

Chapter 1

Tiling Hubbard

1.1 The Philosophy of Auxiliary Models

In the previous chapter, we extended the Anderson impurity model to host a correlation-driven delocalisation-localisation transition on the impurity site, from a local Fermi liquid state to a local moment state. We demonstrated that this transition captures very well the phenomenology of the Hubbard dimension in infinite dimensions (as seen from, say, dynamical mean-field theory (DMFT)). In this chapter, we extend this approach by developing a formalism to study the more realistic case of finite-dimensional interacting models by using appropriately chosen impurity models as auxiliary models. The key to an *auxiliary model method* is to construct an appropriate auxiliary model that while being tractable captures some essential property of the full lattice model [1]. This involves separating the complete degrees of freedom into a system part (H_S) which one treats exactly and the rest of the system (H_R) that one might simplify in order to be able to solve the problem. The non-trivial nature of the problem arises of course from the hybridisation H_{SR} between the system and the bath:

$$H = \begin{bmatrix} H_R & H_{RS} \\ H_{RS}^* & H_S \end{bmatrix}. \quad (1.1)$$

This separation can always be done exactly, if one does not care about tractability. For example, one can take the Hubbard model that describes electrons hopping on a lattice and interacting when two electrons reside on the same lattice site:

$$H_{\text{hub}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1.2)$$

and separate this into parts, the system being the local orbitals of a specific site l and the rest of the system being all the other sites:

$$H_S = U n_{l\uparrow} n_{l\downarrow}, \quad H_R = -t \sum'_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad H_{SR} + H_{RS} = -t \sum_{i,\sigma} (c_{l,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}), \quad (1.3)$$

where the primed summation is carried out over all nearest-neighbour pairs that do not involve l and the summation in $H_{SR} + H_{RS}$ is over all sites adjacent to l .

The smaller system H_S (often called the *cluster*) is typically chosen such that its eigenstates are known exactly. Progress is then made by choosing a simpler form for H_R and its coupling H_{RS} with the smaller system. This combination of the cluster and the simpler bath is then called the *auxiliary system*. A tractable auxiliary system for the Hubbard model is the single-impurity Anderson model (SIAM); the correlated impurity site represents the set of local orbitals of any given site, while the conduction bath represents the rest of the lattice sites in an approximate fashion. Such a construction is shown in fig. 1.1.

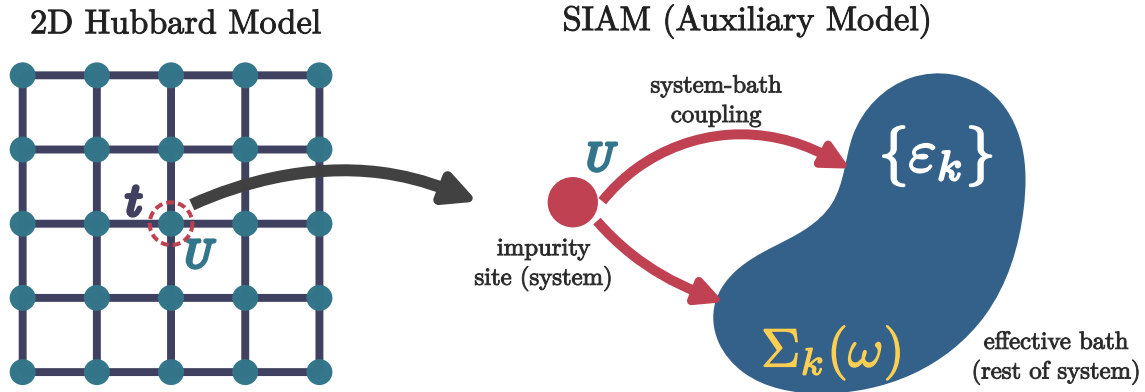


Figure 1.1: *Left:* Full Hubbard model lattice with onsite repulsion U^H on all sites and hopping between nearest neighbour sites with strength t^H . *Right:* Extraction of the auxiliary (cluster+bath) system from the full lattice. The central site on left becomes the impurity site (red) on the right (with an onsite repulsion ϵ_d), while the rest of the $N - 1$ sites on the left form a conduction bath (green circles) (with dispersion ϵ_k and correlation modelled by the self-energy $\Sigma_k(\omega)$) that hybridizes with the impurity through the coupling V .

It should be noted that any reasonable choice of the cluster and bath would break the translational symmetry of the full model: To allow computing quantities, one would need to make the bath (which is a much larger system) simpler than the cluster (which is a single site). This distinction breaks the translational symmetry of the Hubbard model. As a result, calculations that make use of the translation symmetry of the full model (such as k -space objects) will require a periodisation operation of an auxiliary model quantity.

The present work is aimed towards developing a new auxiliary model method to study correlated electronic systems. As described above, the first step is to identify the correct impurity model which can faithfully capture the physics of the lattice model we are trying to solve. The local behaviour of this impurity model should reflect the essential local physics of the lattice model. Typically, we will consider impurity model geometries where the real-space bath site connected directly to the impurity hosts some local interaction. We will henceforth refer to this site as the *zeroth site*. This model must be solved using an impurity solver. In the present work, we use the recently-developed unitary renormalisation group method [2–7]. The leap to the bulk model is then made by applying **manybody lattice translation operators** on the auxiliary model. This process, referred to as *tiling* here, allows us to reconstruct the lattice model Hamiltonian from that of the auxiliary model and restores the translation invariance of the full lattice model. Once the Hamiltonians can be mapped onto one another, it is possible to relate the eigenstates and correlations functions between the auxiliary model and lattice model, using a manybody version of **Bloch’s theorem**.

1.2 What Is The Correct Auxiliary Model For Correlated Electrons on a 2D Square Lattice?

As discussed in more detail in the previous chapter, it was necessary to extend the single-impurity Anderson model (SIAM) in order to obtain a phase transition on the impurity site. Without any modification, the standard Anderson model (at particle-hole symmetry) leads to the emergence of an $\omega = 0$ Kondo resonance in the impurity ($d\sigma$) spectral function at any value of the impurity correlation U_d , at sufficiently low temperatures:

$$H_{\text{SIAM}} = \sum_{k,\sigma} \varepsilon_k n_{k,\sigma} - V \sum_{\sigma} (c_{0,\sigma}^\dagger c_{d,\sigma} + \text{h.c.}) + \varepsilon_d \sum_{\sigma} n_{d,\sigma} + U_d n_{d,\uparrow} n_{d,\downarrow}. \quad (1.4)$$

The operator $c_{0,\sigma}$ acts on the local conduction bath density that couples with the impurity site. The low-energy is one of local Fermi liquid for all parameter regimes. Increasing U_d only serves to reduce the width of the central peak at the cost of the appearance of side bands at energy scales of the order of U_d , but the resonance never disappears. The extended Anderson model that we developed augments the SIAM by allowing for local correlation in the local conduction bath charge density that couples with the impurity spin:

$$H_{\text{ESIAM}} = H_{\text{SIAM}} + J_K \mathbf{S}_d \cdot \mathbf{S}_0 - \frac{U_b}{2} (n_{0,\uparrow}^2 - n_{0,\downarrow}^2); \quad (1.5)$$

tuning this bath correlation to large attractive values (see [8] for some recent findings of non-local effective attractive interactions within the Hubbard model) *does* lead to a localisation transition on the impurity where the local Fermi liquid excitations are replaced by the physics of a gapped local moment on the impurity. We note that the generation of such correlations in the bath is something that occurs in DMFT as well – the conduction bath acquires a *non-trivial self-energy* during the convergence to self-consistency.

While this modified impurity model captures well the Mott metal-insulator transition of the Hubbard model in infinite dimensions, it *lacks any knowledge of the underlying lattice geometry*, and is therefore ill-suited to address the phenomenology of more realistic low-dimensional models. Examples of such phenomenology include the pseudogap phase of the cuprates (with nodal-antinodal dichotomy), strange metal (with T -linear resistivity) and high- T_c superconducting phases observed in several families of quantum materials as well as graphene. This leads us to propose the framework of *lattice-embedded quantum impurity models*. Upon embedding the impurity site within the underlying lattice, the coupling between it and its environment must be consistent with the lowered symmetry of the lattice (see Fig. 1.2). Impurity-bath correlations calculated within such an impurity model are sensitive to the lattice geometry, and are much better suited to address the phenomenology mentioned above.

As a concrete example, we take the extended SIAM defined in eq. 1.5, and write down its lattice-embedded form on a 2D square lattice, with the impurity placed at the site r_d . This is done by allowing the impurity to hybridise with the four nearest-neighbours, through V and J_K . The same

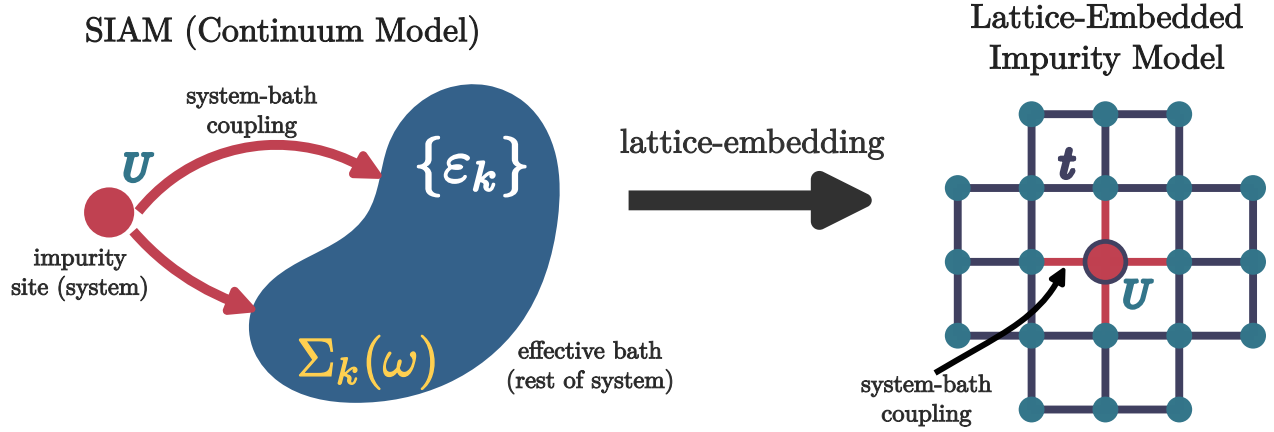


Figure 1.2

four sites also carry the local bath interaction. The complete auxiliary model is

$$\begin{aligned}
 H = & -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + \sum_{\langle i,r_d \rangle} \left[-\frac{V}{Z} \sum_{\sigma} (c_{r_d,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) + \frac{J_K}{Z} \mathbf{S}_{r_d} \cdot \mathbf{S}_i - \frac{W}{2Z} (n_{i,\uparrow}^2 - n_{i,\downarrow}^2) \right] \\
 & + \varepsilon_d \sum_{\sigma} n_{r_d,\sigma} + U_d n_{r_d,\uparrow} n_{r_d,\downarrow},
 \end{aligned} \tag{1.6}$$

where Z is the coordination number of the lattice, and the second summation $\sum_{\langle i,r_d \rangle}$ is carried out over all sites i that are nearest-neighbour to the site r_d . Note that the one-particle hybridisation V and the spin-exchange coupling J_K have their *symmetry lowered* from the s -wave spherical symmetry of the continuum impurity models to a C_4 -symmetry consistent with the underlying lattice. This feature is crucial in explaining the phenomenology of the various low-dimensional materials.

Various enhancements can be applied to such a model. The lattice can be modified to study different materials. More complicated geometries such as a two-layer model can be studied using a two-impurity auxiliary model, where each impurity couples with its own conduction bath as well as to each other.

1.3 Mapping Auxiliary Model To Lattice Model: Tiling Formalism

In this subsection, we provide an explicit example of constructing a lattice model from a lattice-embedded impurity model. This will involve the use of manybody lattice translation operators, so we begin with a brief discussion of them.

1.3.1 Manybody Translation Operators

In order to create the bulk model, we need to translate the local auxiliary model over the entire lattice. For this, we define *many-particle global* translation operators $T(\mathbf{a})$ that translate all positions by a

vector \mathbf{a} . In terms of manybody states and operators, their action is defined as

$$\begin{aligned} T^\dagger(\mathbf{a}) |\mathbf{r}_1, \mathbf{r}_2, \dots\rangle &= |\mathbf{r}_1 + \mathbf{a}\rangle \otimes |\mathbf{r}_2 + \mathbf{a}\rangle \dots \otimes |\mathbf{r}_n + \mathbf{a}\rangle \\ T^\dagger(\mathbf{a}) O(\mathbf{r}_1, \mathbf{r}_2, \dots) T(\mathbf{a}) &= O(\mathbf{r}_1 + \mathbf{a}, \mathbf{r}_2 + \mathbf{a}, \dots) , \end{aligned} \quad (1.7)$$

where $|\mathbf{r}_1, \mathbf{r}_2, \dots\rangle$ is a state in the manyparticle Fock-space basis with the particles localised at the specified positions. For example, for a local fermionic creation operator $c^\dagger(\mathbf{r})$, we have

$$T^\dagger(\mathbf{a}) c^\dagger(\mathbf{r}) T(\mathbf{a}) = c^\dagger(\mathbf{r} + \mathbf{a}) . \quad (1.8)$$

It acts similarly on the auxiliary model Hamiltonian:

$$T^\dagger(\mathbf{a}) H_{\text{aux}}(\mathbf{r}_d) T(\mathbf{a}) = H_{\text{aux}}(\mathbf{r}_d + \mathbf{a}) , \quad (1.9)$$

translating all sites by the vector \mathbf{a} . By introducing the Fourier transform to momentum space,

$$|\mathbf{r}_1, \mathbf{r}_2, \dots\rangle = \otimes_{j=1}^N \int d\mathbf{k}_j e^{i\mathbf{r}_j \cdot \mathbf{k}_j} |\mathbf{k}_j\rangle , \quad (1.10)$$

it is easy to see that the total momentum states are eigenstates of the global translation operators:

$$\begin{aligned} T^\dagger(\mathbf{a}) |\mathbf{k}_1, \mathbf{k}_2, \dots\rangle &= \otimes_{j=1}^N \int d\mathbf{r}_j e^{-i\mathbf{r}_j \cdot \mathbf{k}_j} T^\dagger(\mathbf{a}) |\mathbf{r}_j\rangle , \\ &= \otimes_{j=1}^N \int d\mathbf{r}_j e^{-i\mathbf{r}_j \cdot \mathbf{k}_j} |\mathbf{r}_j + \mathbf{a}\rangle \\ &= \otimes_{j=1}^N e^{i\mathbf{a} \cdot \mathbf{k}_j} \int d\mathbf{r}_j e^{-i\mathbf{r}_j \cdot \mathbf{k}_j} |\mathbf{r}_j\rangle \\ &= e^{i\mathbf{a} \cdot \mathbf{k}_{\text{tot}}} |\mathbf{k}_1, \mathbf{k}_2, \dots\rangle , \end{aligned} \quad (1.11)$$

where $\mathbf{k}_{\text{tot}} = \sum_j \mathbf{k}_j$ is the total momentum. This gives a compact form for the translation operator:

$$T^\dagger(\mathbf{a}) = e^{i\mathbf{a} \cdot \hat{\mathbf{k}}_{\text{tot}}} , \quad (1.12)$$

where $\hat{\mathbf{k}}_{\text{tot}}$ is the total momentum operator.

We end this section by calculating the effect of the translation operators on the k -space annihilation operators. We have

$$c(\mathbf{k}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} c(\mathbf{r}) . \quad (1.13)$$

Applying the translation operator to this decomposition, we get

$$\begin{aligned} T(\vec{a}) c(\mathbf{k}) T^\dagger(\vec{a}) &= \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} T(\vec{a}) c(\mathbf{r}) T^\dagger(\vec{a}) \\ &= \frac{1}{\sqrt{N}} \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} c(\mathbf{r} - \vec{a}) \\ &= e^{-i\mathbf{k} \cdot \vec{a}} c(\mathbf{k}) . \end{aligned} \quad (1.14)$$

1.3.2 Periodisation of Auxiliary Model Into Extended Hubbard Model

We recall the lattice-embedded impurity model defined in eq. 1.6. As discussed above, the route to restoring translation symmetry and reconstructing the lattice model is to translate the auxiliary model using manybody translation operators. Accordingly, we identify the “unit cell” of translation. Since we expect the impurity site to capture most of the physics arising from the correlated electrons, a good choice for the unit cell is the impurity site and its surrounding correlated environment. In order to retain information of the lattice geometry, we convert the hybridisation and bath interaction terms from real space to k -space. The Hamiltonian for the unit cell is therefore

$$H_{\text{clust}}(\mathbf{r}_d) = - \sum_{\mathbf{k}, \sigma} e^{i\mathbf{k} \cdot \mathbf{r}_d} V(\mathbf{k}) (c_{\mathbf{r}_d, \sigma}^\dagger c_{\mathbf{k}, \sigma} + \text{h.c.}) + \sum_{\mathbf{k}_1, \mathbf{k}_2} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}_d} J_K(\mathbf{k}_1, \mathbf{k}_2) \mathbf{S}_{\mathbf{r}_d} \cdot \mathbf{S}_{\mathbf{k}_1, \mathbf{k}_2} + \varepsilon_d n_{\mathbf{r}_d} \\ + U_d n_{\mathbf{r}_d, \uparrow} n_{\mathbf{r}_d, \downarrow} - \frac{1}{2} \sum_{\{\mathbf{k}_i\}, \sigma, \sigma'} \sigma \sigma' e^{i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}_d} W(\{\mathbf{k}_i\}) c_{\mathbf{k}_1, \sigma}^\dagger c_{\mathbf{k}_2, \sigma} c_{\mathbf{k}_3, \sigma'}^\dagger c_{\mathbf{k}_4, \sigma'}, \quad (1.15)$$

where $\mathbf{S}_{\mathbf{k}_1, \mathbf{k}_2} = \sum_{\alpha, \beta} \sigma_{\alpha, \beta} c_{\mathbf{k}_1, \alpha}^\dagger c_{\mathbf{k}_2, \beta}$, and the Fourier transforms are defined by the following relations:

$$\sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_d} V(\mathbf{k}) c_{\mathbf{r}_d, \sigma}^\dagger c_{\mathbf{k}, \sigma} = \frac{V}{Z} \sum_{\mathbf{r} \rightarrow \text{NN of } \mathbf{r}_d} c_{\mathbf{r}_d, \sigma}^\dagger c_{\mathbf{r}, \sigma}, \\ \sum_{\mathbf{k}_1, \mathbf{k}_2} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}_d} J_K(\mathbf{k}_1, \mathbf{k}_2) \vec{S}_{\mathbf{r}_d} \cdot \vec{S}_{\mathbf{k}_1, \mathbf{k}_2} = \frac{J_K}{Z} \sum_{\mathbf{r} \rightarrow \text{NN of } \mathbf{r}_d} \mathbf{S}_{\mathbf{r}_d} \cdot \mathbf{S}_{\mathbf{r}}, \quad (1.16) \\ \sum_{\mathbf{k}_1, \mathbf{k}_2, \mathbf{q}_1, \mathbf{q}_2} e^{i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}_d} W(\{\mathbf{k}_i\}) c_{\mathbf{k}_1, \sigma}^\dagger c_{\mathbf{k}_2, \sigma} c_{\mathbf{k}_3, \sigma'}^\dagger c_{\mathbf{k}_4, \sigma'} = \frac{W}{2Z} \sum_{\mathbf{r} \rightarrow \text{NN of } \mathbf{r}_d} n_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma'},$$

We now translate this unit cell to all sites of the lattice, and reconstruct a translationally-invariant correlated lattice model:

$$H_{\text{latt}} = \sum_{\mathbf{r}} T^\dagger(\mathbf{r} - \mathbf{r}_d) H_{\text{clust}}(\mathbf{r}_d) T(\mathbf{r} - \mathbf{r}_d). \quad (1.17)$$

We consider the effect of the translation operations on each part of the Hamiltonian. The purely local terms translate directly into a chemical potential term and a Hubbard interaction term:

$$\sum_{\mathbf{r}} T^\dagger(\mathbf{r} - \mathbf{r}_d) (\varepsilon_d \sum_{\sigma} n_{\mathbf{r}_d, \sigma} + U_d n_{\mathbf{r}_d, \uparrow} n_{\mathbf{r}_d, \downarrow}) T(\mathbf{r} - \mathbf{r}_d) = \varepsilon_d \sum_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma} + U_d \sum_{\mathbf{r}} n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow}. \quad (1.18)$$

The one-particle hybridisation term maps onto a tight-binding hopping term:

$$\sum_{\mathbf{r}} T^\dagger(\mathbf{r} - \mathbf{r}_d) \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}_d} V(\mathbf{k}) c_{\mathbf{r}_d, \sigma}^\dagger c_{\mathbf{k}, \sigma} T(\mathbf{r} - \mathbf{r}_d) = \sum_{\mathbf{r}} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} V(\mathbf{k}) c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{k}, \sigma} \\ = \frac{V}{Z} \sum_{\mathbf{r}} \sum_{\mathbf{r}' \rightarrow \text{NN of } \mathbf{r}} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} \quad (1.19) \\ = \frac{2V}{Z} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma},$$

where we used eq. 1.14 and the first equation from 1.16, and the fact that each nearest-neighbour pair \mathbf{r}, \mathbf{r}' appears twice in the summation.

The Kondo terms map onto a nearest-neighbour spin-exchange term:

$$\begin{aligned} \sum_{\mathbf{r}, \mathbf{k}_1, \mathbf{k}_2} T^\dagger(\mathbf{r} - \mathbf{r}_d) e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}_d} J_K(\mathbf{k}_1, \mathbf{k}_2) \vec{S}_{\mathbf{r}_d} \cdot \vec{S}_{\mathbf{k}_1, \mathbf{k}_2} T(\mathbf{r} - \mathbf{r}_d) &= \sum_{\mathbf{r}, \mathbf{k}_1, \mathbf{k}_2} e^{i(\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{r}} J_K(\mathbf{k}_1, \mathbf{k}_2) \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{k}_1, \mathbf{k}_2} \\ &= \frac{J_K}{Z} \sum_{\mathbf{r}} \sum_{\mathbf{r}' \rightarrow \text{NN of } \mathbf{r}} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'} , \\ &= \frac{2J_K}{Z} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'} , \end{aligned} \quad (1.20)$$

where we used the second equation from 1.16. Finally, the bath interaction term W maps onto another Hubbard term

$$\begin{aligned} &\sum_{\mathbf{r}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} T^\dagger(\mathbf{r} - \mathbf{r}_d) e^{i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}_d} W(\{\mathbf{k}_i\}) c_{\mathbf{k}_1, \sigma}^\dagger c_{\mathbf{k}_2, \sigma} c_{\mathbf{k}_3, \sigma'}^\dagger c_{\mathbf{k}_4, \sigma'} T(\mathbf{r} - \mathbf{r}_d) \\ &= \sum_{\mathbf{r}, \mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4} e^{i(\mathbf{k}_1 - \mathbf{k}_2 + \mathbf{k}_3 - \mathbf{k}_4) \cdot \mathbf{r}} W(\{\mathbf{k}_i\}) c_{\mathbf{k}_1, \sigma}^\dagger c_{\mathbf{k}_2, \sigma} c_{\mathbf{k}_3, \sigma'}^\dagger c_{\mathbf{k}_4, \sigma'} \\ &= \frac{W}{2Z} \sum_{\mathbf{r}} \sum_{\mathbf{r}' \rightarrow \text{NN of } \mathbf{r}} n_{\mathbf{r}', \sigma} n_{\mathbf{r}', \sigma'} \\ &= \frac{W}{2} \sum_{\mathbf{r}} n_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma'} , \end{aligned} \quad (1.21)$$

where we used the fact that each point \mathbf{r}' (which we relabel as \mathbf{r}) appears Z times in the summation.

The complete lattice Hamiltonian, after applying the translation operators, is

$$H_{\text{latt}} = \varepsilon_d \sum_{\mathbf{r}, \sigma} n_{\mathbf{r}, \sigma} + U_d \sum_{\mathbf{r}} n_{\mathbf{r}, \uparrow} n_{\mathbf{r}, \downarrow} - \frac{2V}{Z} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} + \frac{2J_K}{Z} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \vec{S}_{\mathbf{r}} \cdot \vec{S}_{\mathbf{r}'} - \frac{W}{2} \sum_{\mathbf{r}} (n_{\mathbf{r}, \uparrow} - n_{\mathbf{r}, \downarrow})^2 . \quad (1.22)$$

This is clearly an extended Hubbard model, with both 1-particle and spin-exchange nearest-neighbour hybridisation. The general form of the model is

$$H_{\text{ex-Hub}} = -t \sum_{\langle i, j \rangle, \sigma} (c_{i, \sigma}^\dagger c_{j, \sigma} + \text{h.c.}) + J \sum_{\langle i, j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + U \sum_i n_{i, \uparrow} n_{i, \downarrow} - \mu \sum_{i, \sigma} n_{i, \sigma} , \quad (1.23)$$

such that the effective couplings resulting from the tiling operation is

$$t = \frac{2V}{Z}, \quad J = \frac{2J_K}{Z}, \quad U = U_d - W, \quad \mu = -\varepsilon_d + \frac{W}{2} . \quad (1.24)$$

1.3.3 Form Of The Eigenstates: Bloch's Theorem

The tiled Hamiltonian defined in eq. 1.17 is manifestly symmetric under discrete translation, given that it's expressed in terms of the translation operators. The fact that the Hamiltonian H_{latt} commutes

with the manybody translation operator implies that the total crystal momentum is a conserved quantity. We will now use this to write down a “tiling” relation between the eigenstates of the auxiliary model and those of the lattice model.

In the tight-binding approach to lattice problems, the full Hamiltonian is obtained by translating the dynamics of the localised orbitals at each site over the entire lattice. The full eigenstate $|\Psi\rangle$ is obtained by constructing linear combinations of the eigenstates $|\psi(i)\rangle$ of the local Hamiltonians. According to Bloch’s theorem, $|\Psi\rangle$ is of the form $|\Psi_{n,K}\rangle = \sum_i e^{i\mathbf{K}\cdot\mathbf{r}_i} |\psi_n(i)\rangle$, where \mathbf{K} is the single-particle crystal momentum, n is the band-index that labels various states within the local orbital, and \mathbf{r}_i sums over the positions of the local Hamiltonians. Bloch’s theorem ensures that eigenstates satisfy the following relation under a translation operation by an arbitrary number of lattice spacings na :

$$T^\dagger(la) |\Psi_{n,K}\rangle = \sum_i e^{i\mathbf{K}\cdot\mathbf{r}_i} |\psi_n(i+l)\rangle = e^{-il\mathbf{K}\cdot\mathbf{a}} |\Psi_{n,K}\rangle . \quad (1.25)$$

As discussed earlier, the eigenstates $|\Psi_{n,K}\rangle$ of the lattice Hamiltonian obtained using eq. 1.17 enjoy the discrete translation symmetry of the lattice, and therefore enjoy a *many-body* Bloch’s theorem [9]. This means that the *local* eigenstates $|\psi_n(\mathbf{r}_d)\rangle$ (with the impurity located at an arbitrary position \mathbf{r}_d) of the unit cell auxiliary model Hamiltonian $H_{\text{clust}}(\mathbf{r}_d)$ defined in eq. 1.15 can be used to construct eigenstates of the lattice Hamiltonian. The index $n(= 0, 1, \dots)$ in the subscript indicates that it is the n^{th} eigenstate of the auxiliary model. The following combination of the auxiliary model eigenstates satisfies a many-particle equivalent of Bloch’s theorem [9]:

$$|\Psi_s\rangle \equiv |\Psi_{K,n}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_d} e^{i\mathbf{K}\cdot\mathbf{r}_d} |\psi_n(\mathbf{r}_d)\rangle , \quad (1.26)$$

where N is the total number of lattice sites and \mathbf{r}_d is summed over all lattice spacings. The set of $n = 0$ states form the lowest band in the spectrum of the lattice, while higher values of n produce the more energetic bands.

1.4 Mapping Greens Functions from Auxiliary Model to Lattice Model

1.4.1 One-particle k -space Greens functions

In the previous part, we proposed a form for the eigenstates $|\Psi_s\rangle$ of the bulk Hamiltonian in terms of the ground-states $|\psi_n\rangle$ of the auxiliary models. In this section, we will relate one-particle Greens functions of the lattice model to those of the auxiliary model. We define the retarded time-domain lattice k -space Greens function at zero temperature as

$$G(\mathbf{k}\sigma; t) = -i\theta(t) \langle \Psi_{\text{gs}} | \{c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}^\dagger\} | \Psi_{\text{gs}} \rangle . \quad (1.27)$$

where $|\Psi_{\text{gs}}\rangle$ is the lattice groundstate. Time evolution of the operators is governed by the lattice Hamiltonian H_{latt} :

$$c_{\mathbf{k}\sigma}(t) = e^{itH_{\text{latt}}} c_{\mathbf{k}\sigma} e^{-itH_{\text{latt}}} . \quad (1.28)$$

By using eq. 1.14 and the fact that the translation operators commute with H_{latt} , we have the relation

$$T(\vec{a}) c(\mathbf{k})(t) T^\dagger(\vec{a}) = e^{-i\mathbf{k} \cdot \vec{a}} c(\mathbf{k})(t), \quad (1.29)$$

which combined with eq. 1.14 gives

$$T(\mathbf{a}) c(\mathbf{k})(t) c^\dagger(\mathbf{k}) T^\dagger(\mathbf{b}) = e^{i\mathbf{k} \cdot (\mathbf{b} - \mathbf{a})} c(\mathbf{k})(t) T^\dagger(\mathbf{b} - \mathbf{a}) c^\dagger(\mathbf{k}). \quad (1.30)$$

In order to make use of the mapping between auxiliary model and lattice model Hamiltonians, we would like to express this lattice Greens function in terms of auxiliary model Greens functions – objects that can be computed purely from within a single auxiliary model. This will be a major simplification in our computations, because it is easier to work with a quantum impurity model, as compared to an interacting lattice model.

To make progress towards this, we express the lattice groundstate in terms of the auxiliary model groundstates (using eq. 1.26):

$$G(\mathbf{k}\sigma; t) = -i\theta(t) \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | \{c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}^\dagger\} | \psi_{\text{gs}}(\mathbf{r}_1) \rangle. \quad (1.31)$$

We take one of the terms in the anticommutator and proceed to simplify it:

$$\begin{aligned} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_1) \rangle &= \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_d) | T(\mathbf{r}_2 - \mathbf{r}_d) c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger T^\dagger(\mathbf{r}_1 - \mathbf{r}_d) | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &= \sum_{\mathbf{r}_1, \mathbf{r}_2} e^{i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}(t) T^\dagger(\mathbf{r}_1 - \mathbf{r}_2) c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &= N \sum_{\mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}(t) T^\dagger(\mathbf{r}) c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \end{aligned} \quad (1.32)$$

where \mathbf{r}_d is a reference lattice site, and we used eq. 1.30 in the second step. The other term in the anticommutator gives

$$\begin{aligned} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}(t) | \psi_{\text{gs}}(\mathbf{r}_1) \rangle &= \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_d) | T(\mathbf{r}_2 - \mathbf{r}_d) c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}(t) T^\dagger(\mathbf{r}_1 - \mathbf{r}_d) | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &= \sum_{\mathbf{r}_1, \mathbf{r}_2} e^{-i\mathbf{k} \cdot (\mathbf{r}_1 - \mathbf{r}_2)} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger T^\dagger(\mathbf{r}_1 - \mathbf{r}_2) c_{\mathbf{k}\sigma}(t) | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &= N \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger T^\dagger(\mathbf{r}) c_{\mathbf{k}\sigma}(t) | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \end{aligned} \quad (1.33)$$

To resolve the time evolution of the operators, we insert $1 = \sum_m |\psi_m(\mathbf{r}_d)\rangle \langle \psi_m(\mathbf{r}_d)|$ into the equation. We again work with just the first term of the anticommutator for convenience:

$$\begin{aligned} &\sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_1) \rangle \\ &= N \sum_{\mathbf{r}, n_1, n_2} e^{i\mathbf{k} \cdot \mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}(t) | \psi_{n_1}(\mathbf{r}_d) \rangle \langle \psi_{n_1}(\mathbf{r}_d) | T^\dagger(\mathbf{r}) | \psi_{n_2}(\mathbf{r}_d) \rangle \langle \psi_{n_2}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &= N \sum_{\mathbf{r}, n_1, n_2} e^{i\mathbf{k} \cdot \mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}(t) | \psi_{n_1}(\mathbf{r}_d) \rangle \langle \psi_{n_1}(\mathbf{r}_d) | \psi_{n_2}(\mathbf{r}_d + \mathbf{r}) \rangle \langle \psi_{n_2}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \end{aligned} \quad (1.34)$$

The overlap $\langle \psi_{n_1}(\mathbf{r}_d) | \psi_{n_2}(\mathbf{r}_d + \mathbf{r}) \rangle$ between the eigenstates of the auxiliary models at \mathbf{r}_d and $\mathbf{r}_d + \mathbf{r}$ are appreciable only for $n_1 = n_2$. This is because, for small \mathbf{r} , the auxiliary models are very similar and the states are therefore almost orthogonal. For large \mathbf{r} , the overlap is again suppressed because the auxiliary model eigenstates are localised around the impurity. We therefore make the simplifying assumption: $\langle \psi_{n_1}(\mathbf{r}_d) | \psi_{n_2}(\mathbf{r}_d + \mathbf{r}) \rangle = \delta_{n_1, n_2} \langle \psi_{n_1}(\mathbf{r}_d) | \psi_{n_1}(\mathbf{r}_d + \mathbf{r}) \rangle = \delta_{n_1, n_2} F_{n_1}(\mathbf{r})$. Substituting this, we get

$$\sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_1) \rangle = N \sum_n F_n(\mathbf{k}) \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{k}\sigma}(t) | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle, \quad (1.35)$$

where we have defined the Fourier transform $F_n(\mathbf{k}) = \sum_{\mathbf{r}} e^{i\mathbf{k} \cdot \mathbf{r}} F_n(\mathbf{r})$ of the overlap function.

We now consider more carefully the transition operator $c_{\mathbf{k}\sigma}$ for the 1-particle excitation giving rise to the above Greens function. Within our auxiliary model approach, gapless excitations within the lattice model are represented by gapless excitations of the impurity site, specifically those that try to screen the impurity site. As a result, the uncoordinated scattering process $c_{\mathbf{k}\sigma}$ for the lattice model must be replaced by a coherent excitation \mathcal{T} within the impurity model that captures those gapless excitations that occur in connection with the impurity, and projects out the uncorrelated excitations that take place even when the impurity site is decoupled from the bath.

In order to construct this auxiliary model \mathcal{T} -matrix, we allow for all excitations of the impurity site in conjunction with those of the k -state:

$$\mathcal{T}_{\mathbf{k},\sigma} = \left[\left(\sum_{\sigma'} c_{\mathbf{r}_d\sigma'}^\dagger + \text{h.c.} \right) + \left(S_{\mathbf{r}_d}^+ + \text{h.c.} \right) + \left(C_{\mathbf{r}_d}^+ + \text{h.c.} \right) \right] c_{\mathbf{k}\sigma}, \quad (1.36)$$

where $S_{\mathbf{r}_d}^+$ and $C_{\mathbf{r}_d}^+$ are spin and charge flip operators on the impurity site that cause transition from $|\downarrow\rangle \rightarrow |\uparrow\rangle$ and $|0\rangle \rightarrow |\uparrow\downarrow\rangle$ respectively.

Apart from modifying the excitation operator, we will now simplify the time-evolution as well. The first overlap on the right-hand side of eq. 1.35 expands to

$$\langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma}(t) | \psi_n(\mathbf{r}_d) \rangle = \langle \psi_{\text{gs}}(\mathbf{r}_d) | e^{i(H_{\text{aux}}(\mathbf{r}_d) + H_{\text{cav}}(\mathbf{r}_d))t} \mathcal{T}_{\mathbf{k},\sigma} e^{-i(H_{\text{aux}}(\mathbf{r}_d) + H_{\text{cav}}(\mathbf{r}_d))t} | \psi_n(\mathbf{r}_d) \rangle, \quad (1.37)$$

where $H_{\text{aux}}(\mathbf{r}_d)$ (eq. 1.6) is the auxiliary model Hamiltonian consisting of the cluster Hamiltonian $H_{\text{clust}}(\mathbf{r}_d)$ along with all one-particle terms H_{1p} in the Hamiltonian (in a typical lattice model, this will be the tight-binding hopping terms), and $H_{\text{cav}}(\mathbf{r}_d)$ is the ‘‘cavity’’ Hamiltonian consisting of all interaction (2-particle and beyond) terms in the Hamiltonian. Together, they create the full lattice Hamiltonian: $H_{\text{latt}} = H_{\text{aux}}(\mathbf{r}_d) + H_{\text{cav}}(\mathbf{r}_d)$. Using the Zassenhaus form of the Baker-Campbell-Hausdorff formula, we have

$$e^{i(H_{\text{aux}}(\mathbf{r}_d) + H_{\text{cav}}(\mathbf{r}_d))t} \approx e^{iH_{\text{aux}}(\mathbf{r}_d)t} e^{iH_{\text{cav}}(\mathbf{r}_d)t} e^{[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2}, \quad (1.38)$$

where we have dropped the higher-order terms because the commutators involve only the boundary degrees of freedom and become subsequently smaller as the order increases. One can think of the operator $e^{iH_{\text{cav}}(\mathbf{r}_d)t} e^{[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2}$ as renormalising the auxiliary model \mathcal{T} -matrix through hybridisation with the rest of the system and formally leading to a new \mathcal{T} -matrix:

$$\mathcal{T}_{\mathbf{k},\sigma}^* = e^{iH_{\text{cav}}(\mathbf{r}_d)t} e^{[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2} \mathcal{T}_{\mathbf{k},\sigma} e^{-[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2} e^{-iH_{\text{cav}}(\mathbf{r}_d)t}. \quad (1.39)$$

One can also absorb the modulating phase factor $F_n(\mathbf{k})$ (defined above and appearing in eq. 1.35) into this renormalisation:

$$\mathcal{T}_{\mathbf{k},\sigma}^* = e^{iH_{\text{cav}}(\mathbf{r}_d)t} e^{[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2} \mathcal{T}_{\mathbf{k},\sigma} F_n(\mathbf{k}) \mathcal{P}_n(\mathbf{r}_d) e^{-[H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)]t^2/2} e^{-iH_{\text{cav}}(\mathbf{r}_d)t}, \quad (1.40)$$

where $\mathcal{P}_n(\mathbf{r}_d)$ projects onto the n^{th} eigenstate $|\psi_n(\mathbf{r}_d)\rangle$.

Since the overlap is calculated in the eigenstates of the auxiliary model at \mathbf{r}_d , we adopt the zeroth order approximation of ignoring this renormalisation. Later, we will specify a prescription of systematically improving our computation. The overlap expression becomes

$$\langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma}(t) | \psi_n(\mathbf{r}_d) \rangle = \langle \psi_{\text{gs}}(\mathbf{r}_d) | e^{i(H_{\text{clust}}(\mathbf{r}_d) + H_{1\text{p}})t} \mathcal{T}_{\mathbf{k},\sigma} e^{-i(H_{\text{clust}}(\mathbf{r}_d) + H_{1\text{p}})t} | \psi_n(\mathbf{r}_d) \rangle. \quad (1.41)$$

To make the problem tractable, we treat the effect of $H_{1\text{p}}$ at the level of an expectation value and note that the effect of the transition operator is to create a hole of momentum \mathbf{k} (eq. 1.36). Let the Hamiltonian $H_{1\text{p}}$ be diagonal in certain modes $c_{\nu,\sigma}$ with energies ϵ_ν , and the operator $c_{\mathbf{k},\sigma}$ can be expressed in terms of these modes: $c_{\mathbf{k},\sigma} = \sum_\nu C_{\nu,\mathbf{k}} c_{\nu,\sigma}^\dagger$. A similar decomposition will hold for the \mathcal{T} -matrix. Substituting it gives

$$\langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma}(t) | \psi_n(\mathbf{r}_d) \rangle = \sum_\nu C_{\nu,\mathbf{k}} \langle \psi_{\text{gs}}(\mathbf{r}_d) | e^{i(H_{\text{clust}}(\mathbf{r}_d) + H_{1\text{p}})t} \mathcal{T}_{\nu,\sigma} e^{-i(H_{\text{clust}}(\mathbf{r}_d) + H_{1\text{p}})t} | \psi_n(\mathbf{r}_d) \rangle. \quad (1.42)$$

Each excitation $\mathcal{T}_{\nu,\sigma}$ therefore leads to an energy cost $-\epsilon_\nu$. Moreover, $|\psi_n(\mathbf{r}_d)\rangle$ and $|\psi_{\text{gs}}(\mathbf{r}_d)\rangle$ are eigenstates of $H_{\text{clust}}(\mathbf{r}_d)$ with energies E_n and E_0 . This leads to the following simplified expression:

$$\langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma}(t) | \psi_n(\mathbf{r}_d) \rangle = \sum_\nu C_{\nu,\mathbf{k}} e^{-i(E_n - E_0 + \epsilon_\nu)t} \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\nu,\sigma} | \psi_n(\mathbf{r}_d) \rangle. \quad (1.43)$$

Treating the other overlap in eq. 1.35 in an identical fashion gives

$$\langle \psi_n(\mathbf{r}_d) | c_{\mathbf{k}\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle = \sum_\nu C_{\nu,\mathbf{k}} \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\nu,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \quad (1.44)$$

Substituting the expression back into 1.35 and then into 1.31, we get an expression for one half of the retarded Greens function:

$$\begin{aligned} & -i\theta(t) \langle \Psi_{\text{gs}} | c_{\mathbf{k}\sigma}(t) c_{\mathbf{k}\sigma}^\dagger | \Psi_{\text{gs}} \rangle \\ &= -i\theta(t) \sum_{\nu,n} C_{\nu,\mathbf{k}} e^{-i(E_n - E_0 + \epsilon_\nu)t} \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma} | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\nu,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \end{aligned} \quad (1.45)$$

Working through the other term with the same strategy, we get the full expression:

$$\begin{aligned} & -i\theta(t) \langle \Psi_{\text{gs}} | \{c_{\mathbf{k}\sigma}(t), c_{\mathbf{k}\sigma}^\dagger\} | \Psi_{\text{gs}} \rangle \\ &= -i\theta(t) \sum_{\nu,n} C_{\nu,\mathbf{k}} e^{-i(E_n - E_0 + \epsilon_\nu)t} \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma} | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\nu,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ & \quad - i\theta(t) \sum_{\nu,n} C_{\nu,\mathbf{k}} e^{i(E_n - E_0 - \epsilon_\nu)t} \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k},\sigma}^\dagger | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\nu,\sigma} | \psi_{\text{gs}}(\mathbf{r}_d) \rangle. \end{aligned} \quad (1.46)$$

Changing from time to frequency domain using $g(\omega) = \int dt e^{i\omega T} f(t)$ gives

$$G(\mathbf{k}, \sigma; \omega) = \sum_{v,n} C_{v,k} \left[\frac{\langle \psi_{gs}(\mathbf{r}_d) | \mathcal{T}_{v,\sigma} | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^\dagger | \psi_{gs}(\mathbf{r}_d) \rangle}{\omega - (E_n - E_0 + \epsilon_v)} + \frac{\langle \psi_{gs}(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^\dagger | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{v,\sigma} | \psi_{gs}(\mathbf{r}_d) \rangle}{\omega + (E_n - E_0 - \epsilon_v)} \right]. \quad (1.47)$$

We recognise that the two parts of the lattice model Greens function are the greater and lesser Greens functions of the operator $\mathcal{T}_{\mathbf{k},\sigma}$, calculated within the auxiliary model at \mathbf{r}_d , but at shifted frequencies $\omega \mp \epsilon_{\mathbf{k}}$:

$$G(\mathbf{k}, \sigma; \omega) = \sum_v C_{v,k} [\mathcal{G}^>(\mathcal{T}_{v,\sigma}; \omega - \epsilon_v) + \mathcal{G}^<(\mathcal{T}_{v,\sigma}; \omega + \epsilon_v)] . \quad (1.48)$$

We now discuss how to systematically improve this estimate. One way is to include the effect of other auxiliary models in the overlap function $F_n(\mathbf{r})$. This will of course require us to calculate an off-diagonal Greens function. As a concrete example, upon including the effects of the auxiliary models nearest to the reference point \mathbf{r}_d , the expression for the Greens function becomes

$$G(\mathbf{k}, \sigma; \omega) = \sum_{v,n} C_{v,k} \left[\frac{\langle \psi_{gs}(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^* | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^\dagger | \psi_{gs}(\mathbf{r}_d) \rangle}{\omega - (E_n - E_0 + \epsilon_v)} + \frac{\langle \psi_{gs}(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^\dagger | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{v,\sigma}^* | \psi_{gs}(\mathbf{r}_d) \rangle}{\omega + (E_n - E_0 - \epsilon_v)} \right], \quad (1.49)$$

with $\tau_{v,\sigma}^* = \mathcal{T}_{v,\sigma}(F_n(0) + \sum_{\mathbf{a}} F_n(\mathbf{a}) e^{i\mathbf{k} \cdot \mathbf{a}})$ where \mathbf{a} sums over the primitive lattice vectors. Another way to include more non-local contributions is by considering the effects of the cavity Hamiltonian in eq. 1.40:

$$\mathcal{T}_{\mathbf{k},\sigma}^*(t) = e^{iH_{\text{cav}}(\mathbf{r}_d)t} (\mathcal{T}_{\mathbf{k},\sigma} + t^2/2 [H_{\text{aux}}(\mathbf{r}_d), H_{\text{cav}}(\mathbf{r}_d)], \mathcal{T}_{\mathbf{k},\sigma}) e^{-iH_{\text{cav}}(\mathbf{r}_d)t} . \quad (1.50)$$

The time-domain Greens function associated with this operator will then need to be calculated, which can then be used to calculate frequency-domain functions.

1.4.2 One-particle real-space Greens functions

We now work with Greens functions for real-space excitations. The retarded Greens function in this case is

$$G(\mathbf{r}\sigma; t) = -i\theta(t) \langle \Psi_{gs} | \{c_{\mathbf{r}_d+\mathbf{r},\sigma}(t), c_{\mathbf{r}_d,\sigma}^\dagger\} | \Psi_{gs} \rangle . \quad (1.51)$$

Since our lattice model has discrete translation symmetry, we instead calculate the equivalent quantity

$$G(\mathbf{r}\sigma; t) = -i\theta(t) \sum_{\mathbf{r}_d} \langle \Psi_{gs} | \{c_{\mathbf{r}_d+\mathbf{r},\sigma}(t), c_{\mathbf{r}_d,\sigma}^\dagger\} | \Psi_{gs} \rangle . \quad (1.52)$$

Similar to the k -space Greens functions, express the groundstates as a superposition of auxiliary model Greens functions. We take the first term in the anticommutator and proceed to simplify it:

$$\begin{aligned} \sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d+\mathbf{r},\sigma}(t) c_{\mathbf{r}_d,\sigma}^\dagger | \Psi_{\text{gs}} \rangle &= \frac{1}{N} \sum_{\mathbf{R}, \Delta, \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{R} + \Delta) | c_{\mathbf{r}_d+\mathbf{r},\sigma}(t) c_{\mathbf{r}_d,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{R}) \rangle \\ &= \frac{1}{N} \sum_{\mathbf{R}, \Delta} \langle \psi_{\text{gs}}(-\mathbf{r}_d) | c_{\mathbf{r}-\mathbf{R}-\Delta,\sigma}(t) T(\Delta) c_{-\mathbf{R},\sigma}^\dagger | \psi_{\text{gs}}(-\mathbf{r}_d) \rangle . \end{aligned} \quad (1.53)$$

Local Greens function: $\mathbf{r} = 0$

We first consider the case of local Greens function, by setting $\mathbf{r} = 0$. We also change the dummy variable \mathbf{r}_d , \mathbf{R} and Δ to $-\mathbf{r}_d$, \mathbf{R} and $-\Delta$ to make the expressions tidier:

$$\sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d,\sigma}(t) c_{\mathbf{r}_d,\sigma}^\dagger | \Psi_{\text{gs}} \rangle = \frac{1}{N} \sum_{\mathbf{R}, \Delta, \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{R}+\Delta,\sigma}(t) T^\dagger(\Delta) c_{\mathbf{R},\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle . \quad (1.54)$$

We split the full summation into four parts, based on whether $\mathbf{R} = \mathbf{r}_d$ and whether $\Delta + \mathbf{R} = \mathbf{r}_d$:

$$\begin{aligned} \sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d,\sigma}(t) c_{\mathbf{r}_d,\sigma}^\dagger | \Psi_{\text{gs}} \rangle &= \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d,\sigma}(t) c_{\mathbf{r}_d,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &+ \sum_{\Delta \neq 0} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d+\Delta,\sigma}(t) T^\dagger(\Delta) c_{\mathbf{r}_d,\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &+ \sum_{\mathbf{R} \neq \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d,\sigma}(t) T^\dagger(\mathbf{r}_d - \mathbf{R}) c_{\mathbf{R},\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\ &+ \sum_{\mathbf{R} \neq \mathbf{r}_d, \Delta \neq \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\Delta,\sigma}(t) T^\dagger(\Delta - \mathbf{R}) c_{\mathbf{R},\sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle , \end{aligned} \quad (1.55)$$

where we have used the fact that the location of the auxiliary model does not affect the correlation calculated within the auxiliary model in order to cancel out the summation over \mathbf{r}_d with the factor of $1/N$. The reason for splitting the expression into these parts is to explicitly write out which operators act on the impurity site \mathbf{r}_d and which act on other real-space sites away from the impurity site. We will now replace the real-space excitation operators away from the impurity site with the associated T -matrices, following the discussion above eq. 1.36:

$$\mathcal{T}_{\mathbf{r},\sigma} = \left[\left(\sum_{\sigma'} c_{\mathbf{r}_d\sigma'}^\dagger + \text{h.c.} \right) + \left(S_{\mathbf{r}_d}^+ + \text{h.c.} \right) + \left(C_{\mathbf{r}_d}^+ + \text{h.c.} \right) \right] c_{\mathbf{r}\sigma} = \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} \mathcal{T}_{\mathbf{k},\sigma} . \quad (1.56)$$

We also insert a complete basis of states of the auxiliary model at \mathbf{r}_d , $1 = \sum_n |\psi_n(\mathbf{r}_d)\rangle \langle \psi_n(\mathbf{r}_d)|$, generating an overlap factor F_n as before:

$$\begin{aligned}
& \sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle \\
&= \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\mathbf{k}, n} F'_n(\mathbf{k}) \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k}, \sigma}(t) | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | c_{\mathbf{r}_d, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\mathbf{k}, n} F'_n(\mathbf{k})^* \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d, \sigma}(t) | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k}, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\mathbf{k}_1, \mathbf{k}_2} F'_n(\mathbf{k}_1) F'_n(\mathbf{k}_2)^* \langle \psi_{\text{gs}}(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k}_1, \sigma}(t) | \psi_n(\mathbf{r}_d) \rangle \langle \psi_n(\mathbf{r}_d) | \mathcal{T}_{\mathbf{k}_2, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle ,
\end{aligned} \tag{1.57}$$

where $F'_n(\mathbf{k})$ is the truncated Fourier transform $\sum_{\mathbf{r} \neq 0} e^{i\mathbf{k} \cdot \mathbf{r}} F_n(\mathbf{r})$ of the overlap factor.

We next treat the time-evolution of the operators exactly as in the k -space Greens function. Without repeating the details, we state the final result here, for the frequency-domain real-space local Greens function:

$$\begin{aligned}
G_{\text{loc}}(\omega) &= \mathcal{G}(d\sigma; \omega) + \sum_{\mathbf{k}, \nu} C_{\nu, \mathbf{k}} \left[\mathcal{G}^>(\mathcal{T}_{\nu, \sigma}, d\sigma; \omega - \epsilon_\nu) + \mathcal{G}^<(\mathcal{T}_{\nu, \sigma}, d\sigma; \omega + \epsilon_\nu) \right] \\
&+ \sum_{\mathbf{k}} \mathcal{G}(d\sigma, \mathcal{T}_{\mathbf{k}, \sigma}; \omega) + \sum_{\mathbf{k}, \nu, \mathbf{q}} C_{\nu, \mathbf{k}} \left[\mathcal{G}^>(\mathcal{T}_{\nu, \sigma}, \mathcal{T}_{\mathbf{q}, \sigma}; \omega - \epsilon_\nu) + \mathcal{G}^<(\mathcal{T}_{\nu, \sigma}, \mathcal{T}_{\mathbf{q}, \sigma}; \omega + \epsilon_\nu) \right] ,
\end{aligned} \tag{1.58}$$

where $\mathcal{G}(d\sigma; \omega)$ is the retarded Greens function of the impurity site, $\mathcal{G}^>(\mathcal{T}_{\nu, \sigma}, d\sigma; \omega)$ is the off-diagonal retarded Greens function between the impurity site and the bath state $\nu\sigma$. $\mathcal{G}^>(\mathcal{T}_{\nu, \sigma}, \mathcal{T}_{\mathbf{q}, \sigma}; \omega)$ is the same but between multiple states in the bath.

Non-local Greens function: $\mathbf{r} \neq 0$

We next consider the case of non-local Greens function, where the excitations propagate a non-zero distance \mathbf{r} :

$$\sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d + \mathbf{r}, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle = \frac{1}{N} \sum_{\mathbf{R}, \Delta, \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{R} + \Delta + \mathbf{r}, \sigma}(t) T^\dagger(\Delta) c_{\mathbf{R}, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle . \tag{1.59}$$

To bring this expression closer to the one for the local Greens function, we redefine $\Delta + \mathbf{r} \rightarrow \Delta$:

$$\sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d + \mathbf{r}, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle = \frac{1}{N} \sum_{\mathbf{R}, \Delta, \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{R} + \Delta, \sigma}(t) T^\dagger(\Delta) T(\mathbf{r}) c_{\mathbf{R}, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle . \tag{1.60}$$

This allows to again split the full summation based on whether $\mathbf{R} = \mathbf{r}_d$ and whether $\Delta + \mathbf{R} = \mathbf{r}_d$:

$$\begin{aligned}
\sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d + \mathbf{r}, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle &= \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d, \sigma}(t) T(\mathbf{r}) c_{\mathbf{r}_d, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\Delta \neq 0} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d + \Delta, \sigma}(t) T^\dagger(\Delta - \mathbf{r}) c_{\mathbf{r}_d, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\mathbf{R} \neq \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\mathbf{r}_d, \sigma}(t) T^\dagger(\mathbf{r}_d - \mathbf{R} - \mathbf{r}) c_{\mathbf{R}, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle \\
&+ \sum_{\mathbf{R} \neq \mathbf{r}_d, \Delta \neq \mathbf{r}_d} \langle \psi_{\text{gs}}(\mathbf{r}_d) | c_{\Delta, \sigma}(t) T^\dagger(\Delta - \mathbf{R} - \mathbf{r}) c_{\mathbf{R}, \sigma}^\dagger | \psi_{\text{gs}}(\mathbf{r}_d) \rangle .
\end{aligned} \tag{1.61}$$

Introducing Fourier transforms of the operators and inserting eigenstates of the auxiliary models leads to

$$\sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d + \mathbf{r}, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle = F_n^*(\mathbf{r}) \sum_{\mathbf{r}_d} \langle \Psi_{\text{gs}} | c_{\mathbf{r}_d, \sigma}(t) c_{\mathbf{r}_d, \sigma}^\dagger | \Psi_{\text{gs}} \rangle . \tag{1.62}$$

The net difference from the diagonal Greens function is the presence of the overlap factor $F_n^*(\mathbf{r})$.

1.4.3 Equal-Time Ground State Correlators: Real-space

We first consider a real-space operator $O(\mathbf{r} + \Delta)O^\dagger(\mathbf{r})$ that quantifies the presence of correlations over a distance Δ . The correlation function itself is given by the expectation value of this operator in the ground state:

$$C_O(\Delta) = \langle \Psi_{\text{gs}} | O(\mathbf{r} + \Delta) O^\dagger(\mathbf{r}) | \Psi_{\text{gs}} \rangle . \tag{1.63}$$

To obtain a tractable expression for this, we first replace the full ground state with its expression in terms of the auxiliary model ground states (eq. ??):

$$C_O(\Delta) = \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}'} \langle \psi_{\text{gs}}(\mathbf{r}_1 + \mathbf{r}' + \mathbf{r}_c + \mathbf{r}) | O(\mathbf{r} + \Delta) O^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_1 + \mathbf{r}_c + \mathbf{r}) \rangle e^{-i\mathbf{k}_0 \cdot (\mathbf{r}_1 - \mathbf{r}_2)} , \tag{1.64}$$

where \mathbf{r}_1 and $\mathbf{r}_1 + \mathbf{r}'$ are the positions of the incoming and outgoing auxiliary model states, relative to $\mathbf{r}_c + \mathbf{r}$, and \mathbf{k}_0 is the crystal momentum of the ground state (which we will immediately set to zero). In order to convert the incoming and outgoing states into the same auxiliary mode at a reference location \mathbf{r}_c (which would then allow computations purely within a single auxiliary model), we use the relation: $|\psi_{\text{gs}}(\mathbf{x})\rangle = T^\dagger(\mathbf{x} - \mathbf{r}_c) \psi_{\text{gs}} | \psi(\mathbf{r}_c) \rangle$. Substituting this appropriately for both the auxiliary model states gives:

$$\begin{aligned}
C_O(\Delta) &= \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}'} \langle \psi_{\text{gs}}(\mathbf{r}_c) | T(\mathbf{r}_1 + \mathbf{r}' + \mathbf{r}) O(\mathbf{r} + \Delta) O^\dagger(\mathbf{r}) T^\dagger(\mathbf{r}_1 + \mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \\
&= \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}'} \langle \psi_{\text{gs}}(\mathbf{r}_c) | T(\mathbf{r}') O(\Delta - \mathbf{r}_1) O^\dagger(-\mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \\
&= \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}'} \langle \psi_{\text{gs}}(\mathbf{r}_c + \mathbf{r}') | O(\Delta - \mathbf{r}_1) O^\dagger(-\mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle .
\end{aligned} \tag{1.65}$$

As a final cosmetic change, we transform $\mathbf{r}_1 \rightarrow -\mathbf{r}$:

$$C_O(\Delta) = \frac{1}{N} \sum_{\mathbf{r}, \mathbf{r}'} \langle \psi_{\text{gs}}(\mathbf{r}_c + \mathbf{r}') | O(\Delta + \mathbf{r}) O^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.66)$$

Like in the Greens function calculation, we now consider the various kinds of contributions separately.

Intra-auxiliary model contributions: $\mathbf{r}' = 0$

These terms describe excitations that start and propagate within the same auxiliary model, upto a distance Δ :

$$C_O(\Delta) \rightarrow \frac{1}{N} \sum_{\mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_c) | O(\Delta + \mathbf{r}) O^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.67)$$

With an eye towards introducing the impurity operators into the correlations, we insert a complete basis defined by the eigenstates $\{|\psi_n(\mathbf{r}_c)\rangle\}$ of the auxiliary model into the expression:

$$C_O(\Delta) \rightarrow \frac{1}{N} \sum_{\mathbf{r}} \sum_n \langle \psi_{\text{gs}}(\mathbf{r}_c) | O(\Delta + \mathbf{r}) | \psi_n(\mathbf{r}_c) \rangle \langle \psi_n(\mathbf{r}_c) | O^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.68)$$

For the excitations that exist purely in the conduction bath ($\mathbf{r} \neq \mathbf{r}_c$), the excitation operators must be suitably modified (see the arguments around eq. 1.36) in order to incorporate Kondo screening. The modified excitation operators are generally defined as

$$\tilde{O}(\mathbf{r}) = O(\mathbf{r}) O^\dagger(d) \mathcal{P}_{\text{gs}} , \quad (1.69)$$

where $O^\dagger(d)$ is the hermitian conjugate of the correlation operator O , but applied on the impurity sites. This therefore constitutes a time-reversed scattering process on the impurity site relative to the process in the bath. The operator \mathcal{P}_{gs} projects onto the ground state of the auxiliary model, since we are interested in ground state correlations. The operator multiplying the old correlation operator represents all possible excitations of the impurity site, and ensure that the bath and impurity excitation processes take place coherently. The projector ensures that only tripartite correlations between the impurity site and the two momentum states are captured by the correlation, which is what's desired within the tiling method.

With this modified operator, this class of correlation functions can be written as

$$C_O(\Delta) \rightarrow \frac{1}{N} \sum_{\mathbf{r}} \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}(\Delta + \mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.70)$$

This can be interpreted as the fact that within our auxiliary model formalism, the correlation between the sites \mathbf{r} and $\Delta + \mathbf{r}$ can only occur through a transition process that connect one of the sites with the impurity site and then a return process that connects the impurity site with the other site.

Inter-auxiliary model contributions: $\mathbf{r}' \neq 0$

These are the most non-local contributions, and involve excitations that connect different auxiliary models:

$$C_O(\Delta) \rightarrow \frac{1}{N} \sum_{\mathbf{r}' \neq 0} \langle \psi_{\text{gs}}(\mathbf{r}_c + \mathbf{r}') | \tilde{O}(\Delta + \mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}^\dagger(\mathbf{r}) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.71)$$

1.4.4 Equal-Time Ground State Correlators: Momentum-space

We now consider momentum space correlations, through a general operator $O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1)$:

$$C_O(\mathbf{k}_1, \mathbf{k}_2) = \langle \Psi_{\text{gs}} | O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1) | \Psi_{\text{gs}} \rangle . \quad (1.72)$$

Note that O itself is a two-particle operator. To obtain a tractable expression for this, we first replace the full ground state with its expression in terms of the auxiliary model ground states (eq. ??):

$$C_O(\mathbf{k}_1, \mathbf{k}_2) = \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2) | O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_1) \rangle , \quad (1.73)$$

where \mathbf{r}_1 and \mathbf{r}_2 are the positions of the incoming and outgoing auxiliary model states. In order to convert the incoming and outgoing states into the same auxiliary mode at a reference location \mathbf{r}_c (which would then allow computations purely within a single auxiliary model), we use the relation: $|\psi_{\text{gs}}(\mathbf{x})\rangle = T^\dagger(\mathbf{x} - \mathbf{r}_c) \psi_{\text{gs}} | \psi(\mathbf{r}_c) \rangle$. Substituting this appropriately for both the auxiliary model states gives:

$$C_O(\mathbf{k}_1, \mathbf{k}_2) = \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_c) | T(\mathbf{r}_2 - \mathbf{r}_c) O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1) T^\dagger(\mathbf{r}_1 - \mathbf{r}_c) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.74)$$

In order to simplify the translation operators, we can use eq. 1.14. For that, we would need to know whether the operator O involves a net transfer of momentum. If $O(\mathbf{k})$ commutes with the total number operator $n_{\mathbf{k}} = \sum_{\sigma} n_{\mathbf{k},\sigma}$, there is no momentum transfer. Examples of such operators are spin operators, $S_{\alpha\beta}(\mathbf{k}) \equiv c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\beta}$, and density operators $n_{\mathbf{k}\alpha}$. If $O(\mathbf{k})$ does not commute with $n_{\mathbf{k}}$, there is a net transfer of momentum, and one such operator would be the charge isospin operator $C^+(\mathbf{k}) = c_{\mathbf{k}\uparrow}^\dagger c_{\mathbf{k}\downarrow}^\dagger$. For the first kind of operators, we have $T(\mathbf{a})O(\mathbf{k})T^\dagger(\mathbf{a}) = O(\mathbf{k})$, while for the latter, we get $T(\mathbf{a})O(\mathbf{k})T^\dagger(\mathbf{a}) = e^{-\mathbf{a} \cdot 2\mathbf{k}} O(\mathbf{k})$, where $2\mathbf{k}$ represents the momentum being transferred by the operator. We consider the two cases separately.

Momentum-conserving operators: $[O(\mathbf{k}), n_{\mathbf{k}}] = 0$

For these operators, the expression for the correlation gives

$$\begin{aligned} C_O(\mathbf{k}_1, \mathbf{k}_2) &= \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_c) | T(\mathbf{r}_2 - \mathbf{r}_1) O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \\ &= \sum_{\mathbf{\Lambda}} \langle \psi_{\text{gs}}(\mathbf{r}_c + \mathbf{\Lambda}) | O(\mathbf{k}_2)O^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \end{aligned} \quad (1.75)$$

To obtain the last form, we defined $\mathbf{\Lambda} = \mathbf{r}_2 - \mathbf{r}_1$ as the distance between the incoming and outgoing auxiliary model states, and preformed the sum over the free variable \mathbf{r}_1 to cancel out the factor of $1/N$. Just like before, this expression can be decomposed into a term that involves a single auxiliary model and other terms that involve two distinct auxiliary models. By making the identification of the right transition operator $\tilde{O}(\mathbf{k}) = O(\mathbf{k})O^\dagger(\mathbf{k})\mathcal{P}_{\text{gs}}$, we get

$$C_O(\mathbf{k}_1, \mathbf{k}_2) = \sum_{\mathbf{\Lambda}} \langle \psi_{\text{gs}}(\mathbf{r}_c + \mathbf{\Lambda}) | \tilde{O}(\mathbf{k}_2) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (1.76)$$

Non-momentum-conserving operators: $[O(\mathbf{k}), n_{\mathbf{k}}] \neq 0$

This class of operators incur an additional phase factor of $e^{-\mathbf{a} \cdot 2\mathbf{k}}$ when the translation operators are translated across them:

$$\begin{aligned} C_O(\mathbf{k}_1, \mathbf{k}_2) &= \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_c) | T(\mathbf{r}_2 - \mathbf{r}_1) O(\mathbf{k}_2) O^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle e^{2i(\mathbf{r}_1 - \mathbf{r}_c) \cdot (\mathbf{k}_1 - \mathbf{k}_2)} \\ &= \delta_{\mathbf{k}_1, \mathbf{k}_2} \sum_{\Delta} \langle \psi_{\text{gs}}(\mathbf{r}_c + \Delta) | O(\mathbf{k}_2) O^\dagger(\mathbf{k}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \end{aligned} \quad (1.77)$$

For this expression, we again defined Δ similar to before, and carried out the sum of \mathbf{r}_1 involving the exponential to obtain a factor of $N\delta_{\mathbf{k}_1, \mathbf{k}_2}$. The Kronecker delta factor is a manifestation of translational invariance and the associated total momentum conservation.

As it stands, operators like $O(\mathbf{k}_1)$ act purely on the conduction bath degrees of freedom. In order to incorporate impurity-bath correlation effects, we modify these operators using the appropriate T -matrices, by employing eq. 2.61. The final computations are carried out using these modified operators.

1.4.5 Entanglement Measures

We will now describe the prescription of calculating entanglement measures of the lattice model from within our auxiliary model treatment. In this section, we are interested mainly in two such measures, the entanglement entropy and the mutual information. Given a pure state $|\Psi\rangle$ describing the complete system, the entanglement entropy $S_{\text{EE}}(\nu)$ of a subsystem ν quantifies the entanglement of ν with the rest of the subsystem, and is defined as

$$S_{\text{EE}}(\nu) = -\text{Tr} [\rho(\nu) \log \rho(\nu)] , \quad \rho(\nu) = \text{Tr}_\nu [|\Psi\rangle \langle \Psi|] \quad (1.78)$$

where $\text{Tr} [\cdot]$ is the trace operator, and $\rho(\nu)$ is the reduced density matrix (RDM) for the subsystem ν obtained by taking the partial trace Tr_ν (over the states of ν) of the full density matrix $\rho = |\Psi\rangle \langle \Psi|$. If the subsystem ν describes local regions in real space (or states in k -space), we might be interested in the entanglement between two such subsystems ν_1 and ν_2 . The correct measure to quantify such entanglement is the mutual information:

$$I_2(\nu_1, \nu_2) = S_{\text{EE}}(\nu_1) + S_{\text{EE}}(\nu_2) - S_{\text{EE}}(\nu_1 \cup \nu_2) , \quad (1.79)$$

where $\nu_1 \cup \nu_2$ is a larger subsystem formed by combining ν_1 and ν_2 .

Real-space entanglement

Real-space entanglement measures can be used to probe delocalisation-localisation transitions. The simplest such measure is the entanglement of a local mode. Since the local entanglement entropy will be uniform at each lattice site for a system with translation invariance, it suffices to calculate the real-space averaged entanglement entropy $S_{\text{EE}}^{\text{loc}} = \frac{1}{N} \sum_{\mathbf{r}} S_{\text{EE}}(\mathbf{r})$. By visualising the lattice model as a superposition of auxiliary models placed at various sites (eq. ??), the real space average of the lattice model can be thought of as an average over sites of a particular impurity model, and then a

second average over all the impurity models. But since all impurity models are equivalent to each other, the second average is redundant. Secondly, all correlations must derive from the impurity site, which can be formally encoded by subtracting, from this average, the corresponding contribution obtained in the absence of the impurity site. In total, the lattice-auxiliary model relation for the local entanglement entropy can be written as

$$S_{\text{EE}}^{\text{loc}} = \frac{1}{N} \sum_{\mathbf{r}} \left[S_{\text{EE}}(\mathbf{r}_d + \mathbf{r}) - S_{\text{EE}}^{(0)}(\mathbf{r}_d + \mathbf{r}) \right], \quad (1.80)$$

where \mathbf{r}_d is the impurity site position, \mathbf{r} is the distance of a conduction bath site from the impurity site (can be zero), and $S_{\text{EE}}(\mathbf{r}_d + \mathbf{r})$ is the entanglement entropy, calculated within the impurity model, at the location $\mathbf{r}_d + \mathbf{r}$. $S_{\text{EE}}^{(0)}(\mathbf{r}_d + \mathbf{r})$ is the same entanglement entropy, but calculated for an impurity model with vanishing impurity-bath hybridisation and bath interaction.

Momentum-space entanglement

Entanglement measures in k -space can provide valuable information regarding the Fermi surface structure and the nature of gapless excitations proximate to it. The most elementary measure is the entanglement entropy $S_{\text{EE}}(\mathbf{q})$ of a single excitation carrying momentum \mathbf{q} . Unlike $S_{\text{EE}}^{\text{loc}}$, this does not involve an average, and involves a single computation:

$$\tilde{S}_{\text{EE}}(\mathbf{q}) = S_{\text{EE}}(\mathbf{q}) - S_{\text{EE}}^{(0)}(\mathbf{q}). \quad (1.81)$$

It is possible to improve this by considering inter-auxiliary model contributions in the reduced density matrix $\rho(\mathbf{q})$. On the lattice model, $\rho(\mathbf{q})$ is defined as

$$\rho(\mathbf{q}) = \text{Tr}_{\mathbf{q}} \left[|\Psi_{\text{gs}}\rangle \langle \Psi_{\text{gs}}| \right], \quad (1.82)$$

where $\text{Tr}_{\mathbf{q}} [\cdot]$ is the partial trace over the Hilbert space of \mathbf{q} , and $|\Psi_{\text{gs}}\rangle$ is the tiled ground state. Using eq. ??, we can write the ground state in terms of those of the auxiliary model. These leads to two classes of terms, one purely within a single auxiliary model ground state $|\psi_{\text{gs}}\rangle$, and the other involving transitions across auxiliary models:

$$\rho(\mathbf{q}) \sim \text{Tr}_{\mathbf{q}} \left[|\psi_{\text{gs}}(\mathbf{r}_d)\rangle \langle \psi_{\text{gs}}(\mathbf{r}_d)| \right] + \frac{1}{N} \text{Tr}_{\mathbf{q}} \sum_{\mathbf{r}} \left[|\psi_{\text{gs}}(\mathbf{r}_d)\rangle \langle \psi_{\text{gs}}(\mathbf{r}_d + \mathbf{r})| \right], \quad (1.83)$$

where $|\psi_{\text{gs}}(\mathbf{r}_d)\rangle$ is a reference auxiliary model ground state, and $|\psi_{\text{gs}}(\mathbf{r}_d + \mathbf{r})\rangle$ sums over other auxiliary models at increasing distances from this reference model. The \sim indicates that the RDM needs to be normalised. The first term leads to the expression in eq. 1.82, while the second term can be used to improve this estimate. Away from any quantum critical points, the localised nature of the impurity-bath hybridisation ensures that impurity correlations decay exponentially away from the transition. This ensures that the second term is very small away from a critical point. We therefore restrict ourselves to just the first term in the present work.

1.5 Properties of the Bloch states

1.5.1 Translation invariance

It is easy to verify that $\Psi_{\vec{k}}(\{\mathbf{r}_k\})$ transforms like Bloch functions under translation by a displacement \mathbf{r} :

$$\Psi_{\vec{k}}(\{\mathbf{r}_k + \mathbf{r}\}) = \frac{1}{\lambda_{|\vec{k}\rangle} \mathcal{Z} N} \sum_{\mathbf{r}_i, \mathbf{a}} e^{i\vec{k} \cdot \vec{R}_i} \psi_{\text{aux}}(\mathbf{r}_i - \mathbf{r}, \mathbf{a}) = \frac{1}{\lambda_{|\vec{k}\rangle} \mathcal{Z} N} \sum_{\mathbf{r}_j, \mathbf{a}} e^{i\vec{k} \cdot (\vec{R}_j + \mathbf{r})} \psi_{\text{aux}}(\mathbf{r}_j, \mathbf{a}) = e^{i\vec{k} \cdot \vec{R}} \Psi_{\vec{k}}(\{\mathbf{r}_k\}) \quad (1.84)$$

In the last equation, we transformed $\mathbf{r}_i \rightarrow \mathbf{r}_j = \mathbf{r}_i - \mathbf{r}$. Note that the argument \mathbf{a} does not change under a translation of the system, because that vector always represents the difference between the impurity lattice position and its nearest neighbours, irrespective of the absolute position of the impurity.

The wavefunction can be even brought into the familiar Bloch function form:

$$\begin{aligned} \Psi_{\vec{k}}^n(\{\mathbf{r}_k\}) &= \sum_{\mathbf{r}_i, \mathbf{a}} \frac{e^{i\vec{k} \cdot \vec{R}_i}}{\lambda_{|\vec{k}\rangle} \mathcal{Z} N} \psi_{\text{aux}}(\{\mathbf{r}_d - \mathbf{r}_i, \mathbf{r}_0 - \mathbf{r}_i - \mathbf{a}\}) = \frac{e^{i\vec{k} \cdot \frac{1}{N} \sum_k \vec{r}_k}}{\lambda_{|\vec{k}\rangle} \mathcal{Z} N} \sum_{\mathbf{r}_i, \mathbf{a}} e^{-i\vec{k} \cdot (\frac{1}{N} \sum_k \mathbf{r}_k - \vec{R}_i)} \psi_{\text{aux}}(\{\mathbf{r}_d - \mathbf{r}_i, \mathbf{r}_0 - \mathbf{r}_i - \mathbf{a}\}) \\ &= e^{i\vec{k} \cdot \vec{r}_{\text{COM}}} \eta_{\vec{k}}(\{\mathbf{r}_k\}) \end{aligned} \quad (1.85)$$

where $\mathbf{r}_{\text{COM}} = \frac{1}{N} \sum_k \mathbf{r}_k$ is the center-of-mass coordinate and $\eta_{\vec{k}}(\{\mathbf{r}_k\}) = \frac{1}{\lambda_{|\vec{k}\rangle} \mathcal{Z} N} \sum_{\mathbf{r}_i} e^{-i\vec{k} \cdot (\frac{1}{N} \sum_k \mathbf{r}_k - \vec{R}_i)} \psi_{\text{aux}}^n(\{\mathbf{r}_k - \mathbf{r}_i\})$ is the translation symmetric function. This form of the eigenstate allows the interpretation that tuning the Bloch momentum \vec{k} corresponds to a translation of the center of mass of the system (or in this case, of the auxiliary models that comprise the system).

1.5.2 Orthonormality

It is straightforward to show that these states form an orthonormal basis. We start by writing down the inner product of two distinct such states:

$$\begin{aligned} \langle \Psi_{\vec{k}'} | \Psi_{\vec{k}} \rangle &= \frac{1}{\lambda_{|\vec{k}'\rangle}^* \lambda_{|\vec{k}\rangle} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{a}, \mathbf{a}'} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_j, \mathbf{a}') | \psi_{\text{aux}}(\mathbf{r}_i, \mathbf{a}) \rangle \\ &= \frac{1}{\lambda_{|\vec{k}'\rangle}^* \lambda_{|\vec{k}\rangle} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{a}, \mathbf{a}'} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') T^\dagger(\mathbf{r}_0 - \mathbf{r}_j) T(\mathbf{r}_0 - \mathbf{r}_i) | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \end{aligned} \quad (1.86)$$

At this point, we insert a complete basis of momentum eigenkets $1 = \sum_{\vec{q}} |\vec{q}\rangle \langle \vec{q}|$ to resolve the translation operators:

$$\begin{aligned}
 \langle \Psi_{\vec{k}'} | \Psi_{\vec{k}} \rangle &= \frac{1}{\lambda_{|\vec{k}'}^* \lambda_{|\vec{k}} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{a}, \mathbf{a}', \vec{q}} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') T(\mathbf{r}_j - \mathbf{r}_i) |\vec{q}\rangle \langle \vec{q}| \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
 &= \frac{1}{\lambda_{|\vec{k}'}^* \lambda_{|\vec{k}} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{a}, \mathbf{a}', \vec{q}} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') e^{i\vec{q} \cdot (\mathbf{r}_j - \mathbf{r}_i)} |\vec{q}\rangle \langle \vec{q}| \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
 &= \frac{1}{|\lambda_{|\vec{k}}|^2 \mathcal{Z}^2} \delta_{\vec{k}, \vec{k}'} \sum_{\mathbf{a}, \mathbf{a}'} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') |\vec{k}\rangle \langle \vec{k}| \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle
 \end{aligned} \tag{1.87}$$

At the last step, we used the summation form of the Kronecker delta function: $\sum_{\mathbf{r}_i} e^{i\mathbf{r}_i \cdot (\vec{k} - \vec{q})} \sum_{\mathbf{r}_j} e^{i\mathbf{r}_j \cdot (\vec{q} - \vec{k}')} = N \delta_{\vec{k}, \vec{q}} N \delta_{\vec{k}', \vec{q}}$. The final remaining step is to identify that the inner products inside the summation are actually independent of the direction \mathbf{a}, \mathbf{a}' of the connecting vector, and both are equal to the normalisation factor $\lambda_{|\vec{k}}|$:

$$\langle \Psi_{\vec{k}'} | \Psi_{\vec{k}} \rangle = \frac{1}{|\lambda_{|\vec{k}}|^2 \mathcal{Z}^2} \delta_{\vec{k}, \vec{k}'} \sum_{\mathbf{a}, \mathbf{a}'} |\lambda_{|\vec{k}}|^2 = \frac{1}{|\lambda_{|\vec{k}}|^2 \mathcal{Z}^2} \delta_{\vec{k}, \vec{k}'} \omega^2 |\lambda_{|\vec{k}}|^2 = \delta_{\vec{k}, \vec{k}'} \tag{1.88}$$

This concludes the proof of orthonormality.

1.5.3 Eigenstates

To demonstrate that these are indeed eigenstates of the bulk Hamiltonian, we will calculate the matrix elements of the full Hamiltonian between these states:

$$\begin{aligned}
 \langle \Psi_{\vec{k}'} | H_{\text{H-H}} | \Psi_{\vec{k}} \rangle &= \frac{1}{\lambda_{|\vec{k}'}^* \lambda_{|\vec{k}} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k, \mathbf{a}, \mathbf{a}'} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_j, \mathbf{a}') | H_{\text{aux}}(\mathbf{r}_k) | \psi_{\text{aux}}(\mathbf{r}_i, \mathbf{a}) \rangle \\
 &= \frac{1}{\lambda_{|\vec{k}'}^* \lambda_{|\vec{k}} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k, \mathbf{a}, \mathbf{a}'} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | T_{\mathbf{r}_0 - \mathbf{r}_j}^\dagger T_{\mathbf{r}_0 - \mathbf{r}_k} H_{\text{aux}}(\mathbf{r}_0) T_{\mathbf{r}_0 - \mathbf{r}_k}^\dagger T_{\mathbf{r}_0 - \mathbf{r}_i} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
 &= \frac{1}{\lambda_{|\vec{k}'}^* \lambda_{|\vec{k}} \mathcal{Z}^2 N^2} \sum_{\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k, \mathbf{a}, \mathbf{a}'} e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | T_{\mathbf{r}_k - \mathbf{r}_j}^\dagger H_{\text{aux}}(\mathbf{r}_0) T_{\mathbf{r}_k - \mathbf{r}_i} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle
 \end{aligned} \tag{1.89}$$

To resolve the translation operators, we will now insert the momentum eigenstates $|\vec{k}\rangle$ of the full model: $1 = \sum_{\vec{q}} |\vec{q}\rangle \langle \vec{q}|$ in between the operators.

$$\begin{aligned}
\langle \Psi_{\vec{k}'} | H_{\text{H-H}} | \Psi_{\vec{k}} \rangle &= \sum_{\substack{r_i, r_j, r_k, \\ a, a', \vec{q}, \vec{q}'}} \frac{e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)}}{\lambda_{|\vec{k}'\rangle}^* \lambda_{|\vec{k}\rangle} \mathcal{Z}^2 N^2} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | \vec{q}' \rangle \langle \vec{q}' | T_{\mathbf{r}_k - \mathbf{r}_j}^\dagger H_{\text{aux}}(\mathbf{r}_0) T_{\mathbf{r}_k - \mathbf{r}_i} | \vec{q} \rangle \langle \vec{q} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
&= \sum_{\substack{r_i, r_j, r_k, \\ a, a', \vec{q}, \vec{q}'}} \frac{e^{i(\vec{k} \cdot \vec{R}_i - \vec{k}' \cdot \vec{R}_j)}}{\lambda_{|\vec{k}'\rangle}^* \lambda_{|\vec{k}\rangle} \mathcal{Z}^2 N^2} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | \vec{q}' \rangle e^{-i\vec{q}' \cdot (\mathbf{r}_k - \mathbf{r}_j)} e^{i\vec{q} \cdot (\mathbf{r}_k - \mathbf{r}_i)} \langle \vec{q}' | H_{\text{aux}}(\mathbf{r}_0) | \vec{q} \rangle \langle \vec{q} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
&= \frac{N}{\lambda_{|\vec{k}'\rangle}^* \lambda_{|\vec{k}\rangle} \mathcal{Z}^2} \sum_{a, a', \vec{q}, \vec{q}'} \delta_{\vec{k}, \vec{q}} \delta_{\vec{q}, \vec{q}'} \delta_{\vec{q}', \vec{k}} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | \vec{q}' \rangle \langle \vec{q}' | H_{\text{aux}}(\mathbf{r}_0) | \vec{q} \rangle \langle \vec{q} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
&= \frac{N}{|\lambda_{|\vec{k}\rangle}|^2 \mathcal{Z}^2} \delta_{kk'} \sum_{a, a'} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | \vec{k} \rangle \langle \vec{k} | H_{\text{aux}}(\mathbf{r}_0) | \vec{k} \rangle \langle \vec{k} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle \\
&= \frac{N}{|\lambda_{|\vec{k}\rangle}|^2 \mathcal{Z}^2} \delta_{kk'} \langle \vec{k} | H_{\text{aux}}(\mathbf{r}_0) | \vec{k} \rangle \underbrace{\sum_{a, a'} \langle \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}') | \vec{k} \rangle \langle \vec{k} | \psi_{\text{aux}}(\mathbf{r}_0, \mathbf{a}) \rangle}_{w^2 |\lambda_{|\vec{k}\rangle}|^2} \\
&= N \delta_{kk'} \langle \vec{k} | H_{\text{aux}}(\mathbf{r}_0) | \vec{k} \rangle
\end{aligned} \tag{1.90}$$

The momentum eigenket $|\vec{k}\rangle$ can be expressed as a sum over position eigenkets at varying distances from \mathbf{r}_0 . This form allows a systematic method of improving the energy eigenvalue estimate, because the interacting in the impurity model is extremely localised, so the overlap between two auxiliary models decreases rapidly with distance. The majority of the contribution will come from the state at \mathbf{r}_0 , and improvements are then made by considering auxiliary models at further distances.

Chapter 2

Kondo Breakdown in a Heavy-Fermion Model

2.1 Bilayer extended Hubbard model: Impurity model

[10] 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):

$$H_{\text{aux}} = H_{\text{lp}} + H_f + H_d + H_{fd} , \quad (2.1)$$

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

$$H_{\text{lp}} = -t \sum_{\sigma, \alpha} \sum_{\langle i, j \rangle} \left(c_{i, \sigma, \alpha}^\dagger c_{j, \sigma, \alpha} + \text{h.c.} \right) - \sum_{i, \sigma, \alpha} \mu_\alpha n_{i, \sigma, \alpha} , \quad (2.2)$$

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:

$$\begin{aligned} H_f = & -\frac{U_f}{2} (n_{f, \uparrow} - n_{f, \downarrow})^2 + \sum_{Z \in \text{NN}} \left[-V \sum_{\sigma} \left(c_{f, \sigma}^\dagger c_{Z, \sigma, f} + \text{h.c.} \right) + \frac{J}{2} \sum_{\alpha, \beta} \mathbf{S}_f \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{Z, \alpha, f}^\dagger c_{Z, \beta, f} \right. \\ & \left. - \frac{W_f}{2} (n_{Z, \uparrow, f} - n_{Z, \downarrow, f})^2 \right] , \\ H_d = & -\eta_d n_d - \frac{U_d}{2} (n_{d, \uparrow} - n_{d, \downarrow})^2 + \sum_{Z \in \text{NN}} \left[-V \sum_{\sigma} \left(c_{d, \sigma}^\dagger c_{Z, \sigma, d} + \text{h.c.} \right) + \frac{J}{2} \sum_{\alpha, \beta} \mathbf{S}_d \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{Z, \alpha, d}^\dagger c_{Z, \beta, d} \right] , \end{aligned} \quad (2.3)$$

where $c_{v, \sigma, \alpha}^\dagger$ can refer to creation operator for either the f -layer. Finally, H_{fd} represents the inter-layer hybridisation:

$$H_{fd} = -V_\perp \sum_{\sigma} \left(c_{d, \sigma}^\dagger c_{f, \sigma} + \text{h.c.} \right) . \quad (2.4)$$

2.2 Tiling Into Bilayer Extended Hubbard Model

Tiling the impurity model leads to a bilayer extended Hubbard model on the 2D square lattice. In order to tile our auxiliary model to restore translation invariance, we identify the cluster which acts as the “unit” cell of translation. As discussed in the text surrounding eq. 1.15, a good choice for the unit cell is the impurity site and it’s surrounding correlated environment. Placing the impurity sites at \mathbf{r}_d in each layer, we get

$$H_{\text{clust}}(\mathbf{r}_d) = H_f(\mathbf{r}_d) + H_d(\mathbf{r}_d) + H_{fc}(\mathbf{r}_d) . \quad (2.5)$$

The details of tiling a cluster Hamiltonian were already shown in Sec. 1.3.2; the general idea is to use manybody translation operators (details in Sec. 1.3.1) to center the cluster Hamiltonian at various sites of the lattice, such that combining all such terms leads to a periodised Hamiltonian. we write down the final result here:

$$\begin{aligned} H_{\text{latt}} = & \sum_{\mathbf{r}} T^\dagger(\mathbf{r}) H_{\text{clust}}(\mathbf{r}_d) T(\mathbf{r}) \\ = & -\frac{2V}{Z} \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} \right) - \sum_i \left[\eta_d n_{i,d} + \frac{U_d}{2} (n_{i,\uparrow,d} - n_{i,\downarrow,d})^2 \right] + \frac{2J}{Z} \sum_{\langle i,j \rangle} \mathbf{S}_{i,d} \cdot \mathbf{S}_{j,d} \\ & - \frac{2V}{Z} \sum_{\langle i,j \rangle, \sigma} \left(f_{i,\sigma}^\dagger f_{j,\sigma} + \text{h.c.} \right) - \frac{U_f - W_f}{2} \sum_i (n_{i,\uparrow,f} - n_{i,\downarrow,f})^2 + \frac{2J}{Z} \sum_{\langle i,j \rangle} \mathbf{S}_{i,f} \cdot \mathbf{S}_{j,f} \\ & - V_\perp \sum_{i,\sigma} (f_{i,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) \end{aligned} \quad (2.6)$$

Tiling the impurity model therefore leads to a bilayer extended Hubbard model, with effective couplings that depend on the auxiliary model couplings. The value of η_d defines the effective chemical potential of the d -layer; a non-zero value moves the layer away from half-filling. The f -layer is pinned at half-filling.

Following Sec. 1.4.1, the retarded k -space Greens function in either layer can be expressed in terms of auxiliary model Greens functions:

$$G(\mathbf{k}, \sigma, \alpha; \omega) = \sum_{\nu} C_{\nu, \mathbf{k} \alpha} \left[\mathcal{G}^>(\mathcal{T}_{\nu, \sigma, \alpha}; \omega - \mathcal{E}_\nu(\mathbf{k})) - \mathcal{G}^<(\mathcal{T}_{\nu, \sigma, \alpha}; \omega + \mathcal{E}_\nu(\mathbf{k})) \right] , \quad (2.7)$$

where $\alpha = f, d$ denotes the layer in which the Greens function is being calculated, the modes ν indicate the operators which diagonalise the Hamiltonian H_{1p} , with energies $\mathcal{E}_\nu(\mathbf{k})$:

$$H_{1p} = -\frac{2V}{Z} \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.} + f_{i,\sigma}^\dagger f_{j,\sigma} + \text{h.c.} \right) - V_\perp \sum_{i,\sigma} (f_{i,\sigma}^\dagger c_{i,\sigma} + \text{h.c.}) - \sum_i \eta_d n_{i,d} , \quad (2.8)$$

and the \mathcal{T} -matrices are defined in eq. 1.36:

$$\mathcal{T}_{\nu, \sigma, \alpha} = \left[\left(\sum_{\sigma'} c_{\alpha \sigma'}^\dagger + \text{h.c.} \right) + (S_\alpha^+ + \text{h.c.}) + (C_\alpha^+ + \text{h.c.}) \right] c_{\nu, \sigma} , \quad (2.9)$$

In order to calculate $\mathcal{E}_v(\mathbf{k})$, we introduce the k -space modes via a Fourier transform:

$$c_{i,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}_i} c_{\mathbf{k},\sigma}^\dagger, \quad f_{i,\sigma}^\dagger = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{-i\mathbf{k} \cdot \mathbf{r}_i} f_{\mathbf{k},\sigma}^\dagger. \quad (2.10)$$

In terms of these modes, the 1-particle Hamiltonian decouples in k -space:

$$H_{1p} = \sum_{\mathbf{k},\sigma} \left[(\epsilon_{\mathbf{k}} - \eta_d)(n_{\mathbf{k},\sigma,d} + n_{\mathbf{k},\sigma,f}) - V_\perp (c_{\mathbf{k},\sigma}^\dagger f_{\mathbf{k},\sigma} + \text{h.c.}) \right]. \quad (2.11)$$

The diagonal modes are given by

$$v_{\mathbf{k},\sigma,\pm}^\dagger = C_{\pm,k} c_{\mathbf{k},\sigma}^\dagger + \sqrt{1 - C_{\pm,k}^2} f_{\mathbf{k},\sigma}^\dagger, \quad (2.12)$$

the coefficients obtained from diagonalising the matrix

$$H_{1p}(\mathbf{k}) = \begin{pmatrix} \epsilon_{\mathbf{k}} & -V_\perp \\ -V_\perp & \epsilon_{\mathbf{k}} - \eta_d \end{pmatrix}. \quad (2.13)$$

The energies are given by $\mathcal{E}_\pm(\mathbf{k}) = \epsilon_{\mathbf{k}} - \eta_d/2 \pm \Delta$, with $\epsilon_{\mathbf{k}}$ being $-\frac{4V}{Z}(\cos k_x + \cos k_y)$ for a 2D square lattice and $\Delta = \sqrt{V_\perp^2 + \eta_d^2}/4$. Substituting into the expression for the lattice Greens function, we get

$$G(\mathbf{k}, d; \omega) = \sum_{\alpha=\pm} C_{\alpha,k} \left[\mathcal{G}^>(\mathcal{T}_{\mathbf{k},\alpha,d}; \omega - \epsilon_{\mathbf{k}} + \eta_d/2 + \alpha\Delta) + \mathcal{G}^<(\mathcal{T}_{\mathbf{k},\alpha,d}; \omega + \epsilon_{\mathbf{k}} - \eta_d/2 - \alpha\Delta) \right]. \quad (2.14)$$

Following eq. 1.58, we can similarly write down an expression the local lattice Greens function, in real-space:

$$\begin{aligned} G_{\text{loc}}(\omega) &= \mathcal{G}(d\sigma; \omega) \\ &+ \sum_{\mathbf{k},\alpha=\pm} C_{\alpha,k} \left[\mathcal{G}^>(\mathcal{T}_{\mathbf{k},\alpha,d}, d\sigma; \omega - \epsilon_{\mathbf{k}} + \eta_d/2 + \alpha\Delta) + \mathcal{G}^<(\mathcal{T}_{\mathbf{k},\alpha,d}, d\sigma; \omega + \epsilon_{\mathbf{k}} - \eta_d/2 - \alpha\Delta) \right] \\ &+ \sum_{\mathbf{k}} \mathcal{G}(d\sigma, \mathcal{T}_{\mathbf{k},\sigma}; \omega) \\ &+ \sum_{\mathbf{k},\mathbf{q},\alpha=\pm} C_{\alpha,k} \left[\mathcal{G}^>(\mathcal{T}_{\mathbf{k},\alpha,d}, \mathcal{T}_{\mathbf{q},\sigma,d}; \omega - \epsilon_{\mathbf{k}} + \eta_d/2 + \alpha\Delta) + \mathcal{G}^<(\mathcal{T}_{\mathbf{k},\alpha,d}, \mathcal{T}_{\mathbf{q},\sigma,d}; \omega + \epsilon_{\mathbf{k}} - \eta_d/2 - \alpha\Delta) \right] \end{aligned} \quad (2.15)$$

2.3 Unitary RG Analysis of The Bilayer Lattice-Embedded ESIAM

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

$$H_{\text{aux}} = \sum_{\mathbf{k},\sigma,\alpha} \epsilon_{\mathbf{k},\alpha} n_{\mathbf{k},\sigma,\alpha} + \sum_{\alpha} \sum_{Z \in \text{NN}} \left[\frac{1}{2} J_\alpha \sum_{\sigma,\sigma'} \mathbf{S}_\alpha \cdot \boldsymbol{\sigma}_{\alpha\beta} c_{Z,\sigma,\alpha}^\dagger c_{Z,\sigma',\alpha} - \frac{W_\alpha}{2} (n_{Z,\uparrow,\alpha} - n_{Z,\downarrow,\alpha})^2 \right] + J\mathbf{S}_f \cdot \mathbf{S}_d. \quad (2.16)$$

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. Let the momentum states being decoupled from the two layers be $|\mathbf{q}, \sigma, f\rangle$ and $|\mathbf{q}, \sigma, d\rangle$ if they are above the Fermi energy (unoccupied in the low-energy configuration) and $|\bar{\mathbf{q}}, \sigma, f\rangle$ and $|\bar{\mathbf{q}}, \sigma, d\rangle$ if they are below the Fermi energy (occupied in the low-energy configuration). 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 $J = 0$:

$$\frac{\Delta J_f(\mathbf{k}_1, \mathbf{k}_2)}{\Delta D} = \int_{UV} d\mathbf{q} \rho(\mathbf{q}) [J_f(\mathbf{k}_1, \mathbf{q})J_f(\mathbf{q}, \mathbf{k}_2) + J_f(\mathbf{q}, \bar{\mathbf{q}})W_f(\mathbf{k}_1, \mathbf{q}, \bar{\mathbf{q}}, \mathbf{k}_2)] G_f^{(0)}(\mathbf{q}), \quad (2.17)$$

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 $J = 0$):

$$G_f^{(0)}(\mathbf{q}) = \frac{1}{\omega - |\epsilon_f(\mathbf{q})|/2 + J_f(\mathbf{q})/4 + W_f(\mathbf{q})/2}. \quad (2.18)$$

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

$$G_f(\mathbf{q}) = \frac{1}{1/G_f^{(0)} - J\vec{S}_f \cdot \vec{S}_d}. \quad (2.19)$$

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

$$\vec{S}_f \cdot \vec{S}_d = \frac{-3}{4}\mathcal{P}_0 + \frac{1}{4}\mathcal{P}_1, \quad \mathcal{P}_0 + \mathcal{P}_1 = \mathbb{I}. \quad (2.20)$$

Using these relations, we can write

$$\begin{aligned} G_f(\mathbf{q}) &= \frac{1}{1/G_f^{(0)} + 3J/4}\mathcal{P}_0 + \frac{1}{1/G_f^{(0)} - J/4}\mathcal{P}_1 \\ &= \left(\frac{1/4}{1/G_f^{(0)} + 3J/4} + \frac{3/4}{1/G_f^{(0)} - J/4} \right) \mathbb{I} + \left(\frac{1}{1/G_f^{(0)} + 3J/4} + \frac{1}{1/G_f^{(0)} - J/4} \right) \vec{S}_f \cdot \vec{S}_d. \end{aligned} \quad (2.21)$$

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

$$\frac{\Delta J_\alpha}{\Delta D} = \int_{UV} d\mathbf{q} \rho(\mathbf{q}) [J_\alpha(\mathbf{k}_1, \mathbf{q})J_\alpha(\mathbf{q}, \mathbf{k}_2) + J_\alpha(\mathbf{q}, \bar{\mathbf{q}})W_\alpha(\mathbf{k}_1, \mathbf{q}, \bar{\mathbf{q}}, \mathbf{k}_2)] \left(\frac{1}{4} \frac{1}{1/G_\alpha^{(0)}(\mathbf{q}) + 3J/4} + \frac{3}{4} \frac{1}{1/G_\alpha^{(0)}(\mathbf{q}) - J/4} \right) \quad (2.22)$$

We now turn to the renormalisation of J , arising from hybridisation of f - and d -layers. In order to capture coherent scattering processes between the two layers, we project onto the following rotated basis of excited states:

$$|H\rangle_{\pm} = \frac{1}{\sqrt{2}} \left(|H(\mathbf{q})\rangle_f \pm |H(\mathbf{q})\rangle_d \right), \quad (2.23)$$

$$\mathcal{P}(\mathbf{q})_H = |H\rangle_+ \langle H|_+ + |H\rangle_- \langle H|_- ,$$

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

$$\Delta H = \frac{1}{N^2} \sum_{\mathbf{q} \in \text{UV}} \langle L | \frac{1}{2} J_f(\bar{\mathbf{q}}, \mathbf{q}) S_f^+ c_{\mathbf{q}-\downarrow, f}^{\dagger} c_{\mathbf{q}+\uparrow, f} \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H \frac{1}{2} J_d(\mathbf{q}, \bar{\mathbf{q}}) S_d^- c_{\mathbf{q}\uparrow, d}^{\dagger} c_{\bar{\mathbf{q}}\downarrow, d} | L \rangle , \quad (2.24)$$

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

$$G = \frac{1}{\omega - H_D} , \quad (2.25)$$

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:

$$H_D = \sum_{\mathbf{q}, \sigma \in \mathbf{q}_{\pm}, \alpha} \epsilon_{\alpha}(\mathbf{q}) \tau_{\mathbf{q}, \sigma} + \frac{1}{2} \sum_{\alpha} J_{\alpha} S_{\alpha}^z \sum_{\mathbf{q}, \sigma} \sigma n_{\mathbf{q}, \sigma, \alpha} + J \vec{S}_f \cdot \vec{S}_d . \quad (2.26)$$

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

$$\mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H = \frac{1}{2} (G_f + G_d) (|H\rangle_+ \langle H|_+ + |H\rangle_- \langle H|_-) + \frac{1}{2} (G_f - G_d) (|H\rangle_+ \langle H|_- + |H\rangle_- \langle H|_+) , \quad (2.27)$$

where

$$G_{\alpha}(\mathbf{q}) = \frac{1}{\omega - \frac{1}{2} [\epsilon_{\alpha}(\mathbf{q}) - \epsilon_{\alpha}(\bar{\mathbf{q}})] + \frac{1}{2} J_{\alpha}(\mathbf{q}) + W_{\alpha}(\mathbf{q}) - \frac{1}{4} J} . \quad (2.28)$$

In eq. 2.24, 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

$$\langle L | S_f^+ c_{\mathbf{q}-\downarrow, f}^{\dagger} c_{\mathbf{q}+\uparrow, f} \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H S_d^- c_{\mathbf{q}\uparrow, d}^{\dagger} c_{\bar{\mathbf{q}}\downarrow, d} | L \rangle = S_f^+ S_d^- \langle H_f | \mathcal{P}(\mathbf{q})_H G \mathcal{P}(\mathbf{q})_H | H_d \rangle = \frac{1}{2} (G_f + G_d) S_f^+ S_d^- . \quad (2.29)$$

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

$$\Delta H = \frac{1}{8N^2} \sum_{\mathbf{q} \in \text{UV}} J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}}) (G_f(\mathbf{q}) + G_d(\mathbf{q})) S_f^+ S_d^- . \quad (2.30)$$

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

$$\frac{\Delta H}{\Delta D} = \frac{1}{8N} S_f^+ S_d^- \int_{UV} d\mathbf{q} \rho(\mathbf{q}) J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}}) (G_f(\mathbf{q}) + G_d(\mathbf{q})) . \quad (2.31)$$

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

$$\begin{aligned} \frac{\Delta J}{\Delta D} &= \frac{1}{2} J_f J_d \int_{UV} d\mathbf{q} \rho(\mathbf{q}) J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}}) (G_f(\mathbf{q}) + G_d(\mathbf{q})) \\ &= \frac{1}{2} \int_{UV} d\mathbf{q} \rho(\mathbf{q}) \left[\frac{J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}})}{\omega - \frac{1}{2} \bar{\epsilon}_f(\mathbf{q}) + \frac{1}{2} J_f(\mathbf{q}) + W_f(\mathbf{q}) - \frac{1}{4} J} + \frac{J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}})}{\omega - \frac{1}{2} \bar{\epsilon}_d(\mathbf{q}) + \frac{1}{2} J_d(\mathbf{q}) + W_d(\mathbf{q}) - \frac{1}{4} J} \right], \end{aligned} \quad (2.32)$$

where $\bar{\epsilon}_\alpha(\mathbf{q}) = \epsilon_f(\mathbf{q}) - \epsilon_f(\bar{\mathbf{q}})$ is the total excitation energy for the pair of states $\mathbf{q}, \bar{\mathbf{q}}$.

2.4 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:

$$\begin{aligned} J_f(\mathbf{k}, \mathbf{q}) &= \frac{J_f}{2} [\cos(k_x - q_x) + \cos(k_y - q_y)], \\ W(\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}') &= \frac{W}{2} [\cos(k_x - q_x + k'_x - q'_x) + \cos(k_y - q_y + k'_y - q'_y)]. \end{aligned} \quad (2.33)$$

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. 2.33 is (anti)symmetric under translation of (one)both momentum by either of the two RLVs:

$$\begin{aligned} J_f(\mathbf{k} + \mathbf{Q}_i, \mathbf{q}) &= J_f(\mathbf{k}, \mathbf{q} + \mathbf{Q}_i) = -J_f(\mathbf{k}, \mathbf{q}) ; i = 1, 2 ; \\ J_f(\mathbf{k} + \mathbf{Q}_i, \mathbf{q} + \mathbf{Q}_j) &= J_f(\mathbf{k}, \mathbf{q}) ; i = 1, 2 \quad j = 1, 2 . \end{aligned} \quad (2.34)$$

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. ??) 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:

$$\mathbf{k}_y = \mathbf{q}_y, \quad \mathbf{k}_x = -\mathbf{q}_x . \quad (2.35)$$

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

$$\begin{aligned} J_f(\mathbf{k}, \bar{\mathbf{k}}') &= J_f(\bar{\mathbf{k}}, \mathbf{k}'), \\ J_f(\bar{\mathbf{k}}, \bar{\mathbf{k}}') &= J_f(\mathbf{k}, \mathbf{k}') . \end{aligned} \quad (2.36)$$

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. ??, 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 $\Delta J_f^{(j)}(\bar{\mathbf{k}}_1, \bar{\mathbf{k}}_2) = \Delta J_f^{(j)}(\mathbf{k}_1, \mathbf{k}_2)$.

2.5 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:

$$H^* = \sum_{\alpha, \beta} \mathbf{S}_f \cdot \boldsymbol{\sigma}_{\alpha, \beta} \sum_{\mathbf{k}, \mathbf{q}} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger f_{\mathbf{q}, \beta} . \quad (2.37)$$

We will now obtain a more minimal representation of this interaction. Each momentum label is summed over all four quadrants Q_1 through Q_4 ; eq. 2.34 relates Q_1 with Q_3 and Q_2 with Q_4 :

$$\begin{aligned} \sum_{\mathbf{k}, \mathbf{q}} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger f_{\mathbf{q}, \beta} &= \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in Q_1, Q_2} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger + \sum_{\mathbf{k} \in Q_3, Q_4} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger \right] f_{\mathbf{q}, \beta} \\ &= \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in Q_1, Q_2} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger + \sum_{\mathbf{k} \in Q_1} J_f^*(\mathbf{k} - \mathbf{Q}_1, \mathbf{q}) f_{\mathbf{k} - \mathbf{Q}_1, \alpha}^\dagger + \sum_{\mathbf{k} \in Q_2} J_f^*(\mathbf{k} + \mathbf{Q}_2, \mathbf{q}) f_{\mathbf{k} + \mathbf{Q}_2, \alpha}^\dagger \right] f_{\mathbf{q}, \beta} \\ &= \sum_{\mathbf{q}} \left[\sum_{\mathbf{k} \in Q_1} J_f^*(\mathbf{k}, \mathbf{q}) (f_{\mathbf{k}, \alpha}^\dagger - f_{\mathbf{k} - \mathbf{Q}_1, \alpha}^\dagger) + \sum_{\mathbf{k} \in Q_2} J_f^*(\mathbf{k}, \mathbf{q}) (f_{\mathbf{k}, \alpha}^\dagger - f_{\mathbf{k} + \mathbf{Q}_2, \alpha}^\dagger) \right] f_{\mathbf{q}, \beta} . \end{aligned} \quad (2.38)$$

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

$$A_{\mathbf{k}, \sigma, \pm} = \begin{cases} \frac{1}{\sqrt{2}} (f_{\mathbf{k}, \sigma} \pm f_{\mathbf{k} - \mathbf{Q}_1, \sigma}) , & \mathbf{k} \in Q_1 , \\ \frac{1}{\sqrt{2}} (f_{\mathbf{k}, \sigma} \pm f_{\mathbf{k} + \mathbf{Q}_2, \sigma}) , & \mathbf{k} \in Q_2 , \end{cases} \quad (2.39)$$

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

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

$$\sum_{\mathbf{k}, \mathbf{q}} J_f^*(\mathbf{k}, \mathbf{q}) f_{\mathbf{k}, \alpha}^\dagger f_{\mathbf{q}, \beta} = 2 \sum_{\mathbf{k}, \mathbf{q} \in Q_1, Q_2} J_f^*(\mathbf{k}, \mathbf{q}) A_{\mathbf{k}, \alpha}^\dagger A_{\mathbf{q}, \beta} . \quad (2.40)$$

2.6 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 use eq. 2.39 to express the bare fields $f_{\mathbf{k},\sigma}$ in terms of the new fields $A_{\mathbf{k},\sigma,\pm}$ and $B_{\mathbf{k},\sigma,\pm}$:

$$\begin{aligned} f_{\mathbf{k},\sigma} &= \frac{1}{\sqrt{2}} (A_{\mathbf{k},\sigma,+} + A_{\mathbf{k},\sigma,-}) , \mathbf{k} \in Q_1, Q_2 \\ f_{\mathbf{k}-Q_1,\sigma} &= \frac{1}{\sqrt{2}} (A_{\mathbf{k},\sigma,+} - A_{\mathbf{k},\sigma,-}) , \mathbf{k} \in Q_1 \\ f_{\mathbf{k}+Q_2,\sigma} &= \frac{1}{\sqrt{2}} (A_{\mathbf{k},\sigma,+} - A_{\mathbf{k},\sigma,-}) , \mathbf{k} \in Q_2 \end{aligned} \quad (2.41)$$

where the four relations act on operators in four quadrants. These relations allow us to express correlations $F_{k_i,k_j} = \langle S_d^+ c_{k_i,\uparrow}^\dagger c_{k_j,\downarrow} \rangle$ for the bare fields f in terms of the rotated fields. Using the fact that the Hamiltonian does not couple the fields B_+ and A_+ , we have

$$\begin{aligned} F_{k_1,k_1} &= F_{k_3,k_3} = -F_{k_1,k_3} = \frac{1}{2} \langle S_d^+ A_{k_1,\downarrow,-}^\dagger A_{k_1,\uparrow,-} \rangle , \\ F_{k_2,k_2} &= F_{k_4,k_4} = -F_{k_2,k_4} = \frac{1}{2} \langle S_d^+ A_{k_2,\downarrow,-}^\dagger A_{k_2,\uparrow,-} \rangle , \\ F_{k_1,k_2} &= F_{k_3,k_4} = -F_{k_1,k_4} = -F_{k_2,k_3} = \frac{1}{2} \langle S_d^+ A_{k_1,\downarrow,-}^\dagger A_{k_1,\uparrow,-} \rangle , \end{aligned} \quad (2.42)$$

where the momentum state k_i belongs to the quadrant Q_i .

2.7 Effective Star Graph Representation of Kondo Interaction

To make computation less intensive, we want to make the Hamiltonian in eq. 2.40 sparser, by going to a star graph representation where each node of the graph couples only with the impurity spin (central node) and not to the other nodes of the graph. We therefore consider a rotated basis of excitations

$$\gamma_{i,\sigma}^\dagger = \sum_k \Lambda_{i,k} A_{k,\sigma}^\dagger , \text{ where } \sum_k \Lambda_{i,k}^* \Lambda_{j,k} = \delta_{i,j} . \quad (2.43)$$

These fermions of course satisfy the appropriate algebra:

$$\left\{ \gamma_{i,\sigma}, \gamma_{j,\sigma'}^\dagger \right\} = \sum_{k,q} \Lambda_{i,k}^* \Lambda_{j,q} \left\{ A_{k,\sigma}, A_{q,\sigma'}^\dagger \right\} = \delta_{i,j} \delta_{\sigma,\sigma'} . \quad (2.44)$$

In order to calculate the coefficients $\Lambda_{i,k}$, we impose the star graph simplification condition described above:

$$\sum_{\mathbf{k},\mathbf{q}} J_f^*(\mathbf{k},\mathbf{q}) A_{\mathbf{k},\alpha}^\dagger A_{\mathbf{q},\beta} = \sum_i K_i \gamma_{i,\alpha}^\dagger \gamma_{i,\beta} , \quad (2.45)$$

where K_i are the eigenvalues of the Kondo coupling matrix $J_f^*(\mathbf{k},\mathbf{q})$. Substituting the definition of the γ fields (eq. 2.43) leads to the equation

$$J_f^*(\mathbf{k},\mathbf{q}) = \sum_i \Lambda_{k,i} K_i \Lambda_{i,q}^\dagger \implies \mathcal{J} = \Lambda K \Lambda^\dagger , \quad (2.46)$$

where \mathcal{J} is the Kondo coupling matrix with matrix elements $J_f^*(\mathbf{k}, \mathbf{q})$, K is a diagonal matrix with the eigenvalues (K_i) of \mathcal{J} along its diagonal, and Λ is the matrix $\Lambda_{i,k}$ (the rotated indices i along the row, and the earlier momentum indices along the column). From eq. 2.46, it is clear that since \mathcal{J} is Hermitian, the matrix Λ is simply the unitary matrix which diagonalises the Kondo matrix \mathcal{J} :

$$\Lambda^\dagger \mathcal{J} \Lambda = K . \quad (2.47)$$

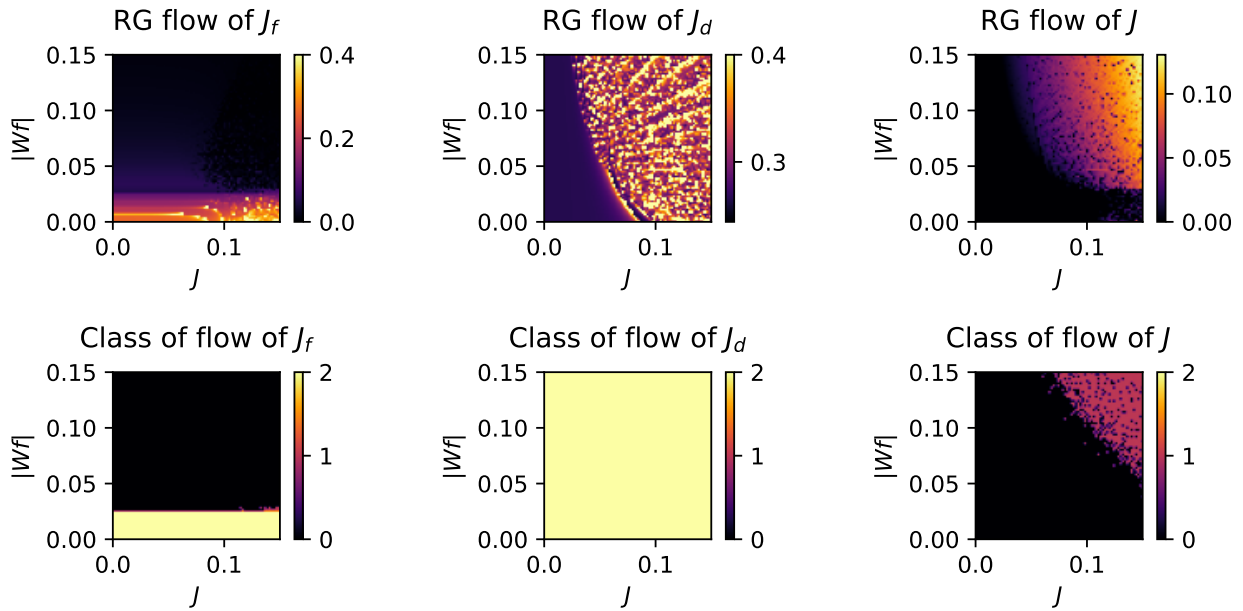
The prescription is therefore as follows. We compute the unitary transformation Λ that diagonalises \mathcal{J} and obtain the eigenvalues $\{K_i\}$. Using the eigenvalues, we work with the sparser Hamiltonian

$$\vec{S}_f \cdot \sum_{\alpha, \beta} \vec{\sigma}_{\alpha, \beta} \sum_i K_i \gamma_{i, \alpha}^\dagger \gamma_{i, \beta} . \quad (2.48)$$

If we have to calculate a certain correlation $C_{k,q}$, we instead calculate the correlation matrix $\tilde{C}_{i,j}$, and then transform back using the unitary transformation:

$$C = \Lambda \tilde{C} \Lambda^\dagger . \quad (2.49)$$

2.8 RG flow simulation on the $d = \infty$ Bethe lattice at half-filling



2.9 RG flow simulation on the 2D square lattice

Kondo coupling and bath interaction acquire k -dependence:

$$J(\mathbf{k}, \mathbf{q}) = \frac{J}{2} [\cos(\mathbf{k}_x - \mathbf{q}_x) + \cos(\mathbf{k}_y - \mathbf{q}_y)] , \quad (2.50)$$

$$W(\mathbf{k}, \mathbf{q}, \mathbf{k}', \mathbf{q}') = \frac{W}{2} [\cos(\mathbf{k}_x - \mathbf{q}_x + \mathbf{k}'_x - \mathbf{q}'_x) + \cos(\mathbf{k}_y - \mathbf{q}_y + \mathbf{k}'_y - \mathbf{q}'_y)] .$$

The particle-hole transformed state $\bar{\mathbf{q}}$ associated with \mathbf{q} is defined as $\bar{\mathbf{q}} = \mathbf{q} + (\pi, \pi)$ if \mathbf{q} is in the first or third quadrant and $\mathbf{q} + (\pi, -\pi)$ is in the second or fourth quadrant.

We first introduce a non-zero chemical potential in the conduction bath of the two layer:

$$H_{\text{aux}} = \sum_{\mathbf{k}, \sigma, \alpha} (\epsilon_{\mathbf{k}, \alpha} - \mu) n_{\mathbf{k}, \sigma, \alpha} + \sum_{\alpha} \sum_{Z \in \text{NN}} \left[\frac{1}{2} J_{\alpha} \sum_{\sigma, \sigma'} \mathbf{S}_{\alpha} \cdot \boldsymbol{\sigma}_{\alpha \beta} c_{Z, \sigma, \alpha}^{\dagger} c_{Z, \sigma', \alpha} - \frac{W_{\alpha}}{2} (n_{Z, \uparrow, \alpha} - n_{Z, \downarrow, \alpha})^2 \right] + J \mathbf{S}_f \cdot \mathbf{S}_d. \quad (2.51)$$

The effect of this is to split the RG equation into contributions from particle and hole sectors:

$$\begin{aligned} \frac{\Delta J_{\alpha}}{\Delta D} = & \frac{1}{2} \int_{PS} d\mathbf{q} \rho(\mathbf{q}) [J_{\alpha}(\mathbf{k}_1, \mathbf{q}) J_{\alpha}(\mathbf{q}, \mathbf{k}_2) + J_{\alpha}(\mathbf{q}, \bar{\mathbf{q}}) W_{\alpha}(\mathbf{k}_1, \mathbf{q}, \bar{\mathbf{q}}, \mathbf{k}_2)] \left(\frac{1/4}{1/G_{\alpha}^{(0)}(\mathbf{q}) + \mu/2 + 3J/4} + \frac{3/4}{1/G_{\alpha}^{(0)}(\mathbf{q}) + \mu/2 - J/4} \right) \\ & + \frac{1}{2} \int_{HS} d\mathbf{q} \rho(\mathbf{q}) [J_{\alpha}(\mathbf{k}_1, \mathbf{q}) J_{\alpha}(\mathbf{q}, \mathbf{k}_2) + J_{\alpha}(\mathbf{q}, \bar{\mathbf{q}}) W_{\alpha}(\mathbf{k}_1, \mathbf{q}, \bar{\mathbf{q}}, \mathbf{k}_2)] \left(\frac{1/4}{1/G_{\alpha}^{(0)}(\mathbf{q}) - \mu/2 + 3J/4} + \frac{3/4}{1/G_{\alpha}^{(0)}(\mathbf{q}) - \mu/2 - J/4} \right) \end{aligned} \quad (2.52)$$

where PS and HS integrate over the particle and hole sectors of the excited states (where the excited states are occupied and unoccupied respectively).

Since the bath interaction doesn't renormalise, its functional form remains unchanged and can be substituted into the RG equations. In fact, we can write the expressions in a compact matrix form for efficient computation:

$$\frac{\Delta J_{\alpha}}{\Delta D} = J_{\alpha} \mathcal{G}_{\alpha} J_{\alpha}^{\dagger} + \mathcal{W}_{\alpha} \text{Tr} [\mathcal{G}'_{\alpha}], \quad (2.53)$$

where all objects are matrices. J_{α} is the Kondo coupling matrix. \mathcal{G}_{α} is a diagonal matrix with matrix elements

$$\mathcal{G}_{\alpha}[q, q] = \begin{cases} \rho(q) \left(\frac{1}{8} \frac{1}{1/G_{\alpha}^{(0)}(\mathbf{q}) + \mu/2 + 3J/4} + \frac{3}{8} \frac{1}{1/G_{\alpha}^{(0)}(\mathbf{q}) + \mu/2 - J/4} \right), & \mathbf{q} \in PS, \\ \rho(q) \left(\frac{1}{8} \frac{1}{1/G_{\alpha}^{(0)}(\mathbf{q}) - \mu/2 + 3J/4} + \frac{3}{8} \frac{1}{1/G_{\alpha}^{(0)}(\mathbf{q}) - \mu/2 - J/4} \right), & \mathbf{q} \in HS, \end{cases} \quad (2.54)$$

if q is in the UV subspace and zero otherwise. \mathcal{W}_{α} is the bath interaction matrix whose matrix elements are given by $\mathcal{W}_{\alpha}[k, k'] = \frac{W}{2} [\cos(k_x - k'_x) + \cos(k_y - k'_y)]$. Finally, \mathcal{G}'_{α} is another diagonal matrix whose matrix elements are defined as $\mathcal{G}'_{\alpha}[q, q] = \mathcal{G}[q, q] J_{\alpha}[q, \bar{q}]$.

The RG equation for the inter-layer coupling J can be written as

$$\frac{\Delta J}{\Delta D} = \frac{1}{2} \mathbf{J} \cdot \mathbf{G}, \quad (2.55)$$

where \mathbf{J} and \mathbf{G} are vectors defined by the elements $\mathbf{J}[q] = J_f(\bar{\mathbf{q}}, \mathbf{q}) J_d(\mathbf{q}, \bar{\mathbf{q}})$ and

$$\mathbf{G}[q] = \rho(\mathbf{q}) \left[\frac{1}{\omega - \frac{1}{2} \bar{\epsilon}_f(\mathbf{q}) + \frac{1}{2} J_f(\mathbf{q}) + W_f(\mathbf{q}) - \frac{1}{4} J} + \frac{1}{\omega - \frac{1}{2} \bar{\epsilon}_d(\mathbf{q}) + \frac{1}{2} J_d(\mathbf{q}) + W_d(\mathbf{q}) - \frac{1}{4} J} \right]. \quad (2.56)$$

2.10 Mapping Correlations from Auxiliary Model to Lattice Model

We follow a similar procedure as the one laid out in the earlier work. Using Bloch's theorem, the eigenstates for the tiled lattice model can be expressed as a superposition of the "local" eigenstates of the auxiliary model. Let $|\psi_{\text{gs}}(\mathbf{r}_d)\rangle$ be the groundstate of the bilayer impurity model with the f - and d -impurity sites located at \mathbf{r}_d (only tracking the horizontal position). The low-lying eigenstates of the tiled model for the total crystal momentum \mathbf{k} are then given by

$$|\Psi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\mathbf{r}_d} e^{i\mathbf{k}\cdot\mathbf{r}_d} |\psi_{\text{gs}}(\mathbf{r}_d)\rangle . \quad (2.57)$$

We first consider intra-layer equal-time correlators, of the form

$$C_{O_\alpha}(\Delta) = \langle \Psi_{\mathbf{k}} | O_\alpha(\mathbf{r} + \Delta) O_\alpha^\dagger(\mathbf{r}) | \Psi_{\mathbf{k}} \rangle , \quad (2.58)$$

where α can be f or d and indicates the layer in which the correlation is being calculated (or equivalently, the layer in which the operators act).

Following arguments identical to the ones laid out in the previous work, we substitute eq. 2.57 into eq. 2.58 and use global translation operators to transfer the sum over the local eigenstates into a sum over the operators, allowing us to compute correlations within a single auxiliary model:

$$C_{O_\alpha}(\Delta) = \frac{1}{N} \sum_{\mathbf{r}_1, \mathbf{r}_2} \langle \psi_{\text{gs}}(\mathbf{r}_2 + \mathbf{r}_c) | O_\alpha(\Delta + \mathbf{r}_1) O_\alpha^\dagger(\mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle e^{-i\mathbf{k}\cdot\mathbf{r}_2} . \quad (2.59)$$

Using the treatment laid out in the previous work, we can extract an intra-auxiliary model component from the full expression (by setting $\mathbf{r}_2 = 0$):

$$\frac{1}{N} \sum_{\mathbf{r}_1} \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}_\alpha(\Delta + \mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}_\alpha^\dagger(\mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (2.60)$$

The modified excitation operators are generally defined as

$$\tilde{O}_\alpha(\mathbf{r}) = O_\alpha(\mathbf{r}) O^\dagger(\alpha) \mathcal{P}_{\text{gs}} , \quad (2.61)$$

where $O^\dagger(d)$ is the hermitian conjugate of the correlation operator O , but applied on the impurity sites. This therefore constitutes a time-reversed scattering process on the impurity site relative to the process in the bath. The operator \mathcal{P}_{gs} projects onto the ground state of the auxiliary model, since we are interested in ground state correlations. The operator multiplying the old correlation operator represents excitation of the impurity site, and ensures that the bath and impurity excitation processes take place coherently. The projector ensures that only tripartite correlations between the impurity site and the two momentum states are captured by the correlation, which is what's desired within the tiling method.

For inter-layer correlations, we have

$$C_O(\Delta) = \langle \Psi_{\mathbf{k}} | O_{\bar{\alpha}}(\mathbf{r} + \Delta) O_\alpha^\dagger(\mathbf{r}) | \Psi_{\mathbf{k}} \rangle , \quad (2.62)$$

where $\bar{\alpha}$ represents the layer opposite to α . An identical treatment leads to the following intra-auxiliary model contribution

$$\frac{1}{N} \sum_{\mathbf{r}_1} \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}_{\bar{\alpha}}(\Delta + \mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle \langle \psi_{\text{gs}}(\mathbf{r}_c) | \tilde{O}_\alpha^\dagger(\mathbf{r}_1) | \psi_{\text{gs}}(\mathbf{r}_c) \rangle . \quad (2.63)$$

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