Quantum criticality in a Kondo-Mott lattice model

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I. IMPURITY MODEL

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

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

II. TILING RECONSTRUCTION

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

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

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

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

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

B. Inter-layer processes

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

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

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

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

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

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

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

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

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:

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

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):

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

C. Complete coupling RG equation

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

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:

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

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:

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

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

$$J_f(\mathbf{k},\bar{\mathbf{k}}') = J_f(\bar{\mathbf{k}},\mathbf{k}'),$$
$$J_f(\bar{\mathbf{k}},\bar{\mathbf{k}}') = J_f(\mathbf{k},\mathbf{k}') \;. \tag{18}$$

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 $J_f^{(j)}(\mathbf{k}_2,\mathbf{q})\,J_f^{(j)}\left(\mathbf{q},\bar{\mathbf{k}}_1\right) = J_f^{(j)}\left(\bar{\mathbf{k}}_2,\bar{\mathbf{q}}\right)J_f^{(j)}(\bar{\mathbf{q}},\mathbf{k}_1)$ 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 $\Delta J_f^{(j)}\left(\bar{\mathbf{k}}_1,\mathbf{k}_2\right) = \Delta J_f^{(j)}\left(\mathbf{k}_1,\bar{\mathbf{k}}_2\right)$. A similar line of argument shows that $\Delta J_f^{(j)}\left(\bar{\mathbf{k}}_1,\bar{\mathbf{k}}_2\right) = \Delta J_f^{(j)}(\mathbf{k}_1,\mathbf{k}_2)$.

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:

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

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:

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

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. For every shell of conduction bath states of width ΔD integrated out, the Hamiltonian couplings renormalise by folding in the effects of virtual excitations to these states. We already have the renormalisation group equations for the couplings J_α in the case of $J=0$:

$$\frac{\Delta J_f}{\Delta D} = J_f^2\int_{UV} d\mathbf{q}\ \rho(\mathbf{q})G_f^{(0)} \ , \tag{34}$$

where $\mathbf{q}$ sums over the UV states being integrated out, $\rho(\mathbf{q})$ is the density of states for the momentum states being integrated out and $G_f^{(0)}$ is the propagator for the excited intermediate state (for $J=0$):

$$G_f^{(0)} = \frac{1}{\omega - \epsilon_f(\mathbf{q})/2 + J_f/4 + W_f/2} \ . \tag{35}$$

An identical equations holds for ΔJ_d, with al $f-$quantities replaced with $d-$quantities. Switching on J modifies the excitation energy in the propagator:

$$G_f = \frac{1}{1/G_f^{(0)} - J\vec{S}_f\cdot\vec{S}_d} \ . \tag{36}$$

This expression can be simplified by noting that the operator in the denominator has only two eigenvalues, $-3/4$ in the singlet sector and $1/4$ in the triplet sector. Defining the projectors $\mathcal{P}_0$ and $\mathcal{P}_1$ for the two sectors, we have

$$\vec{S}_f\cdot\vec{S}_d = \frac{-3}{4}\mathcal{P}_0 + \frac{1}{4}\mathcal{P}_1, \quad \mathcal{P}_0+\mathcal{P}_1 = \mathbb{I} \ . \tag{37}$$

Using these relations, we can write

$$\begin{aligned} G_f &= \frac{1}{1/G_f^{(0)}+3J/4}\mathcal{P}_0 + \frac{1}{1/G_f^{(0)}-J/4}\mathcal{P}_1 \\ &= \left(\frac{1/4}{1/G_f^{(0)}+3J/4} + \frac{3/4}{1/G_f^{(0)}-J/4}\right)\mathbb{I} + \left(\frac{1}{1/G_f^{(0)}+3J/4} + \frac{1}{1/G_f^{(0)}-J/4}\right)\vec{S}_f\cdot\vec{S}_d \ . \end{aligned} \tag{38}$$

Noting that only the first operator renormalises the Kondo interaction, we get the following modified RG equation for the Kondo coupling J_α:

$$\frac{\Delta J_\alpha}{\Delta D} = J_\alpha^2\int_{UV} d\mathbf{q}\ \rho(\mathbf{q})\left(\frac{1/4}{\omega-\epsilon_\alpha(\mathbf{q})/2+J_\alpha/4+W_\alpha/2+3J/4} + \frac{3/4}{\omega-\epsilon_\alpha(\mathbf{q})/2+J_\alpha/4+W_\alpha/2-J/4}\right) \ , \tag{39}$$

We now turn to the renormalisation of J, arising from hybridisation of $f-$ and $d-$layers. Let the momentum states being decoupled from the two layers be $|\mathbf{q}_\pm,\sigma,f\rangle$ and $|\mathbf{q}_\pm,\sigma,d\rangle$, where the subscript indicates the sign of the energy of that state (and hence whether its occupancy in the low-energy configurations $|L\rangle_f$, $|L\rangle_d$). In order to capture coherent scattering processes between the two layers, we project onto the following rotated basis of excited states:

$$\begin{aligned} |H\rangle_\pm &= \frac{1}{\sqrt{2}}\left(|H(\mathbf{q})\rangle_f \pm |H(\mathbf{q})\rangle_d\right) \ , \\ \mathcal{P}(\mathbf{q})_H &= |H\rangle_+\langle H|_+ + |H\rangle_-\langle H|_- \ , \end{aligned} \tag{40}$$

where $|H(\mathbf{q})\rangle_\alpha$ is the state obtained upon exciting both states $|\mathbf{q}\rangle_\pm$ in the layer α: $|H(q)\rangle_\alpha = c^\dagger_{\mathbf{q}+,\alpha}c_{\mathbf{q}-,\alpha}|L\rangle_f|L\rangle_d$, and $\mathcal{P}(\mathbf{q})_H$ projects onto this rotated excited basis. We focus on the spin-flip component $JS_f^+S_d^-$ of the Hamiltonian.

There are two kinds of processes that renormalise this coupling. We first consider one that involves a spin-flip of the $d-$layer followed by a spin-flip of the $f-$layer:

$$\Delta H = \frac{1}{N^2} \sum_{\mathbf{q} \in \mathrm{UV}} \langle L | \frac{1}{2} J_f S_f^+ c^\dagger_{\mathbf{q}-_\downarrow, f} c_{\mathbf{q}+\uparrow, f} \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H \frac{1}{2} J_d S_d^- c^\dagger_{\mathbf{q}+\uparrow, d} c_{\mathbf{q}-\downarrow, d} | L \rangle \ , \tag{41}$$

where $|L\rangle = |L\rangle_f |L\rangle_d$ is the initial configuration for both layers. G is the propagator for the excited state:

$$G = \frac{1}{\omega - H_D} \ , \tag{42}$$

where H_D is the diagonal part of the Hamiltonian corresponding to the excited(intermediate) state. The diagonal part consists of the kinetic energy and the Ising part of the Kondo interaction:

$$H_D = \sum_{\mathbf{q}, \sigma \in \mathbf{q}_\pm, \alpha} \epsilon_\alpha(\mathbf{q}) \tau_{\mathbf{q}, \sigma} + \sum_\alpha J_\alpha S_\alpha^z \sum_{\mathbf{q}, \sigma} \sigma n_{\mathbf{q}, \sigma, \alpha} + J \vec{S}_f \cdot \vec{S}_d \ . \tag{43}$$

Calculating the matrix elements of the propagator in the rotated basis gives

$$\mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H = \frac{1}{2} (G_f + G_d) \left(|H\rangle_+ \langle H|_+ + |H\rangle_- \langle H|_- \right) + \frac{1}{2} (G_f - G_d) \left(|H\rangle_+ \langle H|_- + |H\rangle_- \langle H|_+ \right) \ , \tag{44}$$

where

$$G_\alpha = \frac{1}{\omega - \frac{1}{2} \left[\epsilon_\alpha(q_+) - \epsilon_\alpha(q_-) \right] + \frac{1}{2} J_\alpha + W_\alpha - \frac{1}{4} J} \ . \tag{45}$$

In eq. 41, since the first process is an excitation into a $d-$state and the second process is a de-excitation from an $f-$state, the expression can be simplified into

$$\langle L | S_f^+ c^\dagger_{\mathbf{q}-_\downarrow, f} c_{\mathbf{q}+\uparrow, f} \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H S_d^- c^\dagger_{\mathbf{q}+\uparrow, d} c_{\mathbf{q}-\downarrow, d} | L \rangle = S_f^+ S_d^- \langle H_f | \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H | H_d \rangle = \frac{1}{2} (G_f + G_d) S_f^+ S_d^- \ . \tag{46}$$

The net Hamiltonian renormalisation is finally a sum over the contribution from each mode:

$$\Delta H = \frac{1}{8N^2} J_f J_d \sum_{\mathbf{q} \in \mathrm{UV}} (G_f + G_d) S_f^+ S_d^- \ . \tag{47}$$

Converting the sums to integrals (assuming a density of states $\rho(\mathbf{q})$) gives the final expression

$$\frac{\Delta H}{\Delta D} = \frac{1}{8N} S_f^+ S_d^- J_f J_d \int_{UV} d\mathbf{q} \ \rho(\mathbf{q}) (G_f + G_d) \ . \tag{48}$$

The time-reversed of this process can be obtained simply by exchanging the $d-$interaction with the $f-$interaction. Since the renormalisation itself is symmetric, the contribution is equal to what we obtained here. The total renormalisation in the coupling for the term $S_f^+ S_d^-$ is therefore

$$\begin{aligned} \frac{\Delta J}{\Delta D} &= \frac{1}{2} J_f J_d \int_{UV} d\mathbf{q} \ \rho(\mathbf{q}) (G_f + G_d) \\ &= \frac{1}{2} J_f J_d \int_{UV} d\mathbf{q} \ \rho(\mathbf{q}) \left[\frac{1}{\omega - \frac{1}{2} \left[\epsilon_f(q_+) - \epsilon_f(q_-) \right] + \frac{1}{2} J_f + W_f - \frac{1}{4} J} + \frac{1}{\omega - \frac{1}{2} \left[\epsilon_d(q_+) - \epsilon_d(q_-) \right] + \frac{1}{2} J_d + W_d - \frac{1}{4} J} \right] \end{aligned} \tag{49}$$

VIII. RG FLOW SIMULATION ON THE $d = \infty$ BETHE LATTICE AT HALF-FILLING