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:

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

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:

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

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:

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

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.
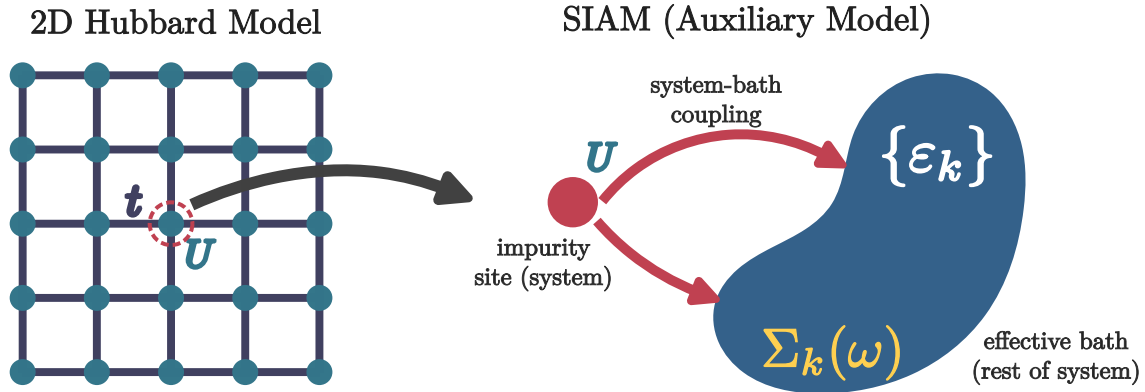
2D Hubbard Model   **SIAM (Auxiliary Model)**

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:

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

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:

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

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
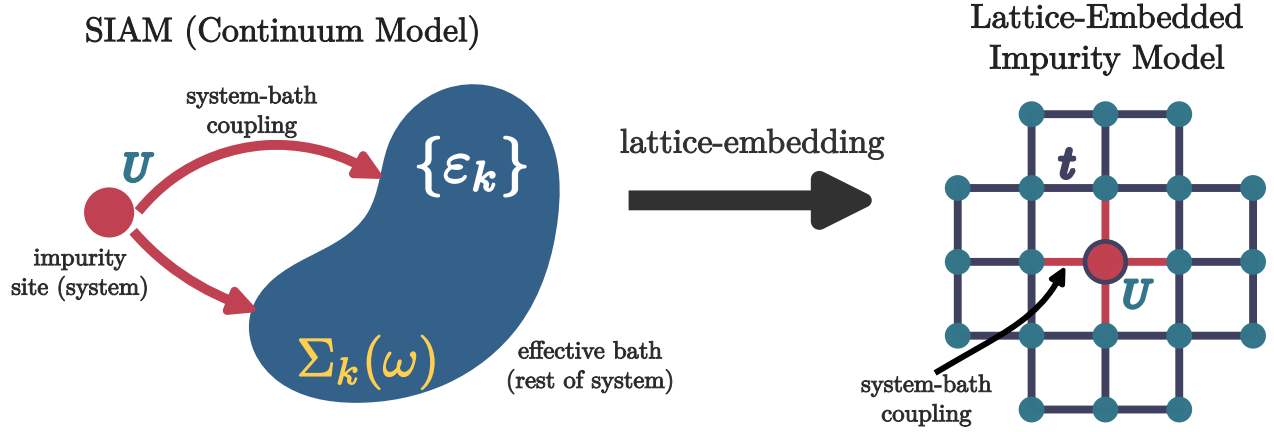
Figure 1.2

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

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

(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 it's 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 $T(\boldsymbol{a})$ that translate all positions by a

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

$$T^\dagger(a) |r_1, r_2, \ldots\rangle = |r_1 + a\rangle \otimes |r_2 + a\rangle \ldots \otimes |r_n + a\rangle$$
$$T^\dagger(a)O(r_1, r_2, \ldots)T(a) = O(r_1 + a, r_2 + a, \ldots) , \tag{1.7}$$

where $|r_1, r_2, \ldots\rangle$ 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 $c^\dagger(r)$, we have

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

It acts similarly on the auxiliary model Hamiltonian:

$$T^\dagger(a)H_{\text{aux}}(r_d)T(a) = H_{\text{aux}}(r_d + a) , \tag{1.9}$$

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

$$|r_1, r_2, \ldots\rangle = \otimes_{j=1}^N \int dk_j e^{ir_j \cdot k_j} |k_j\rangle , \tag{1.10}$$

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

$$\begin{aligned} T^\dagger(a) |k_1, k_2, \ldots\rangle &= \otimes_{j=1}^N \int dr_j e^{-ir_j \cdot k_j} T^\dagger(a) |r_j\rangle , \\ &= \otimes_{j=1}^N \int dr_j e^{-ir_j \cdot k_j} |r_j + a\rangle \\ &= \otimes_{j=1}^N e^{ia \cdot k_j} \int dr_j e^{-ir_j \cdot k_j} |r_j\rangle \\ &= e^{ia \cdot k_{\text{tot}}} |k_1, k_2, \ldots\rangle , \end{aligned} \tag{1.11}$$

where $k_{\text{tot}} = \sum_j k_j$ is the total momentum. This gives a compact form for the translation operator:

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

where $\hat{k}_{\text{tot}}$ 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

$$c(k) = \frac{1}{\sqrt{N}} \sum_r e^{-ik \cdot r} c(r) . \tag{1.13}$$

Applying the translation operator to this decomposition, we get

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

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 it's 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

$$H_{\text{clust}}(\boldsymbol{r}_d) = -\sum_{\boldsymbol{k},\sigma} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_d} V(\boldsymbol{k})(c^\dagger_{\boldsymbol{r}_d,\sigma} c_{\boldsymbol{k},\sigma} + \text{h.c.}) + \sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}_d}\, J_K(\boldsymbol{k}_1,\boldsymbol{k}_2)\boldsymbol{S}_{\boldsymbol{r}_d}\cdot\boldsymbol{S}_{\boldsymbol{k}_1,\boldsymbol{k}_2} + \varepsilon_d n_{\boldsymbol{r}_d}$$

$$+ U_d n_{\boldsymbol{r}_d,\uparrow} n_{\boldsymbol{r}_d,\downarrow} - \frac{1}{2}\sum_{\{\boldsymbol{k}_i\},\sigma,\sigma'} \sigma\,\sigma'\, e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}_d} W(\{\boldsymbol{k}_i\}) c^\dagger_{\boldsymbol{k}_1,\sigma} c_{\boldsymbol{k}_2,\sigma} c^\dagger_{\boldsymbol{k}_3,\sigma'} c_{\boldsymbol{k}_4,\sigma'}\,,$$

$$(1.15)$$

where $\boldsymbol{S}_{\boldsymbol{k}_1,\boldsymbol{k}_2} = \sum_{\alpha,\beta}\boldsymbol{\sigma}_{\alpha,\beta} c^\dagger_{\boldsymbol{k}_1,\alpha} c_{\boldsymbol{k}_2,\beta}$, and the Fourier transforms are defined by the following relations:

$$\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_d} V(\boldsymbol{k}) c^\dagger_{\boldsymbol{r}_d,\sigma} c_{\boldsymbol{k},\sigma} = \frac{V}{Z}\sum_{r\to\text{NN of }\boldsymbol{r}_d} c^\dagger_{\boldsymbol{r}_d,\sigma} c_{\boldsymbol{r},\sigma}\,,$$

$$\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}_d}\, J_K(\boldsymbol{k}_1,\boldsymbol{k}_2)\vec{S}_{\boldsymbol{r}_d}\cdot\vec{S}_{\boldsymbol{k}_1,\boldsymbol{k}_2} = \frac{J_K}{Z}\sum_{r\to\text{NN of }\boldsymbol{r}_d} \boldsymbol{S}_{\boldsymbol{r}_d}\cdot\boldsymbol{S}_r\,, \qquad (1.16)$$

$$\sum_{\boldsymbol{k}_1,\boldsymbol{k}_2,\boldsymbol{q}_1,\boldsymbol{q}_2} e^{i(\boldsymbol{k}_1-\boldsymbol{k}_2+\boldsymbol{k}_3-\boldsymbol{k}_4)\cdot\boldsymbol{r}_d} W(\{\boldsymbol{k}_i\}) c^\dagger_{\boldsymbol{k}_1,\sigma} c_{\boldsymbol{k}_2,\sigma} c^\dagger_{\boldsymbol{k}_3,\sigma'} c_{\boldsymbol{k}_4,\sigma'} = \frac{W}{2Z}\sum_{r\to\text{NN of }\boldsymbol{r}_d} n_{r,\sigma} n_{r,\sigma'}\,,$$

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

$$H_{\text{latt}} = \sum_r T^\dagger(\boldsymbol{r}-\boldsymbol{r}_d) H_{\text{clust}}(\boldsymbol{r}_d) T(\boldsymbol{r}-\boldsymbol{r}_d)\,. \qquad (1.17)$$

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:

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

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

$$\sum_r T^\dagger(\boldsymbol{r}-\boldsymbol{r}_d)\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_d} V(\boldsymbol{k}) c^\dagger_{\boldsymbol{r}_d,\sigma} c_{\boldsymbol{k},\sigma} T(\boldsymbol{r}-\boldsymbol{r}_d) = \sum_r\sum_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} V(\boldsymbol{k}) c^\dagger_{r,\sigma} c_{\boldsymbol{k},\sigma}$$

$$= \frac{V}{Z}\sum_r\sum_{r'\to\text{NN of }r} c^\dagger_{r,\sigma} c_{r',\sigma} \qquad (1.19)$$

$$= \frac{2V}{Z}\sum_{\langle r,r'\rangle} c^\dagger_{r,\sigma} c_{r',\sigma}\,,$$

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

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

$$
\sum_{r,k_1,k_2} T^\dagger(r - r_d)e^{i(k_1-k_2)\cdot r_d} J_K(k_1, k_2)\vec{S}_{r_d} \cdot \vec{S}_{k_1,k_2}T(r - r_d) = \sum_{r,k_1,k_2} e^{i(k_1-k_2)\cdot r} J_K(k_1, k_2)\vec{S}_r \cdot \vec{S}_{k_1,k_2}
$$

$$
= \frac{J_K}{Z} \sum_r \sum_{r'\to\text{NN of } r} \vec{S}_r \cdot \vec{S}_{r'} ,
$$

$$
= \frac{2J_K}{Z} \sum_{\langle r,r'\rangle} \vec{S}_r \cdot \vec{S}_{r'} ,
$$

(1.20)

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

$$
\sum_{r,k_1,k_2,k_3,k_4} T^\dagger(r - r_d)e^{i(k_1-k_2+k_3-k_4)\cdot r_d}W(\{k_i\})c^\dagger_{k_1,\sigma}c_{k_2,\sigma}c^\dagger_{k_3,\sigma'}c_{k_4,\sigma'}T(r - r_d)
$$

$$
= \sum_{r,k_1,k_2,k_3,k_4} e^{i(k_1-k_2+k_3-k_4)\cdot r}W(\{k_i\})c^\dagger_{k_1,\sigma}c_{k_2,\sigma}c^\dagger_{k_3,\sigma'}c_{k_4,\sigma'}
$$

$$
= \frac{W}{2Z} \sum_r \sum_{r'\to\text{NN of } r} n_{r',\sigma}n_{r',\sigma'}
$$

$$
= \frac{W}{2} \sum_r n_{r,\sigma}n_{r,\sigma'} ,
$$

(1.21)

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

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

$$
H_{\text{latt}} = \varepsilon_d \sum_{r,\sigma} n_{r,\sigma} + U_d \sum_r n_{r,\uparrow}n_{r,\downarrow} - \frac{2V}{Z} \sum_{\langle r,r'\rangle} c^\dagger_{r,\sigma}c_{r',\sigma} + \frac{2J_K}{Z} \sum_{\langle r,r'\rangle} \vec{S}_r \cdot \vec{S}_{r'} - \frac{W}{2} \sum_r \left(n_{r,\uparrow} - n_{r,\downarrow}\right)^2 .
$$

(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

$$
H_{\text{ex-Hub}} = -t \sum_{\langle i,j\rangle,\sigma} (c^\dagger_{i,\sigma}c_{j,\sigma} + \text{h.c.}) + J \sum_{\langle i,j\rangle} S_i \cdot S_j + U \sum_i n_{i,\uparrow}n_{i,\downarrow} - \mu \sum_{i,\sigma} n_{i,\sigma} ,
$$

(1.23)

such that the effective couplings resulting from the tiling operation is

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

(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 liner combinations of the eigenstates $|\psi(i)\rangle$ of the local Hamiltonians. According to Bloch's theorem, $|\Psi\rangle$ is of the form $|\Psi_{n,K}\rangle = \sum_i e^{iK\cdot r_i} |\psi_n(i)\rangle$, where K is the single-particle crystal momentum, n is the band-index that labels various states within the local orbital, and 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:

$$T^\dagger(la) |\Psi_{n,K}\rangle = \sum_i e^{iK\cdot r_i} |\psi_n(i+l)\rangle = e^{-ilK\cdot a} |\Psi_{n,K}\rangle \ . \tag{1.25}$$

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 $|\psi_n(r_d)\rangle$ (with the impurity located at an arbitrary position r_d) of the unit cell auxiliary model Hamiltonian $H_{\text{clust}}(r_d)$ defined in eq. 1.15 can be used to construct eigenstates of the lattice Hamiltonian. The index $n(=0,1,\ldots)$ in the subscript indicates that it is the nth eigenstate of the auxiliary model. The following combination of the auxiliary model eigenstates satisfies a many-particle equivalent of Bloch's theorem [9]:

$$|\Psi_s\rangle \equiv |\Psi_{K,n}\rangle = \frac{1}{\sqrt{N}} \sum_{r_d} e^{iK\cdot r_d} |\psi_n(r_d)\rangle \ , \tag{1.26}$$

where N is the total number of lattice sites and 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

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

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

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

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

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

which combined with eq. 1.14 gives

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

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):

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

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

$$\sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}\langle\psi_{\text{gs}}(\boldsymbol{r}_2)|c_{\boldsymbol{k}\sigma}(t)c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_1)\rangle = \sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|T(\boldsymbol{r}_2-\boldsymbol{r}_d)c_{\boldsymbol{k}\sigma}(t)c_{\boldsymbol{k}\sigma}^{\dagger}T^{\dagger}(\boldsymbol{r}_1-\boldsymbol{r}_d)|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$$

$$= \sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}e^{i\boldsymbol{k}(\boldsymbol{r}_1-\boldsymbol{r}_2)}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}(t)T^{\dagger}(\boldsymbol{r}_1-\boldsymbol{r}_2)c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$$

$$= N\sum_{\boldsymbol{r}}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}(t)T^{\dagger}(\boldsymbol{r})c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle . \tag{1.32}$$

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

$$\sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}\langle\psi_{\text{gs}}(\boldsymbol{r}_2)|c_{\boldsymbol{k}\sigma}^{\dagger}c_{\boldsymbol{k}\sigma}(t)|\psi_{\text{gs}}(\boldsymbol{r}_1)\rangle = \sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|T(\boldsymbol{r}_2-\boldsymbol{r}_d)c_{\boldsymbol{k}\sigma}^{\dagger}c_{\boldsymbol{k}\sigma}(t)T^{\dagger}(\boldsymbol{r}_1-\boldsymbol{r}_d)|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$$

$$= \sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}e^{-i\boldsymbol{k}(\boldsymbol{r}_1-\boldsymbol{r}_2)}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}^{\dagger}T^{\dagger}(\boldsymbol{r}_1-\boldsymbol{r}_2)c_{\boldsymbol{k}\sigma}(t)|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$$

$$= N\sum_{\boldsymbol{r}}e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}^{\dagger}T^{\dagger}(\boldsymbol{r})c_{\boldsymbol{k}\sigma}(t)|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle . \tag{1.33}$$

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

$$\sum_{\boldsymbol{r}_1,\boldsymbol{r}_2}\langle\psi_{\text{gs}}(\boldsymbol{r}_2)|c_{\boldsymbol{k}\sigma}(t)c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_1)\rangle$$

$$= N\sum_{\boldsymbol{r},n_1,n_2}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}(t)|\psi_{n_1}(\boldsymbol{r}_d)\rangle\langle\psi_{n_1}(\boldsymbol{r}_d)|T^{\dagger}(\boldsymbol{r})|\psi_{n_2}(\boldsymbol{r}_d)\rangle\langle\psi_{n_2}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$$

$$= N\sum_{\boldsymbol{r},n_1,n_2}e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\langle\psi_{\text{gs}}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}(t)|\psi_{n_1}(\boldsymbol{r}_d)\rangle\langle\psi_{n_1}(\boldsymbol{r}_d)|\psi_{n_2}(\boldsymbol{r}_d+\boldsymbol{r})\rangle\langle\psi_{n_2}(\boldsymbol{r}_d)|c_{\boldsymbol{k}\sigma}^{\dagger}|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle . \tag{1.34}$$

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

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

(1.35)

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

We now consider more carefully the transition operator $c_{\boldsymbol{k}\sigma}$ 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 $c_{\boldsymbol{k}\sigma}$ 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:

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

(1.36)

where $S_{\boldsymbol{r}_d}^+$ and $C_{\boldsymbol{r}_d}^+$ 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

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

(1.37)

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

$$e^{i(H_{\mathrm{aux}}(\boldsymbol{r}_d)+H_{\mathrm{cav}}(\boldsymbol{r}_d))t} \approx e^{iH_{\mathrm{aux}}(\boldsymbol{r}_d)t} e^{iH_{\mathrm{cav}}(\boldsymbol{r}_d)t} e^{[H_{\mathrm{aux}}(\boldsymbol{r}_d),\, H_{\mathrm{cav}}(\boldsymbol{r}_d)]t^2/2} \ ,$$

(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 $e^{iH_{\mathrm{cav}}(\boldsymbol{r}_d)t} e^{[H_{\mathrm{aux}}(\boldsymbol{r}_d),\, H_{\mathrm{cav}}(\boldsymbol{r}_d)]t^2/2}$ 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:

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

(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:

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

where $\mathcal{P}_n(\mathbf{r}_d)$ projects onto the nth 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

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

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

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

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

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

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

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

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

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

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

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

$$G(\boldsymbol{k}, \sigma; \omega) = \sum_{\nu} C_{\nu, \boldsymbol{k}} \left[\mathcal{G}^{>}(\mathcal{T}_{\nu, \sigma}; \omega - \epsilon_\nu) + \mathcal{G}^{<}(\mathcal{T}_{\nu, \sigma}; \omega + \epsilon_\nu) \right] . \tag{1.48}$$

We now discuss how to systematically improve this estimate. One way is to include the effect of other auxiliary models in the overlap function $F_n(\boldsymbol{r})$. 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 $\boldsymbol{r}_d$, the expression for the Greens function becomes

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

with $\tau_{\nu, \sigma}^{*} = \mathcal{T}_{\nu, \sigma}(F_n(0) + \sum_{\boldsymbol{a}} F_n(\boldsymbol{a}) e^{i\boldsymbol{k} \cdot \boldsymbol{a}})$ where $\boldsymbol{a}$ 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:

$$\mathcal{T}_{\boldsymbol{k}, \sigma}^{*}(t) = e^{iH_{\mathrm{cav}}(\boldsymbol{r}_d)t} (\mathcal{T}_{\boldsymbol{k}, \sigma} + t^2/2 \left[[H_{\mathrm{aux}}(\boldsymbol{r}_d), H_{\mathrm{cav}}(\boldsymbol{r}_d)], \mathcal{T}_{\boldsymbol{k}, \sigma} \right]) e^{-iH_{\mathrm{cav}}(\boldsymbol{r}_d)t} . \tag{1.50}$$

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

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

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

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

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:

$$
\sum_{r_d} \langle \Psi_{\text{gs}} | c_{r_d+r,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \Psi_{\text{gs}} \rangle = \frac{1}{N} \sum_{R,\Delta,r_d} \langle \psi_{\text{gs}}(R+\Delta) | c_{r_d+r,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \psi_{\text{gs}}(R) \rangle
$$
$$
= \frac{1}{N} \sum_{R,\Delta} \langle \psi_{\text{gs}}(-r_d) | c_{r-R-\Delta,\sigma}(t) T(\Delta) c^{\dagger}_{-R,\sigma} | \psi_{\text{gs}}(-r_d) \rangle \; .
$$
(1.53)

Local Greens function: $r = 0$

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

$$
\sum_{r_d} \langle \Psi_{\text{gs}} | c_{r_d,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \Psi_{\text{gs}} \rangle = \frac{1}{N} \sum_{R,\Delta,r_d} \langle \psi_{\text{gs}}(r_d) | c_{R+\Delta,\sigma}(t) T^{\dagger}(\Delta) c^{\dagger}_{R,\sigma} | \psi_{\text{gs}}(r_d) \rangle \; .
$$
(1.54)

We split the full summation into four parts, based on whether $R = r_d$ and whether $\Delta + R = r_d$:

$$
\sum_{r_d} \langle \Psi_{\text{gs}} | c_{r_d,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \Psi_{\text{gs}} \rangle = \langle \psi_{\text{gs}}(r_d) | c_{r_d,\sigma}(t) c^{\dagger}_{r_d,\sigma} | \psi_{\text{gs}}(r_d) \rangle
$$
$$
+ \sum_{\Delta \neq 0} \langle \psi_{\text{gs}}(r_d) | c_{r_d+\Delta,\sigma}(t) T^{\dagger}(\Delta) c^{\dagger}_{r_d,\sigma} | \psi_{\text{gs}}(r_d) \rangle
$$
$$
+ \sum_{R \neq r_d} \langle \psi_{\text{gs}}(r_d) | c_{r_d,\sigma}(t) T^{\dagger}(r_d-R) c^{\dagger}_{R,\sigma} | \psi_{\text{gs}}(r_d) \rangle
$$
$$
+ \sum_{R \neq r_d, \Delta \neq r_d} \langle \psi_{\text{gs}}(r_d) | c_{\Delta,\sigma}(t) T^{\dagger}(\Delta-R) c^{\dagger}_{R,\sigma} | \psi_{\text{gs}}(r_d) \rangle \; ,
$$
(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 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 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:

$$
\mathcal{T}_{r,\sigma} = \left[\left(\sum_{\sigma'} c^{\dagger}_{r_d\sigma} + \text{h.c.} \right) + \left(S^{+}_{r_d} + \text{h.c.} \right) + \left(C^{+}_{r_d} + \text{h.c.} \right) \right] c_{r\sigma} = \sum_{k} e^{ik \cdot r} \mathcal{T}_{k,\sigma} \; .
$$
(1.56)

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

$$
\begin{aligned}
\sum_{r_d} &\langle\Psi_{\text{gs}}|c_{r_d,\sigma}(t)c^\dagger_{r_d,\sigma}|\Psi_{\text{gs}}\rangle \\
&= \langle\psi_{\text{gs}}(r_d)|c_{r_d,\sigma}(t)c^\dagger_{r_d,\sigma}|\psi_{\text{gs}}(r_d)\rangle \\
&+ \sum_{k,n} F'_n(k)\,\langle\psi_{\text{gs}}(r_d)|\mathcal{T}_{k,\sigma}(t)|\psi_n(r_d)\rangle\,\langle\psi_n(r_d)|c^\dagger_{r_d,\sigma}|\psi_{\text{gs}}(r_d)\rangle \\
&+ \sum_{k,n} F'_n(k)^*\,\langle\psi_{\text{gs}}(r_d)|c_{r_d,\sigma}(t)|\psi_n(r_d)\rangle\,\langle\psi_n(r_d)|\mathcal{T}^\dagger_{k,\sigma}|\psi_{\text{gs}}(r_d)\rangle \\
&+ \sum_{k_1,k_2} F'_n(k_1)F'_n(k_2)^*\,\langle\psi_{\text{gs}}(r_d)|\mathcal{T}_{k_1,\sigma}(t)|\psi_n(r_d)\rangle\,\langle\psi_n(r_d)|\mathcal{T}^\dagger_{k_2,\sigma}|\psi_{\text{gs}}(r_d)\rangle\ ,
\end{aligned}
\tag{1.57}
$$

where $F'_n(k)$ is the truncated Fourier transform $\sum_{r\neq 0} e^{ik\cdot r} F_n(r)$ 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:

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

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 $\nu\sigma$. $\mathcal{G}^>(\mathcal{T}_{\nu,\sigma}, \mathcal{T}_{q,\sigma};\omega)$ is the same but between multiple states in the bath.

Non-local Greens function: $r \neq 0$

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

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

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

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

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

$$\sum_{\boldsymbol{r}_d} \langle \Psi_{\mathrm{gs}} | c_{\boldsymbol{r}_d + \boldsymbol{r}, \sigma}(t) c_{\boldsymbol{r}_d, \sigma}^{\dagger} | \Psi_{\mathrm{gs}} \rangle = \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_d) | c_{\boldsymbol{r}_d, \sigma}(t) T(\boldsymbol{r}) c_{\boldsymbol{r}_d, \sigma}^{\dagger} | \psi_{\mathrm{gs}}(\boldsymbol{r}_d) \rangle$$

$$+ \sum_{\Delta \neq 0} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_d) | c_{\boldsymbol{r}_d + \Delta, \sigma}(t) T^{\dagger}(\Delta - \boldsymbol{r}) c_{\boldsymbol{r}_d, \sigma}^{\dagger} | \psi_{\mathrm{gs}}(\boldsymbol{r}_d) \rangle$$

$$+ \sum_{\boldsymbol{R} \neq \boldsymbol{r}_d} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_d) | c_{\boldsymbol{r}_d, \sigma}(t) T^{\dagger}(\boldsymbol{r}_d - \boldsymbol{R} - \boldsymbol{r}) c_{\boldsymbol{R}, \sigma}^{\dagger} | \psi_{\mathrm{gs}}(\boldsymbol{r}_d) \rangle$$

$$+ \sum_{\boldsymbol{R} \neq \boldsymbol{r}_d, \Delta \neq \boldsymbol{r}_d} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_d) | c_{\Delta, \sigma}(t) T^{\dagger}(\Delta - \boldsymbol{R} - \boldsymbol{r}) c_{\boldsymbol{R}, \sigma}^{\dagger} | \psi_{\mathrm{gs}}(\boldsymbol{r}_d) \rangle \ .$$

$$(1.61)$$

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

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

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

1.4.3 Equal-Time Ground State Correlators: Real-space

We first consider a real-space operator $O(\boldsymbol{r} + \Delta) O^{\dagger}(\boldsymbol{r})$ 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:

$$C_O(\Delta) = \langle \Psi_{\mathrm{gs}} | O(\boldsymbol{r} + \Delta) O^{\dagger}(\boldsymbol{r}) | \Psi_{\mathrm{gs}} \rangle \ . \qquad (1.63)$$

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. **??**):

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

where $\boldsymbol{r}_1$ and $\boldsymbol{r}_1 + \boldsymbol{r}'$ are the positions of the incoming and outgoing auxiliary model states, relative to $\boldsymbol{r}_c + \boldsymbol{r}$, and $\boldsymbol{k}_0$ 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 $\boldsymbol{r}_c$ (which would then allow computations purely within a single auxiliary model), we use the relation: $| \psi_{\mathrm{gs}}(\boldsymbol{x}) \rangle = T^{\dagger}(\boldsymbol{x} - \boldsymbol{r}_c) \psi_{\mathrm{gs}} | \psi(\boldsymbol{r}_c) \rangle$. Substituting this appropriately for both the auxiliary model states gives:

$$C_O(\Delta) = \frac{1}{N} \sum_{\boldsymbol{r}_1, \boldsymbol{r}'} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_c) | T(\boldsymbol{r}_1 + \boldsymbol{r}' + \boldsymbol{r}) O(\boldsymbol{r} + \Delta) O^{\dagger}(\boldsymbol{r}) T^{\dagger}(\boldsymbol{r}_1 + \boldsymbol{r}) | \psi_{\mathrm{gs}}(\boldsymbol{r}_c) \rangle$$

$$= \frac{1}{N} \sum_{\boldsymbol{r}_1, \boldsymbol{r}'} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_c) | T(\boldsymbol{r}') O(\Delta - \boldsymbol{r}_1) O^{\dagger}(-\boldsymbol{r}_1) | \psi_{\mathrm{gs}}(\boldsymbol{r}_c) \rangle \qquad (1.65)$$

$$= \frac{1}{N} \sum_{\boldsymbol{r}_1, \boldsymbol{r}'} \langle \psi_{\mathrm{gs}}(\boldsymbol{r}_c + \boldsymbol{r}') | O(\Delta - \boldsymbol{r}_1) O^{\dagger}(-\boldsymbol{r}_1) | \psi_{\mathrm{gs}}(\boldsymbol{r}_c) \rangle \ .$$

As a final cosmetic change, we transform $r_1 \to -r$:

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

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

Intra-auxiliary model contributions: $r' = 0$

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

$$C_O(\Delta) \to \frac{1}{N} \sum_{r} \langle \psi_{\text{gs}} (r_c) \, | O(\Delta + r)O^\dagger(r) | \psi_{\text{gs}} (r_c) \rangle \ . \tag{1.67}$$

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

$$C_O(\Delta) \to \frac{1}{N} \sum_{r} \sum_{n} \langle \psi_{\text{gs}} (r_c) \, | O(\Delta + r) \, | \psi_n (r_c) \rangle \langle \psi_n (r_c) | \, O^\dagger(r) | \psi_{\text{gs}} (r_c) \rangle \ . \tag{1.68}$$

For the excitations that exist purely in the conduction bath ($r \neq r_c$), 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

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

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 $\mathcal{P}_{\text{gs}}$ 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

$$C_O(\Delta) \to \frac{1}{N} \sum_{r} \langle \psi_{\text{gs}} (r_c) \, | \tilde{O}(\Delta + r) | \psi_{\text{gs}} (r_c) \rangle \langle \psi_{\text{gs}} (r_c) \, | \tilde{O}^\dagger(r) | \psi_{\text{gs}} (r_c) \rangle \ . \tag{1.70}$$

This can be interpreted as the fact that within our auxiliary model formalism, the correlation between the sites r and $\Delta + r$ 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: $r' \neq 0$

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

$$C_O(\Delta) \to \frac{1}{N} \sum_{r' \neq 0} \langle \psi_{\text{gs}} (r_c + r') \, | \tilde{O}(\Delta + r) | \psi_{\text{gs}} (r_c) \rangle \langle \psi_{\text{gs}} (r_c) \, | \tilde{O}^\dagger(r) | \psi_{\text{gs}} (r_c) \rangle \ . \tag{1.71}$$

1.4.4 Equal-Time Ground State Correlators: Momentum-space

We now consider momentum space correlations, through a general operator $O(k_2)O^\dagger(k_1)$:

$$C_O(k_1, k_2) = \langle \Psi_{\text{gs}} | O(k_2) O^\dagger(k_1) | \Psi_{\text{gs}} \rangle \ . \tag{1.72}$$

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. **??**):

$$C_O(k_1, k_2) = \frac{1}{N} \sum_{r_1, r_2} \langle \psi_{\text{gs}}(r_2) | O(k_2) O^\dagger(k_1) | \psi_{\text{gs}}(r_1) \rangle \ , \tag{1.73}$$

where r_1 and 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 r_c (which would then allow computations purely within a single auxiliary model), we use the relation: $|\psi_{\text{gs}}(x)\rangle = T^\dagger(x - r_c)\psi_{\text{gs}}|\psi(r_c)\rangle$. Substituting this appropriately for both the auxiliary model states gives:

$$C_O(k_1, k_2) = \frac{1}{N} \sum_{r_1, r_2} \langle \psi_{\text{gs}}(r_c) | T(r_2 - r_c) O(k_2) O^\dagger(k_1) T^\dagger(r_1 - r_c) | \psi_{\text{gs}}(r_c) \rangle \ . \tag{1.74}$$

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

Momentum-conserving operators: $[O(k), n_k] = 0$

For these operators, the expression for the correlation gives

$$\begin{aligned} C_O(k_1, k_2) &= \frac{1}{N} \sum_{r_1, r_2} \langle \psi_{\text{gs}}(r_c) | T(r_2 - r_1) O(k_2) O^\dagger(k_1) | \psi_{\text{gs}}(r_c) \rangle \\ &= \sum_{\Delta} \langle \psi_{\text{gs}}(r_c + \Delta) | O(k_2) O^\dagger(k_1) | \psi_{\text{gs}}(r_c) \rangle \ . \end{aligned} \tag{1.75}$$

To obtain the last form, we defined $\Delta = r_2 - r_1$ as the distance between the incoming and outgoing auxiliary model states, and preformed the sum over the free variable 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 $\tilde{O}(k) = O(k)O^\dagger(d)\mathcal{P}_{\text{gs}}$, we get

$$C_O(k_1, k_2) = \sum_{\Delta} \langle \psi_{\text{gs}}(r_c + \Delta) | \tilde{O}(k_2) | \psi_{\text{gs}}(r_c) \rangle \langle \psi_{\text{gs}}(r_c) | \tilde{O}^\dagger(k_1) | \psi_{\text{gs}}(r_c) \rangle \ . \tag{1.76}$$

Non-momentum-conserving operators: $[O(k), n_k] \neq 0$

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

$$
\begin{aligned}
C_O(k_1, k_2) &= \frac{1}{N} \sum_{r_1, r_2} \langle \psi_{\text{gs}}(r_c) | T(r_2 - r_1) O(k_2) O^\dagger(k_1) | \psi_{\text{gs}}(r_c) \rangle \, e^{2i(r_1 - r_c) \cdot (k_1 - k_2)} \\
&= \delta_{k_1, k_2} \sum_{\Delta} \langle \psi_{\text{gs}}(r_c + \Delta) | O(k_2) O^\dagger(k_1) | \psi_{\text{gs}}(r_c) \rangle \ .
\end{aligned}
\tag{1.77}
$$

For this expression, we again defined Δ similar to before, and carried out the sum of r_1 involving the exponential to obtain a factor of $N \delta_{k_1, k_2}$. The Kronecker delta factor is a manifestation of translational invariance and the associated total momentum conservation.

As it stands, operators like $O(k_1)$ 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. 1.69. 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

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

where $\text{Tr}\left[\cdot\right]$ 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:

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

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 $S_{\text{EE}}^{\text{loc}} = \frac{1}{N} \sum_r S_{\text{EE}}(r)$. 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 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

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

where $\boldsymbol{r}_d$ is the impurity site position, $\boldsymbol{r}$ is the distance of a conduction bath site from the impurity site (can be zero), and $S_{\text{EE}}(\boldsymbol{r}_d + \boldsymbol{r})$ is the entanglement entropy, calculated within the impurity model, at the locatiom $\boldsymbol{r}_d + \boldsymbol{r}$. $S_{\text{EE}}^{(0)}(\boldsymbol{r}_d + \boldsymbol{r})$ 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 $S_{\text{EE}}(\boldsymbol{q})$ of a single excitation carrying momentum $\boldsymbol{q}$. Unlike $S_{\text{EE}}^{\text{loc}}$, this does not involve an average, and involves a single computation:

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

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

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

where $\text{Tr}_{\boldsymbol{q}} [\cdot]$ is the partial trace over the Hilbert space of $\boldsymbol{q}$, 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:

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

where $|\psi_{\text{gs}}(\boldsymbol{r}_d)\rangle$ is a reference auxiliary model ground state, and $|\psi_{\text{gs}}(\boldsymbol{r}_d + \boldsymbol{r})\rangle$ 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 $\Psi_{\vec{k}}(\{\boldsymbol{r}_k\})$ transforms like Bloch functions under translation by a displacement $\boldsymbol{r}$:

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

$$(1.84)$$

In the last equation, we transformed $\boldsymbol{r}_i \to \boldsymbol{r}_j = \boldsymbol{r}_i - \boldsymbol{r}$. Note that the argument $\boldsymbol{a}$ 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:

$$\Psi_{\vec{k}}^n(\{\boldsymbol{r}_k\}) = \sum_{\boldsymbol{r}_i,\boldsymbol{a}} \frac{e^{i\vec{k}\cdot\vec{R}_i}}{\lambda_{|\vec{k}\rangle}\mathcal{Z}N}\psi_{\mathrm{aux}}(\{\boldsymbol{r}_d - \boldsymbol{r}_i, \boldsymbol{r}_0 - \boldsymbol{r}_i - \boldsymbol{a}\}) = \frac{e^{i\vec{k}\cdot\frac{1}{N}\sum_k \vec{r}_k}}{\lambda_{|\vec{k}\rangle}\mathcal{Z}N} \sum_{\boldsymbol{r}_i,\boldsymbol{a}} e^{-i\vec{k}\cdot\left(\frac{1}{N}\sum_k \boldsymbol{r}_k - \vec{R}_i\right)}\psi_{\mathrm{aux}}(\{\boldsymbol{r}_d - \boldsymbol{r}_i, \boldsymbol{r}_0 - \boldsymbol{r}_i - \boldsymbol{a}$$

$$= e^{i\vec{k}\cdot\vec{r}_{\mathrm{COM}}}\eta_{\vec{k}}(\{\boldsymbol{r}$$

$$(1.85)$$

where $\boldsymbol{r}_{\mathrm{COM}} = \frac{1}{N}\sum_k \boldsymbol{r}_k$ is the center-of-mass coordinate and $\eta_{\vec{k}}(\{\boldsymbol{r}_k\}) = \frac{1}{\lambda_{|\vec{k}\rangle}\mathcal{Z}N} \sum_{\boldsymbol{r}_i} e^{-i\vec{k}\cdot\left(\frac{1}{N}\sum_k \boldsymbol{r}_k - \vec{R}_i\right)}\psi_{\mathrm{aux}}^n(\{\boldsymbol{r}_k - \boldsymbol{r}$ 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:

$$\langle\Psi_{\vec{k}'}|\Psi_{\vec{k}}\rangle = \frac{1}{\lambda_{|\vec{k}'\rangle}^*\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{a},\boldsymbol{a}'} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)}\langle\psi_{\mathrm{aux}}(\boldsymbol{r}_j, \boldsymbol{a}')|\psi_{\mathrm{aux}}(\boldsymbol{r}_i, \boldsymbol{a})\rangle$$

$$= \frac{1}{\lambda_{|\vec{k}'\rangle}^*\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{a},\boldsymbol{a}'} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)}\langle\psi_{\mathrm{aux}}(\boldsymbol{r}_0, \boldsymbol{a}')T^\dagger(\boldsymbol{r}_0 - \boldsymbol{r}_j)T(\boldsymbol{r}_0 - \boldsymbol{r}_i)|\psi_{\mathrm{aux}}(\boldsymbol{r}_0, \boldsymbol{a})\rangle$$

$$(1.86)$$

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:

$$
\begin{aligned}
\langle\Psi_{\vec{k}'}|\Psi_{\vec{k}}\rangle &= \frac{1}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{r_i, r_j, a, a', \vec{q}} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)} \langle\psi_{\text{aux}}(r_0, a')\, T\,(r_j - r_i)\,|\vec{q}\rangle\langle\vec{q}|\,\psi_{\text{aux}}(r_0, a)\rangle \\
&= \frac{1}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{r_i, r_j, a, a', \vec{q}} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)} \langle\psi_{\text{aux}}(r_0, a')\, e^{i\vec{q}\cdot(r_j - r_i)}\,|\vec{q}\rangle\langle\vec{q}|\,\psi_{\text{aux}}(r_0, a)\rangle \\
&= \frac{1}{|\lambda_{|\vec{k}\rangle}|^2 \mathcal{Z}^2}\delta_{\vec{k},\vec{k}'} \sum_{a, a'} \langle\psi_{\text{aux}}(r_0, a')\,|\vec{k}\rangle\langle\vec{k}|\,\psi_{\text{aux}}(r_0, a)\rangle
\end{aligned}
$$

$$(1.87)$$

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

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

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:

$$
\begin{aligned}
\langle\Psi_{\vec{k}'}|\,H_{\text{H-H}}\,|\Psi_{\vec{k}}\rangle &= \frac{1}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{r_i, r_j, r_k, a, a'} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)} \langle\psi_{\text{aux}}(r_j, a')|\,H_{\text{aux}}(r_k)\,|\psi_{\text{aux}}(r_i, a)\rangle \\
&= \frac{1}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{r_i, r_j, r_k, a, a'} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)} \langle\psi_{\text{aux}}(r_0, a')|\,T^\dagger_{r_0-r_j}T_{r_0-r_k}H_{\text{aux}}(r_0)\,T^\dagger_{r_0-r_k}T_{r_0-r_i}\,|\psi_{\text{aux}}(r_0, a)\rangle \\
&= \frac{1}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \sum_{r_i, r_j, r_k, a, a'} e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)} \langle\psi_{\text{aux}}(r_0, a')|\,T^\dagger_{r_k-r_j}H_{\text{aux}}(r_0)\,T_{r_k-r_i}\,|\psi_{\text{aux}}(r_0, a)\rangle
\end{aligned}
$$

$$(1.89)$$

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\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)}}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \langle \psi_{\text{aux}}\left(r_0, a'\right) |\vec{q}'\rangle \langle \vec{q}'| T^\dagger_{r_k - r_j} H_{\text{aux}}\left(r_0\right) T_{r_k - r_i} |\vec{q}\rangle \langle \vec{q}|\psi_{\text{aux}}\left(r_0, a\right)\rangle \\[6pt]
&= \sum_{\substack{r_i, r_j, r_k, \\ a, a', \vec{q}, \vec{q}'}} \frac{e^{i\left(\vec{k}\cdot\vec{R}_i - \vec{k}'\cdot\vec{R}_j\right)}}{\lambda^*_{|\vec{k}'\rangle}\lambda_{|\vec{k}\rangle}\mathcal{Z}^2 N^2} \langle \psi_{\text{aux}}\left(r_0, a'\right) |\vec{q}'\rangle e^{-i\vec{q}'\cdot\left(r_k - r_j\right)} e^{i\vec{q}\cdot\left(r_k - r_i\right)} \langle \vec{q}'|H_{\text{aux}}\left(r_0\right) |\vec{q}\rangle \langle \vec{q}|\psi_{\text{aux}}\left(r_0, a\right)\rangle \\[6pt]
&= \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}}\left(r_0, a'\right) |\vec{q}'\rangle \langle \vec{q}'|H_{\text{aux}}\left(r_0\right) |\vec{q}\rangle \langle \vec{q}|\psi_{\text{aux}}\left(r_0, a\right)\rangle \\[6pt]
&= \frac{N}{|\lambda_{|\vec{k}\rangle}|^2 \mathcal{Z}^2} \delta_{kk'} \sum_{a, a'} \langle \psi_{\text{aux}}\left(r_0, a'\right) |\vec{k}\rangle \langle \vec{k}|H_{\text{aux}}\left(r_0\right) |\vec{k}\rangle \langle \vec{k}|\psi_{\text{aux}}\left(r_0, a\right)\rangle \\[6pt]
&= \frac{N}{|\lambda_{|\vec{k}\rangle}|^2 \mathcal{Z}^2} \delta_{kk'} \langle \vec{k}|H_{\text{aux}}\left(r_0\right) |\vec{k}\rangle \underbrace{\sum_{a, a'} \langle \psi_{\text{aux}}\left(r_0, a'\right) |\vec{k}\rangle \langle \vec{k}|\psi_{\text{aux}}\left(r_0, a\right)\rangle}_{w^2 |\lambda_{|\vec{k}\rangle}|^2} \\[6pt]
&= N\delta_{kk'} \langle \vec{k}|H_{\text{aux}}\left(r_0\right) |\vec{k}\rangle
\end{aligned}
$$

$$(1.90)$$

The momentum eigenket $|\vec{k}\rangle$ can be expressed as a sum over position eigenkets at varying distances from 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 r_0, and improvements are then made by considering auxiliary models at further distances.

Bibliography

[1] Richard M. Martin, Lucia Reining, and David M. Ceperley. *Interacting Electrons: Theory and Computational Approaches*. Cambridge University Press, 2016.

[2] Anirban Mukherjee and Siddhartha Lal. Scaling theory for mott–hubbard transitions: I. t = 0 phase diagram of the 1/2-filled hubbard model. *New Journal of Physics*, 22(6):063007, jun 2020.

[3] Anirban Mukherjee and Siddhartha Lal. Scaling theory for mott–hubbard transitions-II: quantum criticality of the doped mott insulator. *New Journal of Physics*, 22(6):063008, jun 2020.

[4] Anirban Mukherjee and Siddhartha Lal. Holographic unitary renormalisation group for correlated electrons-i: a tensor network approach. *Nuclear Physics B*, 960:115170, 2020.

[5] Anirban Mukherjee and Siddhartha Lal. Holographic unitary renormalisation group for correlated electrons-ii: insights on fermionic criticality. *Nuclear Physics B*, 960:115163, 2020.

[6] Siddhartha Patra and Siddhartha Lal. Origin of topological order in a cooper-pair insulator. *Phys. Rev. B*, 104:144514, Oct 2021.

[7] Santanu Pal, Anirban Mukherjee, and Siddhartha Lal. Correlated spin liquids in the quantum kagome antiferromagnet at finite field: a renormalization group analysis. *New Journal of Physics*, 21(2):023019, feb 2019.

[8] Daria Gazizova and J. P. F. LeBlanc. Emergent nearest-neighbor attraction in the fully renormalized interactions of the single-band repulsive hubbard model at weak coupling, arxiv:2307.02360, 2023.

[9] Alexandrina Stoyanova. *Delocalized and correlated wave functions for excited states in extended systems*. PhD thesis, University of Groningen, 2006.