Quantum criticality in a Kondo-Mott Lattice Model

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I. IMPURITY MODEL

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

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

II. TILING RECONSTRUCTION

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

III. COUPLING RENORMALISATION GROUP FLOWS

Off-diagonal terms:

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

A. Intra-layer processes

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

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

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

B.   Inter-layer processes

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

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

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

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

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

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

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

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

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:

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

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

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

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:

$$J_f(\mathbf{k}, \mathbf{q}) = \frac{J_f}{2} \left[\cos(k_x - q_x) + \cos(k_y - q_y) \right] \ ,$$

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

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:

$$J_f(\mathbf{k} + \mathbf{Q}_i, \mathbf{q}) = J_f(\mathbf{k}, \mathbf{q} + \mathbf{Q}_i) = -J_f(\mathbf{k}, \mathbf{q}) \ ; \ i = 1, 2 \ ;$$

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

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 $J_f^{(j)}(\mathbf{k}_2, \mathbf{q}) J_f^{(j)}(\mathbf{q}, \bar{\mathbf{k}}_1) = J_f^{(j)}(\bar{\mathbf{k}}_2, \bar{\mathbf{q}}) J_f^{(j)}(\bar{\mathbf{q}}, \mathbf{k}_1)$ 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:

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

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 $\mathcal{Q}_4$:

$$\sum_{\mathbf{k}, \mathbf{q}} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger f_{\mathbf{q}, \beta} = \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in \mathcal{Q}_1, \mathcal{Q}_2} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger + \sum_{\mathbf{k} \in \mathcal{Q}_3, \mathcal{Q}_4} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger \right] f_{\mathbf{q}, \beta}$$

$$= \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in \mathcal{Q}_1, \mathcal{Q}_2} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger + \sum_{\mathbf{k} \in \mathcal{Q}_1} J_f^*(\mathbf{k} - \mathbf{Q_1}, \mathbf{q}) f_{\mathbf{k} - \mathbf{Q_1}, \alpha}^\dagger + \sum_{\mathbf{k} \in \mathcal{Q}_2} J_f^*(\mathbf{k} + \mathbf{Q_2}, \mathbf{q}) f_{\mathbf{k} + \mathbf{Q_2}, \alpha}^\dagger \right] f_{\mathbf{q}, \beta} \tag{20}$$

$$= \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in \mathcal{Q}_1} J_f^*(\mathbf{k}, \mathbf{q}) \left(f_{\mathbf{k}, \alpha}^\dagger - f_{\mathbf{k} - \mathbf{Q_1}, \alpha}^\dagger \right) + \sum_{\mathbf{k} \in \mathcal{Q}_2} J_f^*(\mathbf{k}, \mathbf{q}) \left(f_{\mathbf{k}, \alpha}^\dagger - f_{\mathbf{k} + \mathbf{Q_2}, \alpha}^\dagger \right) \right] f_{\mathbf{q}, \beta} \ .$$

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

$$A_{\mathbf{k},\sigma,\pm} = \frac{1}{\sqrt{2}} \left(f_{\mathbf{k},\sigma} \pm f_{\mathbf{k}-\mathbf{Q_1},\sigma} \right), \mathbf{k} \in \mathcal{Q}_1 ,$$

$$B_{\mathbf{k},\sigma,\pm} = \frac{1}{\sqrt{2}} \left(f_{\mathbf{k},\sigma} \pm f_{\mathbf{k}+\mathbf{Q_2},\sigma} \right), \mathbf{k} \in \mathcal{Q}_2 , \tag{21}$$

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

$$\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f_{\mathbf{k},\alpha}^\dagger f_{\mathbf{q},\beta} = 2 \sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} J_f^*(\mathbf{k},\mathbf{q}) A_{\mathbf{k},\alpha}^\dagger A_{\mathbf{q},\beta} + 2 \sum_{\mathbf{k}\in\mathcal{Q}_2,\mathbf{q}\in\mathcal{Q}_1} J_f^*(\mathbf{k},\mathbf{q}) B_{\mathbf{k},\alpha}^\dagger A_{\mathbf{q},\beta}$$

$$+ 2 \sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) A_{\mathbf{k},\alpha}^\dagger B_{\mathbf{q},\beta} + 2 \sum_{\mathbf{k}\in\mathcal{Q}_2,\mathbf{q}\in\mathcal{Q}_2} J_f^*(\mathbf{k},\mathbf{q}) B_{\mathbf{k},\alpha}^\dagger B_{\mathbf{q},\beta} . \tag{22}$$

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:

$$\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) f_{\mathbf{k},\alpha}^\dagger f_{\mathbf{q},\beta} = 2 \sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} \left[J_f^*(\mathbf{k},\mathbf{q}) A_{\mathbf{k},\alpha}^\dagger A_{\mathbf{q},\beta} + J_f^*(\bar{\mathbf{k}},\mathbf{q}) B_{\mathbf{k},\alpha}^\dagger A_{\bar{\mathbf{q}},\beta} + J_f^*(\mathbf{k},\bar{\mathbf{q}}) A_{\mathbf{k},\alpha}^\dagger B_{\bar{\mathbf{q}},\beta} + J_f^*(\bar{\mathbf{k}},\bar{\mathbf{q}}) B_{\bar{\mathbf{k}},\alpha}^\dagger B_{\bar{\mathbf{q}},\beta} \right]$$

$$= 2 \sum_{\mathbf{k}\in\mathcal{Q}_1,\mathbf{q}\in\mathcal{Q}_1} \left[J_f^*(\mathbf{k},\mathbf{q}) \left(A_{\mathbf{k},\alpha}^\dagger A_{\mathbf{q},\beta} + B_{\mathbf{k},\alpha}^\dagger B_{\bar{\mathbf{q}},\beta} \right) + J_f^*(\bar{\mathbf{k}},\mathbf{q}) \left(B_{\mathbf{k},\alpha}^\dagger A_{\bar{\mathbf{q}},\beta} + A_{\mathbf{k},\alpha}^\dagger B_{\bar{\mathbf{q}},\beta} \right) \right] . \tag{23}$$

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

$$\gamma_{\mathbf{k},\sigma,\pm} = \frac{1}{\sqrt{2}} \left(A_{\mathbf{k},\sigma,-} \pm B_{\bar{\mathbf{k}},\sigma,-} \right), \mathbf{k} \in \mathcal{Q}_1 ,$$

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

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

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

V. CORRELATIONS IN TRUNCATED REPRESENTATION

In order to calculate equal-time correlations (such as $\langle S_d^+ f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}'\uparrow}\rangle$), 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 $\phi_{\mathbf{k},\sigma,\pm}$:

$$f_{\mathbf{k},\sigma} = \frac{1}{2} \left(\phi_{\mathbf{k},\sigma,+} + \phi_{\mathbf{k},\sigma,-} + \gamma_{\mathbf{k},\sigma,+} + \gamma_{\mathbf{k},\sigma,-} \right), \qquad f_{\bar{\mathbf{k}},\sigma} = \frac{1}{2} \left(\phi_{\mathbf{k},\sigma,+} - \phi_{\mathbf{k},\sigma,-} + \gamma_{\mathbf{k},\sigma,+} - \gamma_{\mathbf{k},\sigma,-} \right),$$

$$f_{\mathbf{k}-\mathbf{Q_1},\sigma} = \frac{1}{2} \left(\phi_{\mathbf{k},\sigma,+} + \phi_{\mathbf{k},\sigma,-} - \gamma_{\mathbf{k},\sigma,+} - \gamma_{\mathbf{k},\sigma,-} \right), \quad f_{\bar{\mathbf{k}}+\mathbf{Q_2},\sigma} = \frac{1}{2} \left(\phi_{\mathbf{k},\sigma,+} - \phi_{\mathbf{k},\sigma,-} - \gamma_{\mathbf{k},\sigma,+} + \gamma_{\mathbf{k},\sigma,-} \right), \tag{26}$$

where the four relations act on operators in four quadrants. Suppose that both $\mathbf{k}$ and $\mathbf{k}'$ in the correlation $\langle S_d^+ f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}'\uparrow}\rangle$ 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

$$\langle S_d^+ f_{\mathbf{k}\downarrow}^\dagger f_{\mathbf{k}'\uparrow}\rangle = \langle S_d^+ (\gamma_{\mathbf{k},\downarrow,+}^\dagger + \gamma_{\mathbf{k},\downarrow,-}^\dagger)(\gamma_{\mathbf{k}',\uparrow,+} + \gamma_{\mathbf{k}',\uparrow,-})\rangle , \tag{27}$$

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