbf{k}'\uparrow}\rangle = \frac{1}{4}\langle S_d^+ (\gamma^\dagger_{\mathbf{k},\downarrow,+} + \gamma^\dagger_{\mathbf{k},\downarrow,-})(\gamma_{\mathbf{k}',\uparrow,+} + \gamma_{\mathbf{k}',\uparrow,-})\rangle \ , \tag{27}
$$

and so can be computed from the four correlations $\langle S_d^+ \gamma^\dagger_{\mathbf{k},\downarrow,\pm}\gamma_{\mathbf{k}',\uparrow,\pm}\rangle$.

VI. BILAYER EXTENDED HUBBARD MODEL: IMPURITY MODEL

We approach the heavy-fermion problem by starting from a bilayer extended Hubbard model, consisting of two layers (f and c). Towards studying this lattice model, we adopt a two-layer impurity problem that hosts a correlated impurity site in each layer (S_f and S_d):

$$H_{\text{aux}} = H_{\text{iti}} + H_f + H_d + H_{fd} \ , \tag{28}$$

where H_{iti} is the Hamiltonian for the non-interacting itinerant electrons of either layer,

$$H_{\text{iti}} = -\sum_{\sigma,\alpha}\left[t_\alpha \sum_{\langle i,j\rangle}\left(c^\dagger_{i,\sigma,\alpha}c_{j,\sigma,\alpha} + \text{h.c.}\right) + \mu \sum_{i,\sigma,\alpha} n_{i,\sigma,\alpha}\right] \ , \tag{29}$$

such that α sums over the two layers f and d. H_f and H_d describe the dynamics of the correlated impurity sites (and their local neighbourhood) in each layer:

$$H_\alpha = \varepsilon_\alpha \sum_\sigma n_{\alpha,\sigma} + U_\alpha n_{\alpha,\uparrow}n_{\alpha,\downarrow} + \sum_{Z\in\text{NN}}\left[V_\alpha \sum_\sigma \left(\alpha^\dagger_\sigma c_{Z,\sigma,\alpha} + \text{h.c.}\right) + \frac{1}{2}J_\alpha \sum_{\alpha,\beta}\mathbf{S}_\alpha\cdot\boldsymbol{\sigma}_{\alpha\beta}c^\dagger_{Z,\alpha,\alpha}c_{Z,\beta,\alpha} - \frac{W_\alpha}{2}\left(n_{Z,\uparrow,\alpha} - n_{Z,\downarrow,\alpha}\right)^2\right] \ , \tag{30}$$

where $\alpha^\dagger_\sigma$ can refer to creation operator for either the $f-$layer ($f^\dagger_\sigma$) or the $d-$layer ($d^\dagger_\sigma$). Finally, H_{fd} represents the inter-layer hybridisation:

$$H_{fc} = J\mathbf{S}_f\cdot\mathbf{S}_d + V\sum_\sigma\left(f^\dagger_\sigma d_\sigma + \text{h.c.}\right) \ , \tag{31}$$

Tiling the impurity model leads to bilayer extended Hubbard model. In order to tile, we place the impurity sites at a position $\mathbf{r}$ on the lattice, and then we translate the entire model, taking into account the overcounting of the itinerant electrons:

$$\begin{aligned} H_{\text{tiled}} &= \sum_{\mathbf{r}} H_{\text{aux}}(\mathbf{r}) - (N-1)H_{\text{iti}} \\ &= \sum_\alpha\left[-\tilde{t}_\alpha \sum_{\langle i,j\rangle,\sigma}\left(c^\dagger_{i,\sigma,\alpha}c_{j,\sigma,\alpha} + \text{h.c.}\right) + \tilde{J}\sum_{\langle i,j\rangle}\mathbf{S}_{i,\alpha}\cdot\mathbf{S}_{j,\alpha} + \varepsilon_\alpha\sum_{i,\sigma}n_{i,\sigma,\alpha} + U_\alpha\sum_i n_{i,\uparrow,\alpha}n_{i,\downarrow,\alpha}\right] \\ &+ \sum_i\left[J\mathbf{S}_{i,f}\cdot\mathbf{S}_{j,d} + V\sum_\sigma\left(c^\dagger_{i,\sigma,f}c_{i,\sigma,d} + \text{h.c.}\right)\right] \end{aligned} \tag{32}$$

VII. UNITARY RG ANALYSIS OF BILAYER LATTICE-EMBEDDED SIAM

In the limit of large U_α, we carry out a Schrieffer-Wolff transformation and work with the following low-energy Hamiltonian:

$$H_{\text{aux}} = \sum_{\mathbf{k},\sigma,\alpha}\epsilon_{\mathbf{k},\alpha}n_{\mathbf{k},\sigma,\alpha} + \sum_\alpha\sum_{Z\in\text{NN}}\left[\frac{1}{2}J_\alpha\sum_{\alpha,\beta}\mathbf{S}_\alpha\cdot\boldsymbol{\sigma}_{\alpha\beta}c^\dagger_{Z,\alpha,\alpha}c_{Z,\beta,\alpha} - \frac{W_\alpha}{2}\left(n_{Z,\uparrow,\alpha} - n_{Z,\downarrow,\alpha}\right)^2\right] + J\mathbf{S}_f\cdot\mathbf{S}_d \ . \tag{33}$$

In order to study the low-energy physics of the impurity model, we iteratively integrate out high-energy degrees of freedom using the unitary RG method. We already have the renormalisation group equations for the couplings J_α in the case of $J=0$. It turns out that even upon switching on J, no additional processes exist which renormalise J_α. As a result, their RG equations remain unchanged.

We now turn to the renormalisation of J. More specifically, we consider the spin-flip component $JS^+_fS^-_d$. The various processes contributing to its renormalisation can be classified into the following groups.

A. Through spin-flip scattering within $f-$ and $d-$layers

We first consider scattering processes that integrate out particle (occupied) states of the high-energy subspace. One such process is

$$\Delta_1 = \frac{1}{N^2}\sum_{\mathbf{q}\in\text{UV}}\sum_{\mathbf{k}\in\text{IR}}\frac{1}{2}JS^+_fS^-_d G_{2,f}(\epsilon_{\mathbf{q},f} - \epsilon_{\mathbf{k},f})\frac{1}{2}J_fS^-_f c^\dagger_{\mathbf{q}\uparrow}c_{\mathbf{k}\downarrow}G_{1,f}(\epsilon_{\mathbf{k},f} - \epsilon_{\mathbf{q},f}, \mathbf{k}, \mathbf{q})\frac{1}{2}J_fS^+_f c^\dagger_{\mathbf{k}\downarrow}c_{\mathbf{q}\uparrow} \ , \tag{34}$$

where $G_{1,f}$ and $G_{2,f}$ are propagators for the first and second intermediate states:

$$G_{1,f}(E,\mathbf{k},\mathbf{q}) = \frac{1}{\omega - \frac{1}{2}E + \frac{1}{4}\left(J_f(\mathbf{k}) + J_f(\mathbf{q})\right) + \frac{1}{2}\left(W_f(\mathbf{k}) + W_f(\mathbf{q})\right)} \ , \quad G_{2,f}(E) \quad = \frac{1}{\omega - \frac{1}{2}E} \ . \tag{35}$$

Upon contracting the momentum field operators, we get

$$\begin{aligned}
\Delta_1 &= S_f^+ S_d^- \frac{1}{N^2}\frac{1}{8} J J_f^2 \sum_{\mathbf{q}\in\mathrm{UV}}\sum_{\mathbf{k}\in\mathrm{IR}} G_{1,f}(\epsilon_{\mathbf{k},f} - \epsilon_{\mathbf{q},f}, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_{\mathbf{q},f} - \epsilon_{\mathbf{k},f}) n_{\mathbf{q}\uparrow}\left(1 - n_{\mathbf{k}\downarrow}\right) \\
&= S_f^+ S_d^- \frac{1}{8} J J_f^2 \int_{\mathrm{UV}} d\epsilon_1 \int_{\mathrm{IR}} d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_2 - \epsilon_1, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_1 - \epsilon_2) n_{\mathbf{q}\uparrow}\left(1 - n_{\mathbf{k}\downarrow}\right) \\
&= S_f^+ S_d^- \frac{1}{8} J J_f^2 \int_{-D}^{-(D-\delta D)} d\epsilon_1 \int_0^D d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_2 - \epsilon_1, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_1 - \epsilon_2) \ .
\end{aligned} \tag{36}$$

A very similar process can be constructed by reversing the sequence of operations in the present process, while staying in the occupied sector:

$$\Delta_2 = \frac{1}{N^2}\sum_{\mathbf{q}\in\mathrm{UV}}\sum_{\mathbf{k}\in\mathrm{IR}} \frac{1}{2} J_f S_f^+ c^\dagger_{\mathbf{q}\downarrow} c_{\mathbf{k}\uparrow} G_{1,f}(\epsilon_{\mathbf{k},f} - \epsilon_{\mathbf{q},f}, \mathbf{k}, \mathbf{q}) \frac{1}{2} J_f S_f^- c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{q}\downarrow} G_{2,f}(\epsilon_{\mathbf{q},f} - \epsilon_{\mathbf{k},f}) \frac{1}{2} J S_f^+ S_d^- \ . \tag{37}$$

This leads to an exchange of the intermediate states, leaving the product of propagators $G_{1,f}G_{2,f}$ unchanged. Combining with the previous contribution, we get

$$\begin{aligned}
\Delta_1 + \Delta_2 &= S_f^+ S_d^- \frac{1}{8} J J_f^2 \int_{\mathrm{UV}} d\epsilon_1 \int_{\mathrm{IR}} d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_2 - \epsilon_1, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_1 - \epsilon_2) \sum_\sigma n_{\mathbf{q}\sigma}\left(1 - n_{\mathbf{k}\bar\sigma}\right) \\
&= S_f^+ S_d^- \frac{1}{4} J J_f^2 \int_{-D}^{-(D-\delta D)} d\epsilon_1 \int_0^D d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_2 - \epsilon_1, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_1 - \epsilon_2) \ .
\end{aligned} \tag{38}$$

The particle-hole transformed contribution is easily obtained by switching the momentum indices in the propagators. In total, we get

$$\begin{aligned}
\Delta_1 + \Delta_2 = S_f^+ S_d^- \frac{1}{4} J J_f^2 \Bigg[&\int_{-D}^{-(D-\delta D)} d\epsilon_1 \int_0^D d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_2 - \epsilon_1, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_1 - \epsilon_2) \\
&+ \int_{D-\delta D}^{D} d\epsilon_1 \int_{-D}^0 d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_1 - \epsilon_2, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_2 - \epsilon_1) \Bigg] \\
= S_f^+ S_d^- \frac{1}{4} J J_f^2 \int_{D-\delta D}^{D} d\epsilon_1 \int_{-D}^0 d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} &\left[G_{1,f}(\epsilon_1 - \epsilon_2, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_2 - \epsilon_1) + G_{1,f}(\epsilon_1 - \epsilon_2, \mathbf{k} + \mathbf{Q}_2, \mathbf{q} + \mathbf{Q}_2) G_{2,f}(\epsilon_2 - \epsilon_1) \right] \ ,
\end{aligned} \tag{39}$$

where we substituted $\epsilon_i \to -\epsilon_i$ in the first integral and used $\epsilon_{\mathbf{q}} = -\epsilon_{\mathbf{q}+\mathbf{Q}_2}$, with $\mathbf{Q}_2 = (\pi, \pi)$. Using the properties of J and W, we can show that $J(\mathbf{k}_1) = J(\mathbf{k}_1 + \mathbf{Q}_2)$. This property allows us to equate the two products within the integrand:

$$\Delta_{1,f} + \Delta_{2,f} = \frac{1}{2} S_f^+ S_d^- J J_f^2 \int_{D-\delta D}^{D} d\epsilon_1 \int_{-D}^0 d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,f}(\epsilon_1 - \epsilon_2, \mathbf{k}, \mathbf{q}) G_{2,f}(\epsilon_2 - \epsilon_1) \ . \tag{40}$$

where the subscript f indicates that this takes into account spin-flip scattering processes within the $f-$layer.

Carrying out the same computation for the $d-$layer simply requires changing all $f-$quantities to $d-$quantities:

$$\Delta_{1,d} + \Delta_{2,d} = \frac{1}{2} S_f^+ S_d^- J J_d^2 \int_{D-\delta D}^{D} d\epsilon_1 \int_{-D}^0 d\epsilon_2 \sum_{\mathbf{q}\in\epsilon_1}\sum_{\mathbf{k}\in\epsilon_2} G_{1,d}(\epsilon_1 - \epsilon_2, \mathbf{k}, \mathbf{q}) G_{2,d}(\epsilon_2 - \epsilon_1) \ , \tag{41}$$

where

$$G_{1,d}(E,\mathbf{k},\mathbf{q}) = \frac{1}{\omega - \frac{1}{2}E + \frac{1}{4}\left(J_d(\mathbf{k}) + J_d(\mathbf{q})\right) + \frac{1}{2}\left(W_d(\mathbf{k}) + W_d(\mathbf{q})\right)} \ , \quad G_{2,d}(E) \quad = \frac{1}{\omega - \frac{1}{2}E} \ . \tag{42}$$