

Auxiliary Model Approach to Strongly-Correlated Systems

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March 10, 2022

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Chapter 1

Introduction

1.1 Philosophy of the auxiliary model method

The method is closely tied to the auxiliary system approach described in [1]. We can view the full Hamiltonian as a sum of two component Hamiltonians H_1, H_2 connected via the interaction term H_{12} .

$$H = \begin{pmatrix} H_1 & H_{12} \\ H_{12}^* & H_2 \end{pmatrix} = H_1 |1\rangle \langle 1| + H_2 |2\rangle \langle 2| + H_{12} |1\rangle \langle 2| + H_{12}^* |2\rangle \langle 1| \quad (1.1.1)$$

where $|1\rangle$ ($|2\rangle$) actually represents a sum over all basis kets of subsystem 1 (subsystem 2). As an example, we can split the the Hubbard model Hamiltonian between a particular site $i = p$ and the rest of the lattice as follows:

$$\begin{aligned} H_{\text{hubb}} = & \overbrace{U^H \hat{n}_{p\uparrow} \hat{n}_{p\downarrow} - \mu^H \sum_{\sigma} \hat{n}_{p\sigma}}^{H_1} \\ & + \underbrace{U^H \sum_{i \neq p} \hat{n}_{i\uparrow} \hat{n}_{p\downarrow} - \mu^H \sum_{i \neq p, \sigma} \hat{n}_{i\sigma} - t^H \sum_{\substack{\sigma, \langle i, j \rangle \\ i \neq p \neq j}} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.})}_{H_2} \\ & - \underbrace{t^H \sum_{\substack{\sigma, \\ i \in \text{N.N. of } p}} (c_{i\sigma}^\dagger c_{p\sigma} + \text{h.c.})}_{H_{12} + H_{12}^*} \end{aligned} \quad (1.1.2)$$

The Greens function of the full Hamiltonian can also be split in a similar fashion:

$$G(\omega) = \begin{pmatrix} G_1 & G_{12} \\ G_{12}^* & G_2 \end{pmatrix} \quad (1.1.3)$$

The subsystem 1 is usually taken to be the "smaller system", and consequently, subsystem 2 represents the "bath". The smaller system is typically chosen such that its eigenstates are known exactly. Progress is then made by choosing a simpler version of the bath H_2 and a simpler form also for its coupling H_{12} with the smaller system. This combination of the smaller system and the simpler bath is then called the *auxiliary system*. A typical auxiliary system for the Hubbard model would be the SIAM, where the impurity represents an arbitrary site p of the lattice, the bath represents the rest of the lattice sites and the hybridisation term between the impurity and the bath represents the coupling term H_{12} . Such a construction is shown in fig. 1.1. *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*

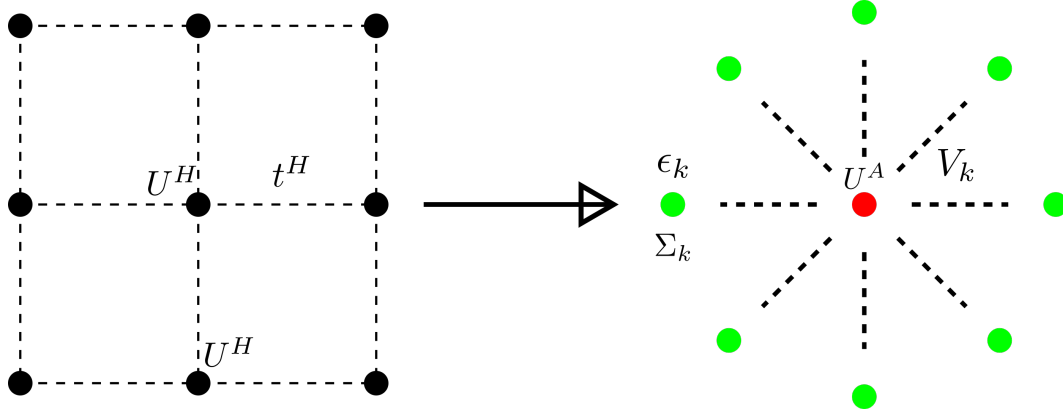


Figure 1.1: *Left*: Full Hubbard model lattice with onsite repulsion U^H on all sites and hopping between nearest neighbour sites with strength t^H . *Right*: Extraction of the auxiliary (cluster+bath) system from the full lattice. The central site on left becomes the impurity site (red) on the right (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 .

(which is a single site). This distinction breaks the translational symmetry of the Hubbard model. For eg., if one chooses eq. 1.2.2 as the auxiliary system, then the fact that the impurity has an onsite correlation while the bath only has a global capacitive cost ($\sim U_b N^2$) means we have broken the symmetry between the cluster and the bath.

The algorithm of DMFT then involves starting with some local self-energy of the bath, $\Sigma(\omega)$, and using an impurity solver to calculate the impurity Greens function in the presence of this self-energy. This impurity Greens function is then used to calculate the impurity self-energy $\Sigma_d(\omega)$, and the self-energy of the bath is then set equal to this impurity self-energy: $\Sigma(\omega) = \Sigma_d(\omega)$, because we expect, on grounds of the lattice symmetry, that the impurity is the same as any other site in the bath. This is said to be the self-consistency step, because the bath self-energy is completely determined only at the end. With this updated bath self-energy, one then repeats the entire process until there is no further change in the bath self-energy at the self-consistency step.

1.2 What is the minimal impurity model for a Mott MIT?

A correlated single impurity site connected with a non-interacting bath with a uniform density of states leads to a well-defined Kondo resonance at low temperatures, as seen in the impurity spectral function. Increasing the impurity correlation U 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 , but the resonance never dies. The situation is however different if the impurity is embedded in a correlated conduction bath with a non-trivial density of states. For the case of a conduction band with the DOS shown in the right of the figure below, the impurity hybridises into a reduced bandwidth because of the correlation on the lattice. This difference is what leads to a metal-insulator transition of a bulk Hubbard model under dynamical mean-field theory (DMFT). Under self-consistency, the non-interacting bath gets modified into one with a highly-correlated self-energy. At low U , the impurity spectral function remains gapless, but at sufficiently large U , the bath is able to kill the Kondo resonance and lead to an insulating state. *This leaves open the following question: What is the minimal correlation one can insert into the non-interacting bath (of a single-impurity Anderson model) that can capture both the metallic and insulating phases of the bulk model?* [2]

This is an attempt to obtain various quantities like Greens functions, self-energies, spectral functions and (if possible) energies and wavefunctions of the Hubbard model, using a cluster-bath approach. The cluster-bath system is taken to be a single-impurity Anderson model with a correlated bath. The correlation will be brought about in two ways: a self-energy $\Sigma(k, \omega)$ of the bath, and a double occupancy repulsion cost U_b . The Hubbard and the correlated single-impurity Anderson models are defined using the Hamiltonians

$$H_{\text{hubb}} = -t^H \sum_{\sigma, \langle i, j \rangle} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U^H \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu^H \sum_{i\sigma} \hat{n}_{i\sigma} \quad (1.2.1)$$

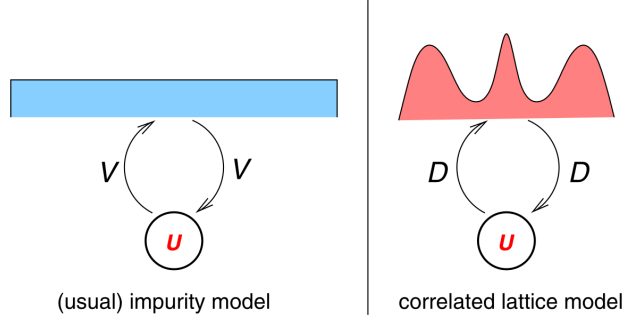


Figure 1.2: "Comparison of the usual Anderson impurity model of a strongly interacting site coupled via V to an uncorrelated featureless and wide conduction-electron band (left-hand side) and the Hubbard model situation (right-hand side). In the latter case, an electron leaving a correlated site moves within the strongly correlated and narrow band of the central peak. In this situation there is a kink at the effective Kondo energy scale which is smaller than the width of the narrow band." Image and caption source in footnote.

$$H_{\text{siam}} = \sum_{k\sigma} [\epsilon_k + \Sigma(k, \omega)] \hat{n}_{k\sigma} + \epsilon_d^A \sum_{\sigma} \hat{n}_{d\sigma} + U^A \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} + U_b \sum_{kk'} \hat{n}_k \hat{n}_{k'} - t^A \sum_{k\sigma} (c_{d\sigma}^\dagger c_{k\sigma} + \text{h.c.}) \quad (1.2.2)$$

Broadly speaking, the method involves first solving the SIAM using a unitary renormalisation group approach, to get the low energy effective theory, and then combining the low energy Hamiltonians in a symmetrized fashion to get the Hamiltonian for the Hubbard model lattice. It is reminiscent of dynamical mean-field theory (DMFT) - both involve an impurity-solver that solves an auxiliary system. The difference, however, lies in the following points:

- While DMFT primarily works with Greens functions and self-energies, this method involves Hamiltonians. The impurity-solver in DMFT provides an impurity Greens function (which is then equated with the local Greens function of the bath), while the impurity-solver in this method actually provides a low energy Hamiltonian.
- The final step of DMFT is the self-consistency equation, where the impurity and bath-local quantities are set equal. This ensures all sites, along with the impurity site, have the same self-energy, something which is required on grounds of translational invariance. The present method, however, brings about the translational invariance in a different way. It symmetrizes the Hamiltonians itself, such that all quantities then derived from the Hamiltonian are then guaranteed to have the symmetry.

The meaning of each of these statements will become clearer when we describe the method in more detail.

Chapter 2

Physics of the generalised single-impurity Anderson model

2.1 Introduction of spin-exchange and charge isospin-exchange interactions into the SIAM: the generalised SIAM

We will now study the generalised SIAM obtained by introducing spin-exchange and charge isospin-exchange interactions between the impurity and the conduction bath. Such terms are generated when one does a Schrieffer-Wolff transformation on the SIAM, but we will find it prudent to keep these terms in the bare model itself.

The spin-exchange interaction has the form

$$J\vec{S}_d \cdot \vec{s} = J \left[S_d^z s^z + \frac{1}{2} (S_d^+ s^- + S_d^- s^+) \right], \quad (2.1.1)$$

where $\vec{S}_d = (S_d^x, S_d^y, S_d^z) = \sum_{\alpha\beta} \vec{\sigma}_{\alpha\beta} c_{d\alpha}^\dagger c_{d\beta}$ is the impurity spin operator, $\vec{s} = \sum_{kk'\alpha\beta} \vec{\sigma}_{\alpha\beta} c_{k\alpha}^\dagger c_{k'\beta}$ is the spin operator for the conduction bath and J is the spin-exchange coupling. The bath spin operator actually acts locally, as can be seen by Fourier transforming to real space (using the definition $f(k) = \frac{1}{\sqrt{N}} \sum_r g(r) \exp(ikr)$):

$$\vec{s} = \sum_{kk'rr'} \frac{1}{N} e^{ikr - ik'r'} \vec{\sigma}_{\alpha\beta} c_{r\alpha}^\dagger c_{r'\beta} = \sum_{rr'} \frac{1}{N} \vec{\sigma}_{\alpha\beta} c_{r\alpha}^\dagger c_{r'\beta} N \delta(r) \delta(r') = \vec{\sigma}_{\alpha\beta} c_{0\alpha}^\dagger c_{0\beta} \quad (2.1.2)$$

In order to introduce the charge isospin coupling, we define the Nambu spinor [3, 4] $\psi^k = \begin{pmatrix} c_{k\uparrow} & c_{k\downarrow}^\dagger \end{pmatrix}$, and the charge isospin [5] for the mobile conduction electrons

$$\vec{C} = \sum_{kk'} \psi^{k\dagger} \vec{S} \psi^{k'} = \frac{1}{2} \sum_{kk'\alpha\beta} \psi_\alpha^{k\dagger} \vec{\sigma}_{\alpha\beta} \psi_\beta^{k'} \quad (2.1.3)$$

The various components of the isospin are

$$\begin{aligned} C^z &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\sigma}^z \psi_\sigma^{k'} = \frac{1}{2} \sum_{kk'\sigma} \left(c_{k\sigma}^\dagger c_{k'\sigma} - \frac{1}{2} \delta_{kk'} \right) \\ C^x &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^x \psi_{\bar{\sigma}}^{k'} = \sum_{kk'\sigma} \frac{\sigma}{4} \left(c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger + \text{h.c.} \right) \\ C^y &= \sum_{kk'\sigma} \frac{1}{2} \psi_\sigma^{k\dagger} \sigma_{\sigma\bar{\sigma}}^y \psi_{\bar{\sigma}}^{k'} = \sum_{kk'\sigma} -\frac{i\sigma}{4} \left(c_{k\sigma}^\dagger c_{k'\bar{\sigma}}^\dagger - \text{h.c.} \right) \end{aligned} \quad (2.1.4)$$

It is easy to verify that these operators satisfy the SU(2) commutation algebra. For example, if we write $C^x = A + A^\dagger$ and $C^y = B + B^\dagger$, then $[C^x, C^y] = [A, B^\dagger] - \text{h.c.}$, where

$$[A, B^\dagger] = \frac{1}{4} \sum_{kk', qq'} \left[c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, i c_{q'\downarrow} c_{q\uparrow} \right] = \frac{i}{4} \sum_{kq} \left(c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger \right) \quad (2.1.5)$$

and therefore

$$\Rightarrow [C^x, C^y] = \frac{i}{2} \sum_{kq} (c_{k\uparrow}^\dagger c_{q\uparrow} - c_{k\downarrow} c_{q\downarrow}^\dagger) = iC^z \quad (2.1.6)$$

There are similar operators for the impurity electron:

$$\psi_d = \begin{pmatrix} c_{d\uparrow} & c_{d\downarrow}^\dagger \end{pmatrix}, \quad \vec{C}_d = \frac{1}{2} \sum_{\beta} \psi_{d,\alpha}^\dagger \vec{\sigma}_{\alpha\beta} \psi_{d,\beta} \quad (2.1.7)$$

The full charge-Kondo interaction can now be written down in terms of these isospins:

$$K \vec{C}_d \cdot \vec{C} = K \left[C_d^z C^z + \frac{1}{2} (C_d^+ C^- + C_d^- C^+) \right] \quad (2.1.8)$$

where $C^\pm \equiv C^x \pm iC^y$.

$$C^+ = \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow}^\dagger, \quad C^- = \sum_{kk'} c_{k'\downarrow} c_{k\uparrow} \quad (2.1.9)$$

The full generalised Anderson model Hamiltonian, at particle-hole symmetry, is

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 + \sum_{k\sigma} (V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c.) + J \vec{S}_d \cdot \vec{s} + K \vec{C}_d \cdot \vec{C} \quad (2.1.10)$$

For the URG analysis, at each RG step, we decouple the electronic states $q\beta$ on the k -space shell of radius Λ_j . For simplicity, we will only consider those diagonal terms in the denominator that either have both $q\beta$ and $q\bar{\beta}$ or both $q\beta$ and d or both $q\bar{\beta}$ and d . Terms that have purely $q\bar{\beta}$ will not be considered. Also, the scattering between just d and $q\bar{\beta}$ can be ignored since it is diagonal in $q\beta$. The diagonal (number-preserving) part is

$$H_D = \sum_{\beta} \epsilon_q \tau_{q\beta} + \epsilon_d (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 + J S_d^z s_q^z + K C_d^z C_q^z \quad (2.1.11)$$

where $s_q^z = \frac{1}{2} (\hat{n}_{q\uparrow} - \hat{n}_{q\downarrow})$ and $C_q^z = \frac{1}{2} (\hat{n}_{q\uparrow} + \hat{n}_{q\downarrow} - 1)$. The off-diagonal part is:

$$H_X = \sum_{\beta=\uparrow,\downarrow} \left[V c_{d\beta}^\dagger c_{q\beta} + \frac{1}{2} J \sum_{k<\Lambda_N} \left\{ (\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}}) \frac{1}{2} c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right\} + \frac{1}{2} K \sum_{k<\Lambda_N} \left\{ (\hat{n}_d - 1) \frac{1}{2} c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}}^\dagger c_{k\bar{\beta}} c_{q\beta} \right\} \right] + \text{h.c.} \quad (2.1.12)$$

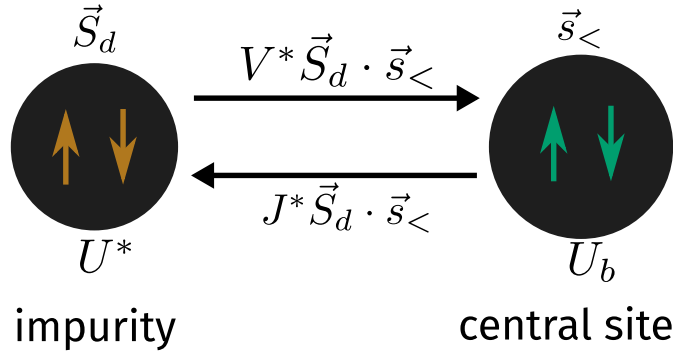


Figure 2.1: While we have studied the full model under renormalisation group, often we will turn to a simplified zero-bandwidth version of the model that is obtained by ignoring the kinetic energy part of the Hamiltonian. This zero-bandwidth model is effectively a two site model.

2.2 RG equations for generalised SIAM

$$\begin{aligned}
\Delta\epsilon_d &= 2V^2 n_j \left(\frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + \frac{n_j}{2} \left(\frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right), \\
\Delta V &= -\frac{3n_j V}{8} \left[J \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + K \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \right], \\
\Delta J &= -\frac{n_j J^2}{\omega - \frac{D}{2} + \frac{J}{4}}, \\
\Delta K &= -\frac{n_j K^2}{\omega - \frac{D}{2} + \frac{K}{4}}
\end{aligned} \tag{2.2.1}$$

In terms of $U = -2\epsilon_d$, the equations become

$$\Delta U = 4V^2 n_j \left(\frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \left(\frac{J^2}{d_2} - \frac{K^2}{d_3} \right), \tag{2.2.2}$$

$$\Delta V = -\frac{3n_j V}{8} \left[J \left(\frac{1}{d_2} + \frac{1}{d_1} \right) + K \left(\frac{1}{d_3} + \frac{1}{d_0} \right) \right], \tag{2.2.3}$$

$$\Delta J = -\frac{n_j J^2}{d_2}, \quad \Delta K = -\frac{n_j K^2}{d_3} \tag{2.2.4}$$

d_i are the denominators:

$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{K}{4} \tag{2.2.5}$$

2.3 Nature of coupling RG flows

2.3.1 Repulsive interaction on impurity: $U > 0$

For the Hamiltonians with positive on-site correlation, we will assume that the spin-exchange coupling is positive and charge isospin-exchange coupling is negative: $J > 0, K < 0$. This choice is motivated by the signs of the corresponding terms when they are generated via a Schrieffer-Wolff transformation [6]. The impurity-bath hybridisation V is always positive. The sign of the couplings lead to inequalities among the denominators which we will utilise at various points. First of all, since $U > 0$, we have $d_1 - d_2 = \frac{U}{2} > 0$. Secondly, since $K < 0$, we have $d_2 - d_3 = \frac{J-K}{4} > 0$. And finally, we have $d_3 - d_0 = \frac{U}{2} > 0$. Combining these, we can write

$$d_1 > d_2 > d_3 > d_0 \tag{2.3.1}$$

The strong-coupling regime is defined as the range of values of ω where the hybridisation is relevant. This is ensured by the assumption $d_1 < 0$. From eq. 2.3.1, we can then conclude that all denominators are negative: $d_i = -|d_i|$. The simplest consequence of this is the RG flow of K :

$$\Delta K = -\frac{n_j K^2}{d_3} = \frac{n_j K^2}{|d_3|} > 0 \implies K_{j+1} > K_j \implies K_0 = -|K_0|, K^* \rightarrow 0 \tag{2.3.2}$$

K_j is the value of K after the j^{th} RG step, K_0 representing the bare value. In other words, since $d_3 < 0$, the RG equation for K provides an algebraic increment, and the negative K increases and flows towards zero. The $*$ indicates a fixed point value. The isospin coupling is irrelevant in this regime, and we will ignore it.

The coupling J , on the other hand, is relevant and flows from a small positive value towards a large value at strong-coupling.

$$\Delta J = -\frac{n_j J^2}{d_2} = \frac{n_j J^2}{|d_2|} > 0 \implies J_{j+1} > J_j \implies J_0 \rightarrow \text{large } J^* \text{ (strong-coupling)} \tag{2.3.3}$$

The value of J^* is obtained when the denominator d_2 vanishes.

Because of the RG irrelevance of K , we can simplify the RG equation for V :

$$\Delta V = -\frac{3n_j V J}{8} \left(\frac{1}{d_2} + \frac{1}{d_1} \right) = \frac{3n_j V J}{8} \left(\frac{1}{|d_2|} + \frac{1}{|d_1|} \right) > 0 \quad (2.3.4)$$

Since both the denominators are positive, V is relevant. The fixed point value V^* is attained when the denominator d_1 vanishes (d_1 will vanish earlier than d_2).

We can compare the rate of flows of V and J :

$$\frac{\Delta V}{\Delta J} = \frac{3V}{8J} \left(1 + \frac{|d_2|}{|d_1|} \right) > \frac{3V}{4J} \quad (2.3.5)$$

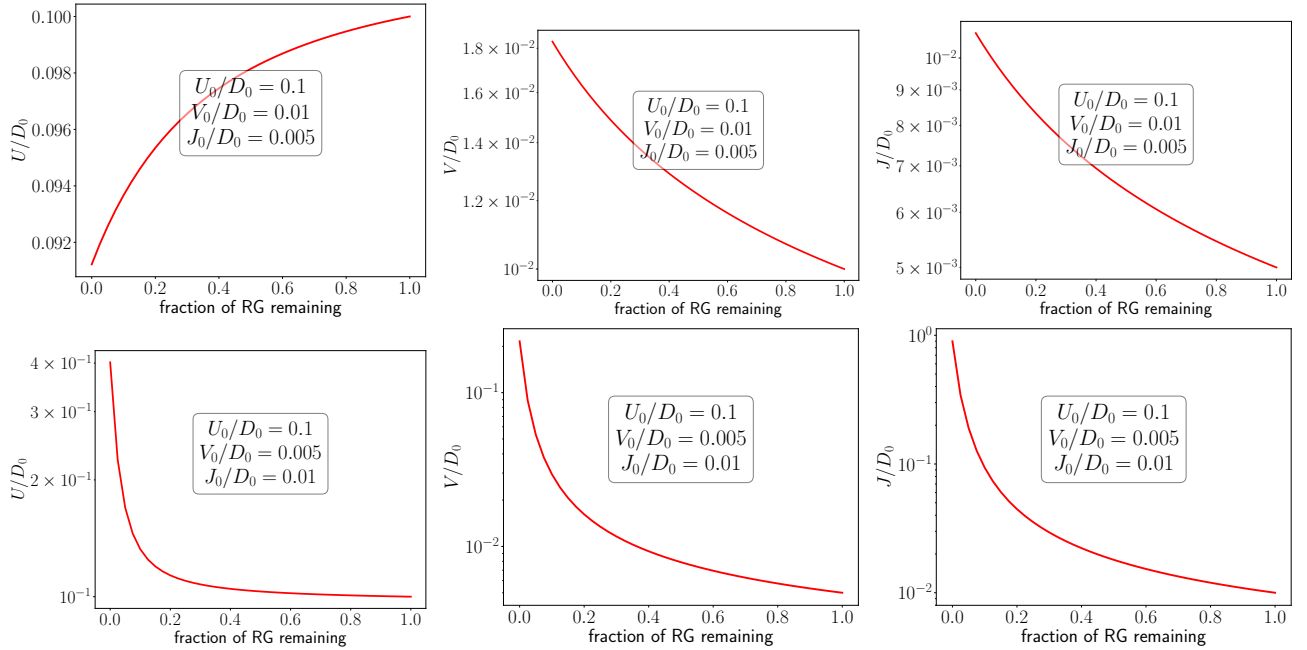
There we used the fact that $|d_2| > |d_1|$. We finally come to the RG equation for U :

$$\Delta U = 4V^2 n_j \left(\frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \frac{J^2}{d_2} = -4V^2 \left(U + \frac{J}{4} \right) \frac{n_j}{d_0 d_1} - \frac{n_j J^2}{d_2} \quad (2.3.6)$$

For $V > J$, we can expect U to be irrelevant. On the other hand, $V < J$ makes U relevant.

In short, the $U > 0$ regime is characterised by an irrelevant isospin-exchange coupling K and a relevant spin-exchange coupling J , and the following set of RG equations for the remaining couplings U and V :

$$\Delta U = 4V^2 n_j \left(\frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \frac{J^2}{d_2}, \quad \Delta V = -\frac{3n_j V J}{8} \left(\frac{1}{d_2} + \frac{1}{d_1} \right) \quad (2.3.7)$$

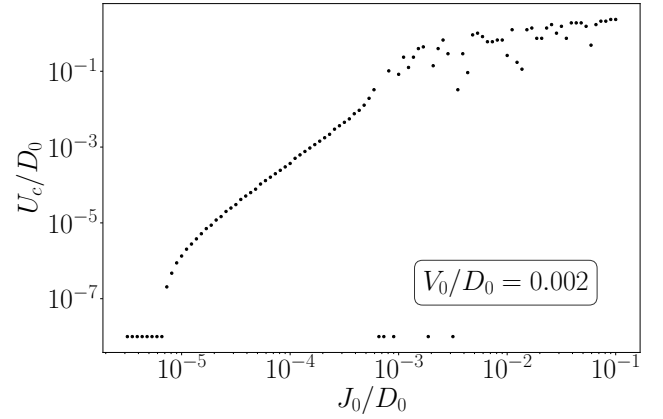
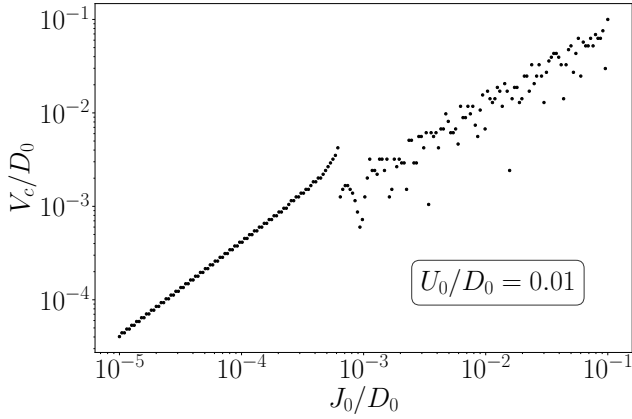
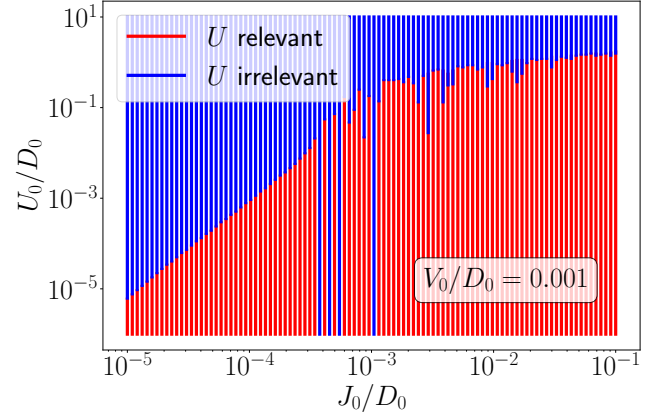
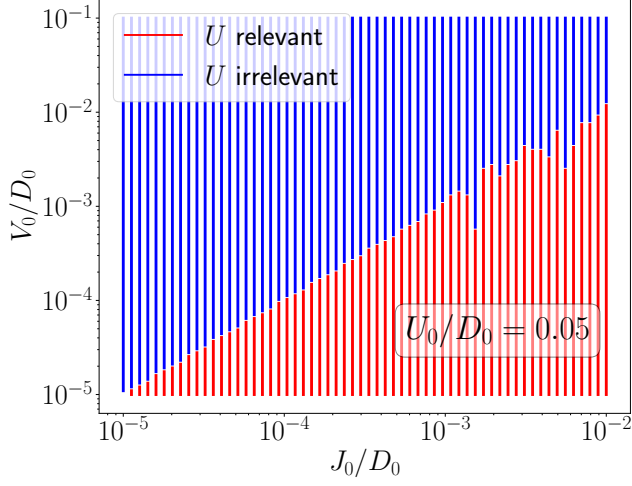


2.3.2 Attractive interaction on impurity: $U < 0$

Here, we have $J < 0$ and $K > 0$. The denominators satisfy the following inequality in this regime:

$$d_0 > d_3 > d_2 > d_1 \quad (2.3.8)$$

The strong-coupling regime here corresponds to $d_0 < 0$. This again means that all the denominators are negative. The spin-exchange coupling J is now irrelevant, because its bare value is negative while its RG equation



is positive: $\Delta J > 0$. Moreover, the isospin coupling K is now positive and so is its RG equation: $\Delta K > 0$, which means it flows to strong-coupling. V also flows to strong-coupling. The RG equation for U can be written as

$$\Delta U = 4V^2 \left(\frac{K}{4} - U \right) \frac{n_j}{d_0 d_1} + \frac{n_j K^2}{d_3} \quad (2.3.9)$$

The first term is necessarily positive, while the second term is negative. This means that for roughly $V_0 > J_0$, we will have $\Delta U > 0$, and since $U_0 < 0$, this amounts to an irrelevant flow of U towards zero. On the other hand, for $J_0 > V_0$, we will have $\Delta U < 0$, and this corresponds to a relevant flow of U towards large negative value.

In other words, the RG flows in this regime can be exactly mapped to those in the positive U regime. The general statement is: in the strong-coupling regime of positive(negative) U , V is always relevant, $J(K)$ is relevant, $K(J)$ is irrelevant, and U is relevant when $J(K) > V$, otherwise U is irrelevant.

2.4 Effective Hamiltonian and ground state

The fixed point Hamiltonian can, in general, be written as

$$\mathcal{H}^* = \sum_{\sigma,k} \epsilon_k \tau_{k\sigma} - \frac{U^*}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 + \sum_{\sigma,k < \Lambda^*} \left(V^* c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} + K^* \vec{C}_d \cdot \vec{C} \quad (2.4.1)$$

The first term is the kinetic energy of all the electrons. The next two terms are the impurity-diagonal pieces, featuring the renormalised interaction U^* . The next three terms are the residual interactions between the impurity and the metal, with the renormalised couplings V^* , J^* and K^* . The summations in these terms extend from the fixed point momentum cutoff Λ^* to 0. This is the region of momentum space which the URG was unable to decouple. The operators \vec{s} and \vec{C} represent the macroscopic magnetic and charge spins formed by the remaining electrons that are lying inside the window $[0, \Lambda^*]$:

$$\vec{s} = \sum_{\substack{k, k' < \Lambda^* \\ \alpha \beta}} c_{k\alpha}^\dagger \vec{\sigma}_{\alpha\beta} c_{k'\beta} \quad (2.4.2)$$

Our goal here is to write down the ground state wavefunction for this low-energy Hamiltonian.

To make progress, we will simplify the effective Hamiltonian by taking the zero bandwidth limit. This reduces it to a two-site problem. One site is of course the impurity site, and this site will be labeled as site 1. The other site will be formed by the center of mass degree of freedom of the conduction electrons, and will be labeled as site 2. The Hamiltonian for this two-site problem is

$$\mathcal{H}_{IR} = -\frac{U^*}{2} (\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow})^2 + V^* \sum_{\sigma} \left(c_{1\sigma}^\dagger c_{2\sigma} + \text{h.c.} \right) + J^* \vec{S}_1 \cdot \vec{S}_2 + K^* \vec{C}_1 \cdot \vec{C}_2 \quad (2.4.3)$$

The subscripts on the operators designate the site on which they act; \hat{n}_1 is the number operator for the first site.

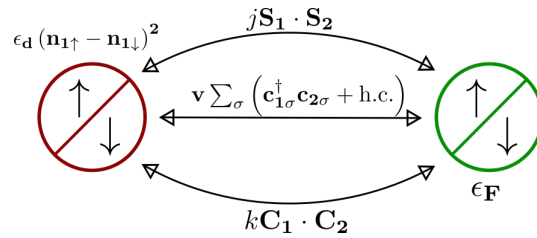


Figure 2.2: Two-site effective problem of fixed point Hamiltonian

We will adopt the following notation to represent the states in this Hilbert space. A general state will be represented in the Fock space basis as $|n_{1\uparrow} n_{1\downarrow} n_{2\uparrow} n_{2\downarrow}\rangle$. For example,

$$|1101\rangle = c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow}^\dagger |-\rangle \quad (2.4.4)$$

$|-\rangle$ is the vacuum state.

For $U > 0$, the ground state is given by

$$|\Psi\rangle_1 = c_s \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_c \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle), \quad E_1 = -V^* \sqrt{\gamma^2 + 4} - \frac{1}{4}U^* - \frac{3}{8}J^* \quad (2.4.5)$$

where $\gamma = \frac{1}{2V^*} \left[\frac{1}{4} (3J^* + K^*) + \frac{1}{2}U^* \right]$. The probabilities for the spin and charge sectors for the ground state are

$$(c_s)^2 = \frac{1}{2\sqrt{\gamma^2 + 4}} (\sqrt{\gamma^2 + 4} + \gamma), \quad (c_c)^2 = \frac{1}{2\sqrt{\gamma^2 + 4}} (\sqrt{\gamma^2 + 4} - \gamma). \quad (2.4.6)$$

For (roughly) $J_0 > V_0$, we get $J^* \gg V^*$ and $U^* \gg U_0$ so that $\gamma \gg 1$. This gives $(c_s)^2 \sim 1$ and $(c_c)^2 \sim 0$. The entire contribution to the ground state then comes from the spin sectors of the two sites. This is calculated numerically in fig. 2.3.

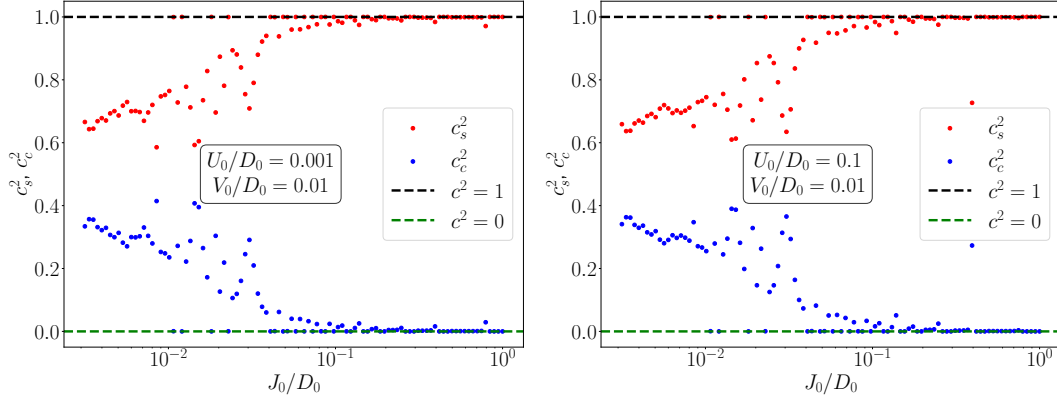


Figure 2.3: Variation of relative weights c_s and c_c with J_0

In the other regime of $U < 0$, the two competing states are $|\Psi\rangle_1$ defined above (with energy E_1), and $|\Psi\rangle_2$, the charge singlet: $|\Psi\rangle_2 = \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle)$ having energy E_2 .

$$E_2 = -\frac{3}{4}K^*, \quad E_1 - E_2 = -\frac{1}{4} \sqrt{\left(\frac{1}{2}K^* + U^*\right)^2 + (4V^*)^2} - \frac{1}{4}U^* + \frac{3}{4}K^* \quad (2.4.7)$$

For $V_0 \gg K_0$, the largest energy scale will be V^* , and we can then approximate this difference as

$$E_1 - E_2 \simeq -V^* < 0 \quad (2.4.8)$$

In such a case, $|\Psi\rangle_1$ will therefore be the ground state. In the other regime $V_0 \ll K_0$, the largest energy scale will be K^* , and we can then write

$$E_1 - E_2 \simeq -\frac{1}{8}K^* + \frac{3}{4}K^* > 0 \quad (2.4.9)$$

In this case, the ground state will be $|\Psi\rangle_2$. There exists, therefore, a phase transition at a critical plane (U_c, K_c, V_c) , where the ground state changes between the charge singlet $|\Psi\rangle_2$ and the spin singlet + charge triplet $|\Psi\rangle_1$.

2.5 Approach towards the thermodynamic limit

The URG method works strictly on finite systems and leads to finite values of fixed point couplings. The behaviour of the Hamiltonian in the thermodynamic limit can then be determined using finite-size scaling where we increase the bandwidth and decrease the width of each RG step. When applied to the fixed point value of the impurity-bath hybridisation parameter V (fig. 2.4), it can be seen that the fixed point value increases as the system size is increased, implying that the continuum limit of V^* is ∞ . This holds for both $V_0 > J_0$ and $V_0 < J_0$, as shown in the two panels of fig. 2.4.

In a similar manner, we checked the variation of the spin and charge probabilities, c_s and c_c , in the ground state, with increasing bandwidth. The result is shown in fig. 2.5. For both $V_0 < J_0$ and $V_0 > J_0$, we see that

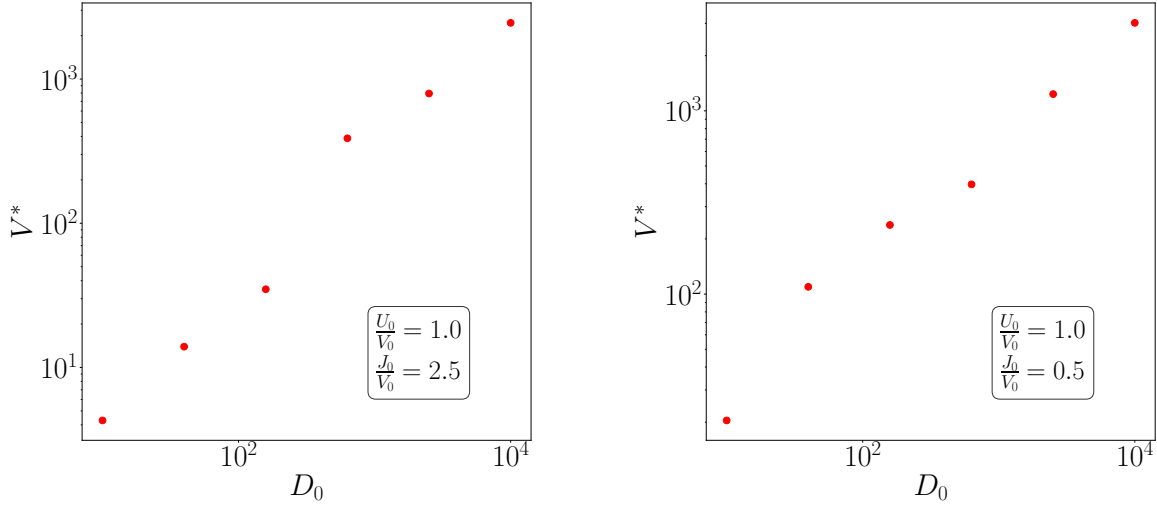


Figure 2.4: Variation of fixed point value V^* with increasing bandwidth D_0 , for both $V_0 > J_0$ and $V_0 < J_0$.

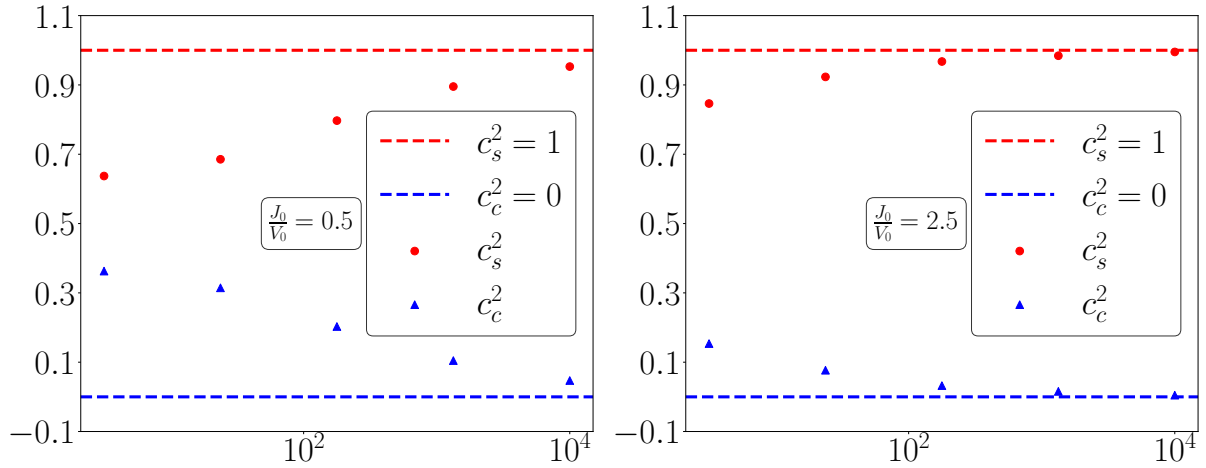


Figure 2.5: Variation of spin and charge fractions, c_s and c_c , of the ground state, as a function of bare bandwidth D_0 . Left and right panels show the cases of $J_0 < V_0$ and $J_0 > V_0$ respectively.

the spin contribution increases towards unity while the charge contribution vanishes. This indicates that at large bandwidth, the ground state becomes purely a spin singlet, formed purely by singly-occupied impurity states.

$$\lim_{D_0 \rightarrow \infty} |\Psi\rangle_1 = \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) \quad (2.5.1)$$

2.6 Effective temperature scale at the fixed point

We will first change the discrete RG equation to a continuum equation by interpreting ΔJ as $\frac{\Delta J}{\Delta \ln D}$, where the denominator is unity: $\Delta \ln D = 1$. Now, since the bandwidth is decreasing under the RG, we can write $\Delta \ln D = -d \ln D$. The continuum equation (for $K = 0$) becomes

$$\frac{dJ}{d \ln D} = n(0)J^2 \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (2.6.1)$$

where we have replaced by the number of states at each shell with that at the Fermi surface (uniform DOS). We can define a dimensionless quantity $g \equiv \frac{J}{\frac{D}{2}} - \omega$. In terms of g , the continuum RG equation becomes

$$-\frac{dg}{d \ln D} + \frac{Dg}{2\omega - D} = \frac{n(0)g^2}{1 - \frac{g}{4}} \quad (2.6.2)$$

Now, for the specific case where D is small ($D \rightarrow 0$), we can simplify and integrate this equation:

$$\begin{aligned} \frac{dg}{d \ln D} &= \frac{n(0)g^2}{\frac{g}{4} - 1} \\ \Rightarrow \left[\frac{1}{g} + \frac{1}{4} \ln g \right]_{g_0}^{g^*} &= n(0) \ln D \Big|_{D_0}^{D^*} \end{aligned} \quad (2.6.3)$$

$g^*(0), D^*(0)$ are the fixed point (bare) values of g, D . From the denominator structure, the fixed-point value is $g^* = 4$. This gives an estimate of the bandwidth of the emergent window:

$$D^* = D_0 \left(\frac{4}{g_0} \right)^{\frac{1}{4n(0)}} \exp \left\{ -\frac{1}{n(0)} \left(\frac{1}{g_0} - \frac{1}{4} \right) \right\} \quad (2.6.4)$$

We can now define a temperature scale for the fixed-point theory:

$$T_K \equiv \frac{2N^*}{\pi} D^* = \frac{2N^*}{\pi} D_0 \left(\frac{4}{g_0} \right)^{\frac{1}{4n(0)}} \exp \left\{ -\frac{1}{n(0)} \left(\frac{1}{g_0} - \frac{1}{4} \right) \right\} \quad (2.6.5)$$

The factor of $2N^*$ is inserted to make the Kondo temperature intensive (we will see below that the N^* allows it to be written in terms of parameters of the two-site Hamiltonian) - $2N^*$ is the total number of momentum states in the fixed point theory. The factor of $\frac{1}{\pi}$ is for aesthetic reasons. Since we have and will primarily work with $\omega = 0$, the fixed point condition can be used to write $D^* = \frac{J^* + K^*}{2}$.

$$T_K = \frac{2N^*}{\pi} \frac{1}{2} (J^* + K^*) = \frac{1}{\pi} (j + k) \quad (2.6.6)$$

2.7 Impurity susceptibilities

2.7.1 Spin susceptibility

The spin susceptibility is defined as

$$\chi(\beta) = \beta \left(\left\langle (S_d^z)^2 \right\rangle - \langle S_d^z \rangle^2 \right) \quad (2.7.1)$$

There is an alternate way of calculating this. We insert a fictitious magnetic field that couples only to the impurity site. The Hamiltonian in the presence of this field is

$$\mathcal{H}'(B) = \mathcal{H} + BS_d^z \quad (2.7.2)$$

The susceptibility is then given by

$$\chi(\beta) = \lim_{B \rightarrow 0} \frac{1}{\beta} \left[\frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 \right] \quad (2.7.3)$$

where $Z(B)$ is the partition function of the Hamiltonian $\mathcal{H}'(B)$. The following is to prove that the RHS of eqs. 2.7.1 and 2.7.3 are the same. We start with 2.7.3. The first derivative can be written as

$$\frac{\partial Z(B)}{\partial B} = \text{Trace} \left[\frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[-\beta S_d^z \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (2.7.4)$$

which means the first term becomes

$$\lim_{B \rightarrow 0} -\frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 = - \left(\beta \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} [S_d^z \exp \{-\beta \mathcal{H}\}] \right)^2 = -\beta^2 \langle S_d^z \rangle^2 \quad (2.7.5)$$

The second derivative is

$$\frac{\partial^2 Z(B)}{\partial B^2} = \text{Trace} \left[-\beta S_d^z \frac{\partial}{\partial B} \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] = \text{Trace} \left[\beta^2 (S_d^z)^2 \exp \left\{ -\beta (\mathcal{H} + BS_d^z) \right\} \right] \quad (2.7.6)$$

so the second term becomes

$$\lim_{B \rightarrow 0} \frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} = \beta^2 \frac{1}{\text{Trace} [\exp \{-\beta \mathcal{H}\}]} \text{Trace} [(S_d^z)^2 \exp \{-\beta \mathcal{H}\}] = \beta^2 \langle (S_d^z)^2 \rangle \quad (2.7.7)$$

The full thing becomes

$$\begin{aligned} \lim_{B \rightarrow 0} \frac{1}{\beta} \left[\frac{1}{Z(B)} \frac{\partial^2 Z(B)}{\partial B^2} - \frac{1}{Z(B)^2} \left(\frac{\partial Z(B)}{\partial B} \right)^2 \right] &= \frac{1}{\beta} \left(-\beta^2 \langle S_d^z \rangle^2 + \beta^2 \langle (S_d^z)^2 \rangle \right) \\ &= \beta \left(\langle (S_d^z)^2 \rangle - \langle S_d^z \rangle^2 \right) \end{aligned} \quad (2.7.8)$$

This completes the proof.

To calculate the impurity susceptibility, we take the zero bandwidth Hamiltonian \mathcal{H}_{IR} and insert a magnetic field to obtain the Hamiltonian in eq. (2.7.2). For a particular regime of U , only one of J or K will be non-zero. We then numerically diagonalise this Hamiltonian to obtain the partition function $Z(B)$ and its derivatives. The spin susceptibility can then be calculated using eq. (2.7.3). The results for $U > 0$ are shown in fig. 2.6.

2.7.2 Charge susceptibility

We can similarly define the charge susceptibility as

$$\chi(\beta) = \beta \left(\langle (C_d^z)^2 \rangle - \langle C_d^z \rangle^2 \right) = \lim_{B_c \rightarrow 0} \frac{1}{\beta} \left[\frac{1}{Z(B_c)} \frac{\partial^2 Z(B_c)}{\partial B_c^2} - \frac{1}{Z(B_c)^2} \left(\frac{\partial Z(B_c)}{\partial B_c} \right)^2 \right] \quad (2.7.9)$$

where B_c is now a field that couples to the impurity charge-isospin:

$$\mathcal{H}'(B_c) = \mathcal{H} + B_c C_d^z \quad (2.7.10)$$

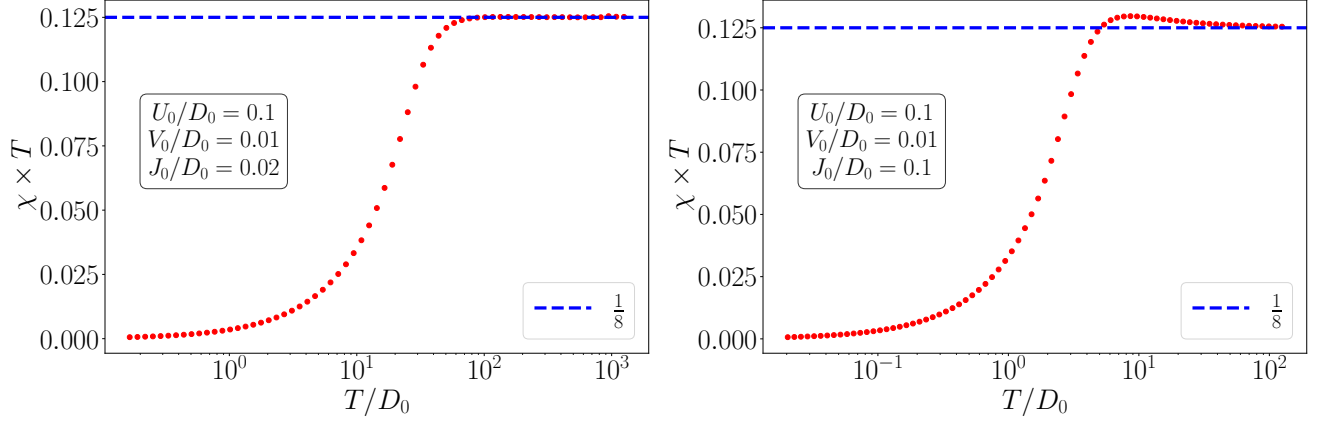


Figure 2.6: Spin susceptibility of the impurity times temperature, for two sets of bare parameters, in $U > 0$. At low temperatures, it becomes linear because χ itself becomes constant (screening), while at high temperatures, $\chi \times T$ becomes constant because of the paramagnetic $\sim 1/T$ form of χ . For the right panel with a larger value of the spin-exchange coupling, the χ tries to go towards the local moment value of $1/4$ but eventually drops back to the free orbital value of $1/8$.

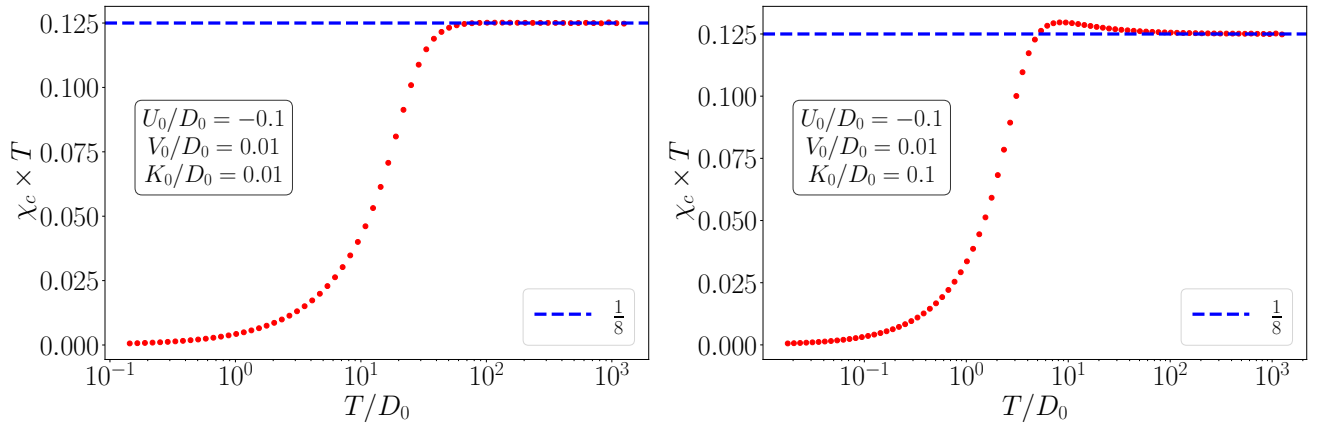


Figure 2.7: Charge susceptibility for the impurity at $U < 0$, for two sets of bare parameters. The physics is very similar to that of the spin susceptibility in $U > 0$.

The charge susceptibility for $U < 0$ is shown in fig. 2.7.

It is interesting to look at the behaviour of the charge susceptibility in the positive U regime, fig. 2.8. It is seen that for $J_0 < V_0$, the charge susceptibility is very similar to the spin susceptibility, with a reduced saturation value. This is because, for that range of bare values, the ground state consists of a comparable mixture of the spin and charge states (see fig. 2.3). This means that the magnetic field term in eq. (2.7.10) can couple to the charge component of the ground state, and give a non-zero charge susceptibility at zero temperature. On the other hand, for $J_0 > V_0$, we see that χ_c vanishes at low temperatures. This can again be understood from the ground state. For that range of bare values, the ground state can be approximated by purely the singlet, because the charge fraction c_-^c becomes very small. This means that the field B_c has nothing to couple with. Alternatively, it can be said that since the ground state has only terms with $\hat{n}_d = 1$, no number fluctuation is possible, and the impurity isospin is not susceptible at all to charge polarisation.

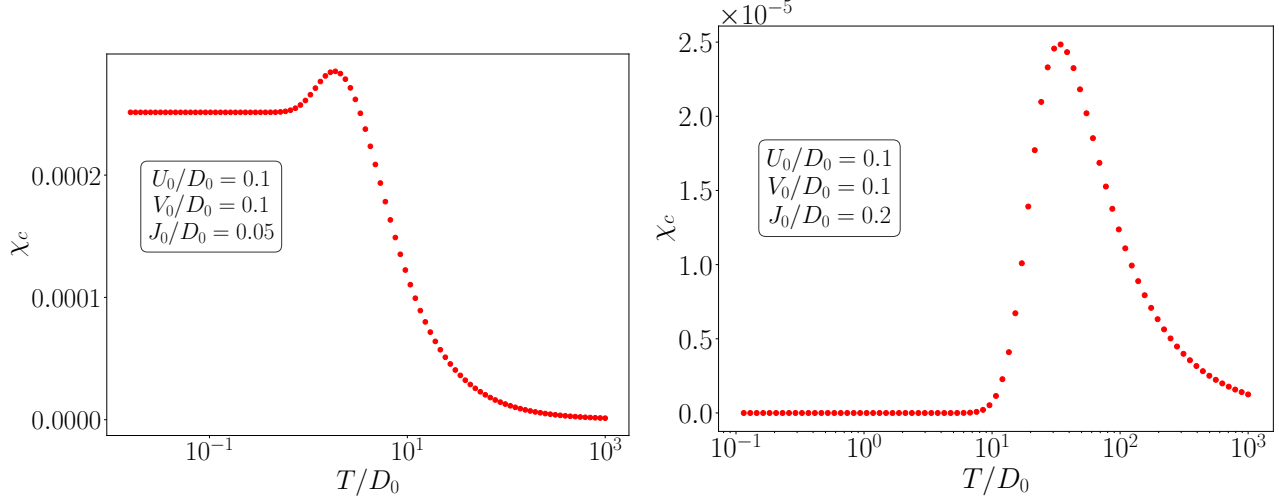


Figure 2.8: Charge susceptibility of the impurity in the positive U regime, for two values of J_0 . The smaller bare value leads to a spin+charge mixed ground state, and hence a non-zero χ_c at zero temperature. The larger J_0 , however, leads to a purely spin ground state without any number fluctuation, and this gives vanishing χ_c at zero temperature.

From eq. (2.5.1), we know that in the thermodynamic limit, the ground state of $U > 0$ regime reduces to a screened local moment. That then implies that the charge susceptibility vanishes at low temperatures, owing to lack of any charge content in the ground state in the large bandwidth limit.

$$\lim_{D_0 \rightarrow \infty} \chi_c(U > 0, T \rightarrow 0) = 0 \quad (2.7.11)$$

2.8 Specific heat

The specific heat is calculated by diagonalizing the fixed point Hamiltonian, numerically. The obtained spectrum is denoted by $\{\mathcal{E}_i\}$. The total average energy of the impurity+cloud at temperature T is then

$$\langle \mathcal{E} \rangle = \frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \quad (2.8.1)$$

where $Z = \sum_i e^{-\beta E_i}$ is the partition function. The specific heat of this system is thus

$$\begin{aligned} C_V &= \frac{\partial \langle \mathcal{E} \rangle}{\partial T} \\ &= -\frac{1}{k_B T^2} \frac{\partial \langle \mathcal{E} \rangle}{\partial \beta} \\ &= \frac{1}{k_B T^2} \left[\frac{1}{Z} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i} - \left(\frac{1}{Z} \sum_i \mathcal{E}_i e^{-\beta \mathcal{E}_i} \right)^2 \right] \end{aligned} \quad (2.8.2)$$

In the absence of impurity, the eigenvalues of the Hamiltonian are $\{\mathcal{E}_i^0\}$ with a partition function $Z^0 = \sum_i e^{-\beta \mathcal{E}_i^0}$, so the bath specific heat is

$$C_V^0 = \frac{1}{k_B T^2} \left[\frac{1}{Z_0} \sum_i \mathcal{E}_i^2 e^{-\beta \mathcal{E}_i^0} - \left(\frac{1}{Z_0} \sum_i \mathcal{E}_i^0 e^{-\beta \mathcal{E}_i^0} \right)^2 \right] \quad (2.8.3)$$

The impurity specific heat is the difference.

$$C_V^{\text{imp}} = C_V - C_V^0 \quad (2.8.4)$$

These values were calculated numerically and plotted against temperature in fig. 2.9.

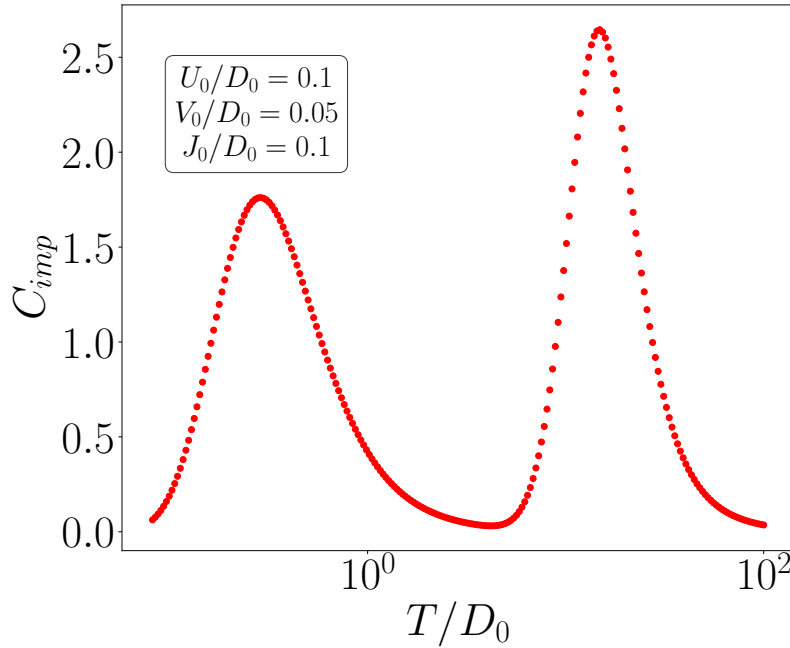


Figure 2.9: Impurity specific heat

2.9 Renormalization of impurity spectral function

In this section we will obtain the impurity spectral function, which is defined in terms of the impurity Green's function as

$$\mathcal{A}(\omega) = -\frac{1}{\pi} \text{Im} [G_{dd}^{\sigma}(\omega)] \quad (2.9.1)$$

The zero temperature retarded Green's function for the impurity, in the frequency domain, can be written as (see Appendix. E)

$$\mathcal{A}(\omega) = \frac{1}{d_0} \sum_{n,0} \left[\|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \delta(\omega + E_0 - E_n) + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \delta(\omega - E_0 + E_n) \right] \quad (2.9.2)$$

where $\mathcal{O}_\sigma = c_{d\sigma} + S_d^- c_{0\bar{\sigma}} + S_d^z c_{0\sigma}$ is the excitation whose spectral function we are interested in. The excitations defined in \mathcal{O} incorporates both single-particle excitations brought about by the hybridisation as well as two-particle spin excitations brought about by the spin-exchange term. Since this is in terms of the exact eigenstates, it is a discrete sum of delta-functions. In practice, we get a continuous distribution. To compare with experiment, we need to convert the discrete sum into a continuous function. Following [7], we replace the delta-functions at $\pm x_n \equiv \pm(E_n - E_0)$ by normalized Gaussian functions

$$\delta(\omega \pm x_n) \rightarrow \frac{1}{\eta_n \sqrt{\pi}} e^{-\left(\frac{\omega \pm x_n}{\eta_n}\right)^2} \quad (2.9.3)$$

The parameter η_n determines the height and width of the Gaussian, and is chosen such that the higher energy poles are broader than the lower energy ones:

$$\eta_n = 4\Delta + \frac{1}{2}|x_n| \quad (2.9.4)$$

$\Delta = \pi\rho(0)V^2$ is the relevant energy scale for the non-interacting ($U = 0$) problem, $\rho(0)$ being the density of states of the conduction bath at the Fermi energy. As a result, the function that we will numerically compute and plot is

$$\mathcal{A}(\omega) = \sum_{n,0} \frac{1}{d_0 \sqrt{\pi} \eta_n} \left[\|\langle 0 | c_{d\sigma} | n \rangle\|^2 e^{-\left(\frac{\omega - x_n}{\eta_n}\right)^2} + \|\langle n | c_{d\sigma} | 0 \rangle\|^2 e^{-\left(\frac{\omega + x_n}{\eta_n}\right)^2} \right] \quad (2.9.5)$$

From the results of Langreth [8], we know that the spectral function at zero frequency is fixed by the occupancy of the impurity. Since we are in the particle-hole symmetric regime, this occupancy is fixed at 1, and hence so is the spectral function height at $\omega = 0$. This result has been used to fix the spectral function height at the center during the computations. The fixed-point Hamiltonian H^* is diagonalized numerically to obtain $\{E_n, |n\rangle\}$, for various values of the couplings. The intention here is to get an idea of how the spectral function morphs under the RG. Doing an actual reverse RG (described in 2.15) would require us to diagonalize a huge Hamiltonian. We take the simpler route of tuning the U from zero to soem large value. This should mimic the journey from the IR theory ($U = 0$) to the UV theory ($U \gg 0$).

The spectral function is plotted for three sets of values in fig. 2.10. For low values of U , the profile is that of a single peak at zero frequency. This is expected because at the low energy effective theory, the high energy Hubbard side bands have been integrated out. As U increases, shoulder-like structures appear on either side of the peak, which finally, at larger U , develop into two side-peaks. This is the microscopic theory, where high energy features are also relevant.

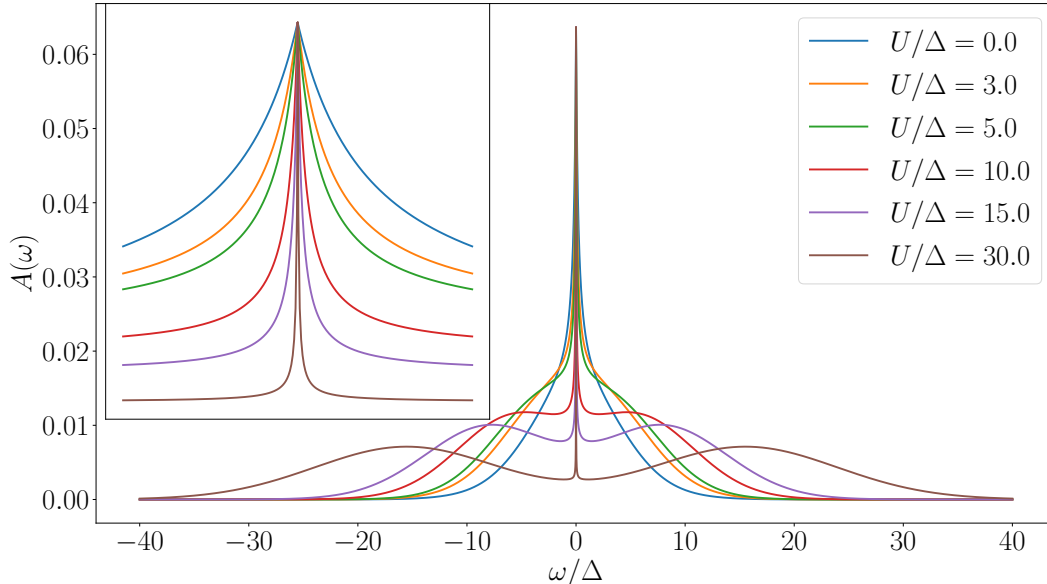


Figure 2.10: Impurity spectral function for multiple values of U . The increase in value of U is accompanied by the appearance of the side-peaks.

The physics of the three peaks can now be looked into. Since the central peak is at zero energy, it has to do with excitations that do not cost any energy. There are two such excitations: excitations within the spin sector and within the charge sector.

$$\begin{array}{cc} JS_d^- & KC_d^- \\ |\uparrow\rangle \xleftrightarrow{\quad} |\downarrow\rangle, & |\uparrow\rangle \xleftrightarrow{\quad} |\downarrow\rangle \\ JS_d^+ & KC_d^+ \end{array} \quad (2.9.6)$$

The thick arrow \uparrow represents the charge isospin. At particle-hole symmetry, both the spin configurations has energy of ϵ_d , while the charge configurations have energy of $2\epsilon_d + U = 0$ and 0 . Hence, no energy is required for these excitations, which is why see a macroscopic number of cloud electrons resonating with the impurity at the Fermi surface. Also note that if \hat{S}_i and \hat{C}_j are two operators of the spin and charge sector ($i, j \in \{x, y, z\}$), then

$$\hat{S}_i \hat{C}_j = \hat{C}_j \hat{S}_i = 0 \quad (2.9.7)$$

We can see this by applying that operator on a basis state. Since the set of four states

$$|\hat{S}_i = \pm \frac{1}{2}, \hat{C}_j = 0\rangle, |\hat{S}_i = 0, \hat{C}_j = \pm \frac{1}{2}\rangle \quad (2.9.8)$$

are all independent, they form a basis. If we apply the operator on these states:

$$\begin{aligned} \hat{S}_i \hat{C}_j |\hat{S}_i\rangle &= 0, & \hat{C}_j \hat{S}_i |S_i\rangle &= S_i \hat{C}_j |S_i\rangle = 0 \\ \hat{C}_j \hat{S}_i |C_j\rangle &= 0, & \hat{S}_i \hat{C}_j |\hat{C}_j\rangle &= C_j \hat{S}_i |\hat{C}_j\rangle = 0 \end{aligned} \quad (2.9.9)$$

This shows that each operator acts only on its own subspace. S_i does not act on the charge sector, and vice-versa. There is no single-particle excitation here.

The physics of the side-peaks is that of single number fluctuations on the impurity. These are brought about by the term $V c_{0\sigma}^\dagger c_{d\sigma} + \text{h.c.}$

$$(\epsilon_d) |\sigma\rangle \xleftrightarrow[V c_{d\bar{\sigma}}/V c_{d\sigma}^{\dagger}]{V c_{d\bar{\sigma}}^\dagger/V c_{d\sigma}} |n_d = 2, 0\rangle (0) \quad (2.9.10)$$

These transitions involve energy transfer of the order of ϵ_d . This is why, at very small U , they remain absorbed inside the central peak. These transitions do not involve any spin or charge-flip, rather they take the impurity between the spin and charge sectors.

2.10 Effective Hamiltonian for excitations of the Kondo cloud

To find an effective Hamiltonian for the excitations of the Kondo cloud, we will integrate out the impurity part of the wavefunction. The Schrodinger equation for the $J > K$ ground state is

$$\begin{aligned} E_g & \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &= \mathcal{H}_0^* \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ V \sum_{\beta} \left[c_{2\beta}^\dagger c_{1\beta} - c_{2\beta} c_{1\beta}^\dagger \right] \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ J \vec{S}_d \cdot \vec{s} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \\ &+ K \vec{C}_d \cdot \vec{c} \left[c_-^s (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_-^c (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \end{aligned} \quad (2.10.1)$$

The last two lines gives

$$\frac{1}{2}Jc_-^s \left[s^z (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) + s^+ |\downarrow, \downarrow\rangle - s^- |\uparrow, \uparrow\rangle \right] + \frac{1}{2}Kc_-^c \left[c^z (|\uparrow\downarrow, 0\rangle - |0, \uparrow\downarrow\rangle) + c^+ |0, 0\rangle + c^- |2, 2\rangle \right] \quad (2.10.2)$$

The second line gives

$$\begin{aligned} & Vc_{2\uparrow}^\dagger \left[c_-^s (|0, \downarrow\rangle) + c_-^c (|\downarrow, 0\rangle) \right] + Vc_{2\downarrow}^\dagger \left[c_-^s (-|0, \uparrow\rangle) + c_-^c (|\uparrow, 0\rangle) \right] \\ & - Vc_{2\uparrow} \left[c_-^s (-|\uparrow\downarrow, \uparrow\rangle) + c_-^c (|\uparrow, \uparrow\downarrow\rangle) \right] - Vc_{2\downarrow} \left[c_-^s (-|\uparrow\downarrow, \downarrow\rangle) + c_-^c (|\downarrow, \uparrow\downarrow\rangle) \right] \end{aligned} \quad (2.10.3)$$

We will now write down four equations by comparing the coefficients of $|\uparrow\rangle, |\downarrow\rangle, |0\rangle$ and $|2\rangle$ of the impurity sector:

$$\begin{aligned} (E_g - H_0^*) c_-^s |\downarrow\rangle &= Vc_-^c (c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle) + \frac{1}{2}Jc_-^s (s^z |\downarrow\rangle - s^- |\uparrow\rangle) \quad [\text{eq. from } |\uparrow\rangle] \\ (-E_g + H_0^*) c_-^s |\uparrow\rangle &= Vc_-^c (c_{2\uparrow}^\dagger |0\rangle - c_{2\downarrow}^\dagger |2\rangle) + \frac{1}{2}Jc_-^s (s^z |\uparrow\rangle + s^+ |\downarrow\rangle) \quad [\text{eq. from } |\downarrow\rangle] \\ (E_g - H_0^*) c_-^c |2\rangle &= Vc_-^s (c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle) + \frac{1}{2}Kc_-^c (-c^z |2\rangle + c^+ |0\rangle) \quad [\text{eq. from } |0\rangle] \\ (E_g - H_0^*) c_-^c |0\rangle &= Vc_-^s (c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle) + \frac{1}{2}Kc_-^c (c^z |0\rangle + c^- |2\rangle) \quad [\text{eq. from } |2\rangle] \end{aligned} \quad (2.10.4)$$

These can be rearranged into

$$\begin{aligned} (E_g - H_0^* - \frac{1}{2}Js^z) |\downarrow\rangle &= V\lambda^{-1} (c_{2\downarrow}^\dagger |0\rangle - c_{2\uparrow} |2\rangle) - \frac{1}{2}Js^- |\uparrow\rangle \\ (E_g - H_0^* + \frac{1}{2}Js^z) |\uparrow\rangle &= V\lambda^{-1} (c_{2\downarrow} |2\rangle - c_{2\uparrow}^\dagger |0\rangle) - \frac{1}{2}Js^+ |\downarrow\rangle \\ (E_g - H_0^* + \frac{1}{2}Kc^z) |2\rangle &= V\lambda (c_{2\uparrow}^\dagger |\downarrow\rangle - c_{2\downarrow}^\dagger |\uparrow\rangle) + \frac{1}{2}Kc^+ |0\rangle \\ (E_g - H_0^* - \frac{1}{2}Kc^z) |0\rangle &= V\lambda (c_{2\uparrow} |\uparrow\rangle + c_{2\downarrow} |\downarrow\rangle) + \frac{1}{2}Kc^- |2\rangle \end{aligned} \quad (2.10.5)$$

where $\lambda = \frac{c_-^s}{c_-^c}$. We want to find the effective Hamiltonian in the subspace of $|\downarrow\rangle$. We first eliminate the charge sector from these equations:

$$\begin{aligned} |0\rangle &= V\lambda \left[\frac{1}{A_-^K} c_{2\uparrow} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) \right] |\uparrow\rangle \\ &+ V\lambda \left[\frac{1}{A_-^K} c_{2\downarrow} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) \right] |\downarrow\rangle \\ |2\rangle &= \frac{V\lambda}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left[\left(c_{2\uparrow}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\downarrow} \right) |\downarrow\rangle + \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\uparrow} - c_{2\downarrow}^\dagger \right) |\uparrow\rangle \right] \end{aligned} \quad (2.10.6)$$

where

$$A_\pm^K = E_g - H_0^* \pm \frac{1}{2}Kc^z \quad (2.10.7)$$

For ease of labeling, we will think of these equations as

$$|0\rangle = a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle, |2\rangle = a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle \quad (2.10.8)$$

The remaining two equations can then be written as

$$\begin{aligned} A_-^J |\downarrow\rangle &= \frac{V}{\lambda} \left[c_{2\downarrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) - c_{2\uparrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^- |\uparrow\rangle \\ A_+^J |\uparrow\rangle &= \frac{V}{\lambda} \left[c_{2\downarrow} (a_2^\uparrow |\uparrow\rangle + a_2^\downarrow |\downarrow\rangle) - c_{2\uparrow}^\dagger (a_0^\uparrow |\uparrow\rangle + a_0^\downarrow |\downarrow\rangle) \right] - \frac{J}{2} s^+ |\downarrow\rangle \end{aligned} \quad (2.10.9)$$

where

$$A_\pm^J = E_g - H_0^* \pm \frac{1}{2} J s^z \quad (2.10.10)$$

Eliminating $|\downarrow\rangle$ and solving for $|\uparrow\rangle$ gives

$$\begin{aligned} A_+^J |\uparrow\rangle &= \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) |\uparrow\rangle + \left(\frac{V}{\lambda} c_{2\downarrow} a_2^\downarrow - \frac{V}{\lambda} c_{2\uparrow}^\dagger a_0^\downarrow - \frac{J}{2} s^+ \right) |\downarrow\rangle \\ &= \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) |\uparrow\rangle \\ &\quad + \left[\frac{V}{\lambda} (c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow} a_2^\downarrow)} \left[\frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow) - \frac{J}{2} s^- \right] |\uparrow\rangle \end{aligned} \quad (2.10.11)$$

The effective Hamiltonian for the $|\uparrow\rangle$ state is

$$\begin{aligned} H_0^* - \frac{J}{2} s^z + \frac{V}{\lambda} (c_{2\downarrow} a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow) &+ \left[\frac{V}{\lambda} (c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow) - \frac{J}{2} s^+ \right] \frac{1}{A_-^J - \frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow} a_2^\downarrow)} \\ &\times \left[\frac{V}{\lambda} (c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow) - \frac{J}{2} s^- \right] \end{aligned} \quad (2.10.12)$$

To get a clearer picture of this effective Hamiltonian, we will keep up to two-particle interactions. We first write down the full forms of $a_{0,2}^\sigma$:

$$\begin{aligned} a_0^\sigma &= V\lambda \left[\frac{1}{A_-^K} c_{2\sigma} + \frac{K}{2} \frac{1}{A_-^K} c^- \frac{1}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(\frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} - \sigma c_{2\sigma}^\dagger \right) \right] \\ a_2^\sigma &= \frac{V\lambda}{A_+^K - \left(\frac{K}{2}\right)^2 c^+ \frac{1}{A_-^K} c^-} \left(-\sigma c_{2-\sigma}^\dagger + \frac{K}{2} c^+ \frac{1}{A_-^K} c_{2\sigma} \right) \end{aligned} \quad (2.10.13)$$

We will first look at the special case of $K = 0$. There, the above expressions simplify to

$$\begin{aligned} a_0^\sigma &= V\lambda \frac{1}{A_-^K} c_{2\sigma} = \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2\sigma} + \mathcal{O}(H_0^{*3}) \\ a_2^\sigma &= -\sigma V\lambda \frac{1}{A_+^K} c_{2-\sigma}^\dagger = -\sigma \frac{V\lambda}{E_g} \left[1 + \frac{1}{E_g} (H_0^*) + \frac{1}{E_g^2} (H_0^*)^2 \right] c_{2-\sigma}^\dagger + \mathcal{O}(H_0^{*3}) \end{aligned} \quad (2.10.14)$$

We will make use of the following commutators:

$$\begin{aligned} [(H_0^*)^m, c_{2\sigma}] &= -\sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}, & [(H_0^*)^m, c_{2\sigma}^\dagger] &= \sum_k \frac{\epsilon_k^m}{\sqrt{N^*}} c_{k\sigma}^\dagger, & m &= 1, 2 \\ [(H_0^*)^m, s^+] &= \sum_{kk'} (\epsilon_k^m - \epsilon_{k'}^m) c_{k\beta}^\dagger c_{k'\beta}, & & & m &= 1, 2 \\ [(s^z)^m, c_{2\sigma}] &= -\left(\frac{\sigma}{2}\right)^m c_{2\sigma}, & [(s^z)^m, c_{2\sigma}^\dagger] &= \left(\frac{\sigma}{2}\right)^m c_{2\sigma}^\dagger, & m &= 1, 2 \\ [(c^z)^m, c_{2\sigma}] &= -\left(\frac{1}{2}\right)^m c_{2\sigma}, & [(c^z)^m, c_{2\sigma}^\dagger] &= \left(\frac{1}{2}\right)^m c_{2\sigma}^\dagger, & m &= 1, 2 \end{aligned} \quad (2.10.15)$$

Now we evaluate the various terms in the effective Hamiltonian.

$$\begin{aligned}
c_{2\downarrow}a_2^\uparrow &= -\frac{V\lambda}{E_g}c_{2\downarrow}\left[1 + \frac{1}{E_g}(H_0^*) + \frac{1}{E_g^2}(H_0^*)^2\right]c_{2\downarrow}^\dagger \\
&= -\frac{V\lambda}{E_g}\left[c_{2\downarrow} + \frac{1}{E_g}(H_0^*)c_{2\downarrow} + \sum_k \frac{\epsilon_k}{E_g\sqrt{N^*}}c_{k\downarrow} + \frac{1}{E_g^2}(H_0^*)^2c_{2\downarrow} + \sum_k \frac{\epsilon_k^2}{E_g^2\sqrt{N^*}}c_{k\downarrow}\right]c_{2\downarrow}^\dagger \\
&= -\frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right]c_{2\downarrow}c_{2\downarrow}^\dagger - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\downarrow}c_{k'\downarrow}^\dagger \\
c_{2\uparrow}a_2^\downarrow &= -\frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right]c_{2\uparrow}c_{2\uparrow}^\dagger - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\uparrow}c_{k'\uparrow}^\dagger \\
c_{2\uparrow}^\dagger a_0^\uparrow &= c_{2\uparrow}^\dagger \frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}(H_0^*) + \frac{1}{E_g^2}(H_0^*)^2\right]c_{2\uparrow} \\
&= \frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right]c_{2\uparrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\uparrow}^\dagger c_{k'\uparrow} \\
c_{2\downarrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right]c_{2\downarrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\downarrow}^\dagger c_{k'\downarrow} \\
c_{2\downarrow}a_2^\downarrow &= \frac{V\lambda}{E_g}c_{2\downarrow}\left[1 + \frac{1}{E_g}(H_0^*) + \frac{1}{E_g^2}(H_0^*)^2\right]c_{2\uparrow}^\dagger \\
&= \frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}(H_0^*)\right]c_{2\downarrow}c_{2\uparrow}^\dagger + \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\downarrow}c_{k'\uparrow}^\dagger \\
c_{2\uparrow}a_2^\uparrow &= -\frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}(H_0^*)\right]c_{2\uparrow}c_{2\downarrow}^\dagger - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\uparrow}c_{k'\downarrow}^\dagger \\
c_{2\uparrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g}\right]c_{2\uparrow}^\dagger c_{2\downarrow} - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\uparrow}^\dagger c_{k'\downarrow} \\
c_{2\downarrow}^\dagger a_0^\uparrow &= \frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g}\right]c_{2\downarrow}^\dagger c_{2\uparrow} - \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)c_{k\downarrow}^\dagger c_{k'\uparrow} \\
c_{2\downarrow}a_2^\uparrow - c_{2\uparrow}^\dagger a_0^\uparrow &= -\frac{V\lambda}{E_g}\left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g}\right)^2\right]\times 2 + \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}c_{k'\downarrow}^\dagger) \\
c_{2\downarrow}a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow &= \frac{V\lambda}{E_g}\left[1 + \frac{1}{E_g}(H_0^*)\right]c_{2\downarrow}c_{2\uparrow}^\dagger \times 2 + \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)(c_{k\downarrow}c_{k'\uparrow}^\dagger + c_{k\uparrow}^\dagger c_{k'\downarrow}) \\
c_{2\downarrow}^\dagger a_0^\downarrow - c_{2\uparrow}a_2^\downarrow &= \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)(c_{k\uparrow}c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}) \\
c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow}a_2^\uparrow &= \frac{V\lambda}{E_gN^*}\sum_{kk'}\left(\frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}\right)(c_{k\uparrow}c_{k'\downarrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\uparrow})
\end{aligned}$$

In all the expressions, we have dropped terms that have more than 4 operators in product. Also, in the last four equations, we have substituted $\hat{n}_{2\uparrow} - \hat{n}_{2\downarrow} = 1$, because this is the effective Hamiltonian for the state with $s^z = \frac{1}{2}$.

We now substitute these expressions into the effective Hamiltonian:

$$\begin{aligned}
H_0^* - \frac{J}{2}s^z - \frac{2V^2}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] &+ \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \\
&+ \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[\frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow \right) \right] \\
&+ \left[\frac{V}{\lambda} \left(c_{2\downarrow} a_2^\downarrow - c_{2\uparrow}^\dagger a_0^\downarrow \right) \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[-\frac{J}{2}s^- \right] \\
&+ \left[-\frac{J}{2}s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[\frac{V}{\lambda} \left(c_{2\downarrow}^\dagger a_0^\uparrow - c_{2\uparrow} a_2^\uparrow \right) \right] \\
&+ \frac{J^2}{4} \left[s^+ \right] \frac{1}{A_-^J - \frac{V^2}{E_g N^*} \sum_{kk'} \xi_k \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right)} \left[s^- \right]
\end{aligned} \tag{2.10.16}$$

where $\xi_k = \frac{\epsilon_k}{E_g} + \frac{\epsilon_k^2}{E_g^2}$. We first consider only zeroth order terms of the central propagator.

$$\begin{aligned}
H_0^* - \frac{J}{2} \underbrace{s^z}_{\frac{1}{2}} - \frac{2V^2}{E_g} \left[1 + \frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] &+ \frac{V^2}{E_g N^*} \sum_{kk'} (\xi_k) \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \\
&+ \frac{V^4}{E_g^2 N^{*2} \left(E_g + \frac{J}{4} \right)} \sum_{kk'} (\xi_{k'} + 2 - \xi_k) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} (\xi_k + \xi_{k'}) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{V^2 J}{2E_g \left(E_g + \frac{J}{4} \right) N^*} \sum_{kk'} (\xi_{k'} + 2 - \xi_k) c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{J V^2}{2E_g \left(E_g + \frac{J}{4} \right) N^*} \sum_{kk'} c_{k\uparrow}^\dagger c_{k'\downarrow} \sum_{kk'} (\xi_k + \xi_{k'}) c_{k\downarrow}^\dagger c_{k'\uparrow} \\
&+ \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \underbrace{s^+ s^-}_{s^z + \frac{1}{2} = 1}
\end{aligned} \tag{2.10.17}$$

We have set $s^z = -\frac{1}{2}$ in the denominator, hence the $E_g = \frac{J}{4}$. If we also consider the first and second order terms from the central propagator, note that they will produce terms of more than quartic interactions in the first three terms. For the last term, we get

$$\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} s^+ \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] s^- \tag{2.10.18}$$

Using the commutator of H_0^* with s^+ to bring H_0^* to the left, and using $s^+ s^- = s^z + \frac{1}{2} = 1$, we get

$$\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 - \sum_{kk'qq'} \left(\xi_k^J - \xi_{k'}^J \right) c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \right] \tag{2.10.19}$$

where $\xi_k^J = \frac{\epsilon_k}{E_g + \frac{J}{4}} + \frac{\epsilon_k^2}{(E_g + \frac{J}{4})^2}$. The full effective Hamiltonian, for $K = 0$, up to quartic interactions, is

$$\begin{aligned} H_0^* + \frac{J}{4} \left(\frac{J}{E_g + \frac{J}{4}} - 1 \right) - \frac{2V^2}{E_g} + \frac{V^2}{E_g N^*} \sum_{kk'} (\xi_k) (c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow} c_{k'\downarrow}^\dagger) - \frac{2V^2}{E_g} \left[\frac{H_0^*}{E_g} + \left(\frac{H_0^*}{E_g} \right)^2 \right] \\ + \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} \left[\frac{H_0^*}{E_g + \frac{J}{4}} + \left(\frac{H_0^*}{E_g + \frac{J}{4}} \right)^2 \right] + \sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \end{aligned} \quad (2.10.20)$$

The coefficient $F_{kk'qq'}$ is

$$\begin{aligned} F_{kk'qq'} = \frac{V^2}{E_g N^* (E_g + \frac{J}{4})} \left[\frac{V^2}{E_g N^*} (\xi_{k'} + 2 - \xi_k) (\xi_q + \xi_{q'}) + \frac{J}{2} (\xi_{k'} + 2 - \xi_k + \xi_q + \xi_{q'}) \right] \\ + \frac{J^2}{4 \left(E_g + \frac{J}{4} \right)} (\xi_{k'}^J - \xi_k^J) \end{aligned} \quad (2.10.21)$$

There are two main types of interactions that gets generated upon integrating out the impurity. One is the Fermi liquid type interactions arising from the H_0^{*2} terms. The Fermi liquid part of the Hamiltonian is

$$\begin{aligned} \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] H_0^* + \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^3} \right] H_0^{*2} \\ = \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right] \left[H_0^* + \sum_{kk'\sigma\sigma'} f_{kk'} \hat{n}_{k\sigma} \hat{n}_{k'\sigma'} \right] \end{aligned} \quad (2.10.22)$$

where the Landau parameter is given by

$$f_{kk'} = \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^2} - \frac{2V^2}{E_g^2} \right]^{-1} \left[\frac{J^2}{4 \left(E_g + \frac{J}{4} \right)^3} - \frac{2V^2}{E_g^3} \right] \epsilon_k \epsilon_{k'} \quad (2.10.23)$$

The more interesting interaction is the off-diagonal term

$$\sum_{kk'qq'} F_{kk'qq'} c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \quad (2.10.24)$$

This interaction arises from the enhanced entanglement between the impurity and the conduction electrons; removing the impurity from the singlet and the triplet generates these off-diagonal scatterings. As such, this is an indicator of the macroscopic entanglement of the singlet formed at the IR fixed point, and plotted in fig. 2.13.

We also wish to point out that this scattering is a signature of the change in Luttinger's count in going from the free orbital or local moment fixed point to the strong-coupling fixed point, as shown in eq. (2.14.28). Both this off-diagonal scattering as well as the change in Luttinger's count are a direct consequence of the non-number conserving term $V c_k^\dagger c_d$ in the full Hamiltonian. The topological change of Luttinger's count is concomitant with the presence of the off-diagonal scattering term in the effective Hamiltonian. *Just the Fermi liquid piece in eq. (2.10.23) will give neither the enhanced mutual information nor the change in Luttinger's count.*

2.11 Obtaining the real space low energy Hamiltonian: the local Fermi liquid

The next step is to obtain the lowest excitations of the fixed point Hamiltonian, in real space. We will work in the $U > 0$ regime. For $V, J \gg 1$, the impurity couples very strongly with the zeroth site, and at zeroth order, it

suffices to say that the zeroth site decouples from the rest of the lattice. This zeroth Hamiltonian then consists of two sites interacting with each other through V and J (the two site problem analysed before).

$$H_0^* = \sum_{\sigma} \left(V^* c_{0\sigma}^{\dagger} c_{d\sigma} + \text{h.c.} \right) + J^* \vec{S}_d \cdot \vec{s} - \frac{1}{2} U^* \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 \quad (2.11.1)$$

$$|\Psi\rangle_1 = c_s \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + c_c \frac{1}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle), \quad E_1 = -V^* \sqrt{\gamma^2 + 4} - \frac{1}{4} U^* - \frac{3}{8} J^* \quad (2.11.2)$$

These were obtained in eq. (2.4.5). The quantities γ and $c_{s,c}$ were defined in and around eq. (2.4.6).

We start with the ground state $|\Psi\rangle_1$ and the star graph as the zeroth level ground state and Hamiltonian, and then add a nearest-neighbour hopping term as a perturbation of the zeroth Hamiltonian. We know that the ground state for the interacting part is predominantly the spin-singlet (it was shown while calculating the ground states of the effective zero-mode Hamiltonian that the ground state is a mixture of singlet and triplet, and the triplet part dies out at large system sizes, see eq. (2.5.1)), so we will take that as our reference state and treat the hopping part that connects the origin to the first site,

$$H_X = t \sum_{\vec{r}_1, \sigma} c_{0\sigma}^{\dagger} c_{\vec{r}_1, \sigma} + \text{h.c.} \equiv v^{\dagger} + v \quad (2.11.3)$$

as a weak perturbation. \vec{r}_1 here sums over the sites that are nearest to the origin. Once this perturbation is taken care of up to a certain order, we will have a decoupled singlet formed by the impurity and the zeroth site, and the rest of the lattice formed by $N - 1$ sites along with the interaction induced by the perturbation. To be precise, the goal is to integrate out the perturbation and generate an effective Hamiltonian in the subspace of the minimal energy states of the two site Hamiltonian, and this effective Hamiltonian will therefore describe the lowest excitations on top of the ground state $|\Psi\rangle_1$. The minimal energy subspace is given by the states:

$$|\Phi\rangle_i = |\Psi\rangle_1 \otimes |\hat{n}_{1\uparrow}, \hat{n}_{1\downarrow}\rangle, \quad \text{where } i \in \begin{cases} 0: & \hat{n}_{1\uparrow} = \hat{n}_{1\downarrow} = 0 \\ 1: & 1 - \hat{n}_{1\uparrow} = \hat{n}_{1\downarrow} = 0 \\ 2: & \hat{n}_{1\uparrow} = 1 - \hat{n}_{1\downarrow} = 0 \\ 3: & 1 - \hat{n}_{1\uparrow} = 1 - \hat{n}_{1\downarrow} = 0 \end{cases} \quad (2.11.4)$$

The effective Hamiltonian will be calculated using perturbation theory in $\frac{H_X^n}{H_0^{*n-1}}$. Since an odd number of scattering processes cannot bring the initial state back to itself, such orders will be absent from the effective Hamiltonian.

2.11.1 Second order effective Hamiltonian

We first consider the case of $n = 2$. The renormalisation of the effective Hamiltonian in the ground state subspace, at this order, is given by

$$\Delta H = \sum_{ij, n} |\Phi\rangle_i \langle \Phi_i| H_X |\Psi\rangle_n \frac{1}{E_{\text{gs}} - E_n} \langle \Psi|_n H_X |\Phi\rangle_j \langle \Phi_j| = \sum_{ij} |\Phi\rangle_i \langle \Phi_j| \langle \Phi_i| v + v^{\dagger} |\Psi\rangle_n \frac{1}{E_{\text{gs}} - E_n} \langle \Psi|_n v + v^{\dagger} |\Phi\rangle_j. \quad (2.11.5)$$

Here, $|\Psi\rangle_n$ are the eigenstates of the two site problem, with eigenvalue E_n . The total scattering process can be described as H_X acting on $|\Phi\rangle_j$ to excite to $|\Psi\rangle_n$, and then a subsequent H_X acting on $|\Psi\rangle_n$ to decay back to $|\Phi\rangle_j$ and into the ground state manifold. Since $|\Phi\rangle_{i,j}$ are eigenstates of the two site Hamiltonian, they are all eigenstates of the total number operator $\hat{n}_{d0} = \sum_{\sigma} (\hat{n}_{d\sigma} + \hat{n}_{0\sigma})$ for the two site model, with eigenvalue 2. Since we are to finally return to the ground state manifold, only those processes in H_X^2 are allowed that conserve \hat{n}_{d0} . These processes are v, v^{\dagger} and v^{\dagger}, v . This also means that the total number of particles on site 1 will remain constant in the process, and we will have $|\Phi\rangle_i = |\Phi\rangle_j$.

$$\Delta H = \sum_i |\Phi\rangle_i \langle \Phi_i| \frac{1}{E_{\text{gs}} - E_n} \left(\langle \Phi_i| v^{\dagger} |\Psi\rangle_n \langle \Psi|_n v |\Phi\rangle_i + \langle \Phi_i| v |\Psi\rangle_n \langle \Psi|_n v^{\dagger} |\Phi\rangle_i \right). \quad (2.11.6)$$

If we define the matrix element $v_{ni} \equiv \langle \Psi|_n v |\Phi\rangle_i$ of v and the excitation energy $\delta E_n = E_n - E_{\text{gs}}$, we can write the renormalisation as

$$\Delta H = \sum_{i, n} \frac{|v_{ni}|^2 + |v_{in}|^2}{-\delta E_n} |\Phi\rangle_i \langle \Phi_i|. \quad (2.11.7)$$

We now look at each $|\Phi_i\rangle$ separately. For $|\Phi_i\rangle = |\Phi\rangle_0 = |\Psi\rangle_1 \otimes |0,0\rangle$, we can write

$$v^\dagger |\Phi\rangle_i = 0, \quad v |\Phi\rangle_i = \frac{t}{\sqrt{2}} \sum_{\sigma} \bar{\sigma} \left(c_s^- |\sigma, 0\rangle + c_c^- |0, \sigma\rangle \right) |\bar{\sigma}\rangle \quad (2.11.8)$$

The first relation gives $v_{in} = \langle \Phi |_i v |\Psi\rangle_n = \left(\langle \Psi |_n v^\dagger |\Phi\rangle_i \right)^* = 0$. The set of states that give non-zero v_{in}^\dagger are specific elements of the set of eigenstates that have a total of either 1 or 3 electrons on the impurity and zeroth sites:

$$|\Psi\rangle_n = |\Psi\rangle_{\pm, \sigma}^{s, p} = -\sqrt{2} \left(a_{1, \pm} |\sigma, p\rangle + a_{2, \pm} |p, \sigma\rangle \right) \otimes |s\rangle, \quad \sigma = \uparrow, \downarrow, \quad E_{\pm, \sigma}^{s, p} = -\frac{U}{4} \pm \frac{1}{2} \Delta; \quad (2.11.9)$$

here, s is a string from the set $\{0, \uparrow, \downarrow, 2\}$ and represents the configuration of the first site $|s\rangle$ in direct product with the impurity and zeroth site entangled composite state, and p is either 2 or 0 such that $p+1 (= 1 \text{ or } 3)$ represents the total number of electrons on the impurity and zeroth sites. For $|\Phi\rangle_0$, only $s = \bar{\sigma}$ and $p = 0$ give non-zero inner product. The coefficients are defined as $a_{1, \pm} = \frac{4V}{\sqrt{2}\mathcal{N}_{\pm}}, a_{2, \pm} = \frac{U \pm 2\Delta}{\sqrt{2}\mathcal{N}_{\pm}}$. The inner product is

$$v_{\pm \sigma, i} = \langle \Psi_{\pm, \sigma}^{\bar{\sigma}, 0} | v |\Phi_i\rangle = \sigma t \left[a_{1, \pm} c_s^- + a_{2, \pm} c_c^- \right] \quad (2.11.10)$$

$\mathcal{N}_{\pm} = \sqrt{16V^2 + (U \pm 2\Delta)^2}$ is the normalisation factor and $\Delta = \frac{1}{2} \sqrt{U^2 + 16V^2}$. The renormalisation for this value of i then becomes

$$(\Delta H)_{i=0} = |\Phi\rangle_0 \langle \Phi |_0 \sum_n \frac{|v_{ni}|^2}{-\delta E_n} = |\Phi\rangle_0 \langle \Phi |_0 \sum_{\sigma, \pm} \frac{|v_{\pm \sigma, i}|^2}{-\delta E_{\pm}^{\sigma}} = -|\Phi\rangle_0 \langle \Phi |_0 2t^2 \sum_{\pm} \frac{\left[a_{1, \pm} c_s^- + a_{2, \pm} c_c^- \right]^2}{\delta E_{\pm}^{\sigma}} \quad (2.11.11)$$

where $\delta E_{\pm}^{\sigma} = E_{\pm}^{\sigma} - E_{\text{gs}}$.

For $i = 1$, we have $|\Phi\rangle_1 = |\Psi\rangle_1 \otimes |\uparrow\rangle$. Carrying out a similar calculation above, we get

$$v |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left(c_s^- |\uparrow, 0, 2\rangle + c_c^- |0, \uparrow, 2\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm, \uparrow}^{2, 0}, \quad v_{ni} = -t \left(c_s^- a_{1, \pm} + c_c^- a_{2, \pm} \right) \quad (2.11.12)$$

$$v^\dagger |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left(c_s^- |\uparrow, 2, 0\rangle - c_c^- |2, \uparrow, 0\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm, \uparrow}^{0, 2}, \quad v_{in} = -t \left(c_s^- a_{1, \pm} - c_c^- a_{2, \pm} \right) \quad (2.11.13)$$

$$(\Delta H)_{i=1} = -|\Phi\rangle_1 \langle \Phi |_1 2t^2 \sum_{\pm} \frac{a_{1, \pm}^2 c_s^{-2} + a_{2, \pm}^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} \quad (2.11.14)$$

The total Hamiltonian $H_0^* + H_X$ is invariant under the transformations $c_\sigma^\dagger \rightarrow c_\sigma, t \rightarrow -t$. Since the renormalisation only involves even powers of t , we can conclude that the renormalisation for $i = 2$ and $i = 3$ will be the same as that of $i = 1$ and $i = 0$ respectively. The total renormalisation at second order is

$$\begin{aligned} \Delta H &= -\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i 2t^2 \sum_{\pm} \frac{a_{1, \pm}^2 c_s^{-2} + a_{2, \pm}^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} - \left(|\Phi\rangle_0 \langle \Phi |_0 + |\Phi\rangle_3 \langle \Phi |_3 \right) 4t^2 \sum_{\pm} \frac{a_{1, \pm} a_{2, \pm} c_s^- c_c^-}{\delta E_{\pm}^{\sigma}} \\ &= -\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i t^2 \sum_{\pm} \frac{1}{\mathcal{N}_{\pm}^2} \frac{\left(4V c_s^- \right)^2 + (U \pm 2\Delta)^2 c_c^{-2}}{\delta E_{\pm}^{\sigma}} - \left(|\Phi\rangle_0 \langle \Phi |_0 + |\Phi\rangle_3 \langle \Phi |_3 \right) \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \end{aligned} \quad (2.11.15)$$

Since the $|\hat{n}_{1\sigma}, \hat{n}_{1\bar{\sigma}}\rangle$ form a complete set, we have $\sum_{i=0}^3 |\Phi\rangle_i \langle \Phi |_i = |\Psi\rangle_1 \langle \Psi |_1$, and the first term becomes a constant. The second term is a local Fermi liquid term on the first site:

$$\begin{aligned} \Delta H &= |\Psi\rangle_1 \langle \Psi |_1 \left[\text{constant} - \left\{ \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} + (1 - \hat{n}_{1\uparrow}) (1 - \hat{n}_{1\downarrow}) \right\} \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \right] \\ &= |\Psi\rangle_1 \langle \Psi |_1 \left[\text{constant} + \left(\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow} \right)^2 \sum_{\pm} \frac{t^2}{\mathcal{N}_{\pm}^2} \frac{8V c_s^- (U \pm 2\Delta) c_c^-}{\delta E_{\pm}^{\sigma}} \right] \end{aligned} \quad (2.11.16)$$

In the strong-coupling regime, we have $J, V \gg U$, and we can then approximate:

$$\delta E_{\pm}^{\sigma} \simeq \frac{3J}{8} + \sqrt{4V^2 - \left(\frac{3J}{8}\right)^2} \mp V, \quad U \pm 2\Delta \simeq \pm 4V, \quad \text{and} \quad \mathcal{N}_{\pm}^2 \simeq 32V^2 \quad (2.11.17)$$

Substituting this gives

$$\Delta H = |\Psi\rangle_1 \langle \Psi|_1 \left[\text{constant} - (\hat{n}_{1\uparrow} - \hat{n}_{1\downarrow})^2 \frac{2t^2 V c_s^- c_c^-}{2 \left(\frac{3J}{8}\right)^2 + 3V^2 + \frac{3J}{4} \sqrt{4V^2 + \left(\frac{3J}{8}\right)^2}} \right] \quad (2.11.18)$$

2.11.2 Fourth order effective Hamiltonian

Using fourth order perturbation theory, we can write the effective Hamiltonian renormalisation at that order in the form

$$\begin{aligned} \Delta H &= - \sum_i |\Phi\rangle_i \langle \Phi|_i \left[\sum_{lmn} \frac{\langle \Phi_i | H_X | \Psi_l \rangle \langle \Psi_l | H_X | \Psi_m \rangle \langle \Psi_m | H_X | \Psi_n \rangle \langle \Psi_n | H_X | \Phi_i \rangle}{\delta E_l \delta E_m \delta E_n} + \Delta^{(2)} H \sum_n \frac{|\langle \Psi_n | H_X | \Phi_i \rangle|^2}{(\delta E_n)^2} \right], \\ &= - \sum_i |\Phi\rangle_i \langle \Phi|_i \left[\sum_m \frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 + \Delta^{(2)} H \sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 \right]. \end{aligned} \quad (2.11.19)$$

We can have at most two successive v^\dagger or two successive v act on a particular state. Any more would lead to $c_\sigma^\dagger |\hat{n}_\sigma = 2\rangle = 0$. This limits the possible scattering processes (in the first term) to the following channels:

$$a. vv^\dagger vv^\dagger, \quad b. v^\dagger vv^\dagger v, \quad c. vvv^\dagger v^\dagger, \quad d. v^\dagger v^\dagger vv. \quad (2.11.20)$$

We start with $i = 0$. Out of the four channels a through d , only b and d survive. For $i = 0$, we already know the relevant $|\Psi\rangle_n$ and hence the $(H_X)_{ni} = v_{ni}$, from eq. (2.11.10).

$$v_{\pm\sigma,i} = \langle \Psi_{\pm,\sigma}^{\bar{\sigma},0} | v | \Phi_i \rangle = \sigma t \left[a_{1,\pm} c_s^- + a_{2,\pm} c_c^- \right] = \sigma t \mathcal{S}_{\pm}^- \quad (2.11.21)$$

where we have defined the sum and difference $\mathcal{S}_{\pm}^{\pm} = a_{1,\pm} c_s^{\pm} + a_{2,\pm} c_c^{\pm}$, $\mathcal{D}_{\pm}^{\pm} = a_{1,\pm} c_s^{\pm} - a_{2,\pm} c_c^{\pm}$. For channel b , we then proceed as follows:

$$|\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = -\sqrt{2} \left(a_{1,\pm} |\sigma, 0\rangle + a_{2,\pm} |0, \sigma\rangle \right) \otimes |\bar{\sigma}\rangle \quad (2.11.22)$$

$$v^\dagger |\Psi\rangle_n = v^\dagger |\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = \sqrt{2} t \left(a_{1,\pm} |\sigma, \bar{\sigma}\rangle + a_{2,\pm} |0, \sigma \bar{\sigma}\rangle \right) \otimes |0\rangle \quad (2.11.23)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |0\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |0\rangle \\ \left[\frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_c^+}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \otimes |0\rangle \end{cases} \implies (H_X)_{m,\pm\sigma} = \begin{cases} ta_{1\pm} \\ \bar{\sigma} ta_{2\pm} \\ \sigma t (a_{1\pm} c_s^+ + a_{2\pm} c_c^+) = \sigma t \mathcal{S}_{\pm}^+ \end{cases} \quad (2.11.24)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{1}{\delta E_{ST}} \left(\sum_{\sigma,\pm} \frac{t^2}{\delta E_{\pm}} \sigma a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 = 0 \\ \frac{1}{\delta E_{CS}} \left(\sum_{\pm,\sigma} \frac{t^2}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 = \frac{4t^4}{\delta E_{CS}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{1}{\delta E_2} \left(- \sum_{\pm,\sigma} \frac{t^2}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 = \frac{4t^4}{\delta E_2} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 \end{cases} \quad (2.11.25)$$

E_{ST}, E_{CS} and E_2 are the energies of the spin triplet zero, charge singlet and spin singlet+charge triplet excited states of the set $|\Psi\rangle_m$ in eq. (2.11.24).

We now turn to channel d :

$$v|\Psi\rangle_n = v|\Psi\rangle_{\pm,\sigma}^{\bar{\sigma},0} = \sqrt{2}t\sigma a_{2\pm}|0,0\rangle \otimes |2\rangle, \quad |\Psi\rangle_m = |0,0,2\rangle, \quad (H_X)_{m,\pm\sigma} = \sqrt{2}t\sigma a_{2\pm} \quad (2.11.26)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \frac{8t^4}{\delta E_{00}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \quad (2.11.27)$$

E_{00} is the energy of the state $|0,0,2\rangle$.

Having accounted for both channels, we will calculate the second part of the effective Hamiltonian in eq. (2.11.19), the part involving $\Delta^{(2)}H$. We already know, from eq. (2.11.11), that

$$\Delta^{(2)}H_{i=0} = -2t^2 \sum_{\pm} \frac{1}{\delta E_{\pm}} (\mathcal{S}_{\pm}^-)^2 \quad (2.11.28)$$

Also, from the expression of $v_{\pm\sigma,i}$, we get

$$\sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 = \sum_{\pm} \frac{2t^2}{(\delta E_{\pm})^2} (\mathcal{S}_{\pm}^-)^2 \quad (2.11.29)$$

Combining it all, the total renormalisation in $i=0$ is

$$-|\Phi\rangle_0 \langle \Phi|_0 4t^4 \left[\left(\frac{1}{\delta E_{CS}} + \frac{2}{\delta E_{00}} \right) \left(\sum_{\pm} \frac{a_{2\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \frac{1}{\delta E_2} \left(\sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 - \sum_{\pm} \frac{(\mathcal{S}_{\pm}^-)^2}{\delta E_{\pm}} \sum_{\pm} \left(\frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right] \quad (2.11.30)$$

We now come to $i=1$: $|\Phi\rangle_1 = |\Psi\rangle_1 \otimes |\uparrow\rangle$. Channels a and b are non-zero here. We start with channel b : $v^\dagger v v^\dagger v$. We already know, from eq. (2.11.12), that

$$v|\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left(c_s^- |\uparrow, 0, 2\rangle + c_c^- |0, \uparrow, 2\rangle \right), \quad |\psi\rangle_n = |\Psi\rangle_{\pm,\uparrow}^{2,0} = -\sqrt{2} \left(a_{1,\pm} |\uparrow, 0\rangle + a_{2,\pm} |0, \uparrow\rangle \right) \otimes |2\rangle, \quad (H_X)_{ni} = -t \mathcal{S}_{\pm}^- \quad (2.11.31)$$

Moving forward:

$$v^\dagger |\Psi\rangle_n = \sqrt{2}t \left(a_{1,\pm} |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle - a_{1,\pm} |\uparrow, \downarrow\rangle \otimes |\uparrow\rangle - a_{2,\pm} |0, 2\rangle \otimes |\uparrow\rangle \right) \quad (2.11.32)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |\uparrow\rangle \\ \left[\frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_c^+}{\sqrt{2}} (|\uparrow, 0\rangle + |0, \uparrow\rangle) \right] \otimes |\uparrow\rangle \\ |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle \end{cases} \implies (H_X)_{m,\pm} (H_X)_{\pm,i} = \begin{cases} t^2 a_{1\pm} \mathcal{S}_{\pm}^- \\ -t^2 a_{2\pm} \mathcal{S}_{\pm}^- \\ t^2 \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \\ -\sqrt{2}t^2 a_{1\pm} \mathcal{S}_{\pm}^- \end{cases} \quad (2.11.33)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{t^4}{\delta E_{ST}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_{CS}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{S}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_2} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^- \right)^2 \\ \frac{2t^4}{\delta E_{\uparrow\uparrow}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{S}_{\pm}^- \right)^2 \end{cases} \quad (2.11.34)$$

$E_{\uparrow\uparrow}$ is the energy of the upwards polarised state $|\uparrow, \uparrow\rangle \otimes |\downarrow\rangle$.

Next is channel a : $vv^\dagger vv^\dagger$. Using eq. (2.11.13) and following the same steps as above, we get:

$$v^\dagger |\Phi\rangle_1 = t \frac{1}{\sqrt{2}} \left(c_s^- |\uparrow, 2, 0\rangle - c_c^- |2, \uparrow, 0\rangle \right), \quad |\Psi\rangle_n = |\Psi\rangle_{\pm,\uparrow}^{0,2} = -\sqrt{2} \left(a_{1,\pm} |\uparrow, 2\rangle + a_{2,\pm} |2, \uparrow\rangle \right) \otimes |0\rangle, \quad (H_X)_{ni} = -t \mathcal{D}_{\pm}^- \quad (2.11.35)$$

$$v|\Psi\rangle_n = \sqrt{2}t \left(a_{1,\pm} |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle - a_{1,\pm} |\uparrow, \downarrow\rangle \otimes |\uparrow\rangle + a_{2,\pm} |2, 0\rangle \otimes |\uparrow\rangle \right) \quad (2.11.36)$$

$$|\Psi\rangle_m = \begin{cases} \frac{1}{\sqrt{2}} (|\uparrow, \downarrow\rangle + |\downarrow, \uparrow\rangle) \otimes |\uparrow\rangle \\ \frac{1}{\sqrt{2}} (|2, 0\rangle - |0, 2\rangle) \otimes |\uparrow\rangle \\ \left[\frac{c_s^+}{\sqrt{2}} (|\uparrow, \downarrow\rangle - |\downarrow, \uparrow\rangle) + \frac{c_e^+}{\sqrt{2}} (|\uparrow\downarrow, 0\rangle + |0, \uparrow\downarrow\rangle) \right] \otimes |\uparrow\rangle \\ |\uparrow, \uparrow\rangle \otimes |\downarrow\rangle \end{cases} \implies (H_X)_{m,\pm} (H_X)_{\pm,i} = \begin{cases} t^2 a_{1\pm} \mathcal{D}_{\pm}^- \\ -t^2 a_{2\pm} \mathcal{D}_{\pm}^- \\ t^2 \mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^- \\ -\sqrt{2} t^2 a_{1\pm} \mathcal{D}_{\pm}^- \end{cases} \quad (2.11.37)$$

$$\frac{1}{\delta E_m} \left\| \sum_n \frac{1}{\delta E_n} (H_X)_{mn} (H_X)_{ni} \right\|^2 = \begin{cases} \frac{1}{\delta E_{ST}} \left(\sum_{\pm} \frac{t^2}{\delta E_{\pm}} a_{1\pm} \mathcal{D}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_{CS}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{2\pm} \mathcal{D}_{\pm}^- \right)^2 \\ \frac{t^4}{\delta E_2} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} \mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^- \right)^2 \\ \frac{2t^4}{\delta E_{\uparrow\uparrow}} \left(\sum_{\pm} \frac{1}{\delta E_{\pm}} a_{1\pm} \mathcal{D}_{\pm}^- \right)^2 \end{cases} \quad (2.11.38)$$

For the final part, we again use $\Delta^{(2)} H_{i=1} = -t^2 \sum_{\pm} \frac{1}{\delta E_{\pm}} \left[(\mathcal{S}_{\pm}^-)^2 + (\mathcal{D}_{\pm}^-)^2 \right]$. Also, since $(H_X)_{ni} = (v + v^\dagger)_{ni}$, we have

$$\sum_n \frac{1}{(\delta E_n)^2} \left\| (H_X)_{ni} \right\|^2 = t^2 \sum_{\pm} \left[\left(\frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left(\frac{\mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right] \quad (2.11.39)$$

Combining all the terms, we get

$$\begin{aligned} -|\Phi\rangle_1 \langle \Phi|_1 4t^4 & \left[\left(\frac{1}{\delta E_{ST}} + \frac{2}{\delta E_{\uparrow\uparrow}} \right) \left\{ \left(\frac{1}{2} \sum_{\pm} \frac{a_{1\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left(\frac{1}{2} \sum_{\pm} \frac{a_{1\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} + \frac{1}{\delta E_{CS}} \left\{ \left(\frac{1}{2} \sum_{\pm} \frac{a_{2\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right. \right. \\ & \left. \left. + \left(\frac{1}{2} \sum_{\pm} \frac{a_{2\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} + \frac{1}{\delta E_2} \left\{ \left(\frac{1}{2} \sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left(\frac{1}{2} \sum_{\pm} \frac{\mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} \right. \\ & \left. - \sum_{\pm} \frac{1}{\delta E_{\pm}} \frac{1}{2} \left\{ (\mathcal{S}_{\pm}^-)^2 + (\mathcal{D}_{\pm}^-)^2 \right\} \sum_{\pm} \frac{1}{2} \left\{ \left(\frac{\mathcal{S}_{\pm}^-}{\delta E_{\pm}} \right)^2 + \left(\frac{\mathcal{D}_{\pm}^-}{\delta E_{\pm}} \right)^2 \right\} \right] \quad (2.11.40) \end{aligned}$$

If we define some quantities: $F_{(1,2)} = \sum_{\pm} \frac{a_{(1,2)\pm} \mathcal{S}_{\pm}^-}{\delta E_{\pm}}$, $G_{(1,2)} = \sum_{\pm} \frac{a_{(1,2)\pm} \mathcal{D}_{\pm}^-}{\delta E_{\pm}}$, $P = \sum_{\pm} \frac{\mathcal{S}_{\pm}^+ \mathcal{S}_{\pm}^-}{\delta E_{\pm}}$, $Q = \sum_{\pm} \frac{\mathcal{D}_{\pm}^+ \mathcal{D}_{\pm}^-}{\delta E_{\pm}}$, $X_n = \sum_{\pm} \frac{(\mathcal{S}_{\pm}^-)^2}{(\delta E_{\pm})^n}$, $Y_n = \sum_{\pm} \frac{(\mathcal{D}_{\pm}^-)^2}{(\delta E_{\pm})^n}$, the total renormalisation from second and fourth order can be written as

$$\begin{aligned} & -(|\Phi\rangle_0 \langle \Phi|_0 + |\Phi\rangle_3 \langle \Phi|_3) 4t^4 \left[\frac{1}{2t^2} X_1 + \left(\frac{1}{\delta E_{CS}} + \frac{2}{\delta E_{00}} \right) F_2^2 + \frac{1}{\delta E_2} P^2 - X_1 X_2 \right] \\ & -(|\Phi\rangle_1 \langle \Phi|_1 + |\Phi\rangle_2 \langle \Phi|_2) t^4 \left[\frac{1}{t^2} (X_1 + Y_1) + \left(\frac{1}{\delta E_{ST}} + \frac{2}{\delta E_{\uparrow\uparrow}} \right) (F_1^2 + G_1^2) + \frac{1}{\delta E_{CS}} (F_2^2 + G_2^2) \right. \\ & \left. + \frac{1}{\delta E_2} (P^2 + Q^2) - (X_1 + Y_1) (X_2 + Y_2) \right] \quad (2.11.41) \end{aligned}$$

The excitation energies are given by

$$\delta E_{CS} = \delta E_{00} = \frac{3J}{8} + \frac{U}{4} + \alpha, \quad \delta E_{\uparrow\uparrow} = \delta E_{ST} = -\frac{U}{4} + \frac{5J}{8} + \alpha, \quad \delta E_2 = 2\alpha, \quad \delta E_{\pm} = \frac{3J}{8} + \alpha \pm \frac{1}{2} \Delta, \quad \alpha \equiv \sqrt{V^2 \gamma^2 + 4V^2} \quad (2.11.42)$$

where $V\gamma = \frac{3J}{8} + \frac{U}{4}$ and $\Delta = \sqrt{\frac{U^2}{4} + 4V^2}$. The effective Hamiltonian can be expressed in the general form

$$H_{\text{eff}} = |\Psi\rangle_1 \langle\Psi|_1 \otimes \left[\text{constant} + \alpha_{\text{spin}} \hat{\mathcal{P}}_{\text{spin}} + \alpha_{\text{charge}} \hat{\mathcal{P}}_{\text{charge}} \right] \quad (2.11.43)$$

$\hat{\mathcal{P}}_{\text{charge}}$ and $\hat{\mathcal{P}}_{\text{spin}}$ are projection operators for, respectively, the charge ($\hat{n}_1 \neq 1$) and spin ($\hat{n}_1 = 1$) sectors of the first site. Since $\hat{\mathcal{P}}_{\text{charge}} + \hat{\mathcal{P}}_{\text{spin}} = 1$, we can eliminate one of the terms and rewrite the effective Hamiltonian in the simpler form

$$H_{\text{eff}} = |\Psi\rangle_1 \langle\Psi|_1 \otimes \left[\text{constant} + \mathcal{F} \hat{\mathcal{P}}_{\text{charge}} \right] \quad (2.11.44)$$

where $\mathcal{F} \equiv \alpha_{\text{charge}} - \alpha_{\text{spin}}$ is the net energy of the charge sector above the spin sector.

We will now look at the extreme strong-coupling regime $J \gg V \gg U, t$. There, all the expressions simplify:

$$\begin{aligned} V\gamma &\simeq \frac{3J}{8}, \quad \Delta \simeq 2V, \quad \alpha \simeq \frac{3J}{8}, \quad c_s^+ = -c_c^- \simeq 0, \quad c_s^- = c_c^+ \simeq 1, \quad \mathcal{N}_{\pm} \simeq 4\sqrt{2}V, \quad a_{1,\pm} \simeq \frac{1}{2}, \quad a_{2,\pm} \simeq \pm \frac{1}{2}, \\ \delta E_{\pm} &= \delta E_{\text{CS}} = \delta E_{00} = \delta E_2 \simeq \frac{3J}{4}, \quad \delta E_{\text{ST}} = \delta E_{\uparrow\uparrow} \simeq J, \quad \mathcal{S}_{\pm}^- = \mathcal{D}_{\pm}^- \simeq \frac{1}{2}, \quad \mathcal{S}_{\pm}^+ = -\mathcal{D}_{\pm}^+ \simeq \pm \frac{1}{2}, \\ F_1 &= G_1 \simeq \frac{2}{3J}, \quad F_2 = G_2 \simeq 0, \quad P = Q \simeq 0, \quad X_1 = Y_1 \simeq \frac{2}{3J}, \quad X_2 = Y_2 \simeq \frac{8}{9J^2} \end{aligned} \quad (2.11.45)$$

The effective Hamiltonian becomes

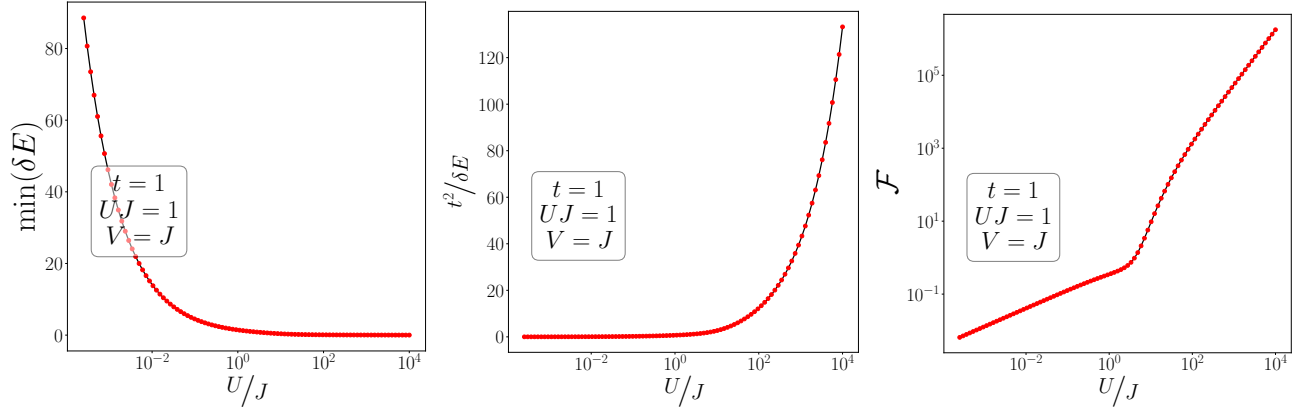
$$\begin{aligned} & - \left(|\Phi\rangle_0 \langle\Phi|_0 + |\Phi\rangle_3 \langle\Phi|_3 \right) \frac{4t^2}{3J} \left[1 - \frac{16t^2}{9J^3} \right] - \left(|\Phi\rangle_1 \langle\Phi|_1 + |\Phi\rangle_2 \langle\Phi|_2 \right) \frac{4t^2}{3J} \left[1 + \frac{2t^2}{9J^2} \right] \\ &= - \frac{4t^2}{3J} \sum_i |\Phi\rangle_i \langle\Phi|_i + \left(|\Phi\rangle_0 \langle\Phi|_0 + |\Phi\rangle_3 \langle\Phi|_3 \right) \frac{64t^4}{27J^3} - \left(|\Phi\rangle_1 \langle\Phi|_1 + |\Phi\rangle_2 \langle\Phi|_2 \right) \frac{8t^4}{27J^3} \\ &= |\Psi\rangle_1 \langle\Psi|_1 \left[\text{constant} + \frac{64t^4}{27J^3} \mathcal{P}_{\text{charge}} - \frac{8t^4}{27J^3} \mathcal{P}_{\text{spin}} \right] \end{aligned} \quad (2.11.46)$$

$\mathcal{P}_{\text{spin}}$ and $\mathcal{P}_{\text{charge}}$ project, respectively, onto the spin and charge sectors of the first site. The fact that the charge sector comes with a positive factor means that the holon-doublon states are repulsive, and this renormalisation of the states generates an effective particle-hole symmetric Fermi liquid interaction on the first site - also known as the local Fermi liquid (LFL) [9].

2.12 Destruction of the Abrikosov-Suhl resonance: passage from strong-coupling to local moment

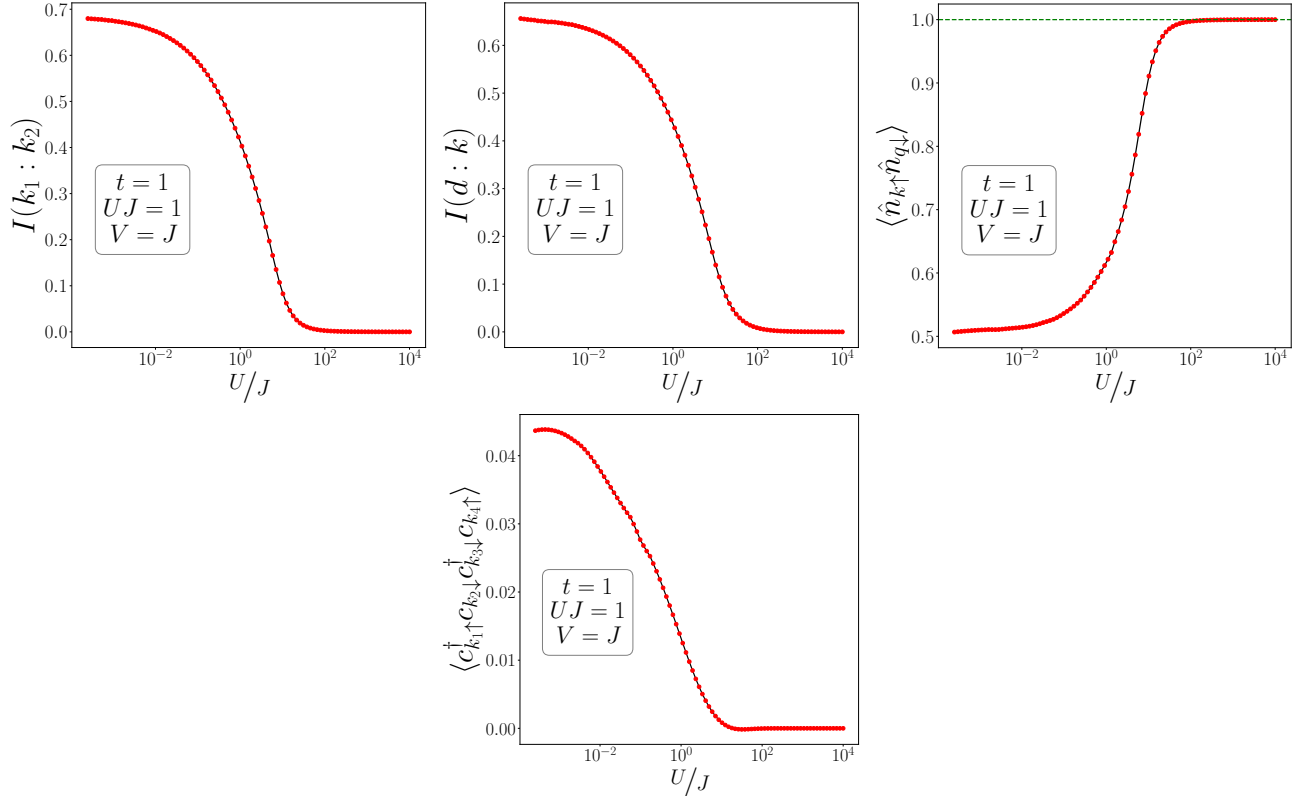
We will now tune the parameters of the fixed point Hamiltonian and study the variation of quantities related to the effective Hamiltonian like the local FL strength \mathcal{F} , the gap in the spectrum of the zeroth Hamiltonian H_0^* and the value of the small parameter $t^2/\delta E$, as well as various measures of entanglement like entanglement entropy, mutual information and spin-spin correlations between various sets of members of the real-space impurity+lattice construction. We will trace a specific path through the space of values of fixed point couplings: we will start from the strong-coupling regime $U \ll J, V$ and go towards the local moment regime $U \gg J, V$. The context of this study is that the technique of dynamical mean-field theory (DMFT) obtains a metal-insulator transition in the 2D Hubbard model by studying the Anderson impurity model as the auxiliary system for the Hubbard; there, the local moment regime of the impurity corresponds to the insulator in the bulk. Our goal here is to study what precisely happens in the effective Hamiltonian in the journey from the metal to the insulator, and draw a concrete connection between this modification of the effective Hamiltonian, and the simultaneous change of the impurity spectral function in fig. 2.10. This is done with the knowledge that the local moment phase of the generalised SIAM is never RG-stable.

Perturbation theory parameters



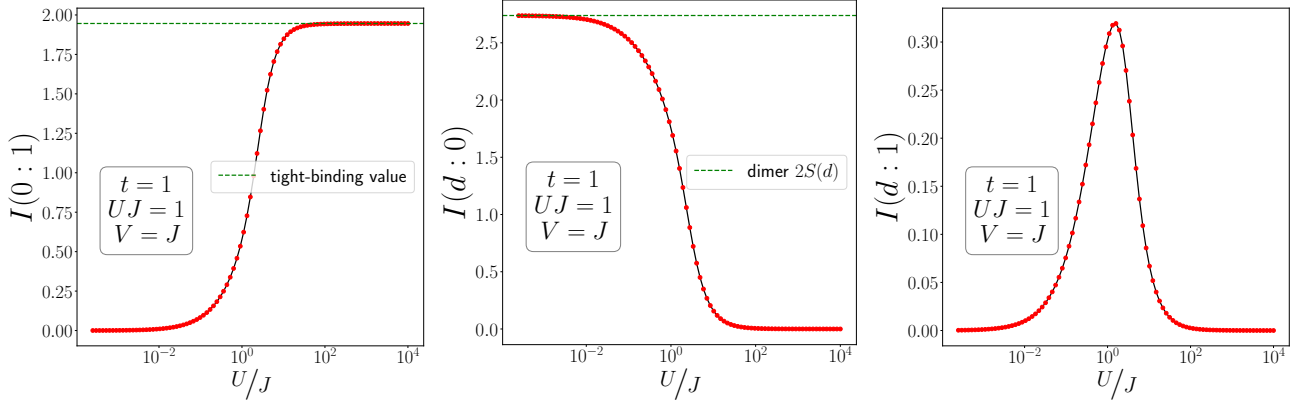
The vanishing of the gap and the growth of the small parameter indicates the breakdown of perturbation theory around the singlet; this simply shows that there is a degeneracy in the local moment regime, and the effective Hamiltonian will have to be obtained using degenerate perturbation theory. The presence of degeneracy also suggests that the effective Hamiltonian will be of the non-Fermi liquid type.

k -space correlations within the Kondo cloud



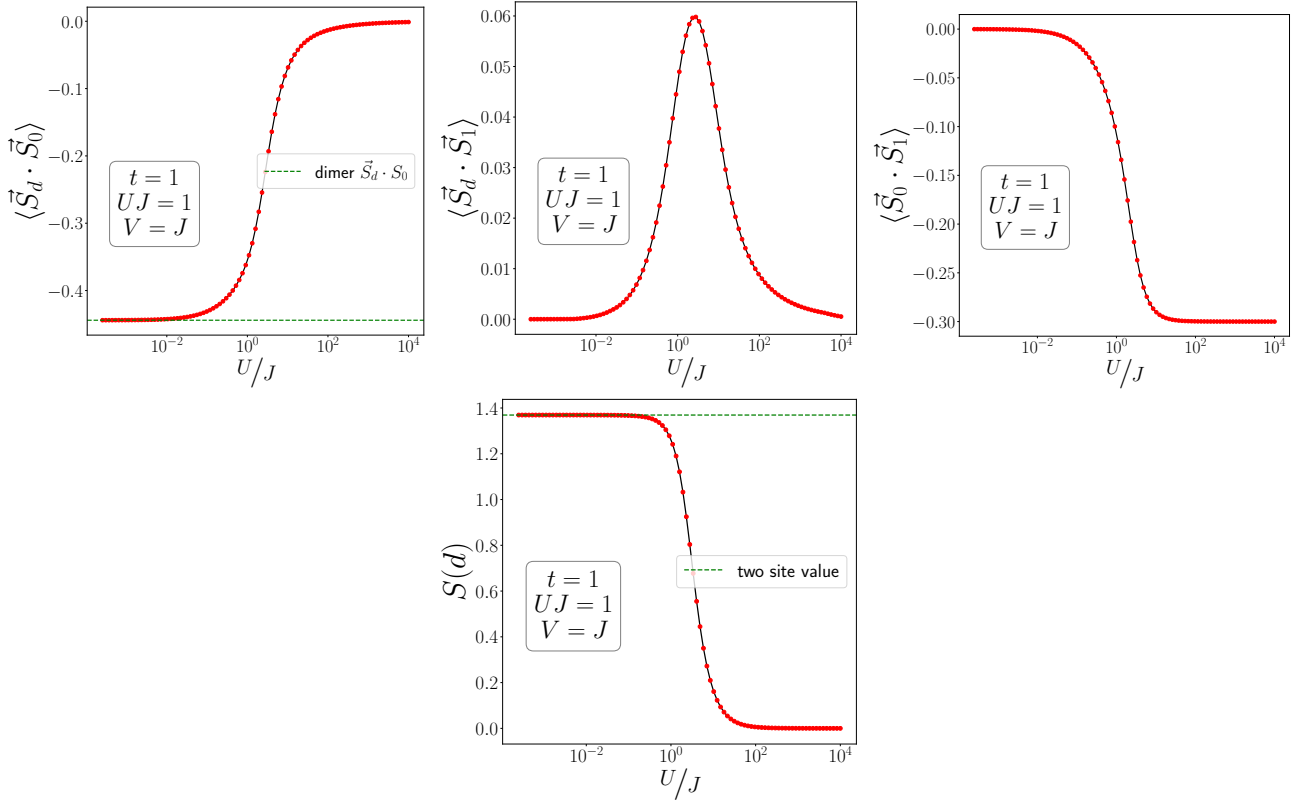
The vanishing of the Kondo cloud at large U/J is clear indication of the destruction of the Kondo cloud and the breakdown of screening. Non-zero mutual information indicates an (impurity-mediated) interaction between the k -states of the conduction bath; seen differently, it is this interaction that is responsively for the screening of the impurity. The disappearance of the mutual information is indicative of the disappearance of this interaction.

Mutual information between various real space members



The impurity-zeroth site mutual information $I(d:0)$ remains unchanged at the maximum for an appreciable range of values, and this shows the stability of the singlet. Meanwhile, the mutual information between the zeroth site and the site nearest to it ($I(0:1)$) grows, because when the singlet weakens, the zeroth site is able to entangle more with the other sites. It finally saturates to its maximum value, which is the value produced as result of the tight-binding hopping. The mutual information between the impurity and sites beyond the zeroth site ($I(d:1)$) show a non-monotonic behaviour; it first increases as the entanglement that was initially restricted to just the impurity and the zeroth sites begins "seeping" into the other sites as well. Beyond a critical value of U/J , $I(d:1)$ starts dropping, because the entanglement has now mostly shifted out of the zero mode and into the conduction bath.

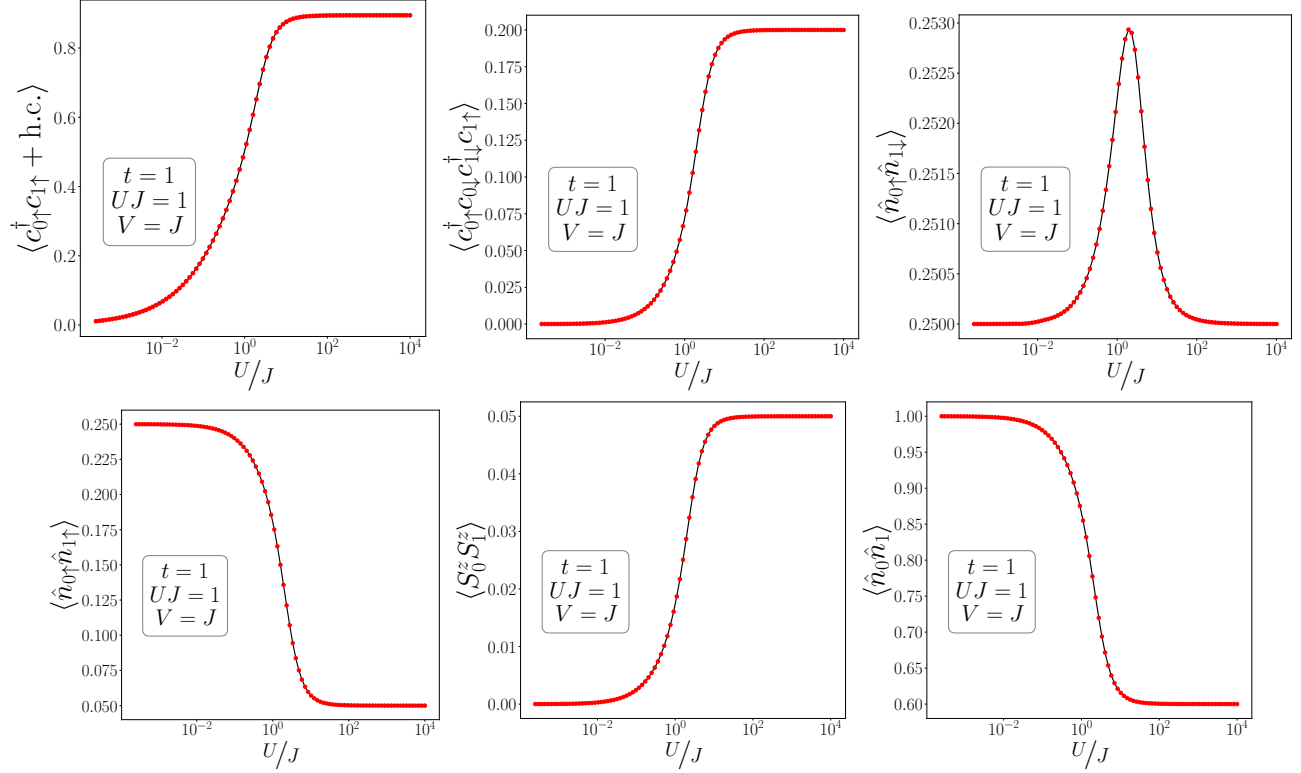
Impurity entanglement entropy and spin-spin correlations



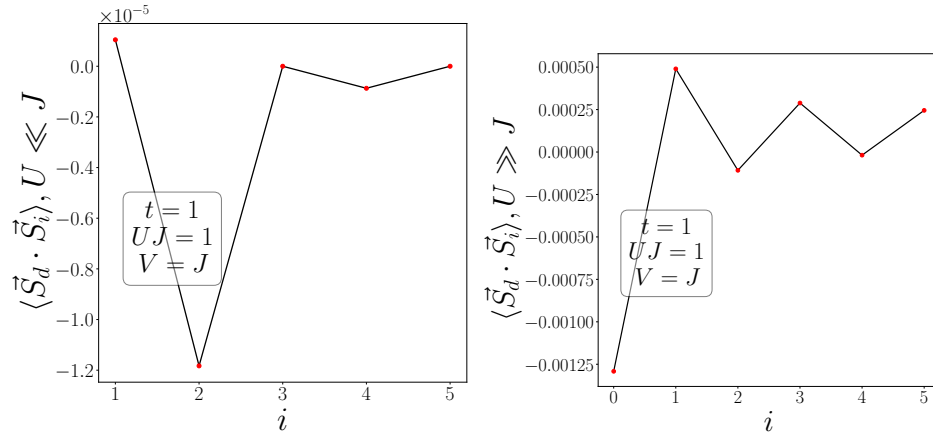
The von-Neumann entanglement entropy $S(d)$ of the impurity shows pretty straightforward behaviour. It is maximum for $U \ll J$ because it is in a singlet configuration. For $U \gg J$, the singlet weakens and the impurity

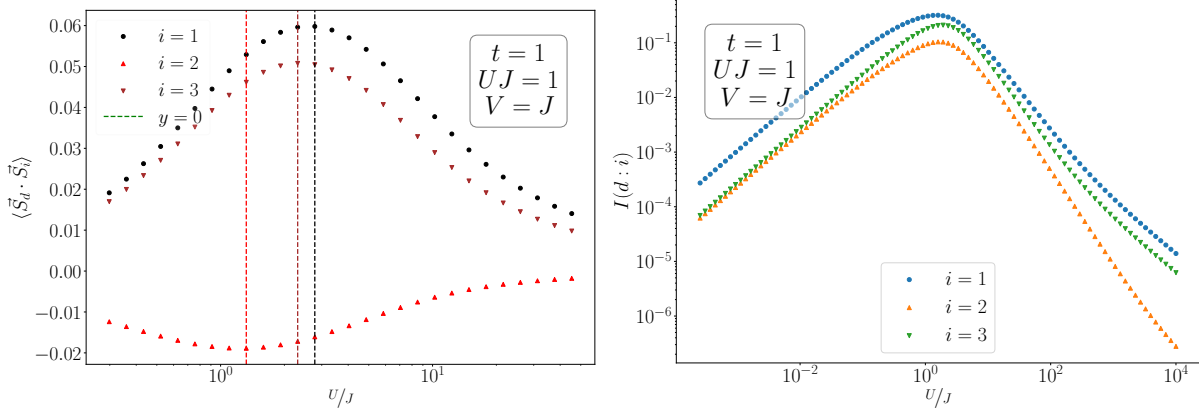
begins to decouple from the bath, leading to a reduction in $S(d)$. At sufficiently low values of J/U , the impurity decouples from the zeroth site and the total system can be factorised into a local moment in product with a tight-binding chain, so that the impurity site will now have zero entanglement entropy.

Real-space correlations

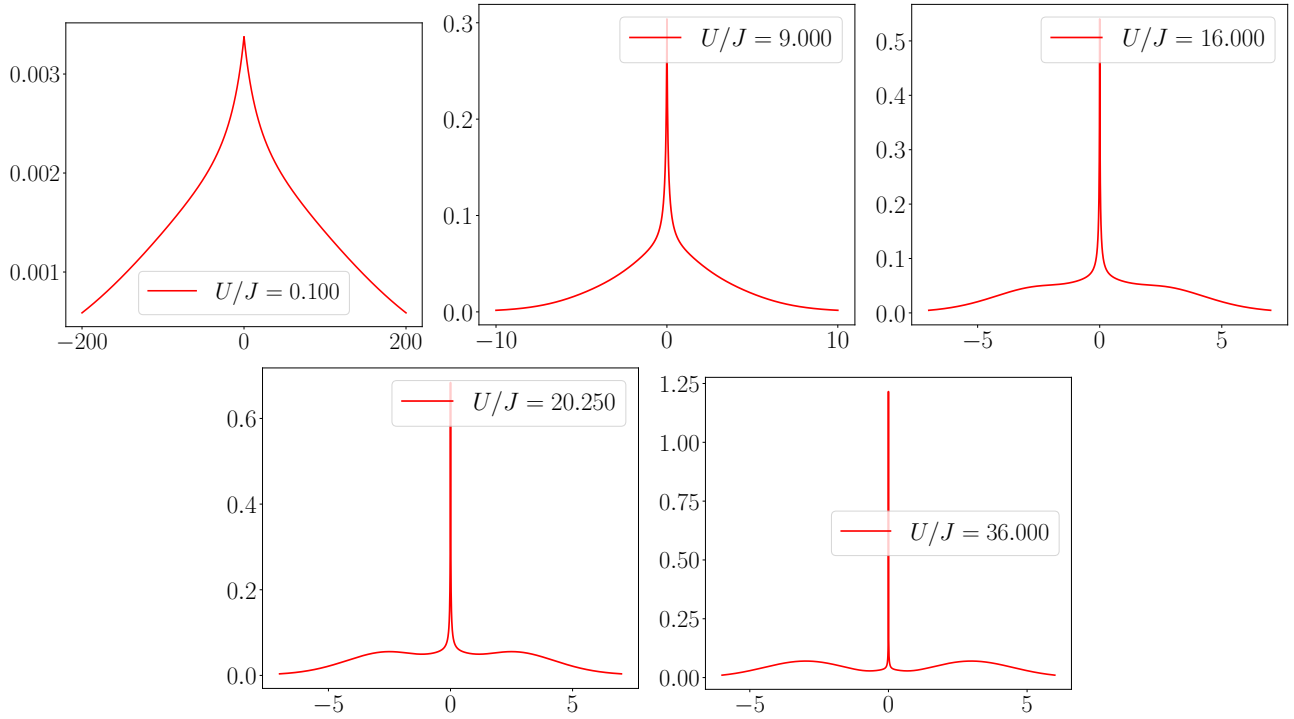


Real-space correlations as function of distance





Impurity spectral function



2.13 Calculating the $T = 0$ Wilson ratio from low energy excitations

The total system now consists of two decoupled parts - the singlet composed of the impurity and the zeroth site, and the remaining lattice composed of $N-1$ sites with a tight-binding dispersion and a local interaction at the 1-th site. The effective Hamiltonian for the remaining lattice is

$$\sum_{i=1}^{\infty} \sum_{\sigma} t \left(c_{i\sigma}^{\dagger} c_{i+1\sigma} + c_{i+1\sigma}^{\dagger} c_{i\sigma} \right) + u \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \quad (2.13.1)$$

We have rewritten the holon term in terms of the spin and doublon operators. We will now invoke the mean-field approximation in simplifying this term. We will be dealing with thermodynamic quantities soon, so the operators will be replaced by their thermodynamic values, that is, the values that minimize the free energy functional.

$$\hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rightarrow \langle \hat{n}_{1\uparrow} \hat{n}_{1\downarrow} \rangle = \langle \delta n_{1\uparrow} \delta n_{1\downarrow} \rangle + \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle \quad (2.13.2)$$

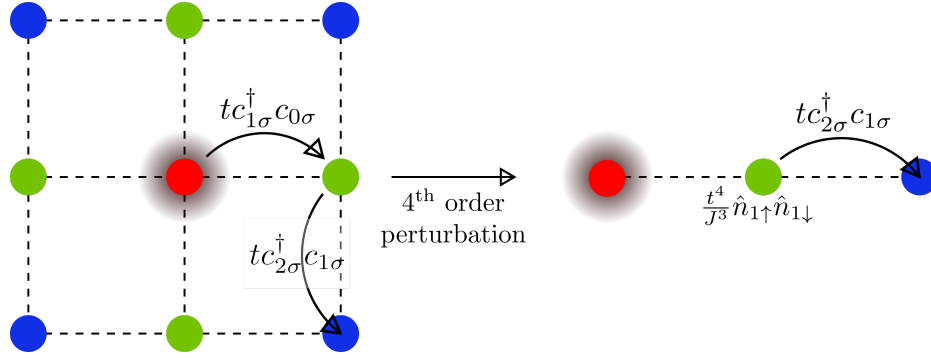


Figure 2.11: *Left*: The nearest-neighbor hopping described by the effective Hamiltonian. The red circle is the impurity. The black cloud at the center demarcates the collection of electrons at the origin of the lattice (which couple to the impurity). The green circles represent lattice sites that are nearest to the origin. The blue circles represent next-nearest sites. *Right*: After treating the hopping between origin and its nearest neighbors as perturbation, we get a system consisting of two decoupled parts: one part is the impurity+cloud singlet, the other part is the rest of the lattice sites. The effect of the hopping between the origin and the green sites is a repulsion term on the green sites.

where $\delta n_{1\sigma} \equiv n_{1\sigma} - \langle n_{1\sigma} \rangle$ is the fluctuation of the particle number above the ground state. The mean-field approximation then involves dropping the first term which is a quadratic fluctuation - since we are interested in values of quantities at $T \rightarrow 0$, this quadratic fluctuation is very small. The interaction we are left with is

$$u \langle n_{1\uparrow} \rangle \langle n_{1\downarrow} \rangle = \sum_{kq\sigma} f_{kq} \langle n_{k\sigma} \rangle \langle n_{q\bar{\sigma}} \rangle \quad (2.13.3)$$

This interaction converts the problem to that of a Landau Fermi liquid, with the quasiparticle energy functional being given by

$$\epsilon_{k\sigma} = \epsilon_k + \sum_q f_{kq} \langle \hat{n}_{q\bar{\sigma}} \rangle \quad (2.13.4)$$

From the form of the quasiparticle energy functional, we can see that there is no spin-parallel term, so we can write

$$f_{kk'\sigma\sigma} = 0, f_{kk'\sigma\bar{\sigma}} = f_{kk'} \quad (2.13.5)$$

We will now use this Fermi liquid form to extract the Wilson ratio. We will make use of the following definitions/results:

$$dn_{k\sigma} = \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) \quad [\text{follows from differentiating FD distribution}] \quad (2.13.6)$$

$$C_V = \frac{d\epsilon}{dT}, \quad \chi^{s,c} = \frac{d}{d(B, \mu)} (n_{\uparrow} \mp n_{\downarrow}), \quad 2f_0^{s,a} = \sum_k (f_{kk'\uparrow\uparrow} \pm f_{kk'\uparrow\downarrow}), \quad F_0^{s,a} = \rho(0)f_0^{s,a} \quad (2.13.7)$$

2.13.1 Low- T Specific heat

$$\begin{aligned} C &= \frac{d}{dT} \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} \\ &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{no quasiparticles at ground state}] \\ &\approx \sum_{k\sigma} \epsilon_{k\sigma}^0 \frac{dn_{k\sigma}}{dT} \quad [\text{same expression as Fermi gas but with modified distribution function}] \\ &= \rho(0)T \end{aligned} \quad (2.13.8)$$

where ρ is the total quasiparticle DOS with contributions from conduction bath and impurity.

$$\rho \sim \text{Im Trace} [G] = \text{Im} \sum_{d\sigma} G_{dd}^\sigma + \text{Im} \sum_{k\sigma} G_{kk}^\sigma = \rho_0 + \rho_{\text{imp}} \quad (2.13.9)$$

which gives

$$C_{imp} \equiv C - C_0 = \rho_{imp}(0)T \quad (2.13.10)$$

2.13.2 Low- T Charge Susceptibility

$$\chi^c = \frac{dN}{d\mu} \quad (2.13.11)$$

Due to change in chemical potential, $\delta\epsilon_{k\sigma}$ is isotropic and SU(2)-symmetric. Hence

$$\begin{aligned} d\epsilon_{k\sigma} &= \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\ &= dn \sum_{k'} \left(f_{kk'\uparrow\uparrow} + f_{kk'\uparrow\downarrow} \right) \quad [dn = dn_{k'\uparrow} = dn_{k'\downarrow}] \\ &= 2dn f_0^s \end{aligned} \quad (2.13.12)$$

Therefore,

$$\begin{aligned} dN &= \sum_{k\sigma} dn_{k\sigma} = \sum_{k\sigma} \frac{\partial n}{\partial \epsilon_{k\sigma}} (d\epsilon_{k\sigma} - d\mu) = \sum_{k\sigma} -\frac{1}{2}\rho (2dn f_0^s - d\mu) = -\rho(0)dN f_0^s + d\mu\rho(0) \\ &\approx d\mu\rho(0) - \rho(0)f_0^s d\mu\rho(0) \quad [\text{substitute } dN \text{ back into itself}] \\ \implies \frac{dN}{d\mu} &= \rho(0) (1 - \rho(0)f_0^s) \implies \chi_{imp}^c = \rho(0)_{imp} - \rho(0)f_0^s \end{aligned} \quad (2.13.13)$$

At an intermediate state, we substituted dN back into itself and kept only the leading order term. This is justified because $f_{kk'}$ goes as $\frac{1}{NJ}$. At the fixed point and for a thermodynamically large system, both J and N are very large, so keeping only the leading order suffices.

From a previous calculation, we know that the charge susceptibility at $T = 0$ is zero (eq. (2.7.9)), so we can write down the following relation:

$$f_0^s = \frac{\rho(0)_{imp}}{\rho(0)} \quad (2.13.14)$$

2.13.3 Low- T Spin Susceptibility

$$\chi^s = \frac{dm}{dB} \quad (2.13.15)$$

Due to change in magnetic field, change in $\epsilon_{k\sigma}$ should be isotropic and SU(2)-antisymmetric. Hence

$$\begin{aligned} d\epsilon_{k\sigma} &= -\frac{1}{2}dB\sigma + \sum_{k'\sigma'} f_{kk'\sigma\sigma'} dn_{k'\sigma'} \\ &= -\frac{1}{2}dB\sigma + dn_\sigma \sum_{k'} \left(f_{kk'\uparrow\uparrow} - f_{kk'\uparrow\downarrow} \right) \quad [dn_{k'\uparrow} = -dn_{k'\downarrow}] \\ &= -\frac{1}{2}dB\sigma + 2dn_\sigma f_0^a \end{aligned} \quad (2.13.16)$$

Since the total number remains constant, $\mu = 0$. Therefore,

$$\begin{aligned} dm &= \sum_k (dn_{k\uparrow} - dn_{k\downarrow}) = -\frac{1}{2} \sum_k \rho (d\epsilon_{k\uparrow} - d\epsilon_{k\downarrow}) = -\frac{1}{2} \sum_k \rho \left(-dB + 2f_0^a (dn_{k\uparrow} - dn_{k\downarrow}) \right) \\ &= dB\rho(0) - dm\rho(0)f_0^a \approx dB\rho(0) - \rho(0)f_0^a B\rho(0) \quad [\text{substitute } dm \text{ back into itself}] \\ \implies \frac{dm}{dB} &= \rho(0) (1 - \rho(0)f_0^a) \implies \chi_{imp}^s = \rho(0)_{imp} - \rho(0)f_0^a \end{aligned} \quad (2.13.17)$$

2.13.4 Wilson ratio

The Wilson ratio for the impurity is defined as

$$R = \frac{\chi_{imp}^s}{\frac{C_{imp}}{T}} \quad (2.13.18)$$

From eq. (2.13.5), we have $f_0^s = -f_0^a$, which, when combined with eq. (2.13.14), gives

$$\chi_{imp}^s = 2\rho(0)_{imp} \quad (2.13.19)$$

The Wilson ratio becomes

$$R = \frac{2\rho(0)_{imp}}{\rho(0)_{imp}} = 2 \quad (2.13.20)$$

2.14 Luttinger's and Friedel's sum rules

The subsequent discussions are for the first quadrant where $U^* = 0$ and $J^* > K^*$. At high temperatures, we see that the impurity susceptibility attains the value of

$$\frac{1}{8k_B T} \quad (2.14.1)$$

which implies that the impurity behaves as a free orbital in this limit, having no coupling with the bath. We can write down the following effective Hamiltonian for such a limit:

$$\mathcal{H}_{\text{high-T}} = \tilde{\epsilon}_d \hat{n}_d + \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} \quad (2.14.2)$$

Since the impurity is decoupled from the bath, we can immediately write down the Hamiltonian just for the impurity:

$$\mathcal{H}_{\text{high-T, imp}} = \tilde{\epsilon}_d \hat{n}_d \quad (2.14.3)$$

We consider the resonant-level model:

$$\mathcal{H}_{\text{res}} = \sum_{k\sigma} \epsilon_k \hat{n}_{k\sigma} + \epsilon_d \hat{n}_d + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + \text{h.c.} \right) \quad (2.14.4)$$

The total Green's function is

$$G(z) = \frac{1}{z - \mathcal{H}_{\text{res}}} \quad (2.14.5)$$

The impurity diagonal Green's function is

$$G_{dd}(z) = \frac{1}{z - \epsilon_d - \Sigma_d(z)}, \quad G_d(z) = G_{dd} |d\rangle \langle d| \quad (2.14.6)$$

where $\Sigma_d(z)$ is in general complex and is zero at the free orbital fixed point. The conduction electron Green's function is

$$G_{kk}(z) = G_k^0(z) + \left[G_k^0(z) V_k \right]^2 G_{dd}(z), \quad G_c(z) \equiv \sum_k |k\rangle \langle k| G_{kk}(z), \quad G_{c0}(z) \equiv \sum_k G_{kk}^0(z) |k\rangle \langle k| \quad (2.14.7)$$

The total Green's function can be written as

$$\begin{aligned} G(z) &= \left(\sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) G \left(\sum_k |k\rangle \langle k| + |d\rangle \langle d| \right) \\ &= \sum_k |k\rangle \langle k| G_{kk}(z) + G_{dd}(z) |d\rangle \langle d| + \text{off-diagonal terms} \\ &= G_c(z) + G_d(z) + \text{off-diagonal terms} \end{aligned} \quad (2.14.8)$$

The total number of electrons is given by

$$\begin{aligned} N &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G(z)] \\ &= \oint \frac{dz}{2\pi i} n_F(z) \text{Tr} [G_d(z) + G_c(z)] \end{aligned} \quad (2.14.9)$$

The contour Γ counts all the singularities of $\text{Tr} G(z)$, and thus encloses only the real axis of the complex plane (since $G(z)$ comes from a Hermitian matrix \mathcal{H}_{res} , all its singularities are real). At this point, we can use an identity:

$$\begin{aligned} \text{Tr} [G_d(z)] &= \text{Tr} \left[\frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \right] = \text{Tr} \left[\frac{|d\rangle \langle d|}{z - \epsilon_d - \Sigma_d(z)} \frac{\partial(z - \epsilon_d)}{\partial z} \right] = \text{Tr} \left[|d\rangle \langle d| G_{dd} \frac{\partial \{G_{dd}^{-1}(z) + \Sigma_d(z)\}}{\partial z} \right] \\ &= \text{Tr} \left[G_d(z) \frac{\partial G_d^{-1}(z)}{\partial z} \right] + \text{Tr} \left[G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right] = \frac{\partial}{\partial z} [\ln \text{Det} G_d^{-1}(z)] + \text{Tr} \left[G_d(z) \frac{\partial \Sigma_d(z)}{\partial z} \right] \end{aligned} \quad (2.14.10)$$

In the last step, we converted the trace to a determinant using

$$\text{Tr} \left[A \frac{\partial A^{-1}}{\partial z} \right] = \frac{\partial}{\partial z} \text{Tr} \ln A^{-1} = \frac{\partial}{\partial z} \sum_i \ln \lambda_i = \frac{\partial}{\partial z} \ln \prod_i \lambda_i = \frac{\partial}{\partial z} \ln \text{Det} A^{-1} \quad (2.14.11)$$

where λ_i are the eigenvalues of A^{-1} . Substituting $\text{Tr} [G_d(z)]$ into the total number of particles gives

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) + \text{Tr} G_c(z) \right] \quad (2.14.12)$$

The conduction electron part can also be simplified:

$$\text{Tr} G_c(z) = \text{Tr} \left[G_{c0}(z) + \sum_k \left\{ G_k^0(z) V_k \right\}^2 G_{dd}(z) |k\rangle \langle k| \right] = \text{Tr} [G_{c0}(z)] + \sum_k \left[G_k^0(z) V_k \right]^2 G_{dd}(z) \quad (2.14.13)$$

Since $G_{c0}^{-1}(z) = z - \sum_k \epsilon_k \hat{n}_k$, we can write $\text{Tr} [G_{c0}(z)] = \text{Tr} \left[G_{c0}(z) \frac{\partial}{\partial z} G_{c0}^{-1} \right]$ and hence

$$\text{Tr} G_c(z) = \frac{\partial}{\partial z} [\ln \text{Det} G_{c0}^{-1}(z)] + \sum_k \left[G_k^0(z) V_k \right]^2 G_{dd}(z) \quad (2.14.14)$$

Updating the total particles with this leads to

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \frac{\partial}{\partial z} \ln \text{Det} \{G_{c0}^{-1}(z)\} + \text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) + \sum_k \left(V_k G_k^0 \right)^2 G_{dd}(z) \right] \quad (2.14.15)$$

For the resonant-level model, we have

$$\Sigma_d = \sum_k V_k^2 G_k^0 = \sum_k \frac{V_k^2}{z - \epsilon_k} \quad (2.14.16)$$

such that

$$\text{Tr} \left(G_d(z) \frac{\partial}{\partial z} \Sigma_d(z) \right) = -G_{dd}(z) \sum_k \left(V_k G_k^0 \right)^2 \quad (2.14.17)$$

which allows us to write

$$N = \oint \frac{dz}{2\pi i} n_F(z) \left[\frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \frac{\partial}{\partial z} \ln \text{Det} \{G_{c0}^{-1}(z)\} \right] \quad (2.14.18)$$

At $T = 0$, n_F is defined as 1 below the FS, $\frac{1}{2}$ at the FS and 0 above it.

$$N = \left[\oint_{\Gamma_{<}} + \frac{1}{2} \oint_{\Gamma_0} \right] \frac{dz}{2\pi i} \left[\frac{\partial}{\partial z} \ln \text{Det} \{G_d^{-1}(z)\} + \frac{\partial}{\partial z} \ln \text{Det} \{G_{c0}^{-1}(z)\} \right] \quad (2.14.19)$$

Following Seki and Yunoki, we can define a winding number for a Green's function $G(z)$:

$$n_{\text{Det } G^{-1}(C)} = \oint_C \frac{dz}{2\pi i} \frac{\partial \ln \text{Det } G^{-1}(z)}{\partial z} = \oint_{\text{Det } G^{-1}(C)} \frac{d \text{Det } G^{-1}}{\text{Det } G^{-1}} \quad (2.14.20)$$

Since $n_{\text{Det } G^{-1}(C)}$ counts the number of times the curve $\text{Det } G^{-1}(C)$ winds around the origin, it is integer-valued and topological. Seki and Yunoki also show that the this number is given by

$$n_{\text{Det } G^{-1}(C)} = P_{\text{Det } G}(C) - Z_{\text{Det } G}(C) \quad (2.14.21)$$

where $P_{f(z)}(C)$ is the number of poles of $f(z)$ enclosed by the contour C , and Z is the corresponding number of zeros. The total number of particles in the resonant level model can thus be written as

$$N = P_{\text{Det } G_d}(\Gamma_{<}) - Z_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2} [P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0)] + P_{\text{Det } G_{c0}}(\Gamma_{<}) - Z_{\text{Det } G_{c0}}(\Gamma_{<}) + \frac{1}{2} [P_{\text{Det } G_{c0}}(\Gamma_0) - Z_{\text{Det } G_{c0}}(\Gamma_0)] \quad (2.14.22)$$

The average number of particles can thus be expressed purely in terms of the number of poles and zeros of the impurity and the conduction electron Green's functions. As shown by Seki and Yunoki, the second line gives the Luttinger volume V_L :

$$N = P_{\text{Det } G_d}(\Gamma_{<}) - Z_{\text{Det } G_d}(\Gamma_{<}) + \frac{1}{2} [P_{\text{Det } G_d}(\Gamma_0) - Z_{\text{Det } G_d}(\Gamma_0)] + V_L \quad (2.14.23)$$

If we start from a non-interacting model ($V_k = 0$), we can write

$$N = \mathcal{N}_{imp}^0 + V_L^0 \quad (2.14.24)$$

where \mathcal{N}_{imp}^0 is simply the number of singularities of G_d on the real axis, for the non-interacting case. We now turn up the interaction V_k , keeping the total number of particles conserved at N . With a non-zero V_k , the impurity self-energy can be written (assuming a constant density of states) as

$$\Sigma_d(z) = \Sigma_d^{\text{real}}(z) - i\Delta \quad (2.14.25)$$

so that the impurity Greens function becomes

$$G_d(z) = \frac{1}{z - \epsilon_d - \Sigma_d^{\text{real}}(z) + i\Delta} \quad (2.14.26)$$

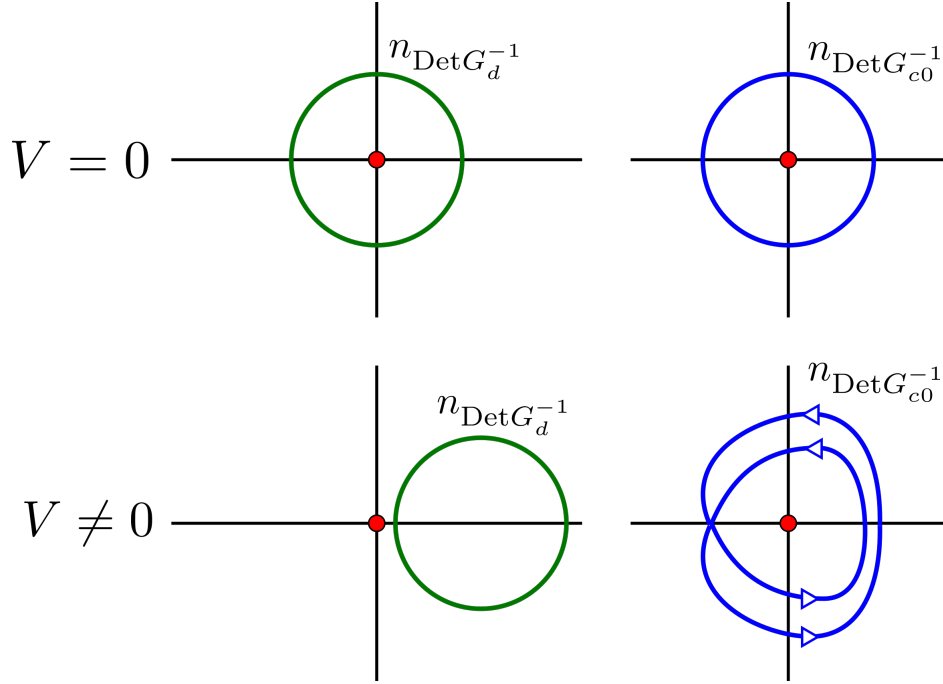
We can see that the presence of an imaginary part lifts the pole of $G_d(z)$ off the real axis, and since the contour Γ_0 encloses only the real axis, this will count as a loss in the number of poles of $G_d(z)$. Also, if we specialize to the case where the renormalized impurity site energy $\epsilon_d^* = \epsilon_d + \Sigma_d^{\text{real}} = 0$, this loss will happen at the Fermi surface, and will hence be multiplied by a factor of half. We can therefore write

$$N = \mathcal{N}_{imp} + V_L = \mathcal{N}_{imp}^0 - \frac{1}{2} + V_L \implies V_L = V_L^0 + \frac{1}{2} \quad (2.14.27)$$

If we take into account the spin-degeneracy and redefine V_L to mean the Luttinger volume for both momentum and spin degrees of freedom, we get

$$V_L = V_L^0 + 1 \quad (2.14.28)$$

This is a specific case of the more general result for Kondo lattices obtained by Oshikawa using flux-insertion arguments in [10]. One can now ask what happens to this result once we also incorporate the spin-exchange interaction $J\vec{S}_d \cdot \vec{s}$; we can expect that it will complicate the self-energy of the impurity. It cannot, however,



preclude the loss of the real pole, nor can it create a new singularity - to do so would require the self-energy to diverge, and we are working with finite systems here. This suggests that the eq. (2.14.28) would still hold.

We have also not accounted for the RG flow from the local moment fixed point to the strong-coupling fixed point. The local moment fixed point is characterized by a decoupled quantum top:

$$\mathcal{H}_{\text{LM}} = \epsilon_d \hat{n}_d + U \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \quad (2.14.29)$$

It can be shown that the single-particle Green's function for this effective Hamiltonian is similar to the one at the free-orbital fixed point. We will use the equation of motion technique to solve for the Green's function. The time-domain retarded Green's function is defined as

$$G_{d\sigma}(t, t') = -i\theta(t - t') \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(t') \right\} \right\rangle \quad (2.14.30)$$

Since the Hamiltonian is time-translation invariant, we can drop one of the instants:

$$G_{d\sigma}(t, 0) = -i\theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (2.14.31)$$

The time derivative is

$$\begin{aligned} \partial_t G_{d\sigma} &= -i \left[\partial_t \theta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \partial_t \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] \\ &= -i \left[\delta(t) \left\langle \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle + \theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \right] = -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \end{aligned} \quad (2.14.32)$$

From the Heisenberg equations of motion, we get

$$i\partial_t c_{d\sigma}(t) = [c_{d\sigma}(t), \mathcal{H}_{\text{LM}}(t)] = [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) \quad (2.14.33)$$

Substituting this into the time-derivative gives

$$\partial_t G_{d\sigma} = -i\delta(t) - i\theta(t) \left\langle \left\{ -i [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle = -i\delta(t) - i\epsilon_d G_{d\sigma} - U\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (2.14.34)$$

We define another Greens function

$$G' = -i\theta(t) \left\langle \hat{n}_{d\bar{\sigma}}(t) \left\{ c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (2.14.35)$$

which satisfies the equation of motion

$$\partial_t G' = -i\delta(t) - i\theta(t) \left\langle \left\{ \partial_t \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle - i\theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle \quad (2.14.36)$$

The second term vanishes because $[\hat{n}_{d\bar{\sigma}}, \mathcal{H}_{LM}] = 0$ and hence $\partial_t \hat{n}_{d\bar{\sigma}} = 0$. Also,

$$\hat{n}_{d\bar{\sigma}}(t) \partial_t c_{d\sigma}(t) = -i\hat{n}_{d\bar{\sigma}}(t) [\epsilon_d + U \hat{n}_{d\bar{\sigma}}(t)] c_{d\sigma}(t) = -i [\epsilon_d + U] \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t) \quad (2.14.37)$$

Therefore,

$$\partial_t G' = -i\delta(t) \langle \hat{n}_{d\bar{\sigma}}(0) \rangle - [\epsilon_d + U] \theta(t) \left\langle \left\{ \hat{n}_{d\bar{\sigma}}(t) c_{d\sigma}(t), c_{d\sigma}^\dagger(0) \right\} \right\rangle = -i\delta(t) - i(\epsilon_d + U) G' \quad (2.14.38)$$

Changing all quantities to frequency-domain:

$$\begin{aligned} G'(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} G'(\omega) \\ \partial_t G'(t) &= - \int_{-\infty}^{\infty} d\omega i\omega e^{-i\omega t} G'(\omega) \\ \delta(t) &= \int_{-\infty}^{\infty} d\omega e^{-i\omega t} \end{aligned} \quad (2.14.39)$$

Substituting these forms in the equation and comparing the coefficients of $e^{i\omega t}$ gives

$$\omega G'(\omega) = \langle \hat{n}_{d\bar{\sigma}}(0) \rangle + (\epsilon_d + U) G'(\omega) \implies G'(\omega) = \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \quad (2.14.40)$$

The equation of motion $G_{d\sigma}$ can now be solved

$$\begin{aligned} \partial_t G_{d\sigma}(t) &= -i\delta(t) - i\epsilon_d G_{d\sigma}(t) - iU G'_{d\sigma}(t) \implies \omega G_{d\sigma}(\omega) = 1 + \epsilon_d G_{d\sigma}(\omega) + U \frac{\langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{\omega - \epsilon_d - U} \\ \implies G_{d\sigma}(\omega) &= \frac{1}{\omega - \epsilon_d} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega - \epsilon_d)(\omega - \epsilon_d - U)} \end{aligned} \quad (2.14.41)$$

For a particle-hole symmetric system, we can substitute $\epsilon_d = -|\epsilon_d|$ and $\epsilon_d + U = |\epsilon_d|$.

$$G_{d\sigma}(\omega) = \frac{1}{\omega + |\epsilon_d|} + \frac{U \langle \hat{n}_{d\bar{\sigma}}(0) \rangle}{(\omega + |\epsilon_d|)(\omega - |\epsilon_d|)} \quad (2.14.42)$$

which reveals two poles at $\pm|\epsilon_d|$, one above and one below the Fermi surface. Since the RHS of eq. (2.14.23) counts the number of poles on or below the FS, we will still count one pole for $G_{d\sigma}$. Thus, this Green's function is topological similar to the free-orbital one at $T = 0$.

The scattering phase shift suffered by the conduction electrons at the Fermi surface, off the impurity, can be calculated from the impurity occupancy, using the Friedel sum rule. From the ground state wavefunction, we can calculate the average number of particles on the impurity:

$$\langle n_d \rangle = \langle \Psi | \sum_{\sigma} \hat{n}_{d\sigma} | \Psi \rangle_1 \quad (2.14.43)$$

$|\Psi\rangle_1$ is the lower energy state in eq. (2.4.5). Performing the inner product gives

$$\langle n_d \rangle = \left(c_s^- \right)^2 + \left(c_c^- \right)^2 = 1 \quad (2.14.44)$$

The phase shift is thus

$$\frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) = \langle n_d \rangle \implies \delta_{\sigma}(0) = \frac{\pi}{2} \quad (2.14.45)$$

There we used $\delta_{\uparrow} = \delta_{\downarrow}$ because the model is SU(2)-symmetric. This line of arguments was first presented for the Kondo model in [11].

The change in Luttinger's number also allows us to calculate the Wilson ratio of the system, from eq. (F.0.7).

$$R = 1 + \sin^2 \left(\frac{\pi}{2} \Delta N_L \right) = 1 + \sin^2 \frac{\pi}{2} = 2 \quad (2.14.46)$$

2.15 Reverse RG analysis

The goal here is to chart the journey starting from the IR fixed point towards the UV regime, by following one particular wavefunction. We will start with a very simple IR ground state wavefunction, and then go back towards the UV ground state by applying the inverse unitary operator U^{\dagger} :

$$\begin{aligned} U : \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} &\rightarrow |1, 2, \dots, N-1\rangle |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} \\ U^{\dagger} : \underbrace{|1, 2, \dots, N^*\rangle |N^*+1\rangle \dots |N\rangle}_{\text{IR ground state}} &\rightarrow |1, 2, \dots, N^*+1\rangle |N^*+2\rangle \dots |N\rangle \rightarrow \dots \rightarrow \underbrace{|1, 2, \dots, N\rangle}_{\text{UV ground state}} \end{aligned}$$

The first process is the forward RG which we used to obtain the scaling equations. The second process is the reverse RG which we will undertake now. In general, we start with an IR wavefunction that consists a certain number of momentum states n_1 still entangled with the impurity, and the remaining momentum states n_2 disentangled from the impurity. The former are said to be part of the emergent Kondo cloud, while the latter are said to be part of the integrals of motion (IOMs) and appear in direct product with the cloud+impurity system in the ground state wavefunction. Each momentum state is tagged with two conduction bath levels, one above the Fermi surface and one below. These will be represented as k, \pm . If we represent the emergent cloud momentum states as $\{k_i\}$ and the IOM states as $\{q_i\}$, the ground state wavefunction can be written as

$$|\Psi\rangle_0 = \left(\otimes_{i=1}^{n_2} |q_i, -, \uparrow\rangle |q_i, -, \downarrow\rangle \right) |\Phi\rangle_{\text{cloud}} \left(\otimes_{i=1}^{n_2} |q_i, +, \uparrow\rangle |q_i, +, \downarrow\rangle \right) \quad (2.15.1)$$

Throughout, we have assumed that the IOMs below the Fermi surface are occupied while those above are unoccupied. This means:

$$|\Psi\rangle_0 = \left(\otimes_{i=1}^{n_2} |\hat{n}_{q_i, -, \uparrow} = 1\rangle |\hat{n}_{q_i, -, \downarrow} = 1\rangle \right) |\Phi\rangle_{\text{cloud}} \left(\otimes_{i=1}^{n_2} |\hat{n}_{q_i, +, \uparrow} = 0\rangle |\hat{n}_{q_i, +, \downarrow} = 0\rangle \right) \quad (2.15.2)$$

$|\Phi\rangle_{\text{cloud}}$ will be obtained by diagonalising a small system of n_1 conduction bath k states. This completes the construction of the IR ground state $|\Psi\rangle_0$. The algorithm of reverse RG then involves applying unitary transformations on this IR wavefunction; the unitary transformations will be the inverse of those that were applied during the forward RG algorithm. Since the forwards RG transformations decoupled k states and transformed them into the IOMS, the inverse transformations will take the momentum states in the IOMs and re-entangle them with the impurity+cloud system, one at a time. This is shown in fig. 2.12.

The next step is to write down the unitaries that will take us from the IR ground state to the UV ground state. In the forward RG, we used the following unitary for decoupling the shell ϵ_q and spin β is

$$U_{q\beta} = \frac{1}{\sqrt{2}} \left[1 + \eta_{0\beta} + \eta_{1\beta}^{\dagger} \right] . \quad (2.15.3)$$

Here, the subscripts 0 and 1 indicate it decouples an electron above and below the Fermi surface respectively. The inverse transformation for re-entangling $q\beta$ is

$$U_{q\beta}^{\dagger} = \frac{1}{\sqrt{2}} \left[1 + \eta_{0\beta}^{\dagger} + \eta_{1\beta} \right] . \quad (2.15.4)$$

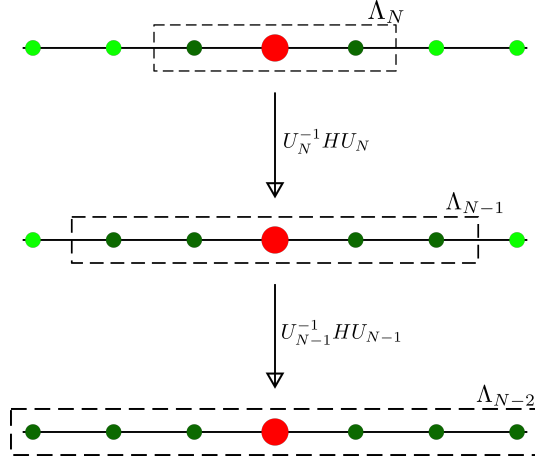


Figure 2.12: We start with a Hamiltonian with an impurity site (red) coupled with two conduction electrons (dark green), with four other decoupled electrons (bright green). The dotted rectangle represents the emergent window $(-\Lambda_j, \Lambda_j)$ at each step; the electrons inside that rectangle are still entangled with the impurity, while the ones inside have been decoupled. The next step of reverse RG involves applying the inverse transformation on the Hamiltonian, which will couple two more electrons from the IOMS (hence four dark green circles in the second step), leading to an enlargement of the emergent window. The unitary varies for each step, hence the notation U_j .

In the $U > 0$ regime, the η s are given by

$$\begin{aligned}\eta_{0\beta}^\dagger &= V \left[\frac{1}{d_0} (1 - \hat{n}_{d\bar{\beta}}) + \frac{1}{d_1} \hat{n}_{d\bar{\beta}} \right] c_{q\beta}^\dagger c_{d\beta} + \frac{1}{d_2} \frac{J}{2} \sum_k \left(S_d^z \beta c_{q\beta}^\dagger c_{k\beta} + c_{d\bar{\beta}}^\dagger c_{d\beta} c_{q\beta}^\dagger c_{k\bar{\beta}} \right), \\ \eta_{1\beta} &= V \left[\frac{1}{d_1} (1 - \hat{n}_{d\bar{\beta}}) + \frac{1}{d_0} \hat{n}_{d\bar{\beta}} \right] c_{d\beta}^\dagger c_{q\beta} + \frac{1}{d_2} \frac{J}{2} \sum_k \left(S_d^z \beta c_{k\beta}^\dagger c_{q\beta} + c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} \right); \end{aligned} \quad (2.15.5)$$

since K is irrelevant, we have set $K = 0$ here. The denominators have already been defined in eq. (2.2.5).

$$d_0 = \omega - \frac{D}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{K}{4} \quad (2.15.6)$$

The wavefunction after reversing one step of the RG will thus be

$$|\Psi\rangle_1 = U_{q\uparrow}^\dagger U_{q\downarrow}^\dagger |\Psi\rangle_0 \quad (2.15.7)$$

Here, q is the first momentum state immediately outside the emergent cloud. Re-entangling further momentum states using their respective unitaries lead to the sequence of wavefunctions $|\Psi\rangle_2, |\Psi\rangle_3$ and so on.

The results of the reverse RG study are depicted in the following plots. We have used two types of quantities in the process - mutual information and correlation functions. The mutual information between two subsystems A and B in a wavefunction with many subsystems is defined as

$$I(A : B) = S_A + S_B - S_{AB} \quad (2.15.8)$$

where $S_{ij\dots q}$ is the von-Neumann entropy of the reduced density matrix obtained after tracing out all degrees of freedom except those in the subscript of S .

The mutual information between two electrons inside the entangled cloud increases as we go towards the IR fixed point. This can be understood in the following manner; as the wavefunction flows towards a smaller sized emergent cloud, the entanglement between those electrons gets distilled out.

We have also computed some correlation functions. All of them increase towards the IR fixed point. The increase in the correlation function $\langle \hat{n}_{k_1\uparrow} \hat{n}_{k_2\downarrow} \rangle$ arises from the crystallization of the spin singlet at the fixed point. The increase in the correlation function $\langle \hat{n}_{k\uparrow} \hat{n}_{k\downarrow} \rangle$ arises from the charge triplet content of the wavefunction, showing the increase of the charge contribution on the momenta. The increase in the off-diagonal correlation function

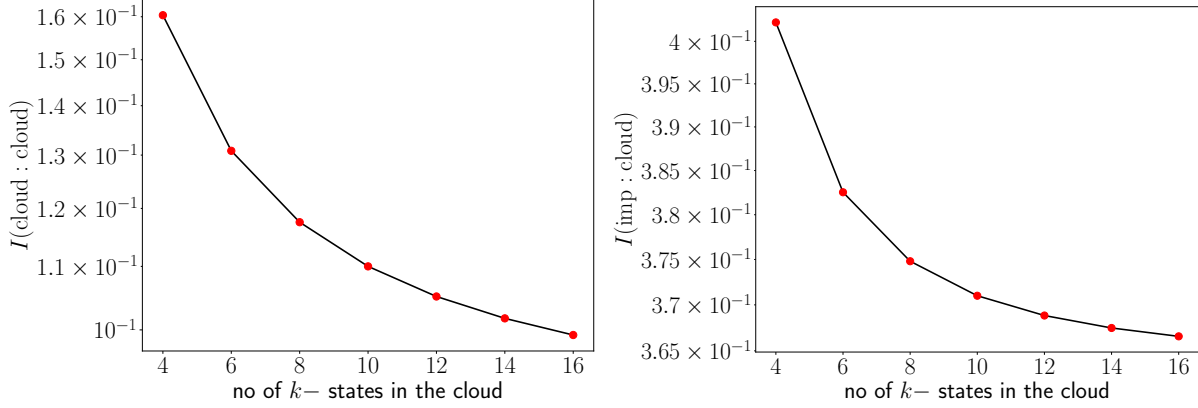


Figure 2.13: *Left*: Mutual information between two conduction electrons inside the cloud. *Right*: Mutual information between a conduction electron inside the cloud and an impurity electron. Both the measures increase towards the strong-coupling fixed point, because of the distillation of the Kondo cloud brought about by the RG flow.

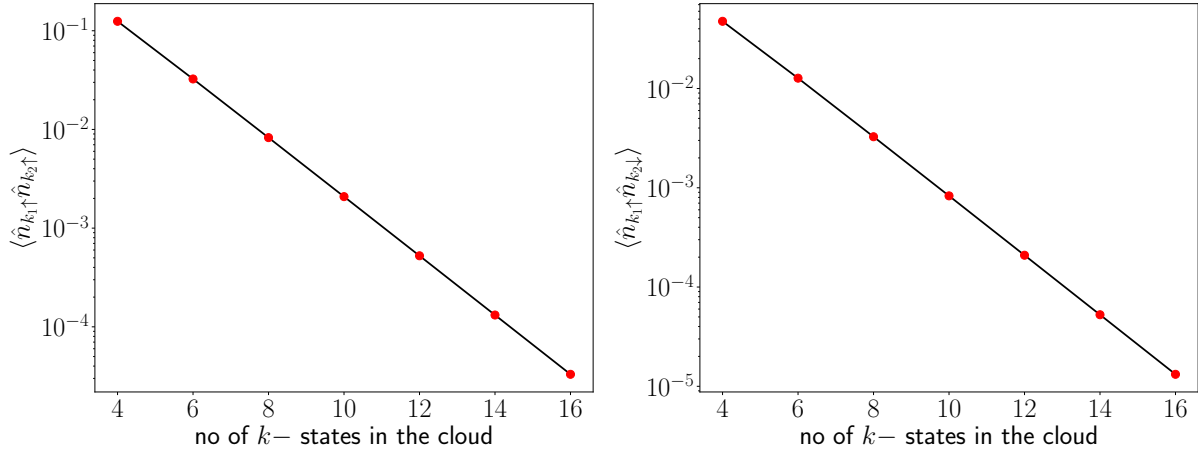


Figure 2.14: Increase in the diagonal correlation functions between cloud electrons under RG flow towards the strong-coupling fixed point. This is consistent with the Fermi liquid pieces generated in the k -space effective Hamiltonian of the Kondo cloud.

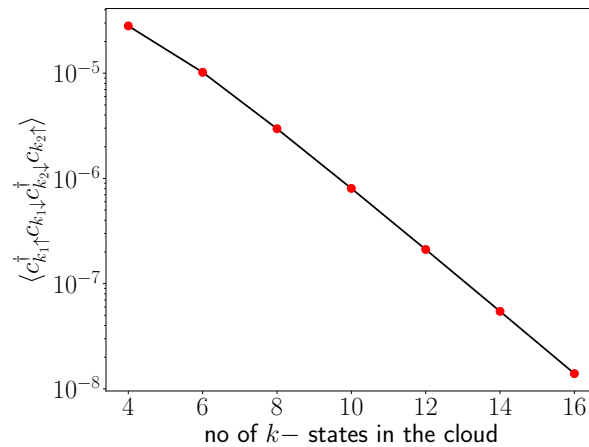


Figure 2.15: Growth of the off-diagonal correlation function between Kondo cloud electrons towards the strong-coupling fixed point. This is the direct cause of the screening of the impurity spin, and is a reflection of the off-diagonal two-particle scattering terms in the k -space effective Hamiltonian of the Kondo cloud.

$\langle c_{k\uparrow}^\dagger c_{k'\downarrow} c_{q\downarrow}^\dagger c_{q'\uparrow} \rangle$ shows that there is a large and non-trivial interaction between the electrons of the cloud that is being mediated by the impurity electron. This interaction is not of the Fermi liquid type, but instead was obtained in the effective Hamiltonian for the Kondo cloud.

Chapter 3

Effect of minimal attractive correlation in the bath

3.1 The modified hamiltonian

We will include a local particle-hole symmetric correlation of strength U_b on the origin of the lattice:

$$\mathcal{H} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} + \epsilon_d \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2 + \sum_{k\sigma} \left(V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c. \right) + J \vec{S}_d \cdot \vec{s} - U_b \left(\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow} \right)^2 \quad (3.1.1)$$

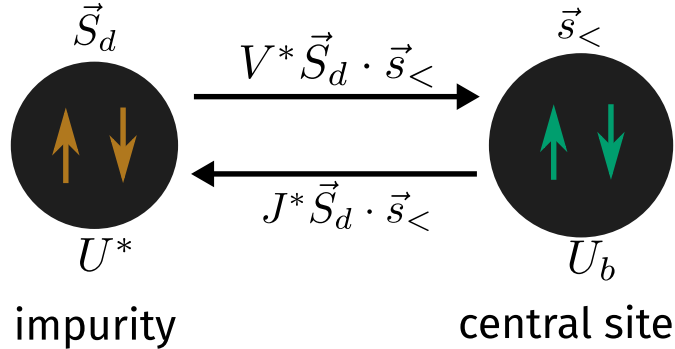


Figure 3.1: While we have studied the full model under renormalisation group, often we will turn to a simplified zero-bandwidth version of the model that is obtained by ignoring the kinetic energy part of the Hamiltonian. This zero-bandwidth model is effectively a two site model.

3.2 RG Equations

The derivation of the RG equations are shown at the end. n_j is the number of k -states at the j^{th} isoenergetic shell.

$$\Delta U_b = 0, \quad \Delta U = 4V^2 n_j \left(\frac{1}{d_1} - \frac{1}{d_0} \right) - n_j \left(\frac{J^2}{d_2} - \frac{K^2}{d_3} \right), \quad (3.2.1)$$

$$\Delta V = -\frac{3n_j V}{8} \left[(J + 4U_b/3) \left(\frac{1}{d_2} + \frac{1}{d_1} \right) + (K + 4U_b/3) \left(\frac{1}{d_3} + \frac{1}{d_0} \right) \right], \quad (3.2.2)$$

$$\Delta J = -\frac{n_j J (J + 4U_b)}{d_2}, \quad \Delta K = -\frac{n_j K (K + 4U_b)}{d_3} \quad (3.2.3)$$

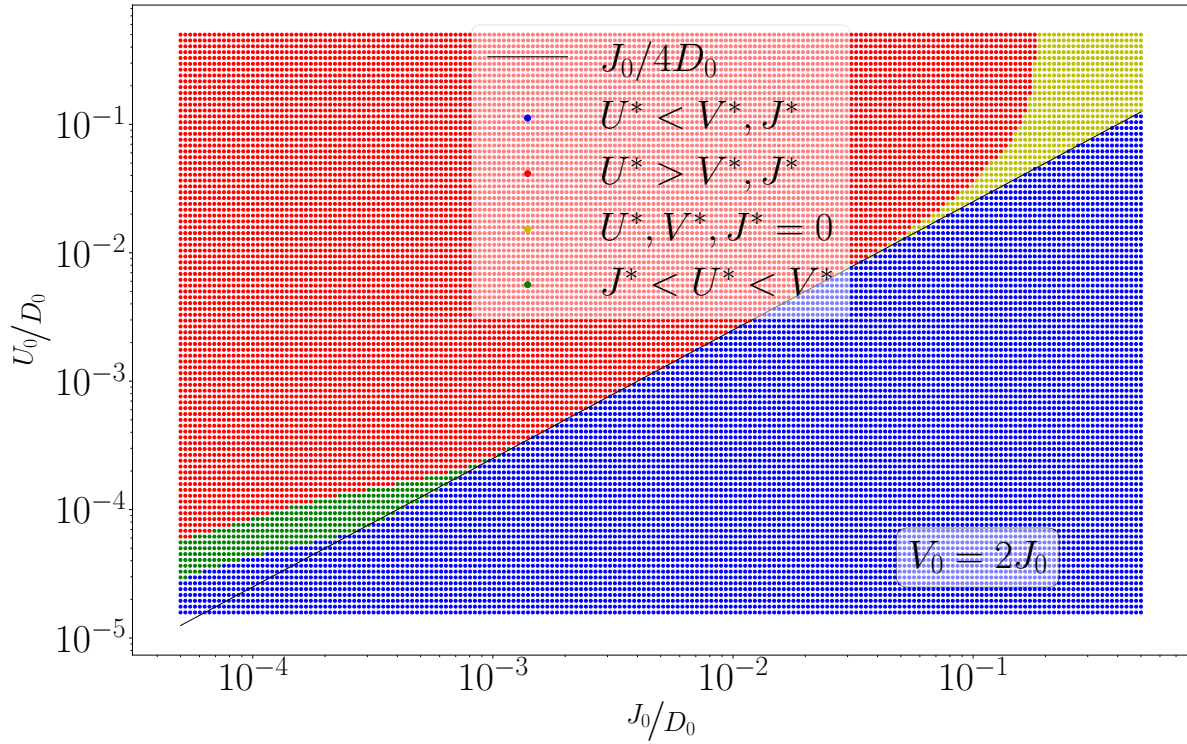
The denominators are

$$d_0 = \omega - \frac{D}{2} + \frac{U_b}{2} - \frac{U}{2} + \frac{K}{4}, \quad d_1 = \omega - \frac{D}{2} + \frac{U_b}{2} + \frac{U}{2} + \frac{J}{4}, \quad d_2 = \omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}, \quad d_3 = \omega - \frac{D}{2} + \frac{U_b}{2} + \frac{K}{4} \quad (3.2.4)$$

Important points regarding notation

- The labels U_0, J_0, V_0 that may occur in the axes of the plots or anywhere else represent the bare values of the couplings U, J and V .
- Throughout the results, the bare value of U_b is set to the negative of the bare value of U_0 : $U_b = -U_0$. This means that whenever we vary U_0 along the axis of a plot, we are simultaneously varying U_b .

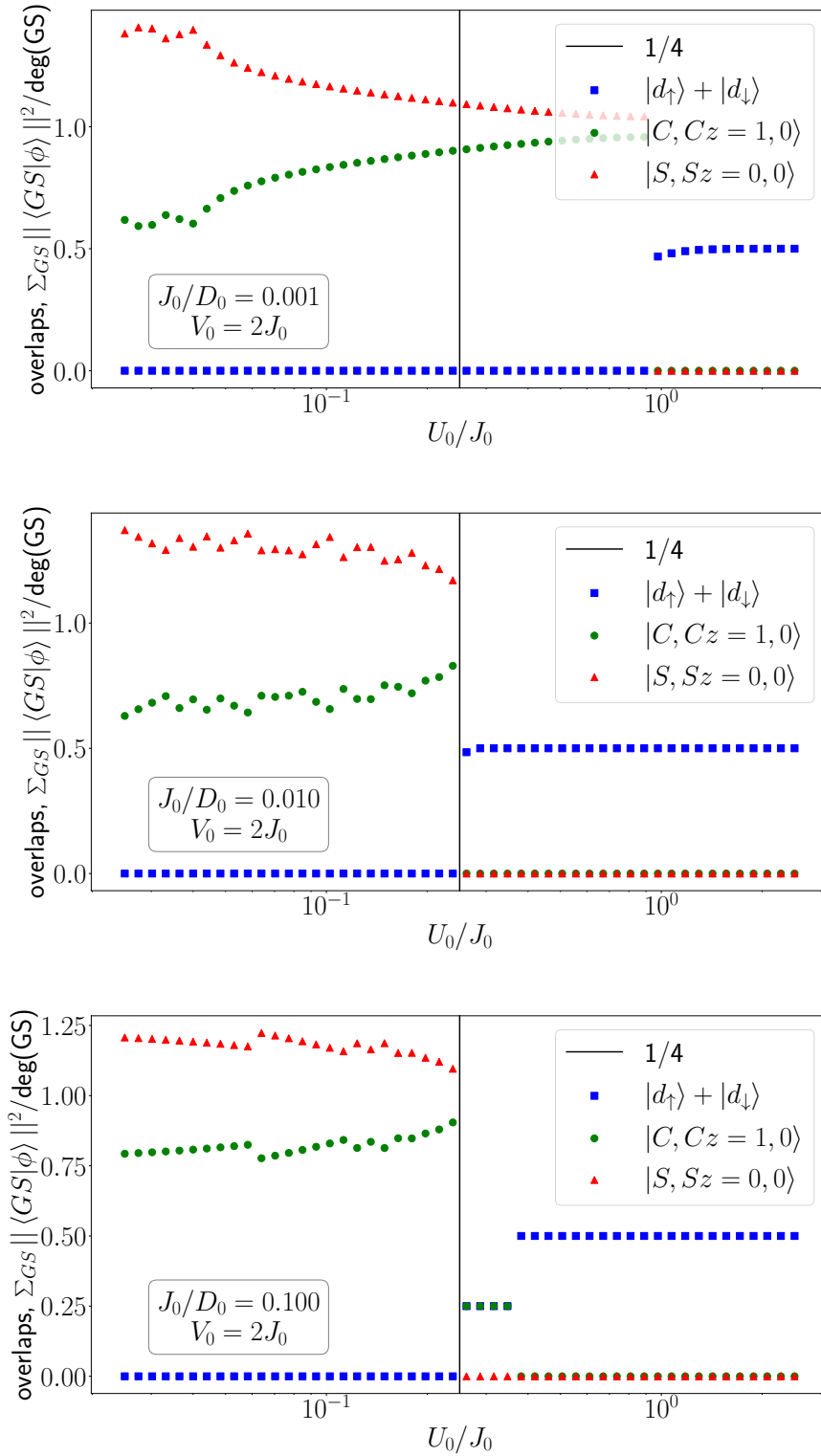
3.3 Phase diagram



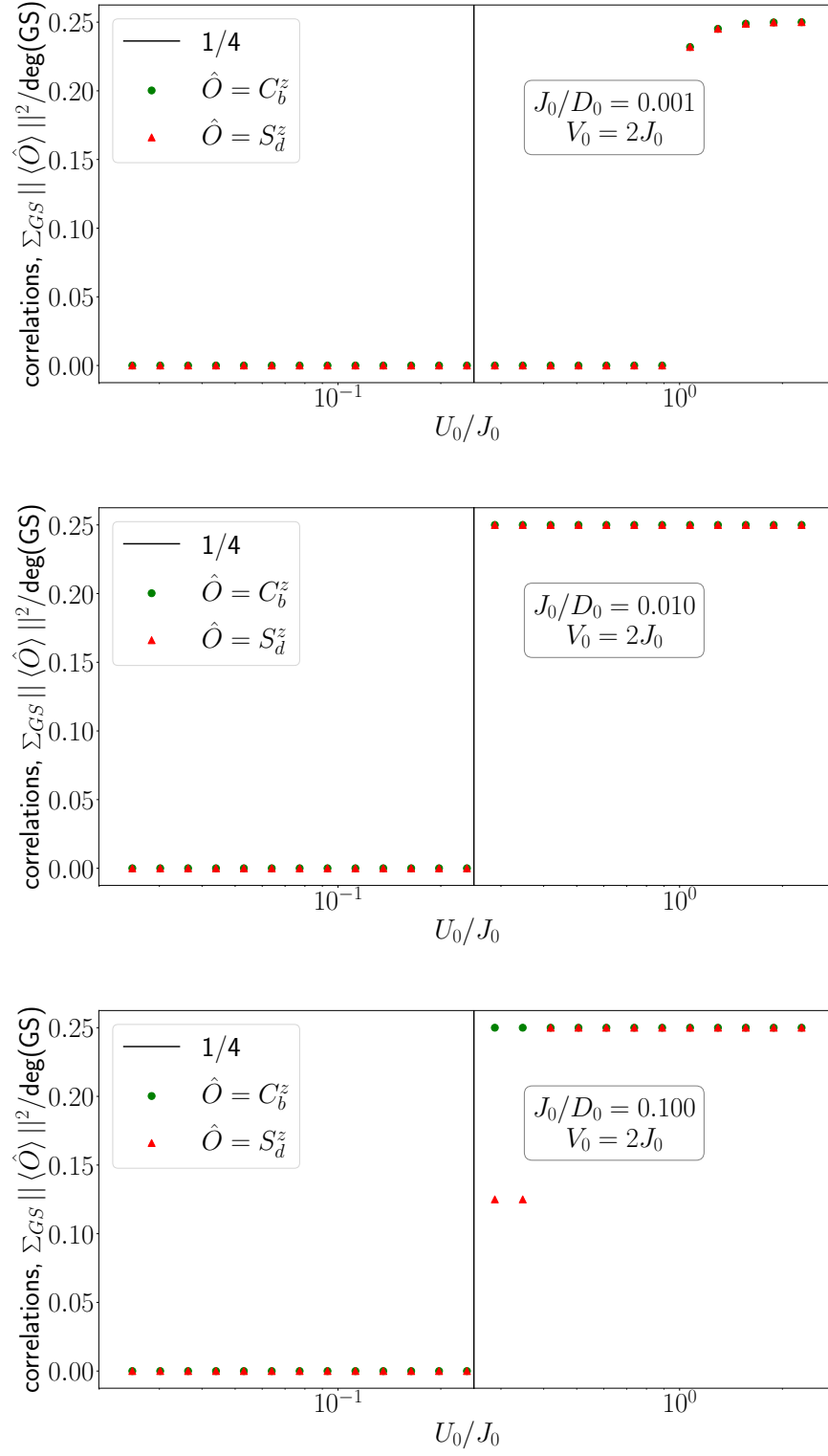
phase	RG flow	fixed point	GS	2-site GS
blue	$\Delta U < 0, \Delta J, \Delta V > 0$	$U^* \ll V^* \ll J^*$	SS	$ SS\rangle = \uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle$
green	$\Delta U < 0, \Delta J < 0, \Delta V > 0$	$J^* < U^* \ll V^*$	SS + CT-0	$c SS\rangle + \sqrt{1-c^2} CT-0\rangle$
red	$\Delta U > 0, \Delta J, \Delta V < 0$	$U^* \gg 1, V^* = J^* = 0$	decoupled LM	$\{ \uparrow\rangle, \downarrow\rangle\} \otimes \{ 0\rangle, 2\rangle\}$
yellow	$\Delta U, \Delta J, \Delta V < 0$	$U^* = V^* = J^* = 0$	lattice	$\{ \uparrow\rangle, \downarrow\rangle, 0\rangle, 2\rangle\} \otimes \{ 0\rangle, 2\rangle\}$

3.4 Evolution of the groundstate across the transition

Overlap of ground state against spin singlet and charge triplet zero states



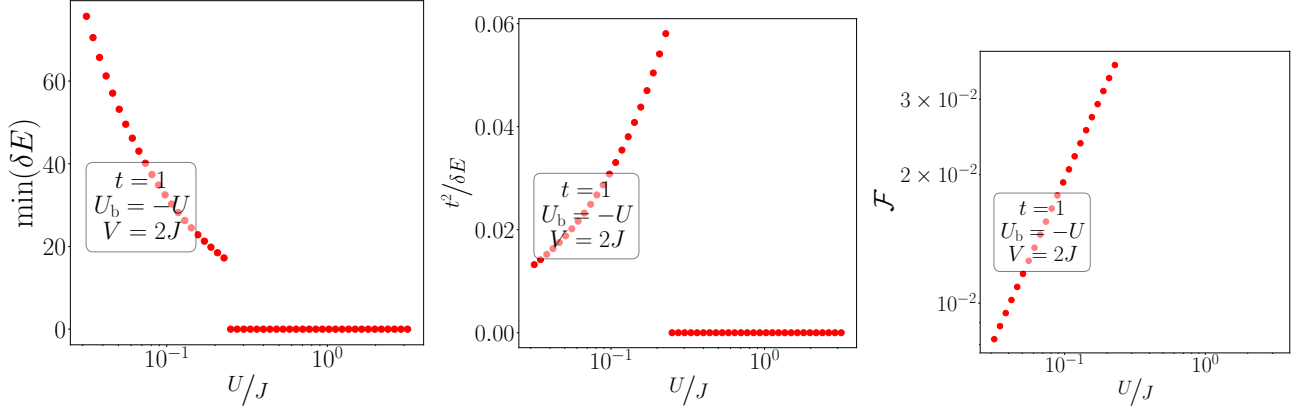
Spin and charge correlations in ground state



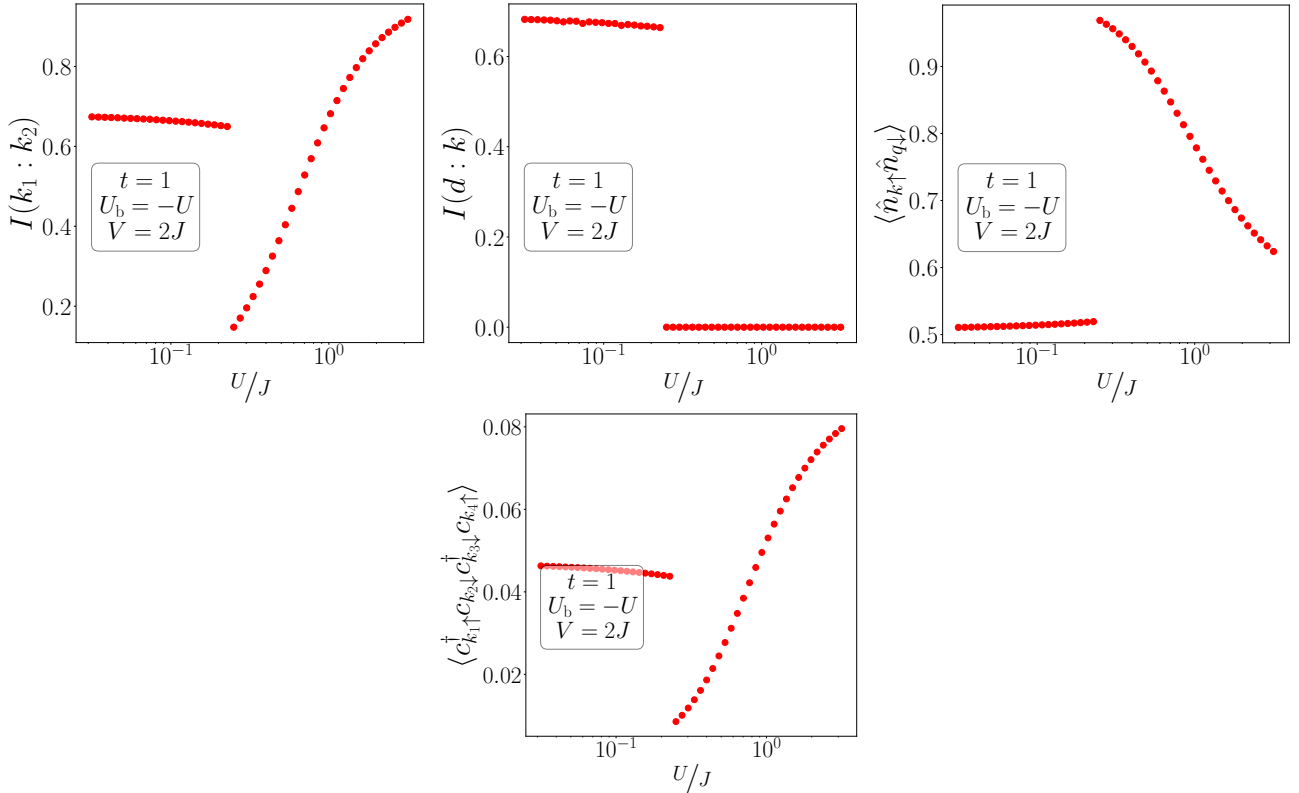
3.5 Evolution of various correlation measures and other quantities

Perturbation theoretic terms

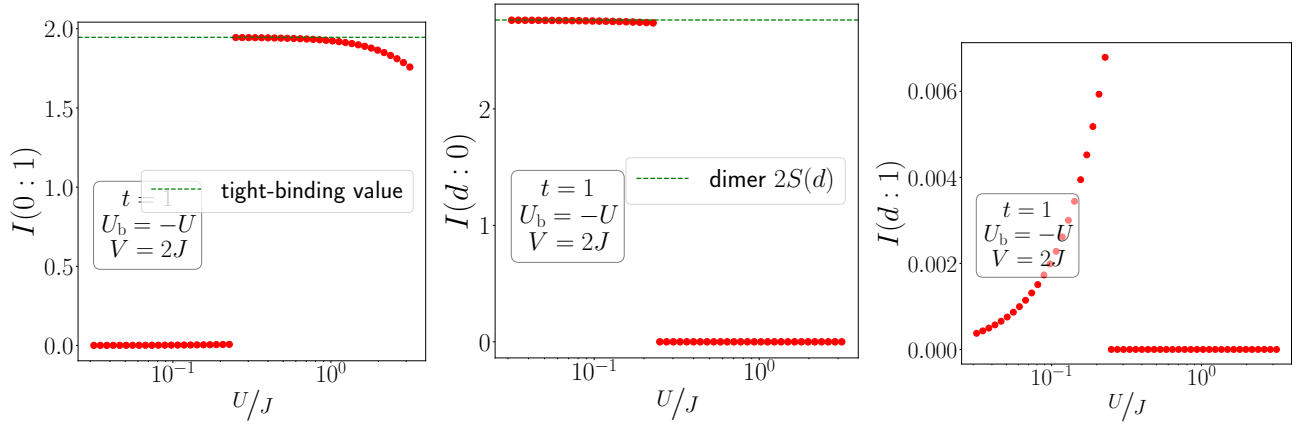
These quantities are related to the local Fermi liquid of the Kondo strong-coupling fixed point and the perturbation theory associated with it. $\min(\delta E)$ is the gap in the spectrum of the two-site Hamiltonian; this which acts as the denominator for the perturbation theoretic calculations. $t^2/\delta E$ is the small parameter for the expansion, t being the tight-binding hopping. \mathcal{F} is the strength of the local Fermi liquid ($\mathcal{F}\hat{n}_{1\uparrow}\hat{n}_{1\downarrow}$).



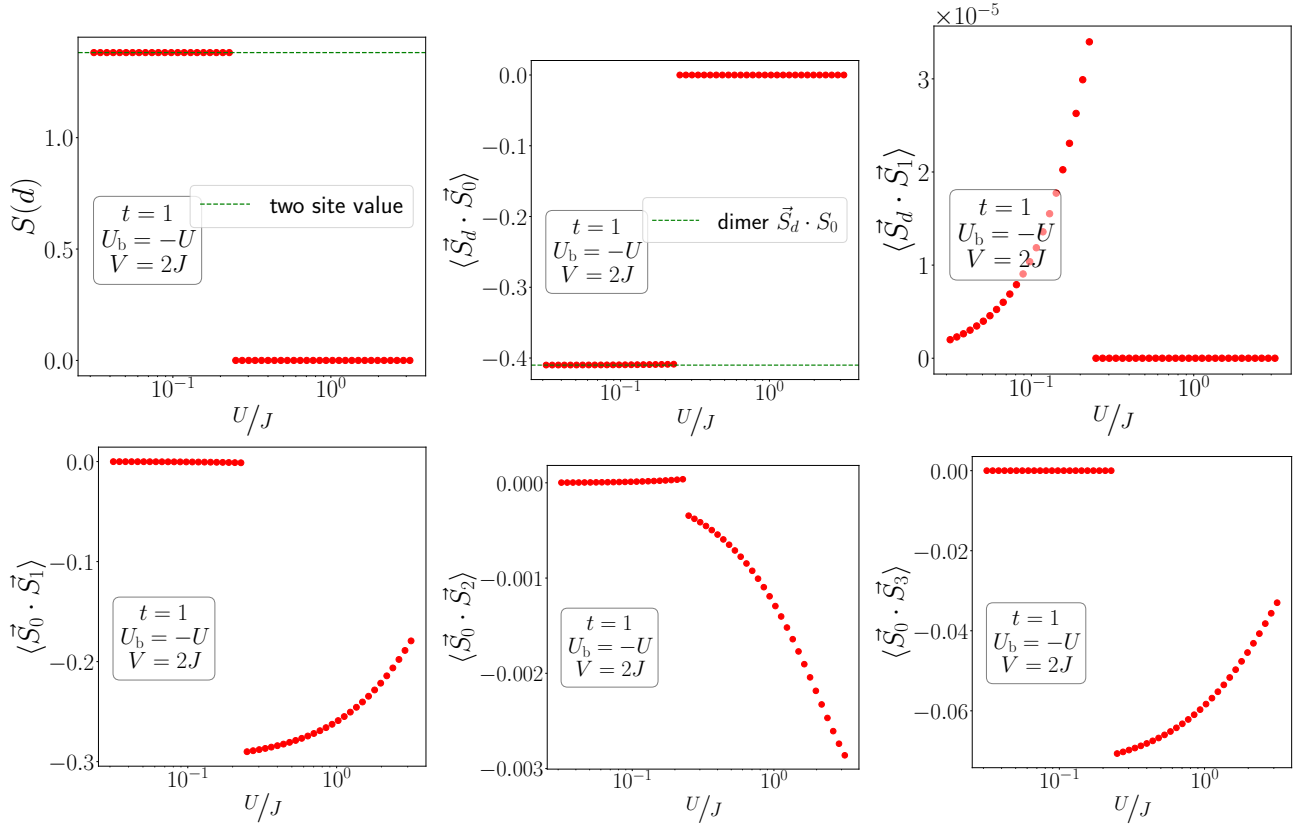
Correlation within the Kondo cloud



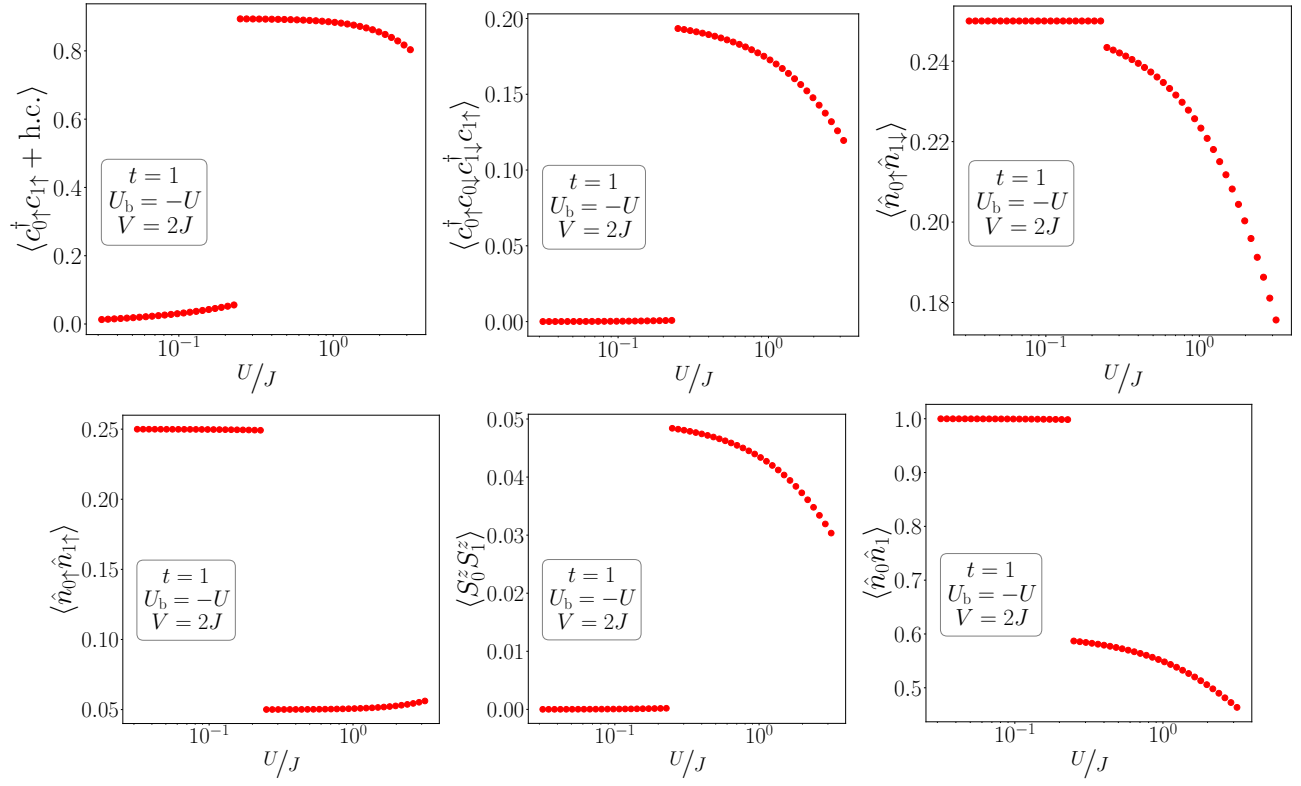
Mutual information between various real space members



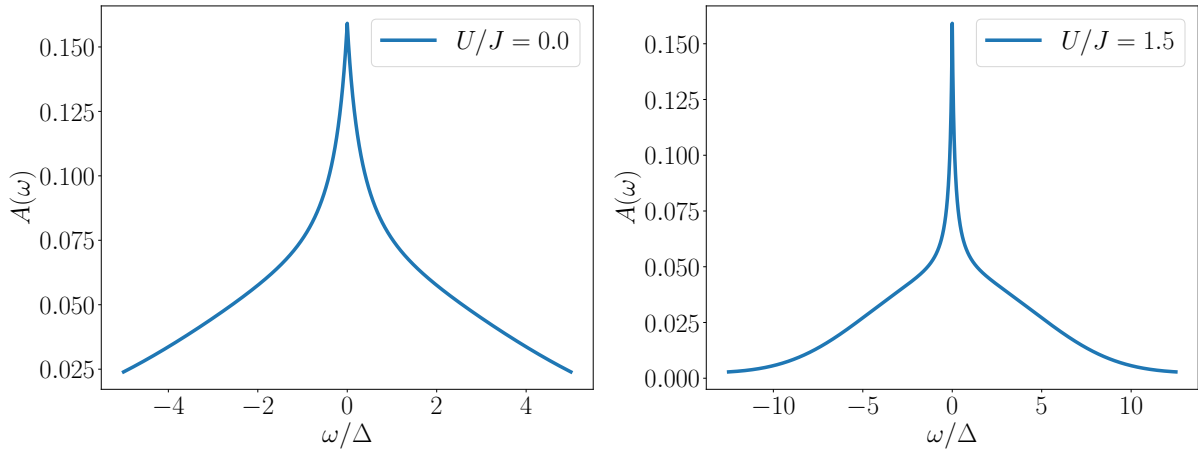
Impurity entanglement entropy and spin-spin correlations

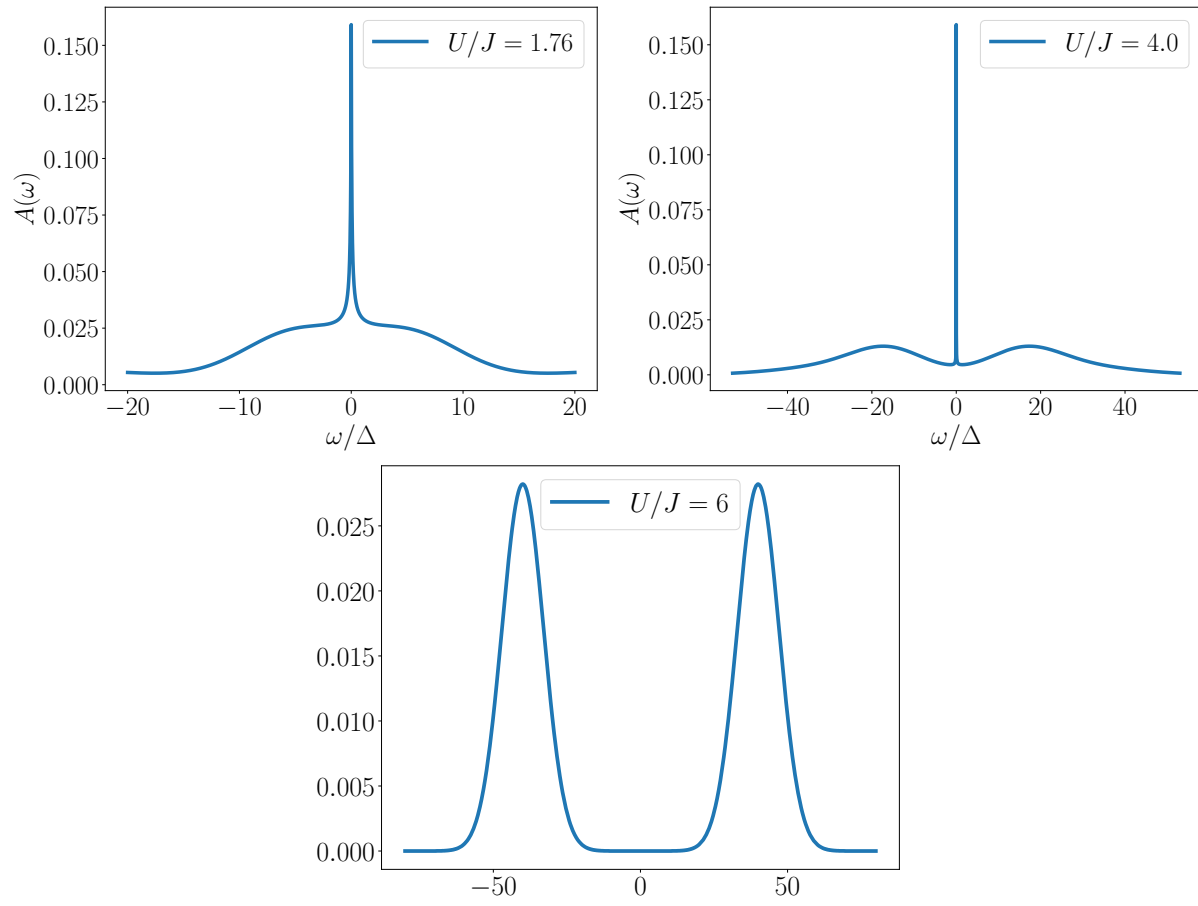


Real-space correlations



Impurity spectral function





Chapter 4

From the auxiliary model to the bulk - single site approach

4.1 Creating General N -site Hubbard Hamiltonian from Anderson molecule embedded in an interacting bath

Previously, we have worked out the groundstate phases of a single-impurity model with an interacting bath:

$$\mathcal{H}_{\text{aux}} = \sum_{k\sigma} \epsilon_k \tau_{k\sigma} - \frac{U}{2} (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 + \sum_{k\sigma} (V_k c_{k\sigma}^\dagger c_{d\sigma} + h.c.) + J \vec{S}_d \cdot \vec{s} - U_b (\hat{n}_{0\uparrow} - \hat{n}_{0\downarrow})^2 \quad (4.1.1)$$

We will use this as the auxiliary model to study the Hubbard model. We do this by first recreating the Hubbard model upon tiling the lattice with instances of this auxiliary model Hamiltonian. To begin this procedure, we first create the unit of tiling - this is done by identifying the impurity as a particular site i of the lattice, and the bath coupled to the impurity as the set of remaining $N - 1$ sites in the lattice. We will also identify the zeroth site of the SIAM lattice as one of the nearest neighbours j of i :

$$\mathcal{H}_{\text{aux}}(i, j) = -2t \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}} (c_{m\sigma}^\dagger c_{n\sigma} + h.c.) - \frac{U}{2} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 + V \sum_{\sigma} (c_{j\sigma}^\dagger c_{i\sigma} + h.c.) + J \vec{S}_i \cdot \vec{S}_j - U_b (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})^2 \quad (4.1.2)$$

The tight-binding term sums over all nearest pairs (m, n) that do not involve the site i . In general i will have w nearest neighbours for a lattice with coordination number w . The total local Hamiltonian for the site i is obtained by averaging over the Hamiltonians $\mathcal{H}_{\text{aux}}(i, j)$ for all nearest neighbours j of i :

$$\begin{aligned} \mathcal{H}_{\text{aux}}(i) &= \frac{1}{w} \sum_{j \in \text{NN of } i} \mathcal{H}_{\text{aux}}(i, j) = -\frac{U}{2} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 + \frac{1}{w} \sum_{j \in \text{NN of } i} \left[-2t \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}} (c_{m\sigma}^\dagger c_{n\sigma} + h.c.) + V \sum_{\sigma} (c_{j\sigma}^\dagger c_{i\sigma} + h.c.) + J \vec{S}_i \cdot \right. \\ &\quad \left. - U_b (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})^2 \right] \\ &= -\frac{U}{2} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 - 2t \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}} (c_{m\sigma}^\dagger c_{n\sigma} + h.c.) + \frac{1}{w} \sum_{j \in \text{NN of } i} \left[V \sum_{\sigma} (c_{j\sigma}^\dagger c_{i\sigma} + h.c.) + J \vec{S}_i \cdot \vec{S}_j \right. \\ &\quad \left. - U_b (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})^2 \right] \end{aligned} \quad (4.1.3)$$

Once we have this local Hamiltonian for a particular site, we translate this over all sites i , and take the average.

$$\begin{aligned}
\mathcal{H}_{\text{full}} &= \frac{1}{N} \sum_i \mathcal{H}_{\text{aux}}(i) = \frac{1}{N} \sum_i \left[-\frac{U}{2} (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 - 2t \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}} (c_{m\sigma}^\dagger c_{n\sigma} + \text{h.c.}) + \frac{1}{w} \sum_{j \in \text{NN of } i} \left[V \sum_{\sigma} (c_{j\sigma}^\dagger c_{i\sigma} + \text{h.c.}) \right. \right. \\
&\quad \left. \left. + J \vec{S}_i \cdot \vec{S}_j - U_b (\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow})^2 \right] \right] \\
&= -\frac{1}{N} \left(\frac{U}{2} + U_b \right) \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 + \frac{1}{N} \sum_i \left[-2t \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}} (c_{m\sigma}^\dagger c_{n\sigma} + \text{h.c.}) + \frac{1}{w} \sum_{j \in \text{NN of } i} \left[V \sum_{\sigma} (c_{j\sigma}^\dagger c_{i\sigma} + \text{h.c.}) \right. \right. \\
&\quad \left. \left. + J \vec{S}_i \cdot \vec{S}_j \right] \right]
\end{aligned} \tag{4.1.4}$$

In the entire tight-binding term $\sum_i \sum_{\substack{m \neq i \neq n \\ \langle m, n \rangle, \sigma}}$, each pair will appear $N - 2$ times, because that is the total number of sites that do not involve either m or n .

$$\begin{aligned}
\mathcal{H}_{\text{full}} &= -\frac{1}{N} \left(\frac{U}{2} + U_b \right) \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 - \frac{2t(N-2)}{N} \sum_{\langle m, n \rangle, \sigma} (c_{m\sigma}^\dagger c_{n\sigma} + \text{h.c.}) + \frac{2}{Nw} \sum_{\langle i, j \rangle} \left[\sum_{\sigma} V (c_{j\sigma}^\dagger c_{i\sigma} + \text{h.c.}) \right. \\
&\quad \left. + J \vec{S}_i \cdot \vec{S}_j \right] \\
&= -\frac{1}{N} \left(\frac{U}{2} + U_b \right) \sum_i (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 - \left(\frac{2t(N-2)}{N} - \frac{2V}{Nw} \right) \sum_{\langle m, n \rangle, \sigma} (c_{m\sigma}^\dagger c_{n\sigma} + \text{h.c.}) + \frac{2J}{Nw} \sum_{\langle i, j \rangle} \vec{S}_i \cdot \vec{S}_j
\end{aligned} \tag{4.1.5}$$

We end up with a Hubbard-Heisenberg model:

$$\mathcal{H}_{H-H} = -\sum_i U_H (\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})^2 - t_H \sum_{\langle i, j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + J_H \sum_{\langle i, j \rangle} \vec{S}_i \cdot \vec{S}_j \tag{4.1.6}$$

The mapping between the parameters is

$$t_{H-H} = \frac{1}{N} \left(2t(N-2) - \frac{2V}{N} \right), \quad U_{H-H} = \frac{1}{N} \left(\frac{U}{2} + U_b \right), \quad J_{H-H} = \frac{2J}{Nw} \tag{4.1.7}$$

The conclusion is that we can tile Anderson models with interacting baths into a Hubbard-Heisenberg model:

$$\frac{1}{N} \sum_i \mathcal{H}_{\text{aux}}(i) = \mathcal{H}_{H-H} \tag{4.1.8}$$

4.2 Single-particle Green's function

We now define the Greens function *operators*:

$$\mathcal{G}_{H-H} = \frac{1}{\omega - (H_{H-H} - E_{\text{gs}})}, \quad \mathcal{G}_{\text{aux}}(i) = \frac{1}{\omega - (H_{\text{aux}}(i) - E_{\text{gs}})} \tag{4.2.1}$$

Rewriting eq. 4.1.8 in terms of these operators, we get

$$\frac{1}{N} \sum_i (\omega - \mathcal{G}_{\text{aux}}^{-1}(i)) = \omega - \mathcal{G}_{H-H}^{-1} \implies \frac{1}{N} \sum_i \mathcal{G}_{\text{aux}}^{-1}(i) = \mathcal{G}_{H-H}^{-1}, \tag{4.2.2}$$

where we used $\frac{1}{N} \sum_i \omega = \omega$. We will now take matrix elements of the full Greens function and obtain these matrix elements in terms of those of the auxiliary model. Let $\{|\Phi\rangle_n\}$ be the set of eigenstates of H_{aux} , and $|\Phi\rangle_0$ be

the groundstate. We assume that the ground state of H_{H-H} is captured well by the auxiliary model, such that the real-space diagonal matrix element for particle propagation is obtained by sandwiching the Greens function between the states $c_{i\sigma}^\dagger |\Phi\rangle_0$:

$$\left(\mathcal{G}_{H-H}^{-1}\right)_{ii}^p \equiv \langle \Phi_0 | c_{i\sigma} \mathcal{G}_{H-H}^{-1} c_{i\sigma}^\dagger | \Phi_0 \rangle = \frac{1}{Nw} \sum_j \sum_{k \in \text{NN of } j} \langle \Phi_0 | c_{i\sigma} \mathcal{G}_{\text{aux}}^{-1}(j, k) c_{i\sigma}^\dagger | \Phi_0 \rangle \quad (4.2.3)$$

The superscript p indicates that this is the particle propagation matrix element. Under the single site approximation, we ignore the hopping between multiple impurity that reside in separate instances of the auxiliary model. Therefore, the only operator $\mathcal{G}_{\text{aux}}^{-1}(j)$ that affects the matrix element is $j = i, k \in \text{NN of } i$. Moreover, because of translation invariance, all k are equivalent.

$$\left(\mathcal{G}_{H-H}^{-1}\right)_{ii}^p = \frac{1}{Nw} w \times \langle \Phi_0 | c_{i\sigma} \mathcal{G}_{\text{aux}}^{-1}(i) c_{i\sigma}^\dagger | \Phi_0 \rangle = \frac{1}{N} \langle \Phi_0 | c_{d\sigma} \mathcal{G}_{\text{aux}}^{-1}(d) c_{d\sigma}^\dagger | \Phi_0 \rangle \quad (4.2.4)$$

where we have identified site i in the auxiliary model as the impurity. By inserting $1 = \sum_n |\Phi_n\rangle \langle \Phi_n|$ on both sides of $\mathcal{G}_{\text{aux}}^{-1}(d)$, we get

$$\left(\mathcal{G}_{H-H}^{-1}(\omega)\right)_{ii}^p = \frac{1}{N} \sum_{m,n} \langle \Phi_0 | c_{d\sigma} | \Phi_m \rangle \langle \Phi_m | \mathcal{G}_{\text{aux}}^{-1}(d) | \Phi_n \rangle \langle \Phi_n | c_{d\sigma}^\dagger | \Phi_0 \rangle = \left(\mathcal{G}_{H-H}^{-1}\right)_{ii} = \frac{1}{N} \sum_n |d_n^p|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d, \omega)\right)_{nn} \quad (4.2.5)$$

There we used the fact that since $|\Phi_m\rangle$ are eigenstates of H_{aux} and hence of $\mathcal{G}_{\text{aux}}^{-1}$, we can set $m = n$. We also defined $d_n^p = \langle \Phi_n | c_{d\sigma}^\dagger | \Phi_0 \rangle$. The hole propagation matrix element can be obtained similarly:

$$\left(\mathcal{G}_{H-H}^{-1}(-\omega)\right)_{ii}^h = \frac{1}{N} \sum_n |d_n^h|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d, -\omega)\right)_{nn} \quad (4.2.6)$$

where $d_n^h = \langle \Phi_n | c_{d\sigma} | \Phi_0 \rangle$. The off-diagonal matrix elements can also be obtained similarly. The difference from the diagonal case is that only one out of the w nearest-neighbour pairs contributes to the matrix element:

$$\left(\mathcal{G}_{H-H}^{-1}\right)_{i,i+1}^p \equiv \langle \Phi_0 | c_{i\sigma} \mathcal{G}_{H-H}^{-1} c_{i+1,\sigma}^\dagger | \Phi_0 \rangle = \frac{1}{Nw} \langle \Phi_0 | c_{i\sigma} \mathcal{G}_{\text{aux}}^{-1}(i, i+1) c_{i+1,\sigma}^\dagger | \Phi_0 \rangle = \frac{1}{Nw} \langle \Phi_0 | c_{d\sigma} \mathcal{G}_{\text{aux}}^{-1}(d) c_{z,\sigma}^\dagger | \Phi_0 \rangle \quad (4.2.7)$$

Here, we identify $i+1$ as the bath zero mode z and i as the impurity d . We again define matrix elements $z_n^p = \langle \Phi_n | c_{z\sigma}^\dagger | \Phi_0 \rangle$, $z_n^h = \langle \Phi_n | c_{z\sigma} | \Phi_0 \rangle$. The matrix element becomes

$$\left(\mathcal{G}_{H-H}^{-1}(\omega)\right)_{i,i+1}^p = \frac{1}{Nw} \sum_n (d_n^p)^* z_n^p \left(\mathcal{G}_{\text{aux}}^{-1}(d, \omega)\right)_{nn} \quad (4.2.8)$$

The hole counterpart is

$$\left(\mathcal{G}_{H-H}^{-1}(-\omega)\right)_{i,i+1}^h = \frac{1}{Nw} \sum_n (d_n^h)^* z_n^h \left(\mathcal{G}_{\text{aux}}^{-1}(d, -\omega)\right)_{nn} \quad (4.2.9)$$

In summary, the four Greens functions are

$$\left(\mathcal{G}_{H-H}^{-1}(\omega)\right)_{ii}^p = \frac{1}{N} \sum_n |d_n^p|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d, \omega)\right)_{nn}, \quad \left(\mathcal{G}_{H-H}^{-1}(-\omega)\right)_{ii}^h = \frac{1}{N} \sum_n |d_n^h|^2 \left(\mathcal{G}_{\text{aux}}^{-1}(d, -\omega)\right)_{nn} \quad (4.2.10)$$

$$\left(\mathcal{G}_{H-H}^{-1}(\omega)\right)_{i,i+1}^p = \frac{1}{Nw} \sum_n (d_n^p)^* z_n^p \left(\mathcal{G}_{\text{aux}}^{-1}(d, \omega)\right)_{nn}, \quad \left(\mathcal{G}_{H-H}^{-1}(-\omega)\right)_{i,i+1}^h = \frac{1}{Nw} \sum_n (d_n^h)^* z_n^h \left(\mathcal{G}_{\text{aux}}^{-1}(d, -\omega)\right)_{nn} \quad (4.2.11)$$

In order to obtain the matrix elements of \mathcal{G}_{H-H} as compared to its inverse, we note that the matrix elements of the inverse are related to the matrix elements of another inverse operator, through some coefficients. We can therefore use the identity

$$\left(\hat{O}\right)_{ij} = \langle i | \hat{O} | j \rangle = \sum_{m,n} \langle i | m \rangle \left(\hat{O}\right)_{mn} \langle n | j \rangle \implies \left(\hat{O}^{-1}\right)_{ij} = \sum_{m,n} \langle i | m \rangle \left(\hat{O}^{-1}\right)_{mn} \langle n | j \rangle \quad (4.2.12)$$

We can identify $(\hat{O}^{-1})_{mn}$ as the matrix elements of $\mathcal{G}_{\text{aux}}^{-1}$ in our expressions. Using the relation, we can therefore write

$$(\mathcal{G}_{H-H}(\omega))_{ii}^p = \frac{1}{N} \sum_n |d_n^p|^2 (\mathcal{G}_{\text{aux}}(d, \omega))_{nn}, \quad (\mathcal{G}_{H-H}(-\omega))_{ii}^h = \frac{1}{N} \sum_n |d_n^h|^2 (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \quad (4.2.13)$$

$$(\mathcal{G}_{H-H}(\omega))_{i,i+1}^p = \frac{1}{Nw} \sum_n (d_n^p)^* z_n^p (\mathcal{G}_{\text{aux}}(d, \omega))_{nn}, \quad (\mathcal{G}_{H-H}(-\omega))_{i,i+1}^h = \frac{1}{Nw} \sum_n (d_n^h)^* z_n^h (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \quad (4.2.14)$$

The single-particle Greens functions can now be written in terms of these matrix elements. Using eq. D.0.6, we write

$$\begin{aligned} (G_{H-H}(\omega))_{\text{loc}} &= (G_{H-H}(\omega))_{ii}^p - (G_{H-H}(-\omega))_{ii}^h = \frac{1}{N} \sum_n \left[|d_n^p|^2 (\mathcal{G}_{\text{aux}}(d, \omega))_{nn} - |d_n^h|^2 (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \right] \\ (G_{H-H}(\omega))_{\text{n-n}} &= (G_{H-H}(\omega))_{i,i+1}^p - (G_{H-H}(-\omega))_{i,i+1}^h = \frac{1}{Nw} \sum_n \left[(d_n^p)^* z_n^p (\mathcal{G}_{\text{aux}}(d, \omega))_{nn} - (z_n^h)^* d_n^h (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \right] \end{aligned} \quad (4.2.15)$$

4.3 Spectral functions and self-energies

The momentum space Greens function can be expressed as a Fourier transform of the real space Greens functions:

$$G_{H-H}(\vec{k}, \omega) = \frac{1}{N} \sum_{\vec{r}, \vec{r}_j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} G_{H-H}(|\vec{r}_i - \vec{r}_j|, \omega) \quad (4.3.1)$$

where \vec{r}_i is the position vector of a particular lattice site. Because of translation invariance, the real space Greens function depends only on the relative vector between any two sites. As a result, $\vec{r} = 0$ gives the local Greens function, $|\vec{r}| = a$ gives the nearest-neighbour Greens function and so on (a being the lattice spacing). As we do not have real space Greens function that are more non-local than nearest neighbour, we will attempt to obtain momentum space Greens function from these two contributions:

$$G_{H-H}(\vec{k}, \omega) \simeq \frac{1}{N} \sum_{\vec{r}_i = \vec{r}_j} (G_{H-H}(\omega))_{\text{loc}} + \frac{1}{N} \sum_{|\vec{r}_i - \vec{r}_j| = a} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} (G_{H-H}(\omega))_{\text{n-n}} \quad (4.3.2)$$

The first summation produces a factor of N , while the second summation can be factorized into a sum over all sites (which again returns N) and a sum over all the primitive vectors connecting any single site with all its nearest neighbours, $\{\vec{a}_i : i \in [1, w]\}$.

$$\begin{aligned} G_{H-H}(\vec{k}, \omega) &\simeq G_{H-H}(\omega)_{\text{loc}} + G_{H-H}(\omega)_{\text{n-n}} \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i} = G_{H-H}(\omega)_{\text{loc}} + G_{H-H}(\omega)_{\text{n-n}} \xi_{\vec{k}} \\ &= \frac{1}{N} \sum_n \left[\left(|d_n^p|^2 + (d_n^p)^* z_n^p \right) (\mathcal{G}_{\text{aux}}(d, \omega))_{nn} - \left(|d_n^h|^2 + (z_n^h)^* d_n^h \right) (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \right] \end{aligned} \quad (4.3.3)$$

where we defined $\xi_{\vec{k}} \equiv \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i}$. For example, on a d-dimensional hypercubic lattice, we obtain

$$\xi_{\vec{k}} = \sum_{i=1}^d \left(e^{ik_i a_i} + e^{-ik_i a_i} \right) = 2 \sum_{i=1}^d \cos k_i a_i \quad (4.3.4)$$

On a 2D square lattice with lattice spacing a , this simplifies to

$$\begin{aligned} \xi_{\vec{q}} &= 2(\cos q_x a + \cos q_y a) \equiv \frac{-\epsilon_{\vec{q}}}{tH}, \\ \epsilon_{\vec{q}} &= -2t^H (\cos q_x a_x + \cos q_y a_y) \end{aligned} \quad (4.3.5)$$

where $\epsilon_{\vec{q}}$ is the tight-binding dispersion.

We can now compute the k -space spectral function $A_H(\vec{k}, \omega)$ and the real-space local spectral function $A_H(\vec{r} = 0, \omega)$ as

$$A_{H-H}(\vec{k}, \omega) = -\frac{1}{\pi} \text{Im}(G_{H-H}(\vec{k}, \omega)) = -\frac{1}{N\pi} \text{Im} \sum_n \left[\left(|d_n^p|^2 + (d_n^p)^* z_n^p \right) (\mathcal{G}_{\text{aux}}(d, \omega))_{nn} - \left(|d_n^h|^2 + (z_n^h)^* d_n^h \right) (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \right] \quad (4.3.6)$$

$$A_{H-H}(\vec{r} = 0, \omega) = -\frac{1}{\pi} \text{Im}(G_{H-H}(\vec{r} = 0, \omega)) = \sum_{\vec{k}} A_{H-H}(\vec{k}, \omega) \quad (4.3.7)$$

With the knowledge of the momentum-space Greens function $G_{H-H}(\vec{k}, \omega)$, we can now use Dyson's equation to calculate the self-energy for propagation of momentum excitations:

$$\Sigma(\vec{k}, \omega) = G_0(\vec{k}, \omega)^{-1} - G(\vec{k}, \omega)^{-1} \quad (4.3.8)$$

where the $G_0(\vec{k}, \omega)^{-1} = \omega - \epsilon_k = \omega + t^{H-H} \xi_k$ is the inverse k -space Greens function for the appropriate non-interacting tight-binding system. Substituting this as well as the full Greens function $G_{H-H}(\vec{k}, \omega)$ into Dyson's equation gives

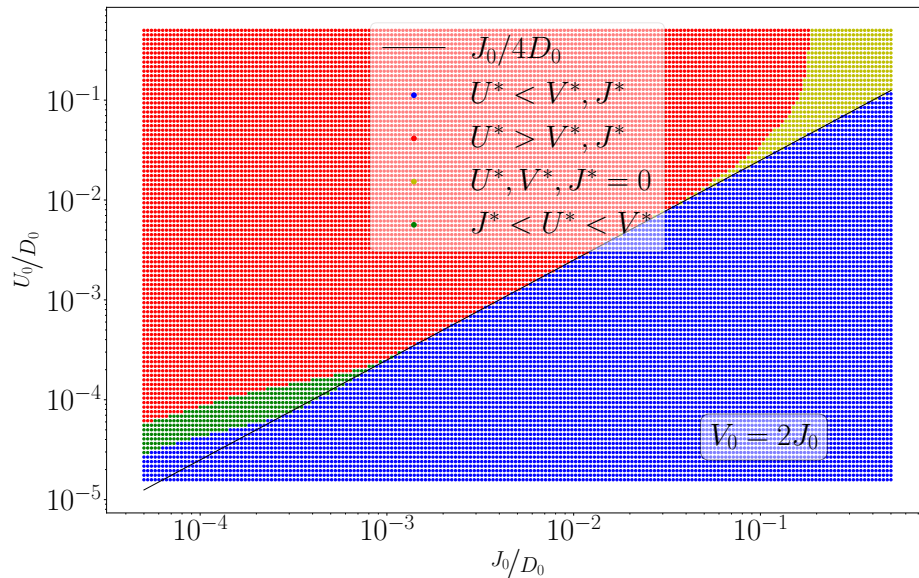
$$\Sigma_{H-H}(\vec{k}, \omega) = \omega + t^{H-H} \xi_k - N \left\{ \sum_n \left[\left(|d_n^p|^2 + (d_n^p)^* z_n^p \right) (\mathcal{G}_{\text{aux}}(d, \omega))_{nn} - \left(|d_n^h|^2 + (z_n^h)^* d_n^h \right) (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn} \right] \right\}^{-1} \quad (4.3.9)$$

This allows us to calculate the full self-energy $\Sigma(\vec{k}, \omega)$ for the Hubbard model on the 2D square lattice.

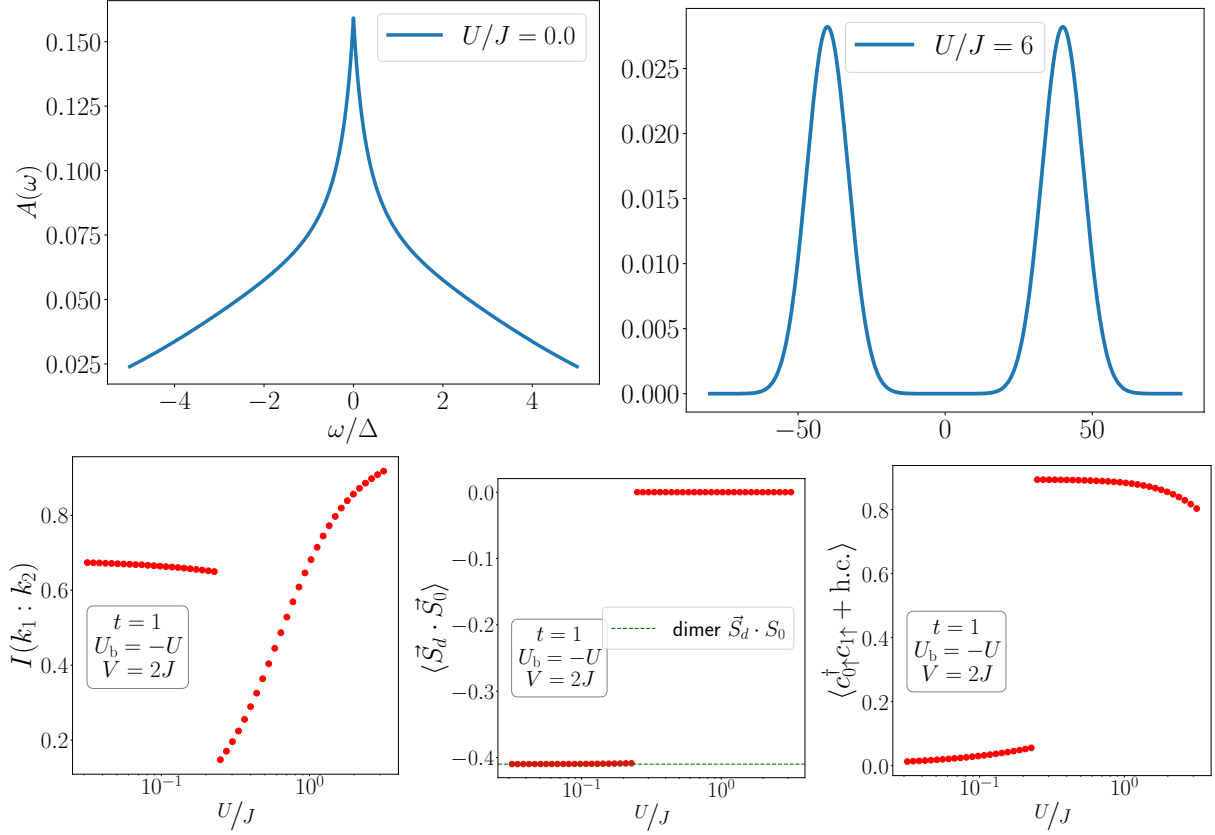
4.4 Evidence for the Mott MIT

Through the URG study of the generalised SIAM with correlation (eq. 4.1.1) shown in chapter 3, we can conclude the following about that model:

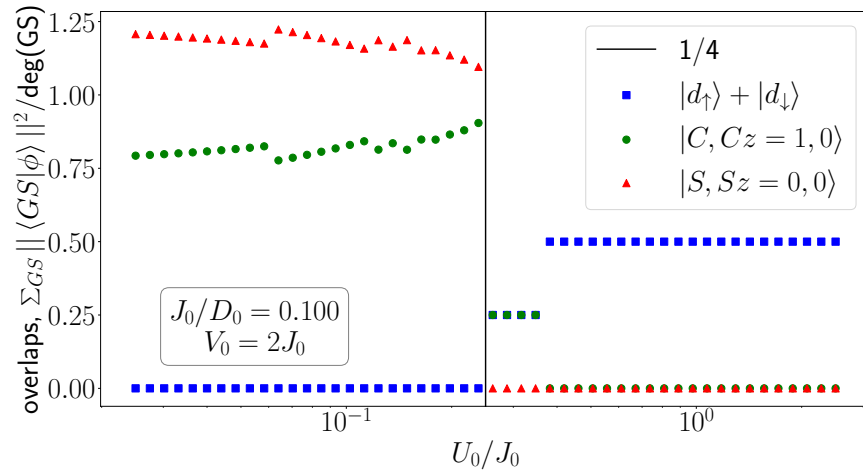
- For $U_b > J/4$, the couplings J and V become irrelevant while U is relevant, which means that **the impurity gets cut off from the bath at low energies**.



- Study of the impurity spectral function shows a gap at low ω for $U_b > J/4$. Other measures like mutual information and spin-spin correlations also show a sharp change on crossing that value, demonstrating **the destruction of the Kondo cloud and the stabilisation of the local moment on the impurity**.



- In the context of the auxiliary model, this represents an **impurity phase transition** from the completely-screened spin-singlet phase to the unscreened local moment phase.



Using the mappings between the auxiliary model parameters and the bulk parameters (eq. 4.1.7), one can define a critical value r_c of the ratio $r = U_{H-H}/J_{H-H}$ at the critical points $-U_b/J = 1/4$ for a given and fixed value of U . We will now argue that this critical point describes a metal-insulator transition. For $r < r_c$, the well-defined low- ω central peak in the impurity spectral function, as well as the large mutual

and information correlations, in the ground state, among the members of the Kondo cloud or between the impurity and the zeroth site show that the impurity and the bath are very strongly entangled, and the weighted poles $\left(|d_n^p|^2 + (d_n^p)^* z_n^p\right) (\mathcal{G}_{\text{aux}}(d, \omega))_{nn}$ and $\left(|d_n^h|^2 + (z_n^h)^* d_n^h\right) (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn}$ are non-zero at low ω . This means that both the local and the nearest-neighbour Greens functions, that are related to these parameters via eq. 4.2.15, have poles at low $-\omega$ and support the propagation of electrons through gapless excitations. Since the spectral function is also very simply related to that of the auxiliary model, the former also shows the same zero-energy resonance.

On the other side $r > r_c$ of the critical point, we know that the impurity gets decoupled from the bath, such that the weighted poles $\left(|d_n^p|^2 + (d_n^p)^* z_n^p\right) (\mathcal{G}_{\text{aux}}(d, \omega))_{nn}$ and $\left(|d_n^h|^2 + (z_n^h)^* d_n^h\right) (\mathcal{G}_{\text{aux}}(d, -\omega))_{nn}$ vanish. This is simply the loss of spectral weight at low- ω because of the removal of the gapless excitations. This then implies that the bulk Greens functions will also gap out at low energies, and that describes an insulating phase where the electrons get "jammed" in the local states. By the same argument as above, the spectral function also sees a gap in this phase.

Chapter 5

From the auxiliary model to the bulk - two site approach

5.1 Solution of the Hubbard dimer using the Anderson molecule

This section tries to see how far we can go if we just work with the Anderson molecule as the smallest unit of tiling. We will attempt to reproduce the entire spectrum of a Hubbard dimer by creating a new Hamiltonian made up purely of Anderson molecules. This will guide us in deciding how to generalize the "tiling method" for a general N -site Hubbard model, as well as give indications as to whether we need a different smallest unit for tiling.

The Hubbard dimer and Anderson molecules (zero-mode) are defined by the following respective Hamiltonians:

$$\begin{aligned} H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - \mu^H \sum_{\sigma, i=1,2} \hat{n}_{i\sigma} \\ H^A &= -t^A \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) + \epsilon_d^A \sum_{\sigma} \hat{n}_{d\sigma} + U^A \hat{n}_{d\uparrow} \hat{n}_{d\downarrow} \end{aligned} \quad (5.1.1)$$

In the first Hamiltonian, the indices $i = 1, 2$ refer to the two lattice sites that constitute the dimer. In the second Hamiltonian, the subscript d indicates the impurity site, while the subscript z indicates the zero-mode site. First, we will assume that the Hubbard dimer is at half-filling ($\frac{1}{2}U^H = \mu^H$):

$$\begin{aligned} H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} + \left(\frac{1}{2}U^H - \mu^H \right) \sum_{\sigma, i=1,2} \hat{n}_{i\sigma} + \text{constant} \\ &= -t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \end{aligned} \quad (5.1.2)$$

Since the Hubbard Hamiltonian is at half-filling, we will also place the impurity at half-filling by setting $\epsilon_d^A = -\frac{1}{2}U^A$:

$$\begin{aligned} H^A &= -t^A \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) + \left(\epsilon_d^A + \frac{1}{2}U^A \right) \sum_{\sigma} \hat{\tau}_{d\sigma} + U^A \hat{\tau}_{d\uparrow} \hat{\tau}_{d\downarrow} + \text{constant} \\ &= -t^A \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) + U^A \hat{\tau}_{d\uparrow} \hat{\tau}_{d\downarrow} \end{aligned} \quad (5.1.3)$$

The first step is to recreate the Hubbard dimer Hamiltonian eq. 5.1.2 using the Anderson molecule Hamiltonian eq. 5.1.3:

$$\begin{aligned}
H^H &= -t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \\
&= \frac{1}{2} \left[-t^H \sum_{\sigma} \left(c_{1\sigma}^{\dagger} c_{2\sigma} + \text{h.c.} \right) + t^H \sum_{\sigma} \left(c_{2\sigma}^{\dagger} c_{1\sigma} + \text{h.c.} \right) \right] + \frac{1}{2} 2U^H \sum_{i=1,2} \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \\
&= \frac{1}{2} \left[-t^A \sum_{\sigma} \left(c_{d\sigma}^{\dagger} c_{z\sigma} + \text{h.c.} \right) \Big|_{\substack{z \rightarrow 2, d \rightarrow 1 \\ t^A \rightarrow t^H}} + t^A \sum_{\sigma} \left(c_{2\sigma}^{\dagger} c_{1\sigma} + \text{h.c.} \right) \Big|_{\substack{d \rightarrow 2, z \rightarrow 1 \\ t^A \rightarrow t^H}} \right] \\
&\quad + \frac{1}{2} \left(U^A \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \Big|_{U^A \rightarrow 2U^H} + U^A \hat{\tau}_{i\uparrow} \hat{\tau}_{i\downarrow} \Big|_{U^A \rightarrow 2U^H} \right) \\
&= \frac{1}{2} \left[H^A \left(t^A \rightarrow t^H, U^A \rightarrow 2U^H, d \rightarrow 1, z \rightarrow 2 \right) + H^A \left(t^A \rightarrow t^H, U^A \rightarrow 2U^H, d \rightarrow 2, z \rightarrow 1 \right) \right]
\end{aligned} \tag{5.1.4}$$

The conclusion we can draw from this is that the Hubbard dimer Hamiltonian can be obtained from the Anderson dimer Hamiltonian in the following fashion:

- The essential idea is that we have to create a local Hubbard Hamiltonian for each site of the Hubbard lattice by replacing the impurity label d in the Anderson dimer with the label of the particular site. So if there are two sites, we will get two local Hamiltonians obtained by replacing d with 1 and 2 respectively. For each local Hamiltonian, the zero-mode label z is replaced by the site that is nearest to the one that d is being replaced by. So, if $d \rightarrow 1(2)$, then $z \rightarrow 2(1)$.
- This, however, is not the only change that we must make, in order to get the local Hamiltonian for a particular site. Along with d and z , we must also make the transformations $t^A \rightarrow t^H, U^A \rightarrow 2U^H$.
- Finally, once we have the local Hamiltonians for sites 1 and 2, we average them to get the total Hubbard Hamiltonian.

Note that we expect most of these "rules" to be specific for the dimer, and there will be generalizations to most of them for a general N -site Hubbard Hamiltonian.

The wavefunctions for the $N = 2$ sector can also be connected through these transformations. Since both the Hamiltonians are analytically solvable, we can write down their groundstate wavefunctions [CITE PAVARINI]:

$$\begin{aligned}
|\Psi_{\text{GS}}^H\rangle &= a_1(U^H, t^H) \frac{1}{\sqrt{2}} (|\uparrow_1, \downarrow_2\rangle - |\downarrow_1, \uparrow_2\rangle) - a_2(U^H, t^H) \sqrt{2} (|\uparrow_1 \downarrow_1\rangle - |\uparrow_2 \downarrow_2\rangle) \\
|\Psi_{\text{GS}}^A\rangle &= a_1\left(\frac{1}{2}U^A, t^A\right) \frac{1}{\sqrt{2}} (|\uparrow_d, \downarrow_z\rangle - |\downarrow_d, \uparrow_z\rangle) - a_2\left(\frac{1}{2}U^A, t^A\right) \sqrt{2} (|\uparrow_d \downarrow_d\rangle - |\uparrow_z \downarrow_z\rangle) \\
E_{\text{GS}}^H &= -\frac{1}{2} \Delta(U^H, t^H), E_{\text{GS}}^A = -\frac{1}{2} \Delta\left(\frac{1}{2}U^A, t^A\right)
\end{aligned} \tag{5.1.5}$$

where

$$a_1(U, t) \equiv \frac{4t}{\sqrt{2\Delta(U, t) (\Delta(U, t) - U)}}, \quad a_2(U, t) \equiv \sqrt{\frac{\Delta(U, t) - U}{2\Delta(U, t)}}, \quad \Delta(U, t) \equiv \sqrt{U^2 + 16t^2} \tag{5.1.6}$$

a_1, a_2 satisfy $a_1(-U, t) = -a_2(U, t)$ and $a_1(U, t)a_2(U, t) = \frac{2t}{\Delta(U, t)}$. From the forms of the wavefunctions and eigenenergies, we can immediately write down

$$\begin{aligned}
|\Psi_{\text{GS}}^H\rangle &= \frac{1}{2} \left[|\Psi_{\text{GS}}^A\rangle \left(t^A, U^A \rightarrow t^H, 2U^H, d \rightarrow 1, z \rightarrow 2 \right) + |\Psi_{\text{GS}}^A\rangle \left(t^A, U^A \rightarrow t^H, 2U^H, d \rightarrow 2, z \rightarrow 1 \right) \right] \\
E_{\text{GS}}^H &= E_{\text{GS}}^A \left(t^A, U^A \rightarrow t^H, 2U^H \right)
\end{aligned} \tag{5.1.7}$$

This shows that the rules laid out before work for the Hamiltonians, as well as the wavefunctions and energy eigenvalues of the $N = 2, 0, 4$ sector. These sectors specifically work because it is only in these sectors can we ensure that $n_d = n_z$, which is required for the Hubbard Hamiltonian because $n_1 = n_2$. In the other sectors ($N = 1, 3$), the impurity site and the zero-mode sites have to be singly-occupied in some part, and since the impurity site incurs a single-occupation cost of $-\frac{U^H}{2}$ which is not borne by the zero-mode site, there is an intrinsic dissimilarity between the two sites of the Anderson molecule in this regime. This dissimilarity does not exist for the Hubbard model, so we cannot hope to connect the two models in this regime. Going forward, we will switch to using Hubbard dimers as the smallest tiling unit for a general Hubbard model.

5.2 Creating General N -site Hubbard Hamiltonian from Hubbard dimers

We will follow the strategy outlined in the previous section. For concreteness, we will consider a lattice of N lattice sites and w nearest neighbours for each site. Note that a uniform number of nearest neighbours means that there is perfect translational invariance on the lattice, which means there cannot be any edge sites. This is achieved by applying periodic boundary conditions on the edges of the lattice. A square 2d lattice is thus placed on a 2-torus.

For each nearest-neighbour pair i, j , we will create a local Hamiltonian $H_{i,j}^D$ from the Hamiltonian of the Hubbard dimer with bath (we will interpret the effective bath as the remaining $N - 2$ sites of the lattice, apart from i, j). We will need to suitably transform the Hamiltonian parameters U^D, t^D , but we will figure those out as we go along. Since the number of nearest neighbour pairs is $\frac{Nw}{2}$, the general Hubbard Hamiltonian should be the average of these local Hamiltonians.

We recall the dimer+bath Hamiltonian here, since we are going to create the full Hamiltonian by combining various realizations of that Hamiltonian:

$$\tilde{H}^D = H^D(0, 1) - t^D \left(c_{0\sigma}^\dagger c_{z\sigma} + c_{1\sigma}^\dagger c_{z\sigma} + \text{h.c.} \right) + \sum_{\vec{k}}^{\text{eff. bath}} \epsilon_{\vec{k}} \hat{n}_{\vec{k}} \quad (5.2.1)$$

We now choose a particular nearest neighbour pair from the full lattice, say (i, j) , and one site that is nearest neighbour to this pair, call that l . We will first create a "local" Hamiltonian, where one particular nearest neighbour pair (i, j) makes up the dimer sites of the Hamiltonian, while the rest $N - 2$ sites of the lattice make up the effective bath and the site l forms the zeroth site of the bath.

$$\tilde{H}^D(i, j, l) \equiv \tilde{H}^D(0 \rightarrow i, 1 \rightarrow j, z \rightarrow l) = H^D(i, j) - t^D \sum_{\sigma} \left(c_{i\sigma}^\dagger c_{l,\sigma} + c_{j\sigma}^\dagger c_{l,\sigma} + \text{h.c.} \right) + \sum_{\vec{k}}^{\text{eff. bath (i,j)}} \epsilon_{\vec{k}} \hat{n}_{\vec{k}} \quad (5.2.2)$$

$H^D(i, j)$ is the Hubbard dimer Hamiltonian in eq. ?? with the indices 0 and 1 replaced by i, j respectively. This is not the total local Hamiltonian for the nearest neighbour pair (i, j) , because it has just one nearest neighbour of the dimer, namely l . To get the full thing, we need to *average* over all the nearest neighbours of the pair i, j , $2(w - 1)$ in number. What we mean by nearest neighbours of the dimer pair (i, j) is made clear in 5.1.

The total Hamiltonian for a particular dimer pair (i, j) then looks like:

$$\begin{aligned} \tilde{H}^D(i, j) &= \frac{1}{2(w-1)} \sum_{l \in \text{NN of (i,j)}} \left[H^D(i, j) - t^D \sum_{\sigma} \left(c_{i\sigma}^\dagger c_{l,\sigma} + c_{j\sigma}^\dagger c_{l,\sigma} + \text{h.c.} \right) + \sum_{\vec{k}}^{\text{eff. bath (i,j)}} \epsilon_{\vec{k}} \hat{n}_{\vec{k}} \right] \\ &= H^D(i, j) + \frac{1}{2(w-1)} \sum_{l \in \text{NN of (i,j)}} \left[-t^D \sum_{\sigma} \left(c_{i\sigma}^\dagger c_{l,\sigma} + c_{j\sigma}^\dagger c_{l,\sigma} + \text{h.c.} \right) + \sum_{\vec{k}, \sigma}^{\text{eff. bath (i,j)}} \epsilon_{\vec{k}} \hat{n}_{\vec{k}} \right] \end{aligned} \quad (5.2.3)$$

We now translate this Hamiltonian over all nearest neighbour pairs on the lattice, and take the average:

$$\tilde{H} = \frac{2}{Nw} \sum_{\langle ij \rangle} \frac{1}{2(w-1)} \sum_{l \in \text{NN of (i,j)}} \tilde{H}^D(i, j, l) = \frac{2}{N} U^D \sum_i \tau_{i\uparrow} \tau_{i\downarrow} - \frac{2}{Nw} \left(1 + \frac{Nw}{2} \right) t^D \sum_{\langle ij \rangle} \left(c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.} \right) \quad (5.2.4)$$

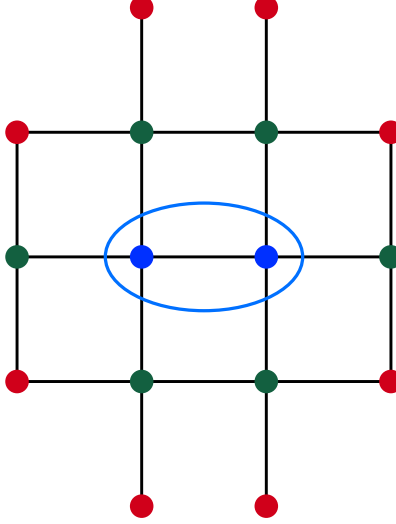


Figure 5.1: Blue circles (enclosed by the oval) indicate the dimer sites. Green circles are the sites that are nearest neighbour to the dimer and the ones that are being summed over under the index l . The red circles are sites that are *not* nearest neighbour to the dimer.

The sum $\langle ij \rangle$ is over all nearest-neighbour pairs. The conclusion is that on tiling the Hubbard dimer+bath Hamiltonians into all the nearest neighbour pairs, we end up with a new Hubbard model Hamiltonian with "renormalised parameters" given by

$$\tilde{t} = \frac{2}{Nw} \left(1 + \frac{Nw}{2}\right) t^D, \quad \tilde{U} = \frac{2}{N} U^D \quad (5.2.5)$$

It is thus apparent that translating the Hubbard dimers throughout the lattice has restored translational invariance, and generated correlations on all sites. With some knowledge of the RG procedure, one can even write down the relation between the Hubbard dimer couplings t^D, U^D and the parent Hubbard model parameters t^H, U^H . We have seen previously in another work that in the absence of any explicit spin or charge isospin exchange couplings, the impurity-bath hybridisation coupling t^A does not flow under the RG. In going from the Hubbard model to the auxiliary model, we replace the non-local operator c_i with the local operator c_d . If we define the normalization of the Fourier transform such that both spaces have $\frac{1}{\sqrt{N}}$, then the auxiliary model coupling can be written as $t^A = \sqrt{N} t^H$. When we write the fixed-point hopping purely in terms of zero mode, another such factor appears: $\sum_k c_k = \sqrt{N} c_0$, such that $t^D = \sqrt{N} (t^A)^*$. Combining these, we get

$$t^D = \sqrt{N} \times (t^A)^* = \sqrt{N} \times t^A = N \times t^H$$

As for the on-site repulsion U^H , we will constrain the RG flows such that the fixed-point value of the impurity on-site repulsion U^A is identical to that of the on-site repulsion of the bath, U_b . A sensible choice for the bath on-site repulsion is simply $U^H \times N$. The factor of N maintains the extensivity of the bath correlation term. We can therefore write

$$U^D \equiv (U^A)^* = U_b = N \times U^H$$

5.3 Formal expressions for single particle Greens functions and other related many-body quantities

5.3.1 Expressing matrix elements of the inverse single particle Greens function in terms of Hubbard dimer counterparts

Since the two Hamiltonians H^H and \tilde{H} are connected via a similarity transformation \mathcal{U} , their ground states are also connected by the same transformation. That is, if the ground states are $|\Phi_0\rangle$ and $|\tilde{\Phi}_0\rangle$ respectively, then $|\tilde{\Phi}_0\rangle = \mathcal{U} |\Phi_0\rangle$. This means that matrix elements of the type in eq. D.0.6 will also be connected. The matrix

elements are of the inverse Greebs function operator defined in eq. D.0.5:

$$\mathcal{G}(\omega, H) = \frac{1}{\omega - (H - E_{\text{GS}})} \quad (5.3.1)$$

Its easy to see that the matrix elements of the original and renormalised versions of this operator, between the original and renormalised states, are equal:

$$\begin{aligned} \left[\mathcal{G}_H^{-1} \right]_{\nu\nu'} &= \langle \nu | \omega - H^H + E_{\text{GS}} | \nu' \rangle = \langle \nu | \mathcal{U}^{-1} \left(\omega - \mathcal{U} H^H \mathcal{U}^{-1} + E_{\text{GS}} \right) \mathcal{U} | \nu' \rangle = \langle \tilde{\nu} | \left(\omega - \tilde{H} + E_{\text{GS}} \right) | \tilde{\nu}' \rangle \\ &= \left[\tilde{\mathcal{G}}^{-1} \right]_{\tilde{\nu}, \tilde{\nu}'} \end{aligned} \quad (5.3.2)$$

where we have defined the renormalised excitation $|\tilde{\nu}'\rangle \equiv \tilde{c}_{\nu'}^\dagger |\tilde{\Phi}_0\rangle \equiv \left(\mathcal{U} c_{\nu'}^\dagger \mathcal{U}^{-1} \right) \mathcal{U} |\Phi_0\rangle = \mathcal{U} |\nu'\rangle$. These equalities are important because they allows us to calculate these matrix elements for \tilde{H} and then equate them to those of H^H , and once we have the matrix elements of $\tilde{\mathcal{G}}$, we can use them to obtain the single-particle Greens functions using eq. D.0.6. More specifically, to calculate the real space single-particle Greens function between the lattice sites i and j , both with spin σ , we will use the relation:

$$G(i\sigma, j\sigma, \omega) = \langle i\sigma | \mathcal{G}(\omega, H) | j\sigma \rangle - \langle \bar{i}\sigma | \mathcal{G}(-\omega, H) | \bar{j}\sigma \rangle = \mathcal{G}(\omega, H)_{i\sigma, j\sigma} - \mathcal{G}(-\omega, H)_{\bar{i}\sigma, \bar{j}\sigma} \quad (5.3.3)$$

where $|i\sigma\rangle = c_{i\sigma}^\dagger |\Phi_0\rangle$ and $|\bar{i}\sigma\rangle = c_{i\sigma} |\Phi_0\rangle$. We can see from the relation that we will need two types of matrix elements, one that propagates a particle excitation ($|i\sigma\rangle$) and the one that propagates a hole excitation ($|\bar{i}\sigma\rangle$).

To this end, we rewrite eq. 5.2.4 in terms of inverse Greens function operators for the new (symmetrized) Hubbard model and the Hubbard dimer respectively:

$$\tilde{\mathcal{G}}(\omega) = \frac{1}{\omega - (\tilde{H} - E_{\text{GS}})}, \quad \mathcal{G}_D(\omega) = \frac{1}{\omega - (\tilde{H}^D(i, j, l) - E_{\text{GS}})} \quad (5.3.4)$$

These are the same operators that appear in the appendix. However, before proceeding, we should note that even though eq. 5.2.4 used the indices i , the correct indices are actually \tilde{i}, \tilde{j} , in light of the fact that operators get renormalised as $c_i \rightarrow \tilde{c}_i \equiv \mathcal{U} c_i$. With this in mind, we can write

$$\omega - \tilde{\mathcal{G}}^{-1}(\omega) = \frac{2}{Nw} \sum_{\langle \tilde{i}, \tilde{j} \rangle} \frac{1}{2(w-1)} \sum_{l \in \text{NN of } j} \left[\omega - \mathcal{G}_D^{-1}(\tilde{i}, \tilde{j}, \tilde{l}) \right] \quad (5.3.5)$$

where $\mathcal{G}_D^{-1}(\tilde{i}, \tilde{j}, \tilde{l})$ is the Greens function inverse matrix of the Hubbard dimer+bath Hamiltonian with \tilde{i}, \tilde{j} as the two sites and \tilde{l} as the zero mode of the bath, eq. 5.2.2, or equivalently, eq. ???. Since the ω on the RHS of eq. 5.3.5 is independent of the summation indices, they can be pulled out along with a factor. The factor is just the total number of nearest neighbour pairs, which is $\frac{Nw}{2}$. This allows it to cancel the ω on the LHS. The equation then simplifies to

$$\tilde{\mathcal{G}}^{-1}(\omega) = \frac{2}{Nw} \sum_{\langle i, j \rangle} \frac{1}{2(w-1)} \sum_{l \in \text{NN of } j} \mathcal{G}_D^{-1}(\omega, \tilde{i}, \tilde{j}, \tilde{l}) \quad (5.3.6)$$

Because of translational invariance, all values of l should give the same Greens function, and we can simplify this to

$$\tilde{\mathcal{G}}^{-1}(\omega) = \frac{2}{Nw} \frac{1}{2(w-1)} \times 2(w-1) \sum_{\langle i, j \rangle} \mathcal{G}_D^{-1}(\omega, \tilde{i}, \tilde{j}) = \frac{2}{Nw} \sum_{\langle i, j \rangle} \mathcal{G}_D^{-1}(\omega, \tilde{i}, \tilde{j}) \quad (5.3.7)$$

We dropped the index \tilde{l} on \mathcal{G}_D^{-1} to mean that any particular choice of \tilde{l} will do. We will now calculate the site-diagonal and site-off-diagonal matrix elements for particle propagation. The site-diagonal matrix element will be calculated between the state $|\tilde{i}, \sigma\rangle = \mathcal{U} c_{i\sigma}^\dagger |\Phi_0\rangle$ and its bra, while the off-diagonal one is between $|\tilde{j}\sigma\rangle$ and $\langle \tilde{i}\sigma|$. Since it has already been shown that the matrix elements of the renormalised Hamiltonian are the same as those of the original Hamiltonian, we will directly replace the former with the latter.

First let's consider the diagonal matrix element at \tilde{i}^{th} site. The only terms that will contribute on the RHS of eq. 5.3.7 are those that have the index \tilde{i} on the dimer. There are w terms that have the index \tilde{i} on the dimer corresponding to the w nearest neighbours of \tilde{i} . Thus, the right hand side will be a sum of w terms, each term being the inverse Greens function of a Hubbard dimer+bath Hamiltonian. Each term will be a real space local Greens function, and because of translational invariance, it will be the same for all choices of the nearest neighbour of \tilde{i} .

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^{\sigma} = \frac{2}{Nw} \sum_{j \in \text{NN of } i} \langle \tilde{\Phi}_0 | c_{i\sigma} \mathcal{G}_D^{-1}(\omega, \tilde{i}, \tilde{j}) c_{i\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle = \frac{2}{N} \langle \tilde{\Phi}_0 | c_{i\sigma} \mathcal{G}_D^{-1}(\omega, \tilde{i}) c_{i\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle \quad (5.3.8)$$

Once we have stripped away the j, l dependence, we can view the RHS as simply the matrix element of the dimer-bath Hamiltonian eq. ?? between the local states of the site zero of the bath:

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^{\sigma} = \frac{2}{N} \langle \tilde{\Phi}_0 | c_{0\sigma} \mathcal{G}_D^{-1}(\omega) c_{0\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle \quad (5.3.9)$$

Just to make it explicit, we repeat once more that $\mathcal{G}_D^{-1}(\omega)$ is the inverse Greens function operator of the Hamiltonian in eq. ?.?. We can expand the state $c_{i\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle$ in terms of a complete set of orthogonal states:

$$c_{0\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle = \sum_n C_n^0 | n \rangle, \quad c_{1\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle = \sum_n C_n^1 | n \rangle \quad (5.3.10)$$

where C^0 and C^1 are coefficients of the linear superposition defined by

$$C_n^0 = \langle n | c_{0\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle, \quad C_n^1 = \langle n | c_{1\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle. \quad (5.3.11)$$

Due to the translation invariance, the coefficients C_n^0 and C_n^1 are independent of the site indices. The index n actually defines a set of quantum numbers that characterize the state $| n \rangle$. For example it might be a combination of number of particles, parity and total spin angular momentum ($n \equiv n, P, S^z$). In light of the Greens function we have in between the states, we choose the orthogonal set to be formed by the eigenstates of the dimer+bath Hamiltonian.

Using this expansion, the matrix element of \mathcal{G} can be written as

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^{\sigma} = \frac{2}{N} \sum_{nn'} \left(C_{n'}^0\right)^* \langle n' | \mathcal{G}_D^{-1}(\omega) | n \rangle C_n^0 \quad (5.3.12)$$

Since $| n \rangle$ is an actual eigenstate of the Hamiltonian that defines $\mathcal{G}_D^{-1}(\omega)$, $\mathcal{G}_D^{-1}(\omega)$ will be diagonal in that basis:

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ii}^{\sigma} = \frac{2}{N} \sum_n |C_n^0|^2 \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn} \quad (5.3.13)$$

Now we come to the off-diagonal Greens function for the nearest neighbour sites i and j . This will receive contribution from only that dimer+bath Hamiltonian that has i, j as the dimer sites. This will not be a real space diagonal Greens function. Instead, it involves two nearest neighbour sites.

$$\left(\mathcal{G}_H^{-1}(\omega)\right)_{ij}^{\sigma} = \frac{2}{Nw} \langle \tilde{\Phi}_0 | c_{0\sigma} \mathcal{G}_D^{-1}(\omega) c_{1\sigma}^{\dagger} | \tilde{\Phi}_0 \rangle = \frac{2}{Nw} \sum_n \left(C_n^0\right)^* C_n^1 \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn} \quad (5.3.14)$$

For convenience, we define $g_n = \left(\mathcal{G}_D^{-1}(\omega)\right)_{nn}$.

The matrix elements for hole propagation are obtained similarly. Here the relevant excitations are $|\bar{i}\sigma\rangle \equiv c_{i\sigma} | \tilde{\Phi}_0 \rangle$, at frequency $-\omega$. To expand these states, we choose the eigenstates with $N - 1$ total particles as the orthonormal basis:

$$c_{0\sigma} | \tilde{\Phi}_0 \rangle = \sum_n \bar{C}_n^0 | \bar{n} \rangle, \quad c_{1\sigma} | \tilde{\Phi}_0 \rangle = \sum_n \bar{C}_n^1 | \bar{n} \rangle \quad (5.3.15)$$

and the counterpart for g_n , here, is

$$\bar{g}_n = \langle \bar{n} | \mathcal{G}_D^{-1}(-\omega) | \bar{n} \rangle \quad (5.3.16)$$

By suitably replacing the symbols, we can write down the matrix elements of $\mathcal{G}_H^{-1}(-\omega)$ for hole propagation:

$$\begin{aligned} \left(\mathcal{G}_H^{-1}(-\omega)\right)_{\bar{i}\bar{i}}^{\sigma} &= \frac{2}{N} \sum_n |\bar{C}_n^0|^2 \bar{g}_n \\ \left(\mathcal{G}_H^{-1}(-\omega)\right)_{\bar{i}\bar{j}}^{\sigma} &= \frac{2}{Nw} \sum_n \left(\bar{C}_n^0\right)^* \bar{C}_n^1 \bar{g}_n \end{aligned} \quad (5.3.17)$$

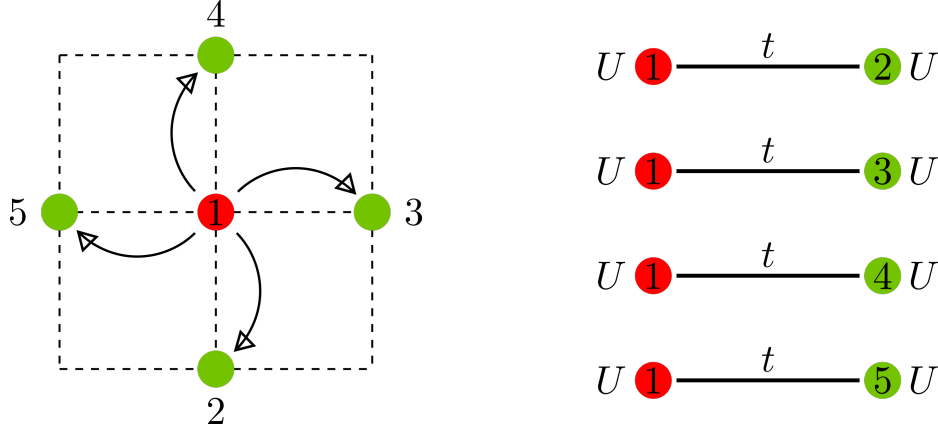


Figure 5.2: *Left*: Part of the lattice that is picked out by the Greens function on the LHS of eq. 5.3.9. *Right*: Hamiltonian whose Greens functions appear on the right hand side of same equation. The two submodels are identical.

5.3.2 Constructing full Greens function matrix from the inverse matrix

The matrix elements $(\mathcal{G}_H^{-1}(\omega))_{ii}^\sigma$ and its nearest neighbour partner can be obtained simply by inverting the internal matrix \mathcal{G}_D^{-1} . This is because,

$$A_{ij} = \sum_{mn} \langle i|n \rangle A_{nm} \langle m|j \rangle \implies A_{ij}^{-1} = \sum_{mn} \langle i|n \rangle A_{nm}^{-1} \langle m|j \rangle \quad (5.3.18)$$

The spectral weights remain unchanged; only the matrix element changes from A_{nm} to $(A^{-1})_{nm}$. Inverting the matrix \mathcal{G}_D is actually simple because it is diagonal in the chosen basis:

$$(\mathcal{G}_D^{-1})_{nn} = \begin{pmatrix} g_0 & 0 & \dots & 0 \\ 0 & g_1 & & \\ & \dots & \dots & \\ 0 & & & g_M \end{pmatrix} \implies (\mathcal{G}_D)_{nn} = \begin{pmatrix} \frac{1}{g_0} & 0 & \dots & 0 \\ 0 & \frac{1}{g_1} & & \\ & \dots & \dots & \\ 0 & & & \frac{1}{g_M} \end{pmatrix} \quad (5.3.19)$$

This allows us to write

$$(\mathcal{G}_H(\omega))_{ii}^\sigma = \frac{4(w-1)}{N} \sum_n |C_n^0|^2 \frac{1}{g_n}, \quad (\mathcal{G}_H(-\omega))_{ii}^\sigma = \frac{4(w-1)}{N} \sum_n |\bar{C}_n^0|^2 \frac{1}{g_n} \quad (5.3.20)$$

and

$$(\mathcal{G}_H(\omega))_{ij}^\sigma = \frac{4(w-1)}{Nw} \sum_n C_n^{0*} C_n^1 \frac{1}{g_n}, \quad (\mathcal{G}_H(-\omega))_{ij}^\sigma = \frac{4(w-1)}{Nw} \sum_n \bar{C}_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \quad (5.3.21)$$

These two expressions can be used to obtain an expression for the real space local and nearest-neighbour Greens functions:

$$\begin{aligned} G_H(\omega)_{\text{loc}} &= (\mathcal{G}_H(\omega))_{ii} - (\mathcal{G}_H(-\omega))_{ii} = \frac{4(w-1)}{N} \sum_n \left(|C_n^0|^2 \frac{1}{g_n} - |\bar{C}_n^0|^2 \frac{1}{g_n} \right) \\ G_H(\omega)_{\text{nn}} &= (\mathcal{G}_H(\omega))_{ij} - (\mathcal{G}_H(-\omega))_{ji} = \frac{4(w-1)}{Nw} \sum_n \left(C_n^{0*} C_n^1 \frac{1}{g_n} - \bar{C}_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \right) \end{aligned} \quad (5.3.22)$$

The momentum space Greens function can be expressed as a Fourier transform of the real space Greens functions:

$$G_H(\vec{k}, \omega) = \frac{1}{N} \sum_{\vec{r}, \vec{r}_j} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} G_H(|\vec{r}_i - \vec{r}_j|, \omega) \quad (5.3.23)$$

where \vec{r}_i is the position vector of a particular lattice site. Because of translation invariance, the real space Greens function depends only on the relative vector between any two sites. As a result, $\vec{r} = 0$ gives the local Greens function, $|\vec{r}| = a$ gives the nearest-neighbour Greens function and so on (a being the lattice spacing). As we do not have real space Greens function that are more non-local than nearest neighbour, we will attempt to obtain momentum space Greens function from these two contributions:

$$G_H(\vec{k}, \omega) \simeq \frac{1}{N} \sum_{\vec{r}_i = \vec{r}_j} G_H(\omega)_{\text{loc}} + \frac{1}{N} \sum_{|\vec{r}_i - \vec{r}_j| = a} e^{i\vec{k} \cdot (\vec{r}_i - \vec{r}_j)} G_H(\omega)_{\text{nn}} \quad (5.3.24)$$

The first summation produces a factor of N , while the second summation can be factorized into a sum over all sites (which again returns N) and a sum over all the primitive vectors connecting any single site with all its nearest neighbours, $\{\vec{a}_i : i \in [1, w]\}$.

$$\begin{aligned} G_H(\vec{k}, \omega) &\simeq G_H(\omega)_{\text{loc}} + G_H(\omega)_{\text{nn}} \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i} \\ &= G_H(\omega)_{\text{loc}} + G_H(\omega)_{\text{nn}} \xi_{\vec{k}} \\ &= \frac{4(w-1)}{N} \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \end{aligned} \quad (5.3.25)$$

where we defined $\xi_{\vec{k}} \equiv \sum_{i=1}^w e^{i\vec{k} \cdot \vec{a}_i}$. For example, on a d -dimensional hypercubic lattice, we obtain

$$\xi_{\vec{k}} = \sum_{i=1}^d \left(e^{ik_i a_i} + e^{-ik_i a_i} \right) = 2 \sum_{i=1}^d \cos k_i a_i \quad (5.3.26)$$

On a 2D square lattice with lattice spacing a , this simplifies to

$$\begin{aligned} \xi_{\vec{q}} &= 2(\cos q_x a + \cos q_y a) \equiv \frac{-\epsilon_{\vec{q}}}{t^H}, \\ \epsilon_{\vec{q}} &= -2t^H(\cos q_x a_x + \cos q_y a_y) \end{aligned} \quad (5.3.27)$$

where $\epsilon_{\vec{q}}$ is the tight-binding dispersion.

We can now compute the k -space spectral function $A_H(\vec{k}, \omega)$ and the real-space local spectral function $A_H(\vec{r} = 0, \omega)$ as

$$\begin{aligned} A_H(\vec{k}, \omega) &= -\frac{1}{\pi} \text{Im}(G_H(\vec{k}, \omega)) = -\frac{4(w-1)}{N\pi} \text{Im} \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \\ A_H(\vec{r} = 0, \omega) &= -\frac{1}{\pi} \text{Im}(G_H(\vec{r} = 0, \omega)) = \frac{1}{N} \sum_{\vec{k}} A_H(\vec{k}, \omega) \end{aligned} \quad (5.3.28)$$

We can again use eqs.(5.3.27), (5.3.9) and (5.3.14) to obtain the spectral functions $A_H(\vec{k}, \omega)$ and $A_H(\vec{r} = 0, \omega)$ for the Hubbard model on the 2D square lattice.

5.3.3 Calculation of self energy matrix from the Dyson equation

With the knowledge of the momentum-space Greens function $G_H(\vec{k}, \omega)$, we can now use Dyson's equation to calculate the self-energy for propagation of momentum excitations:

$$\Sigma(\vec{k}, \omega) = G_0(\vec{k}, \omega)^{-1} - G(\vec{k}, \omega)^{-1} \quad (5.3.29)$$

where the $G_0(\vec{k}, \omega)^{-1} = \omega - \epsilon_k = \omega + t^H \xi_k$ is the inverse k -space Greens function for the appropriate non-interacting tight-binding system. Substituting this as well as the full Greens function $G_H(\vec{k}, \omega)$ into Dyson's equation gives

$$\Sigma_H(\vec{k}, \omega) = \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \left\{ \sum_n \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \right\}^{-1} \quad (5.3.30)$$

Thus, we can use eqs.(5.3.27), (5.3.9) and (5.3.14) to obtain the full self-energy $\Sigma(\vec{k}, \omega)$ for the Hubbard model on the 2D square lattice.

5.4 Calculating the coefficients $C_n^{0,1}$ and $\bar{C}_n^{0,1}$ in practice

The expressions for $C_n^{0,1}$ and $\bar{C}_n^{0,1}$, as mentioned above, involve taking the projection of the exact ground state of the full Hubbard model, $|\tilde{\Phi}_0\rangle$, against the chosen orthogonal basis $|n\rangle$.

1. Since the full Hubbard model ground state wavefunctions are not readily available, one can, as the simplest approximation, assume the ground state has the form

$$|\tilde{\Phi}_0\rangle = \sum_{\langle \tilde{i}\tilde{j} \rangle} |\Phi_{\tilde{i}\tilde{j}}^D\rangle \otimes |\Psi_{\tilde{i}\tilde{j}}\rangle \quad (5.4.1)$$

$|\Phi_{\tilde{i}\tilde{j}}^D\rangle$ would be the ground state of the Hubbard dimer with i, j creating the two sites of the dimer, while $|\Psi_{\tilde{i}\tilde{j}}\rangle$ would be the wavefunction involving the rest of the sites. This of course assumes that the two sets (i, j) and $(a, b, \dots, h, k, \dots)$ are not entangled, and is not true in general. With this assumption, g_0 and g_1 become related to the inverse Greens functions of the Hubbard dimer. Such a choice of the wavefunction is motivated by the fact that in the auxiliary system we chose, the bath had only a diagonal interaction; there was no off-diagonal two particle scattering term. It is further enforced when we extract the zero mode of the entire bath (i.e., we keep just the zeroth site). The zeroth site, along with the impurity, then forms the $|\Phi\rangle$ part of the wavefunction. This will allow for analytic insight, but at the cost of accuracy as discussed above.

2. Another way of approaching the problem is to obtain the ground state wavefunction of a Hubbard model numerically for several values of U^H and t^H , and then computing the matrix elements of H^D against this wavefunction to obtain a family of (g_0, g_1) . This brings the numerical accuracy for a given finite-sized lattice realisation of the Hubbard model. However, this also means we lose any analytical insight into the structure of g_0 and g_1 .
3. The most promising approach of calculating g_0 and g_1 is by systematically improving the required ground state wavefunctions as follows. We obtain numerically the ground state wavefunction of a Hamiltonian that has not just the Hubbard dimer, but also a bath (with dispersion) that connects to both the sites of the dimer:

$$H_{\text{bath}}^D(\tilde{i}, \tilde{j}) = \underbrace{U \left(\tau_{\tilde{i}\uparrow} \tau_{\tilde{i}\downarrow} + \tau_{\tilde{j}\uparrow} \tau_{\tilde{j}\downarrow} \right)}_{\text{Hubbard dimer}} - t \sum_{\sigma} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + \text{h.c.} \right) + \underbrace{\sum_{k\sigma} \epsilon_{k\sigma} \tau_{k\sigma}}_{\text{bath}} - t \sum_{k\sigma} \underbrace{\left(c_{i\sigma}^{\dagger} c_{k\sigma} + c_{j\sigma}^{\dagger} c_{k\sigma} + \text{h.c.} \right)}_{\text{bath-dimer hybridisation}} \quad (5.4.2)$$

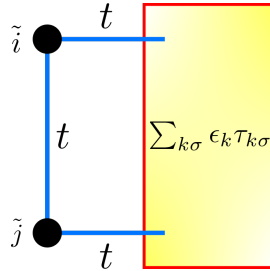


Figure 5.3: Hubbard dimer with dispersion that connects to both sites

By systematically increasing the number of momentum states in the bath dispersion, we can systematically improve the numerical computation of the ground state wavefunction. From here, we can compute matrix elements of H^D , and hence the functions g_0 and g_1 . The presence of the bath can be understood as follow. In the absence of a bath, i.e., we have just a Hubbard dimer, an electron can at most hop between the two

sites and lead to the wavefunction in eq. 5.4.1. However, with a single particle hopping term connecting the dimer to a bath, an electron can also journey between the two sites of the bath via the bath. This leads to entanglement between the dimer's sites and those in the bath; this was clearly ignored in the ground state wavefunction eq. 5.4.1. The introduction of the bath dispersion offers the possibility that we can capture a site diagonal spectral function of the three peak form, because we have previously seen such a spectral function in the fixed point of the URG analysis of the SIAM (where the fixed point effective Hamiltonian was an Anderson molecule with dispersion). If this can be found, then a metal-insulator transition of the full Hubbard model can perhaps be captured by studying the spectral functions of the bath-coupled Hubbard dimer.

4. Another improvement can be made by introducing a self-energy $\Sigma(k, \omega)$ into the bath dispersion. This introduces correlation within the bath. The Hamiltonian that we would need to solve would be the same as eq. 5.4.2, but with ϵ_k replaced by $\tilde{\epsilon}_k \equiv \epsilon_k + \Sigma(k, \omega)$. The self-energy $\Sigma(k, \omega)$ will have to be chosen depending on the phase we want to look at (e.g., metal, insulator etc.). With a Σ that is singular near the Fermi surface at $\omega \rightarrow 0$, the dispersion will become gapped and the phase will be insulating. In such a situation, there are no low-energy bath excitations within a given energy window proximate to its putative Fermi energy. This will localise the bath electrons, as well as confine all journeys between the two sites of the dimer to only the direct path. This is an indication of the localisation of electrons in the Hubbard model to holon-doublon excitations on nearest neighbour sites. In such a circumstance, eq. 5.4.1 will be a very good approximation to the actual insulating ground state of the Hubbard model. On the other hand, if we use a self energy that vanishes near the Fermi surface ($\Sigma(\omega) \sim \omega^2$, i.e., a Fermi liquid bath), then we expect to end up in a metallic phase of the Hubbard model. This is simply due to the possibility of holons and doublons now dispersing throughout the lattice, and be concomitant with the presence of a pole in the single-particle Greens function $G(k, \omega)$ of the Hubbard model. Introducing the self energy therefore gives us a larger variety of wavefunctions and features to work with. Further, this appears to be in line with the original proposals offered by Mott and Kohn for the Mott metal insulator transition as the localisation-delocalisation transition of holon-doublon pairs. With regards to the transition itself, the precise form of the bath $\Sigma(k, \omega)$ (or spectral function) remains to be determined.

Once we have chosen a test Hamiltonian whose wavefunction we can calculate, we can use that to obtain the ground state energy of this state. The wavefunction will act as our $|0\rangle$ and the ground state energy will be our E_{GS} . We can then substitute these into the Lehmann representation form of the Greens function, and calculate the matrix elements $\mathcal{G}_D(\omega)_{\nu\nu'}$ and $\mathcal{G}_D(-\omega)_{\nu\nu'}$ for the Hubbard dimer Hamiltonian. Each set will form a 2×2 matrix, and we can invert them to obtain $\mathcal{G}_D(\omega)$, and then the matrix elements of this inverted matrix will give all the parameters g_0 through \bar{g}_1 .

5.5 Analytic consistency checks

5.5.1 Single-particle Greens function and self energy for the Hubbard dimer

The simplest test involves choosing $H^H = H^D$ and then calculating the momentum space Greens function at $k = 0$, $G(k = 0, \uparrow)$, for the Hubbard dimer ($N = 2, w = 1$). The discrete set of momenta are $\{\vec{k}_n\} = 0, \frac{\pi}{a}$. For $k = 0$, we have

$$\xi_{\vec{k}=0} = e^{ikr} = 1 \quad (5.5.1)$$

Substituting this into eq. 5.3.25 gives

$$G(k = 0, \uparrow) = \sum_n \left[\left(|C_n^0|^2 + C_n^{0*} C_n^1 \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \quad (5.5.2)$$

The expansion in terms of the exact eigenstates takes the form:

$$\begin{aligned} c_{0\uparrow}^\dagger |\tilde{\Phi}_0\rangle &= x |3+ \uparrow\rangle + y |3- \uparrow\rangle, & c_{1\uparrow}^\dagger |\tilde{\Phi}_0\rangle &= x |3+ \uparrow\rangle - y |3- \uparrow\rangle \\ c_{0\uparrow} |\tilde{\Phi}_0\rangle &= y |1+ \downarrow\rangle + x |1- \downarrow\rangle, & c_{1\uparrow} |\tilde{\Phi}_0\rangle &= y |1+ \downarrow\rangle - x |1- \downarrow\rangle \end{aligned} \quad (5.5.3)$$

where $|(3, 1) \pm (\uparrow, \downarrow)\rangle$ are the $N = (3, 1), S^z = (+\frac{1}{2}, -\frac{1}{2})$ eigenstates of even (+) and odd (−) parity:

$$\begin{aligned} H^D |3\pm \uparrow\rangle &= \pm t |3\pm \uparrow\rangle \\ H^D |1\pm \downarrow\rangle &= \mp t |1\pm \downarrow\rangle \end{aligned} \quad (5.5.4)$$

and $x = \frac{a_2 - a_1}{2}, y = \frac{a_2 + a_1}{2}$. The orthogonal basis is therefore

$$\begin{aligned} \{|n\rangle\} &= |3+\uparrow\rangle, |3-\uparrow\rangle \\ \{|\bar{n}\rangle\} &= |1+\downarrow\rangle, |1-\downarrow\rangle \end{aligned} \quad (5.5.5)$$

The coefficients can thus be determined:

$$\begin{aligned} C_{\pm}^0 &= \langle 3\pm\uparrow | c_{0\uparrow}^\dagger | \tilde{\Phi}_0 \rangle = x, y \\ C_{\pm}^1 &= \langle 3\pm\uparrow | c_{1\uparrow}^\dagger | \tilde{\Phi}_0 \rangle = x, -y \\ \bar{C}_{\pm}^0 &= \langle 1\pm\downarrow | c_{0\uparrow} | \tilde{\Phi}_0 \rangle = y, x \\ \bar{C}_{\pm}^1 &= \langle 1\pm\downarrow | c_{1\uparrow} | \tilde{\Phi}_0 \rangle = y, -x \\ g_{\pm} &= \langle 3\pm\uparrow | (\omega + E_{GS} - H^D) | 3\pm\uparrow \rangle = \omega + E_{GS} \mp t \\ \bar{g}_{\pm} &= \langle 1\pm\downarrow | (-\omega + E_{GS} - H^D) | 1\pm\downarrow \rangle = -\omega + E_{GS} \pm t \end{aligned}$$

We can see that $|C_-^0|^2 + C_-^{0*} C_-^1 = y^2 - y^2 = 0$ and $|\bar{C}_-^0|^2 + \bar{C}_-^{0*} \bar{C}_-^1 = x^2 - x^2 = 0$. So we do not need to consider those terms. With this preparation, we can now calculate the Greens function:

$$G(k=0, \omega) = \left(|C_+^0|^2 + C_+^{0*} C_+^1 \right) \frac{1}{g_+} - \left(|\bar{C}_+^0|^2 + \bar{C}_+^{0*} \bar{C}_+^1 \right) \frac{1}{\bar{g}_+} = \frac{2x^2}{\omega + E_{GS} - t} - \frac{2y^2}{-\omega + E_{GS} + t} \quad (5.5.6)$$

The final step is to recognize that $2x^2 = \frac{a_1^2 + a_2^2 - 2a_1 a_2}{2} = \frac{1}{2} - \frac{2t}{\Delta}$, $2y^2 = \frac{a_1^2 + a_2^2 + 2a_1 a_2}{2} = \frac{1}{2} + \frac{2t}{\Delta}$ and $E_{GS} = -\frac{\Delta}{2}$. Then,

$$G(k=0, \omega) = \frac{\frac{1}{2} - \frac{2t}{\Delta}}{\omega - \frac{\Delta}{2} - t} - \frac{\frac{1}{2} + \frac{2t}{\Delta}}{-\omega - \frac{\Delta}{2} + t} = \frac{\frac{1}{2} - \frac{2t}{\Delta}}{\omega - \frac{\Delta}{2} - t} + \frac{\frac{1}{2} + \frac{2t}{\Delta}}{\omega + \frac{\Delta}{2} - t} \quad (5.5.7)$$

5.5.2 On the Bethe lattice

Another test involves considering the case of infinite number of nearest neighbours $w \rightarrow \infty$ (the coordination number, and effectively the dimensionality). Here, as has been argued in the DMFT literature, the correct scaling of the t^H hopping parameter is $t^H \rightarrow t^H/\sqrt{w}$ such that the kinetic energy of the associated tight-binding lattice model is finite. This allows for the competition between the kinetic and potential terms of the Hamiltonian to drive a metal-insulator transition in the limit of $w \rightarrow \infty$ as well. Further, it has been argued in the DMFT literature that the Greens function matrix of the Hubbard model on the Bethe lattice with $w \rightarrow \infty$ becomes purely local (i.e., it has vanishing inter-site matrix elements). We can also see this from eqs.(5.3.21)- the nearest-neighbour inverse Greens function vanishes in the limit of $w \rightarrow \infty$:

$$(\mathcal{G}_H(\omega))_{ij}^\sigma = \frac{2}{Nw} \sum_n \bar{C}_n^{0*} \bar{C}_n^1 \frac{1}{g_n} \implies \lim_{w \rightarrow \infty} (\mathcal{G}_H(\omega))_{ij}^\sigma \rightarrow 0 \quad (5.5.8)$$

There we used the fact since at half-filling on an $SU(2)$ symmetric mode, we expect $\langle \hat{n}_{i\uparrow} \rangle = \frac{1}{2}$, the orthonormal expansion of $c_{i\sigma}^\dagger | \tilde{\Phi}_0 \rangle = \sum_n C_n^i | n \rangle$ to be constrained to $\sum_n |C_n^i|^2 = \frac{1}{2}$, such that the only term that scales with w is w itself. This result then implies that G^H matrix has no k dependence.

In this limit, the self-energy also simplifies:

$$\begin{aligned} \lim_{w \rightarrow \infty} \Sigma_H(\vec{k}, \omega) &= \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \left\{ \sum_n \lim_{w \rightarrow \infty} \left[\left(|C_n^0|^2 + \frac{\xi_{\vec{k}}}{w} C_n^{0*} C_n^1 \frac{1}{g_n} \right) \frac{1}{g_n} - \left(|\bar{C}_n^0|^2 + \frac{\xi_{\vec{k}}}{w} \bar{C}_n^{0*} \bar{C}_n^1 \right) \frac{1}{\bar{g}_n} \right] \right\}^{-1} \\ &= \omega + t^H \xi_{\vec{k}} - \frac{N}{2} \frac{1}{\sum_n \left[\frac{|C_n^0|^2}{g_n} - \frac{|\bar{C}_n^0|^2}{\bar{g}_n} \right]} \end{aligned} \quad (5.5.9)$$

We can now see that even in the limit of $w \rightarrow \infty$, the competition between g_0 (the on-site repulsion) and the hopping related kinetic energy ($t^H \xi_{\vec{k}}$) can lead to a metal-insulator transition.

Chapter 6

Future goals

1. Obtain the metal insulator transition of the 2D Hubbard model on the square lattice from our formalism. Compare with what is obtained from DMFT and its improvements. Also, determine the nature of the bath $\Sigma(k, \omega)$ for the transition point.
2. Once the zero temperature Mott metal-insulator transition is observed, we will investigate its nature.
3. While we have provided expressions for the single particle Greens functions of the N -site Hubbard model from their equivalent single particle Greens functions of the Hubbard dimer, we expect that eq.(4.2.10) holds quite generally for the two-particle Greens function sector as well. We will provide these expressions at a later point in time. More specifically, we will calculate the Greens functions for holon-doublon and spinon-spinon excitations as they are likely to contain more information regarding the ground state.
4. It is also important to benchmark the ground state energy and double occupancy obtained from this method against the ground state wavefunction obtained from exact diagonalisation of small lattices and finite size scaling.
5. It should also prove instructive to investigate the nature of many-particle entanglement in the ground state wavefunction of various phases, and look for signs of a quantum liquid.
6. Once we have a handle on the zero temperature features, we intend to compute Greens functions at non zero temperatures.
7. This method can also be extended to various other models of strong correlation:
 - (a) Heisenberg model, by starting from a Kondo model effective Hamiltonian
 - (b) Periodic Anderson model, by starting from a SIAM with a dispersive bath
 - (c) Periodic Kondo model, by starting from a Kondo model with a dispersive bath
 - (d) Hubbard-Heisenberg model, by starting from a generalized Anderson molecule (Anderson molecule with two-particle spin and charge interactions between the two sites)

Appendix A

Derivation of RG equations: U_b -free terms

A.1 Renormalisation of the impurity energy ϵ_d

The coupling ϵ_d is renormalised by three kinds of vertices: V^2 , J^2 and K^2 . We will consider these processes one after another. We define n_j as the number of states being decoupled on each side of the Fermi surface, at the j^{th} RG step. In order to treat both spin and isospin exchanges democratically, we take $|\Psi\rangle_i = \frac{1}{2}(|0\rangle + |q\uparrow\rangle + |q\downarrow\rangle + |q\uparrow, q\downarrow\rangle)$ as the *initial* state for the scattering processes. The intermediate states $|\Psi\rangle_{\text{int}}$ in the particle sector ($c_{q\beta}|\Psi\rangle_i$) and hole sector ($c_{q\beta}^\dagger|\Psi\rangle_i$) will then have both spin and isospin excitations which can couple with the corresponding impurity degree of freedom. We will assume that states $q > k_F$ ($\epsilon_q > 0$) above the Fermi surface can have only particle excitations and states below the Fermi surface can only have hole excitations. The kinetic energy part $\epsilon_q\tau_{q\beta}$ of H_D for $|\Psi\rangle_i$ is then zero, whereas it is always $D/2$ for $|\Psi\rangle_{\text{int}}$. To demonstrate this for a typical $q < k_F$, the hole excitation is $c_{q\uparrow}|\Psi\rangle_i = \frac{1}{\sqrt{2}}(|0\rangle + |q\downarrow\rangle)$. This has an isospin term in the form of the *holon* and a spin term in the form of the down state. Since $\tau_{q\uparrow} = -\frac{1}{2}$ in the excited state, the kinetic energy for $|\Psi\rangle_{\text{int}}$ is $\epsilon_q\tau_{q\uparrow} = (-D) \times (-\frac{1}{2}) = D/2$.

The renormalisation arising from the first kind of terms, in the particle sector, is

$$\sum_{q\beta} c_{q\beta}^\dagger c_{d\beta} \frac{V^2}{\omega - H_D} c_{d\beta}^\dagger c_{q\beta} = \sum_{q\beta} V^2 \hat{n}_{q\beta} (1 - \hat{n}_{d\beta}) \left(\frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - E_0} + \frac{\hat{n}_{d\bar{\beta}}}{\omega' - E_1} \right) = V^2 n_j \sum_{\beta} (1 - \hat{n}_{d\beta}) \left(\frac{1 - \hat{n}_{d\bar{\beta}}}{\omega_0 - E_0} + \frac{\hat{n}_{d\bar{\beta}}}{\omega_1 - E_1} \right) \quad (\text{A.1.1})$$

q runs over the momentum states that are being decoupled at this RG step: $|q| = \Lambda_j$. $E_{1,0}$ are the diagonal parts of the Hamiltonian at $\hat{n}_{d\bar{\beta}} = 0, 1$ respectively. We have $\hat{n}_{d\beta} = 1$ in the intermediate state because of the $c_{d\beta}^\dagger$ in front of the Greens function. Applying $c_{q\beta}$ on the initial state $|\Psi\rangle_i$ leaves us with $C_q^z = -\frac{1}{2}$ and $s_q^z = \frac{1}{2}\bar{\beta}$. We also know that

$$\hat{n}_{d\beta} = 1, \begin{cases} \hat{n}_{d\bar{\beta}} = 0 & \implies S_d^z = \frac{1}{2}\beta, C_d^z = 0, \epsilon_d (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 = \epsilon_d \\ \hat{n}_{d\bar{\beta}} = 1 & \implies S_d^z = 0, C_d^z = \frac{1}{2}, \epsilon_d (\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow})^2 = 0 \end{cases} \quad (\text{A.1.2})$$

Combining all this, we can write $E_1 = \frac{D}{2} - \frac{K}{4}$ and $E_0 = \frac{D}{2} + \epsilon_d - \frac{J}{4}$. In order to relate ω_0 with ω_1 with the common fluctuation scale ω for the conduction electrons, we will replace these quantum fluctuation scales by the current renormalised values of the single-particle self-energy for the initial state from which we started scattering. For $\hat{n}_{d\bar{\beta}} = 0$, there is no additional self-energy because the impurity does not have any spin: $\omega_0 = \omega$. For $\hat{n}_{d\bar{\beta}} = 1$, we have an additional self-energy of ϵ_d arising from the correlation on the impurity: $\omega_1 = \omega + \epsilon_d$. Substituting the values of $E_{0,1}$ and $\omega_{0,1}$, we get

$$V^2 n_j \sum_{\beta} (1 - \hat{n}_{d\beta}) \left(\frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} + \frac{\hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \quad (\text{A.1.3})$$

Performing a similar calculation for the hole sector gives the contribution:

$$V^2 n_j \sum_{\beta} \hat{n}_{d\beta} \left(\frac{1 - \hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} + \frac{\hat{n}_{d\bar{\beta}}}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \quad (\text{A.1.4})$$

We now come to the second type of terms: spin-spin. We first look at the particle sector:

$$\frac{J^2}{4} \sum_{q\beta} c_{d\bar{\beta}}^{\dagger} c_{d\beta} c_{q\beta}^{\dagger} c_{-q\bar{\beta}} \frac{1}{\omega - H_D} c_{d\beta}^{\dagger} c_{d\bar{\beta}} c_{q\bar{\beta}}^{\dagger} c_{q\beta} = \frac{J^2}{4} n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{\beta} \hat{n}_{d\bar{\beta}} (1 - \hat{n}_{d\beta}) \quad (\text{A.1.5})$$

The diagonal part in the denominator was simple to deduce in this case, because the nature of the scattering requires the spins S_d^z and $\frac{\beta}{2} (\hat{n}_{q\beta} - \hat{n}_{q\bar{\beta}})$ to be anti-parallel. This ensures that the intermediate state has an energy of $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$, and the quantum fluctuation scale is $\omega' = \omega + \epsilon_d$, such that $\omega' - E = \omega - \frac{D}{2} + \frac{J}{4}$. In the hole sector, we have

$$\frac{J^2}{4} n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{\beta} \hat{n}_{d\beta} (1 - \hat{n}_{d\bar{\beta}}) \quad (\text{A.1.6})$$

The final kind of scattering is the K^2 type. Similar to the J^2 term, we get the following contribution:

$$\frac{K^2}{4} \sum_{q\beta} c_{q\beta}^{\dagger} c_{q\bar{\beta}}^{\dagger} c_{d\bar{\beta}} c_{d\beta} \frac{1}{\omega - H_D} c_{d\beta}^{\dagger} c_{d\bar{\beta}}^{\dagger} c_{q\bar{\beta}} c_{q\beta} = \frac{K^2}{2} n_j \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} (1 - \hat{n}_{d\uparrow}) (1 - \hat{n}_{d\downarrow}) \quad (\text{A.1.7})$$

in the particle sector. This is again because $E = \frac{D}{2} - \frac{K}{4}$ in the intermediate state and $\omega' = \omega$. In the hole sector, we get

$$\frac{K^2}{2} n_j \frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} \hat{n}_{d\uparrow} \hat{n}_{d\downarrow}. \quad (\text{A.1.8})$$

We now have all possible renormalisation to the impurity energy ϵ_d . To actually compute the renormalisation, we will first calculate the renormalisation in the energies ϵ_0, ϵ_1 and ϵ_2 of the impurity states $|\hat{n}_d = 0\rangle, |\hat{n}_d = 1\rangle, |\hat{n}_d = 2\rangle$ respectively. The renormalisation of these states are given by the following terms:

- $\Delta\epsilon_0$ is given by the renormalisation of the term $(1 - \hat{n}_{d\uparrow}) (1 - \hat{n}_{d\downarrow})$
- $\Delta\epsilon_1$ is given by the renormalisation of either $(1 - \hat{n}_{d\uparrow}) \hat{n}_{d\downarrow}$ or $(1 - \hat{n}_{d\downarrow}) \hat{n}_{d\uparrow}$
- $\Delta\epsilon_2$ is given by the renormalisation of $\hat{n}_{d\uparrow} \hat{n}_{d\downarrow}$

From eqs. A.1.3, A.1.4, A.1.5, A.1.6, A.1.7 and A.1.8, we write

$$\Delta\epsilon_0 = \Delta\epsilon_2 = \frac{2V^2 n_j}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} + \frac{K^2 n_j / 2}{\omega - \frac{D}{2} + \frac{K}{4}}, \quad \Delta\epsilon_1 = \frac{2V^2 n_j}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} + \frac{J^2 n_j / 2}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (\text{A.1.9})$$

We had started with a particle-hole symmetric Hamiltonian ($2\epsilon_d + U = 0$); the fact that $\Delta\epsilon_0 = \Delta\epsilon_2$ means the RG transformation has preserved that symmetry. The renormalisation of ϵ_d is simply the renormalisation in the energy difference between the singly-occupied and vacant impurity levels: $\Delta\epsilon_d = \Delta\epsilon_1 - \Delta\epsilon_0$. This gives our first RG equation:

$$\Delta\epsilon_d = 2V^2 n_j \left(\frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + \frac{n_j}{2} \left(\frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right) \quad (\text{A.1.10})$$

A.2 Renormalisation of the hybridisation V

Renormalisation of V happens through two kinds of processes: VJ and VK . In other words, the two vertices involve one single-particle scattering and one spin or isospin exchange respectively. We first look at the vertices that involve a spin-exchange scattering.

Within spin-exchange, the scattering can be either via S_d^z or through S_d^\pm . For the first kind, we have the following contribution in the particle sector:

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{4} J \sum_k \left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) c_{k\beta}^\dagger c_{q\beta} = \frac{1}{4} V J n_j \frac{1}{2} \left(\frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right) \sum_{k\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{d\beta} c_{k\beta}^\dagger \quad (\text{A.2.1})$$

The transformation from $\frac{1}{\omega - H_D}$ to $\frac{1}{2} \left(\frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right)$ is made so that we can account for both the initial state and the final state energies through the two fluctuation scales ω'_1 and ω'_2 respectively; we calculate the denominators for both the initial and final states, and then take the mean of the two (hence the factor of half in front). This was not required previously because in the earlier scattering processes, the impurity returned to its initial state at the end, at least in terms of $\epsilon_d \left(\hat{n}_{d\uparrow} - \hat{n}_{d\downarrow} \right)^2$, and so we had $\omega'_1 = \omega'_2 = \omega'$.

Note that the $c_{d\beta}$ in front of the Greens function resulted in $\left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) \rightarrow \left(1 - \hat{n}_{d\bar{\beta}} \right)$. The intermediate state is characterised by $\hat{n}_{d\beta} = 1 - \hat{n}_{d\bar{\beta}} = 1$, which means that $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$. Moreover, the initial state gives $\omega'_1 = \omega + \epsilon_d$ while the final state gives $\omega'_2 = \omega$. Therefore, the renormalisation becomes

$$-\frac{n_j}{4} V J \frac{1}{2} \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) c_{k\beta}^\dagger c_{d\beta} \quad (\text{A.2.2})$$

One can generate another such process by exchanging the single-particle process and the spin-exchange process:

$$\sum_{q\beta} \frac{1}{4} J \sum_k \left(\hat{n}_{d\beta} - \hat{n}_{d\bar{\beta}} \right) c_{q\beta}^\dagger c_{k\beta} \frac{1}{\omega - H_D} V c_{d\beta}^\dagger c_{q\beta} \quad (\text{A.2.3})$$

This is simply the Hermitian conjugate of the previous contribution. Combining this with the previous then gives

$$-\frac{n_j}{8} V J \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left(1 - \hat{n}_{d\bar{\beta}} \right) \left(c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \quad (\text{A.2.4})$$

We now consider the spin-exchange processes involving S_d^\pm :

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{2} J \sum_k c_{d\beta}^\dagger c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger c_{q\beta} = \frac{1}{2} V J n_j \frac{1}{2} \left(\frac{1}{\omega'_1 - E} + \frac{1}{\omega'_2 - E} \right) \sum_{k\beta} \left(1 - \hat{n}_{d\beta} \right) c_{d\bar{\beta}} c_{k\bar{\beta}}^\dagger \quad (\text{A.2.5})$$

We again have $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$, $\omega'_1 = \omega + \epsilon_d$ and $\omega'_2 = \omega$, which gives

$$-\frac{1}{2} V J n_j \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} \sum_{k\beta} \left(1 - \hat{n}_{d\beta} \right) c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} \quad (\text{A.2.6})$$

Combining this with the Hermitian conjugate obtained from exchanging the processes gives

$$-\frac{1}{4} V J n_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left(1 - \hat{n}_{d\beta} \right) \left(c_{k\bar{\beta}}^\dagger c_{d\bar{\beta}} + \text{h.c.} \right) \quad (\text{A.2.7})$$

The contributions from the hole sector are obtained making the transformation $\hat{n}_{d\bar{\beta}} \rightarrow 1 - \hat{n}_{d\bar{\beta}}$ on the particle sector contributions. The total renormalisation to V from VJ processes are

$$-\frac{3n_j}{8} V J \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) \sum_{k\beta} \left(c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \quad (\text{A.2.8})$$

We now look at the VK processes. The first one is

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{4} K \sum_k \left(\hat{n}_d - 1 \right) c_{k\beta}^\dagger c_{q\beta} = -\frac{1}{8} V K n_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} \hat{n}_{d\bar{\beta}} c_{k\beta}^\dagger c_{d\beta} \quad (\text{A.2.9})$$

The exchanged process again gives the Hermitian conjugate, so the combined contribution is

$$-\frac{1}{8}VKn_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} \hat{n}_{d\beta} \left(c_{k\beta}^\dagger c_{d\beta} + \text{h.c.} \right) \quad (\text{A.2.10})$$

The isospin-flip vertex gives

$$\sum_{q\beta} V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \frac{1}{2} K \sum_k c_{d\beta}^\dagger c_{d\beta}^\dagger c_{k\beta} c_{q\beta} = \frac{1}{4} KV n_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} (1 - \hat{n}_{d\beta}) c_{d\beta}^\dagger c_{k\beta} . \quad (\text{A.2.11})$$

Combining with Hermitian conjugate gives

$$\frac{1}{4} KV n_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} (1 - \hat{n}_{d\beta}) \left(c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) . \quad (\text{A.2.12})$$

After obtaining the hole sector contributions, the total renormalisation from VK processes is

$$-\frac{3n_j}{4} VK \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \sum_{k\beta} \left(c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) . \quad (\text{A.2.13})$$

The RG equation for V is

$$\Delta V = -\frac{3n_j V}{8} \left[J \left(\frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) + K \left(\frac{1}{\omega - \frac{D}{2} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} \right) \right] \quad (\text{A.2.14})$$

A.3 Renormalisation of the exchange couplings J and K

We will just note the renormalisation in J^z , which will be equal to J^\pm due to spin-rotation symmetry. The terms that renormalise J^z are of the form $S_d^\pm S_d^\mp$. In the particle sector, we have

$$\sum_q \sum_{kk'} \frac{1}{4} J^2 S_d^\pm c_{q\mp}^\dagger c_{k'\pm} \frac{1}{\omega - H_D} S_d^\mp c_{k\pm}^\dagger c_{q\mp} = -n_j \frac{1}{4} J^2 \left(\frac{1}{2} \pm S_d^z \right) \sum_{kk'} c_{k\pm}^\dagger c_{k\pm} \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (\text{A.3.1})$$

The denominator is determined using $E = \frac{D}{2} + \epsilon_d - \frac{J}{4}$ and $\omega' = \omega + \epsilon_d$. In the hole sector, we similarly have

$$\sum_q \sum_{kk'} \frac{1}{4} J^2 S_d^\mp c_{k\pm}^\dagger c_{q\mp} \frac{1}{\omega - H_D} S_d^\pm c_{q\mp}^\dagger c_{k'\pm} = n_j \frac{1}{4} J^2 \left(\frac{1}{2} \mp S_d^z \right) \sum_{kk'} c_{k\pm}^\dagger c_{k\pm} \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (\text{A.3.2})$$

Adding all four expressions and dropping the constant part, we get

$$-n_j \frac{1}{2} J^2 S_d^z \sum_{kk'} \left(c_{k\uparrow}^\dagger c_{k'\uparrow} - c_{k\downarrow}^\dagger c_{k'\downarrow} \right) \frac{1}{\omega - \frac{D}{2} + \frac{J}{4}} . \quad (\text{A.3.3})$$

We can now directly read off the RG equation for J :

$$\Delta J = -\frac{n_j J^2}{\omega - \frac{D}{2} + \frac{J}{4}} \quad (\text{A.3.4})$$

Since the spin and charge degrees of freedom are treated on an equal footing in the model, we obtain the RG equation for K by simply changing $J \rightarrow K$:

$$\Delta K = -\frac{n_j K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \quad (\text{A.3.5})$$

Appendix B

Derivation of RG equations: U_b -included terms

We first Fourier transform the U_b -term to k -space. In k -space, the diagonal contribution (to H_D) coming from this term is the single-particle self-energy $-U_b \left(\hat{n}_{q\beta} \right)^2$ which can be made particle-hole symmetric in the form:

$$-U_b \left(\tau_{q\beta} \right)^2 \quad (\text{B.0.1})$$

where q is the k -state being decoupled and $\tau \equiv \hat{n} - 1/2$. In the initial state $|\Psi\rangle_i$, we have $\langle \hat{n}_{q\beta} \rangle = 1/2 \implies \tau_{q\beta} = 0$, so the contribution of U_b to that state is 0. For both hole excitations $c_{q\beta} |\Psi\rangle_i$ as well as particle excitations $c_{q\beta}^\dagger |\Psi\rangle_i$, the intermediate state energy lowers to $-U_b/4$.

The off-diagonal part is

$$-\frac{U_b}{2} \sum_{kk'\sigma} c_{k\sigma}^\dagger c_{k'\sigma} + U_b \sum_{k_1, k_2, k'_1, k'_2} c_{k_1\uparrow}^\dagger c_{k_2\uparrow} c_{k'_1\downarrow}^\dagger c_{k'_2\downarrow} \quad (\text{B.0.2})$$

We ignore the potential scattering arising from the first term.

B.1 Renormalisation of U_b

U_b can renormalise only via itself. The relevant renormalisation term in the particle sector is

$$U_b^2 \sum_{q\beta} \sum_{k_1, k_2, k_3, k'_1, k'_2, k'_3} c_{q\beta}^\dagger c_{k_1\beta} c_{k_3\beta}^\dagger c_{k'_1\beta} \frac{1}{\omega - H_D} c_{k'_2\beta}^\dagger c_{k'_3\beta} c_{k_2\beta}^\dagger c_{q\beta} \quad (\text{B.1.1})$$

In order to renormalise U_b , we need to contract one more pair of momenta. There are two choices. The first is by setting $k_3 = k'_3 = q$. The two internal states, then, are $q\beta$ and $q\bar{\beta}$. As discussed above, the intermediate state energy is $-U_b/4$. We therefore have

$$\frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k'_1, k'_2} c_{k_1\beta} c_{k'_1\bar{\beta}} c_{k'_2\bar{\beta}}^\dagger c_{k_2\beta}^\dagger = \frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k'_1, k'_2} c_{k'_2\bar{\beta}}^\dagger c_{k'_1\bar{\beta}} c_{k_2\beta}^\dagger c_{k_1\beta} \quad (\text{B.1.2})$$

Another way to contract the momenta is by setting $k'_1 = k'_2 = q$, which gives a renormalisation of

$$\frac{U_b^2 n_j}{\omega - D/2 + U_b/4} \sum_{\beta} \sum_{k_1, k_2, k_3, k'_3} c_{k_1\beta} c_{k_3\beta}^\dagger c_{k_3'\bar{\beta}} c_{k_2\beta}^\dagger = -\frac{U_b^2 n_j}{\omega - D/2} \sum_{\beta} \sum_{k_1, k_2, k_3, k'_3} c_{k_3'\bar{\beta}}^\dagger c_{k_3'\bar{\beta}} c_{k_2\beta}^\dagger c_{k_1\beta} \quad (\text{B.1.3})$$

The two contributions cancel each other. The same cancellation happens in the hole sector as well.

B.2 Renormalisation of U

U_b does not have any new renormalisation term on account of U_b . U_b does however modify the existing RG equation for U , by shifting the denominator. The existing RG equation is

$$\Delta U = -4V^2 n_j \left(\frac{1}{\omega - \frac{D}{2} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} - \epsilon_d + \frac{J}{4}} \right) - n_j \left(\frac{J^2}{\omega - \frac{D}{2} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{K}{4}} \right). \quad (\text{B.2.1})$$

On accounting for the contribution of U_b to the denominator, we get

$$\Delta U = -4V^2 n_j \left(\frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \epsilon_d + \frac{K}{4}} - \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} - \epsilon_d + \frac{J}{4}} \right) - n_j \left(\frac{J^2}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} - \frac{K^2}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right). \quad (\text{B.2.2})$$

B.3 Renormalisation of V

The single-particle hybridisation V renormalises through terms of VU_b and U_bV kind. The first term gives

$$\begin{aligned} & \sum_{q\beta} \sum_k U_b V c_{q\beta}^\dagger c_{k\beta} \hat{n}_{q\bar{\beta}} \frac{1}{\omega - H_D} c_{d\beta}^\dagger c_{q\beta} \\ &= n_j U_b V \sum_{k\beta} c_{k\beta} \left[\frac{\hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega_1 - E_1} + \frac{1}{\omega'_1 - E_1} \right) + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega_0 - E_0} + \frac{1}{\omega'_0 - E_0} \right) \right] c_{d\beta}^\dagger \end{aligned} \quad (\text{B.3.1})$$

E_1 and E_0 are the intermediate state energies for $\hat{n}_{d\bar{\beta}} = 1$ and 0 respectively. $\omega_{1,0}$ are the quantum fluctuation scales for the corresponding initial states. $\omega'_{1,0}$ are the fluctuation scales for the corresponding final states. The intermediate energies are $E_1 = D/2 - U_b/4 - K/4$, $E_0 = D/2 - U_b/4 - U/2 - J/4$. The fluctuation scales are $\omega_1 = \omega - U/2 = \omega'_0$, $\omega'_1 = \omega = \omega_0$. Substituting these gives

$$\begin{aligned} & -n_j U_b V \sum_{k\beta} c_{d\beta}^\dagger c_{k\beta} \left[\frac{\hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right) \right. \\ & \quad \left. + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \end{aligned} \quad (\text{B.3.2})$$

The second term is of the form

$$\sum_{q\beta} \sum_k U_b V c_{q\beta}^\dagger c_{d\beta} \frac{1}{\omega - H_D} \hat{n}_{q\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \quad (\text{B.3.3})$$

and this is just the Hermitian conjugate of the previous term, so these two terms together lead to

$$\begin{aligned} & -n_j U_b V \sum_{k\beta} \left(c_{d\beta}^\dagger c_{k\beta} + \text{h.c.} \right) \left[\frac{\hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right) \right. \\ & \quad \left. + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \end{aligned} \quad (\text{B.3.4})$$

In the hole sector, we have

$$\begin{aligned} & \sum_{q\beta} \sum_k U_b V \hat{n}_{q\bar{\beta}} c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega - H_D} c_{q\beta}^\dagger c_{d\beta} \\ & - \sum_{q\beta} \sum_k U_b V \left(1 - \hat{n}_{q\bar{\beta}} \right) c_{k\beta}^\dagger c_{q\beta} \frac{1}{\omega - H_D} c_{q\beta}^\dagger c_{d\beta} \\ &= -n_j U_b V \sum_{k\beta} c_{k\beta}^\dagger \left[\frac{\hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega_1 - E_1} + \frac{1}{\omega'_1 - E_1} \right) + \frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega_0 - E_0} + \frac{1}{\omega'_0 - E_0} \right) \right] c_{d\beta} \end{aligned} \quad (\text{B.3.5})$$

$E_1 = D/2 - U_b/4 - U/2 - J/4$, $E_0 = D/2 - U_b/4 - K/4$. The fluctuation scales are $\omega_1 = \omega = \omega'_0$, $\omega'_1 = \omega - U/2 = \omega_0$. Substituting these gives

$$-n_j U_b V \sum_{k\beta} c_{d\beta}^\dagger c_{k\beta} \left[\frac{1 - \hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right) + \frac{\hat{n}_{d\bar{\beta}}}{2} \left(\frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \quad (\text{B.3.6})$$

The other term, obtained by exchanging V and U_b , gives the Hermitian conjugate, so the overall contribution from the hole sector is the same as the total contribution from the particle sector, but with $\hat{n}_{d\bar{\beta}} \rightarrow 1 - \hat{n}_{d\bar{\beta}}$. Combining both the sectors, we get

$$-n_j U_b V \sum_{k\beta} (c_{d\beta}^\dagger c_{k\beta} + \text{h.c.}) \frac{1}{2} \left[\left(\frac{1}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right) + \left(\frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{1}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \quad (\text{B.3.7})$$

Combining with the already existing RG equations, the complete RG equation for V becomes

$$\begin{aligned} \Delta V &= -\frac{3n_j V}{8} \left[\left(\frac{J}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} + \frac{J}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} \right) + K \left(\frac{K}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{K}{\omega - \frac{D}{2} + \frac{U_b}{4} - \frac{U}{2} + \frac{K}{4}} \right) \right] \\ &\quad - \frac{n_j U_b}{2} \left[\left(\frac{V}{\omega - \frac{D}{2} - \frac{U}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{V}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} \right) + \left(\frac{V}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} + \frac{V}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} \right) \right] \\ &= -\frac{n_j V}{8} \left[\left(\frac{3J + 4U_b}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{J}{4}} + \frac{3J + 4U_b}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{U}{2} + \frac{J}{4}} \right) + \left(\frac{3K + 4U_b}{\omega - \frac{D}{2} + \frac{U_b}{4} + \frac{K}{4}} + \frac{3K + 4U_b}{\omega - \frac{D}{2} + \frac{U_b}{4} - \frac{U}{2} + \frac{K}{4}} \right) \right] \end{aligned} \quad (\text{B.3.8})$$

B.4 Renormalisation of J and K

We will track the entire renormalisation purely from that of J^+ , by virtue of the $SU(2)$ symmetry. J^+ renormalises through the JU_b terms. One of the terms is

$$\frac{1}{2} JU_b \sum_q \sum_{k,k'} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} \frac{1}{\omega - H_D} \hat{n}_{q\uparrow} c_{k'\downarrow}^\dagger c_{q\downarrow} = -\frac{1}{2} \frac{JU_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}} \sum_{k,k'} S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (\text{B.4.1})$$

The factor of half in front is the same half factor that appears in front of the $S_1^+ S_2^-, S_1^- S_2^+$ terms when we rewrite $\vec{S}_1 \cdot \vec{S}_2$ in terms of S^z, S^\pm . Another term is obtained by switching J and U_b :

$$\frac{1}{2} JU_b \sum_q \sum_{k,k'} \hat{n}_{q\downarrow} c_{q\uparrow}^\dagger c_{k\uparrow} \frac{1}{\omega - H_D} S_d^+ c_{k'\downarrow}^\dagger c_{q\uparrow} = -\frac{1}{2} \frac{JU_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}} \sum_{k,k'} S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (\text{B.4.2})$$

The corresponding terms in the hole sector are

$$\frac{1}{2} JU_b \sum_q \sum_{k,k'} S_d^+ c_{k'\downarrow}^\dagger c_{q\uparrow} \frac{1}{\omega - H_D} \hat{n}_{q\downarrow} c_{q\uparrow}^\dagger c_{k\uparrow} = -\frac{1}{2} \frac{JU_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}} \sum_{k,k'} S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (\text{B.4.3})$$

$$\frac{1}{2} JU_b \sum_q \sum_{k,k'} \hat{n}_{q\uparrow} c_{k'\downarrow}^\dagger c_{q\downarrow} \frac{1}{\omega - H_D} S_d^+ c_{q\downarrow}^\dagger c_{k\uparrow} = -\frac{1}{2} \frac{JU_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}} \sum_{k,k'} S_d^+ c_{k'\downarrow}^\dagger c_{k\uparrow} \quad (\text{B.4.4})$$

Adding all these terms and combining with the existing RG equation, we get the updated RG equation for J :

$$\Delta J = -J n_j \frac{4U_b + J}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{J}{4}} \quad (\text{B.4.5})$$

We will follow the same strategy with K - we will calculate the renormalisation in K^+ . The first term is

$$\frac{1}{2} K U_b \sum_q \sum_{k,k'} \hat{n}_{q\downarrow} c_{q\uparrow}^\dagger c_{k'\uparrow} \frac{1}{\omega - H_D} C_d^+ c_{k\downarrow} c_{q\uparrow} = -\frac{1}{2} \frac{K U_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{K}{4}} \sum_{k,k'} C_d^+ c_{k\downarrow} c_{k'\uparrow} \quad (\text{B.4.6})$$

The second term in the same sector is obtained by flipping the spins of k and q :

$$\frac{1}{2} K U_b \sum_q \sum_{k,k'} \hat{n}_{q\uparrow} c_{q\downarrow}^\dagger c_{k'\downarrow} \frac{1}{\omega - H_D} C_d^+ c_{q\downarrow} c_{k\uparrow} = -\frac{1}{2} \frac{K U_b n_j}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{K}{4}} \sum_{k,k'} C_d^+ c_{k\downarrow} c_{k'\uparrow} \quad (\text{B.4.7})$$

The terms in the hole sector give identical contributions. The RG equation for K is

$$\Delta K = -K n_j \frac{4U_b + K}{\omega - \frac{D}{2} + \frac{U_b}{2} + \frac{K}{4}} \quad (\text{B.4.8})$$

Appendix C

Analytic results for the Hubbard dimer

Spectrum of the Hubbard dimer

Here we document the spectrum of the Hubbard dimer Hamiltonian in eqs. 5.1.2.

eigenstate	symbol	eigenvalue
$ 0, 0\rangle$	$ 0\rangle$	$\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (\sigma, 0\rangle \pm 0, \sigma\rangle)$	$ 0\sigma_{\pm}\rangle$	$\mp t^H$
$ \sigma, \sigma\rangle$	$ \sigma\sigma\rangle$	$-\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle + \downarrow, \uparrow\rangle)$	$ ST\rangle$	$-\frac{U^H}{2}$
$\frac{1}{\sqrt{2}} (2, 0\rangle - 0, 2\rangle)$	$ CS\rangle$	$\frac{U^H}{2}$
$a_1(U^H, t^H) \frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle) + a_2(U^H, t^H) \frac{1}{\sqrt{2}} (2, 0\rangle + 0, 2\rangle)$	$ -\rangle$	$-\frac{1}{2}\Delta(U^H, t^H)$
$-a_2(U^H, t^H) \frac{1}{\sqrt{2}} (\uparrow, \downarrow\rangle - \downarrow, \uparrow\rangle) + a_1(U^H, t^H) \frac{1}{\sqrt{2}} (2, 0\rangle + 0, 2\rangle)$	$ +\rangle$	$\frac{1}{2}\Delta(U^H, t^H)$
$\frac{1}{\sqrt{2}} (\sigma, 2\rangle \pm 2, \sigma\rangle)$	$ 2\sigma_{\pm}\rangle$	$\pm t^H$
$ 2, 2\rangle$	$ 4\rangle$	$\frac{U^H}{2}$

Table C.1: Spectrum of Hubbard dimer at half-filling

Appendix: Local Greens function for the Hubbard dimer

From the spectral representation, we have the following expression for the local Greens function for the Hubbard dimer at site 0:

$$G_{D,00}^{\sigma}(\omega) = \frac{1}{Z} \sum_{m,n} \|\langle m | c_{i\sigma} | n \rangle\|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \frac{1}{\omega + E_m - E_n} \quad (\text{C.0.1})$$

m, n sum over the exact eigenstates. E_m, E_n are the corresponding energies. We are interested in the $T \rightarrow 0$ Greens function. In that limit, all exponentials except that for the ground state E_{gs} will die out. The exponential inside the summation will then cancel the exponential in the partition function.

$$\begin{aligned} G_{D,00}^{\sigma}(\omega, T \rightarrow 0) &= \sum_n \left[\|\langle GS | c_{i\sigma} | n \rangle\|^2 \frac{1}{\omega + E_{GS} - E_n} + \|\langle n | c_{i\sigma} | GS \rangle\|^2 \frac{1}{\omega + E_n - E_{GS}} \right] \\ &= \sum_n \left[\|\langle n | c_{i\sigma}^{\dagger} | GS \rangle\|^2 \frac{1}{\omega + E_{GS} - E_n} + \|\langle n | c_{i\sigma} | GS \rangle\|^2 \frac{1}{\omega + E_n - E_{GS}} \right] \end{aligned} \quad (\text{C.0.2})$$

The ground state $|GS\rangle$ is just the state $|-\rangle$ in the table C.1. We will choose to look at $\sigma = \uparrow$. Then,

$$\begin{aligned} c_{1\uparrow} |-\rangle &= \frac{a_1}{\sqrt{2}} |0, \downarrow\rangle + \frac{a_2}{\sqrt{2}} |\downarrow, 0\rangle \\ c_{1\uparrow}^\dagger |-\rangle &= -\frac{a_1}{\sqrt{2}} |2, \uparrow\rangle + \frac{a_2}{\sqrt{2}} |\uparrow, 2\rangle \end{aligned} \quad (\text{C.0.3})$$

The set of states $|n\rangle$ that give non-zero inner product $|GS\rangle$ are therefore

$$\begin{aligned} \{|n\rangle\} &= |0 \downarrow_\pm\rangle \\ ||\langle n| c_{\uparrow\sigma} |GS\rangle||^2 &= \frac{1}{4} (a_2 \pm a_1)^2 = \frac{1}{4} (1 \pm 2a_1 a_2) \\ \{E_n\} &= \mp t \end{aligned} \quad (\text{C.0.4})$$

for the second inner product, and

$$\begin{aligned} \{|n\rangle\} &= |2 \uparrow_\pm\rangle \\ ||\langle n| c_{\uparrow\sigma}^\dagger |GS\rangle||^2 &= \frac{1}{4} (a_2 \mp a_1)^2 = \frac{1}{4} (1 \mp 2a_1 a_2) \\ \{E_n\} &= \pm t \end{aligned} \quad (\text{C.0.5})$$

for the first. The Greens function is therefore

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) = \left(\frac{1}{2} + \frac{2t}{\Delta}\right) \frac{\omega}{\omega^2 - \left(t - \frac{\Delta}{2}\right)^2} + \left(\frac{1}{2} - \frac{2t}{\Delta}\right) \frac{\omega}{\omega^2 - \left(t + \frac{\Delta}{2}\right)^2} = G_{D,00}^\downarrow(\omega, T \rightarrow 0). \quad (\text{C.0.6})$$

In the atomic limit ($t = 0$), the Greens function simplifies to

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) \Big|_{\text{atomic}} = \frac{\omega}{\omega^2 - \frac{1}{4}U^2} \quad (\text{C.0.7})$$

In the atomic limit, the singly-occupied state has zero energy:

$$E_1(t = 0) = \langle 1, 0 | \left(U\tau_{0\uparrow}\tau_{0\downarrow} + U\tau_{1\uparrow}\tau_{1\downarrow} \right) | 1, 0 \rangle = 0 \quad (\text{C.0.8})$$

We can write the atomic limit Greens function in terms of this energy and the self energy:

$$G_{D,00}^\uparrow(\omega, T \rightarrow 0) \Big|_{\text{atomic}} = \frac{1}{\omega - E_1(t = 0) - \Sigma(t = 0)} = \frac{1}{\omega - 0 - \frac{U^2}{4\omega}} \quad (\text{C.0.9})$$

The self energy in the atomic limit can be read off as

$$\Sigma(t = 0) = \frac{U^2}{4\omega} \quad (\text{C.0.10})$$

The site local spectral function can also be calculated from the local Greens function:

$$\begin{aligned} A(0 \uparrow, \omega) &= -\frac{1}{\pi} \text{Im } G_{D,00}^\uparrow(\omega) \\ &= \left(\frac{1}{4} - \frac{t}{\Delta}\right) \left[\delta\left(\omega - \frac{1}{2}\Delta - t\right) + \delta\left(\omega + \frac{1}{2}\Delta + t\right) \right] \\ &\quad + \left(\frac{1}{4} + \frac{t}{\Delta}\right) \left[\delta\left(\omega - \frac{1}{2}\Delta + t\right) + \delta\left(\omega + \frac{1}{2}\Delta - t\right) \right] \\ &= A(0 \downarrow, \omega). \end{aligned} \quad (\text{C.0.11})$$

Finally, the inter-site Greens function for the Hubbard dimer is given by

$$G_{D,01}^\uparrow(\omega, T \rightarrow 0) = \left(\frac{1}{2} + \frac{2t}{\Delta}\right) \frac{t - \frac{\Delta}{2}}{\omega^2 - \left(t - \frac{\Delta}{2}\right)^2} + \left(\frac{1}{2} - \frac{2t}{\Delta}\right) \frac{t + \frac{\Delta}{2}}{\omega^2 - \left(t + \frac{\Delta}{2}\right)^2} = G_{D,01}^\downarrow(\omega, T \rightarrow 0). \quad (\text{C.0.12})$$

Using the diagonal and off-diagonal real space Greens functions, we can now compute the momentum-space Greens functions. The two momentum states are $ka = 0, \pi$. By Fourier transforming, these two Greens functions can be written as

$$\begin{aligned} G(k=0, \sigma) &= \sum_r e^{ikr} G(r, \sigma) = G(r=0, \sigma) + G(r=a, \sigma) = \frac{1/2 + 2t/\Delta}{\omega - t + \Delta/2} + \frac{1/2 - 2t/\Delta}{\omega - t - \Delta/2} \\ G(k=\pi, \sigma) &= \sum_r e^{ikr} G(r, \sigma) = G(r=0, \sigma) - G(r=a, \sigma) = \frac{1/2 + 2t/\Delta}{\omega + t - \Delta/2} + \frac{1/2 - 2t/\Delta}{\omega + t + \Delta/2} \end{aligned} \quad (\text{C.0.13})$$

Contributions of various excitations to the site local spectral function

The site local spectral function is

$$A(0 \uparrow, \omega) = \left(\frac{1}{4} - \frac{t}{\Delta} \right) \left[\delta\left(\omega - \frac{\Delta}{2} - t\right) + \delta\left(\omega + \frac{\Delta}{2} + t\right) \right] + \left(\frac{1}{4} + \frac{t}{\Delta} \right) \left[\delta\left(\omega - \frac{\Delta}{2} + t\right) + \delta\left(\omega + \frac{\Delta}{2} - t\right) \right]$$

If the eigenstates of the $N = 1, S^z = -\frac{1}{2}$ sector are $|1\pm\downarrow\rangle$ and those of $N = 3, S^z = \frac{1}{2}$ sector are $|3\pm\uparrow\rangle$, this spectral function originates from the expression:

$$\begin{aligned} A(0 \uparrow, \omega) &= \langle 1 \downarrow_- | c_{0\uparrow} | \text{GS} \rangle \delta\left(\omega + \frac{\Delta}{2} + t\right) + \langle 2 \uparrow_+ | c_{0\uparrow}^\dagger | \text{GS} \rangle \delta\left(\omega - \frac{\Delta}{2} - t\right) \\ &\quad + \langle 1 \downarrow_+ | c_{0\uparrow} | \text{GS} \rangle \delta\left(\omega + \frac{\Delta}{2} - t\right) + \langle 2 \uparrow_- | c_{0\uparrow}^\dagger | \text{GS} \rangle \delta\left(\omega - \frac{\Delta}{2} + t\right) \end{aligned} \quad (\text{C.0.14})$$

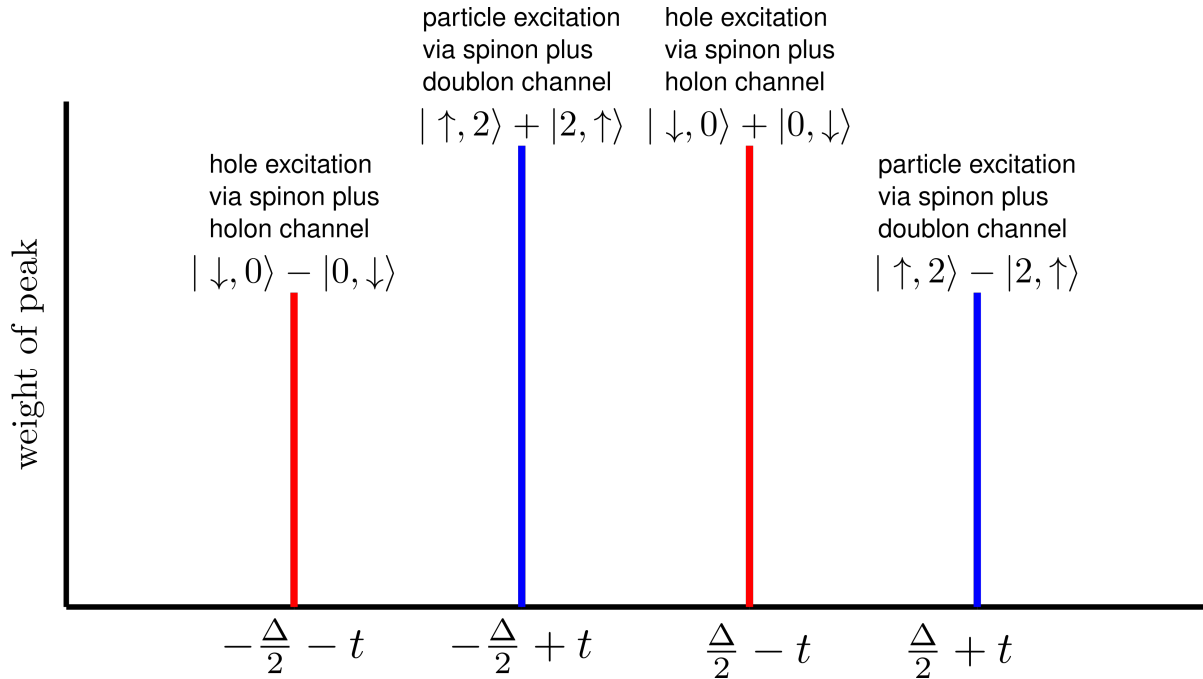


Figure C.1: Position, weight and nature of each of the peaks in the Hubbard dimer site local spectral function

Appendix D

Simple results for the Greens functions

Relation between single-particle Greens function and the Greens function operator ($T = 0$)

The single-particle Greens function is defined as the solution of the equation:

$$(i\partial_t - H(\vec{r})) G(\vec{r}, \vec{r}', t) = \delta(\vec{r} - \vec{r}') \quad (\text{D.0.1})$$

and is given by the expression

$$G(\vec{r}, \vec{r}', t) = -i\theta(t) \left\langle \left\{ c(\vec{r}, t) c^\dagger(\vec{r}', 0) \right\} \right\rangle \quad (\text{D.0.2})$$

This solution can be written in the Lehmann representation and at $T = 0$ as

$$G(\vec{r}\sigma, \vec{r}'\sigma, \omega) = \sum_n \left[\frac{\langle GS | c(\vec{r}, \sigma) | n \rangle \langle n | c^\dagger(\vec{r}', \sigma) | GS \rangle}{\omega + E_{GS} - E_n} + \frac{\langle GS | c^\dagger(\vec{r}', \sigma) | n \rangle \langle n | c(\vec{r}, \sigma) | GS \rangle}{\omega + E_n - E_{GS}} \right] \quad (\text{D.0.3})$$

The sum is over the exact eigenstates of the Hamiltonian. In what follows, we will represent $\vec{r}, \sigma \equiv \nu$ and $\vec{r}', \sigma \equiv \nu'$.

$$\begin{aligned} G(\nu, \nu', \omega) &= \sum_n \left[\frac{\langle GS | c(\nu) | n \rangle \langle n | c^\dagger(\nu') | GS \rangle}{\omega + E_{GS} - E_n} + \frac{\langle GS | c^\dagger(\nu') | n \rangle \langle n | c(\nu) | GS \rangle}{\omega + E_n - E_{GS}} \right] \\ &= \langle GS | c(\nu) \frac{1}{\omega + E_{GS} - H} c^\dagger(\nu') | GS \rangle + \langle GS | c^\dagger(\nu') \frac{1}{\omega + H - E_{GS}} c(\nu) | GS \rangle \end{aligned} \quad (\text{D.0.4})$$

If we now define a Greens function operator

$$\mathcal{G}(\omega, H) = \frac{1}{\omega - (H - E_{GS})} \quad (\text{D.0.5})$$

we can write the single-particle Greens function as a sum of the matrix elements of this operator:

$$G(\nu, \nu', \omega) = \langle \nu | \mathcal{G}(\omega, H) | \nu' \rangle - \langle \bar{\nu}' | \mathcal{G}(-\omega, H) | \bar{\nu} \rangle = \mathcal{G}(\omega, H)_{\nu, \nu'} - \mathcal{G}(-\omega, H)_{\bar{\nu}', \bar{\nu}} \quad (\text{D.0.6})$$

where we have defined the states $|\nu\rangle \equiv c^\dagger(\nu) | GS \rangle$ and $|\bar{\nu}\rangle \equiv c(\nu) | GS \rangle$. The two matrix elements can also be represented in their individual spectral representations:

$$\begin{aligned} \mathcal{G}(\omega, H)_{\nu, \nu'} &= \sum_n \frac{\langle GS | c(\nu) | n \rangle \langle n | c^\dagger(\nu') | GS \rangle}{\omega + E_{GS} - E_n} \\ \mathcal{G}(\omega, H)_{\bar{\nu}', \bar{\nu}} &= \sum_n \frac{\langle GS | c^\dagger(\nu') | n \rangle \langle n | c(\nu) | GS \rangle}{\omega + E_{GS} - E_n} \end{aligned} \quad (\text{D.0.7})$$

Writing single-particle excitations of ground state in terms of $N = 3, S^z = \frac{1}{2}$ eigenstates

The excited state $c_{0\uparrow}^\dagger |\text{GS}\rangle$ can actually be written in terms of the $N = 3, S^z = +\frac{1}{2}$ eigenstates $|3\pm \uparrow\rangle$ defined in table C.1.

$$|3\pm \uparrow\rangle = \frac{1}{\sqrt{2}} (|\uparrow, 2\rangle \pm |2, \uparrow\rangle), \quad H^D |3\pm \uparrow\rangle = \pm t |3\pm \uparrow\rangle \quad (\text{D.0.8})$$

In terms of these eigenstates, we can write

$$\begin{aligned} c_{0\uparrow}^\dagger |\text{GS}\rangle &= c_{0\uparrow}^\dagger [a_1 |SS\rangle + a_2 |CT\rangle] \\ &= a_2 \frac{1}{\sqrt{2}} |\uparrow, 2\rangle - a_1 \frac{1}{\sqrt{2}} |2, \uparrow\rangle \\ &= (x + y) \frac{1}{\sqrt{2}} |\uparrow, 2\rangle + (x - y) \frac{1}{\sqrt{2}} |2, \uparrow\rangle \\ &= x |3+ \uparrow\rangle + y |3- \uparrow\rangle \end{aligned} \quad (\text{D.0.9})$$

where $x + y \equiv a_2$ and $x - y \equiv -a_1$. Similarly, for the other site excitation, we can write

$$\begin{aligned} c_{1\uparrow}^\dagger |\text{GS}\rangle &= c_{1\uparrow}^\dagger [a_1 |SS\rangle + a_2 |CT\rangle] \\ &= a_2 \frac{1}{\sqrt{2}} |2, \uparrow\rangle - a_1 \frac{1}{\sqrt{2}} |\uparrow, 2\rangle \\ &= (x + y) \frac{1}{\sqrt{2}} |2, \uparrow\rangle + (x - y) \frac{1}{\sqrt{2}} |\uparrow, 2\rangle \\ &= x |3+ \uparrow\rangle - y |3- \uparrow\rangle \end{aligned} \quad (\text{D.0.10})$$

Solving for x and y gives

$$x = \frac{a_2 - a_1}{2}, \quad y = \frac{a_2 + a_1}{2} \quad (\text{D.0.11})$$

Similarly, we can also write the single-hole excitation $c_{0\uparrow} |\text{GS}\rangle$ in terms of the $N = 1, S^z = -\frac{1}{2}$ eigenstates, $|1\pm \downarrow\rangle$:

$$|1\pm \downarrow\rangle = \frac{1}{\sqrt{2}} (|\downarrow, 0\rangle \pm |0, \downarrow\rangle), \quad H^D |1\pm \downarrow\rangle = \mp t |1\pm \downarrow\rangle \quad (\text{D.0.12})$$

$$\begin{aligned} c_{0\uparrow} |\text{GS}\rangle &= a_1 \frac{1}{\sqrt{2}} |0, \downarrow\rangle + a_2 \frac{1}{\sqrt{2}} |\downarrow, 0\rangle = y |1+ \downarrow\rangle + x |1- \downarrow\rangle \\ c_{1\uparrow} |\text{GS}\rangle &= a_1 \frac{1}{\sqrt{2}} |\downarrow, 0\rangle + a_2 \frac{1}{\sqrt{2}} |0, \downarrow\rangle = y |1+ \downarrow\rangle - x |1- \downarrow\rangle \end{aligned} \quad (\text{D.0.13})$$

Matrix elements of G^{-1} between single-particle momentum excitations, for the Hubbard dimer

$$G^{-1} \equiv \omega + E_{\text{GS}} - H_D \quad (\text{D.0.14})$$

The particle excitation momentum space kets are $|k_0\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$, $|k_\pi\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$. Therefore,

$$\begin{aligned} \left(G^{-1}\right)_{k_0 k_0} &= \frac{1}{2} (\langle 0| + \langle 1|) (\omega + E_{\text{GS}} - H_D) (|0\rangle + |1\rangle) \\ &= \frac{1}{2} (2x \langle +|) (\omega + E_{\text{GS}} - H_D) (2x |+\rangle) \\ &= 2x^2 (\omega + E_{\text{GS}} - t) \end{aligned} \quad (\text{D.0.15})$$

At the final step, we used $\langle +, +\rangle = 1$ and $\langle +|H_D|+\rangle = t$.

Appendix E

Zero temperature Greens function in frequency domain

The impurity retarded Green's function (assuming the Hamiltonian to be time-independent, which it is) is defined as

$$G_{dd}^\sigma(t) = -i\theta(t) \left\langle \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} \right\rangle \quad (\text{E.0.1})$$

where the average $\langle \rangle$ is over a canonical ensemble at temperature T , and $\mathcal{O}_\sigma = c_{d\sigma} + S_d^- c_{0\bar{\sigma}} + S_d^z c_{0\sigma}$ is the excitation whose spectral function we are interested in. The excitations defined in \mathcal{O} incorporates both single-particle excitations brought about by the hybridisation as well as two-particle spin excitations brought about by the spin-exchange term. What follows is a standard calculation where we write the Green's function in the Lehmann representation. The ensemble average for an arbitrary operator \hat{M} can be written in terms of the exact eigenstates of the fixed point Hamiltonian:

$$H^* |n\rangle = E_n^* |n\rangle, \quad \langle \hat{M} \rangle \equiv \frac{1}{Z} \sum_n \langle n | \hat{M} | n \rangle e^{-\beta E_n^*} \quad (\text{E.0.2})$$

where $Z = \sum_n e^{-\beta E_n^*}$ is the fixed point partition function and $\{|n\rangle\}$ is the set of eigenfunctions of the fixed point Hamiltonian. We can therefore write

$$\begin{aligned} & \left\langle \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} \right\rangle \\ &= \frac{1}{Z} \sum_m e^{-\beta E_m} \langle m | \left\{ \mathcal{O}_\sigma(t), \mathcal{O}_\sigma^\dagger \right\} | m \rangle \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \langle m | \left(\mathcal{O}_\sigma(t) | n \rangle \langle n | \mathcal{O}_\sigma^\dagger + \mathcal{O}_\sigma^\dagger | n \rangle \langle n | \mathcal{O}_\sigma(t) \right) | m \rangle \quad \left[\sum_n |n\rangle \langle n| = 1 \right] \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \langle m | \left(e^{iH^*t} \mathcal{O}_\sigma e^{-iH^*t} | n \rangle \langle n | \mathcal{O}_\sigma^\dagger + \mathcal{O}_\sigma^\dagger | n \rangle \langle n | e^{iH^*t} \mathcal{O}_\sigma e^{-iH^*t} \right) | m \rangle \\ &= \frac{1}{Z} \sum_{m,n} e^{-\beta E_m} \left(e^{i(E_m - E_n)t} \langle m | \mathcal{O}_\sigma | n \rangle \langle n | \mathcal{O}_\sigma^\dagger | m \rangle + e^{i(E_n - E_m)t} \langle m | \mathcal{O}_\sigma^\dagger | n \rangle \langle n | \mathcal{O}_\sigma | m \rangle \right) \\ &= \frac{1}{Z} \sum_{m,n} e^{i(E_m - E_n)t} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \end{aligned} \quad (\text{E.0.3})$$

The time-domain impurity Green's function can thus be written as (this is the so-called Lehmann representation)

$$G_{dd}^\sigma = -i\theta(t) \frac{1}{Z} \sum_{m,n} e^{i(E_m - E_n)t} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \quad (\text{E.0.4})$$

We are interested in the frequency domain form.

$$\begin{aligned} G_{dd}^\sigma(\omega) &= \int_{-\infty}^{\infty} dt e^{i\omega t} G_{dd}^\sigma(t) \\ &= \frac{1}{Z} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t} \end{aligned} \quad (\text{E.0.5})$$

To evaluate the time-integral, we will use the integral representation of the Heaviside function:

$$\theta(t) = \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} \frac{1}{x - i\eta} e^{ixt} dx \quad (\text{E.0.6})$$

With this definition, the integral in $G_{dd}^\sigma(\omega)$ becomes

$$\begin{aligned} (-i) \int_{-\infty}^{\infty} dt \theta(t) e^{i(\omega + E_m - E_n)t} &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} \int_{-\infty}^{\infty} dt e^{i(\omega + E_m - E_n + x)t} \\ &= (-i) \frac{1}{2\pi i} \lim_{\eta \rightarrow 0^+} \int_{-\infty}^{\infty} dx \frac{1}{x - i\eta} 2\pi \delta(\omega + E_m - E_n + x) \\ &= (-i) \frac{1}{i} \lim_{\eta \rightarrow 0^+} \frac{-1}{\omega + E_m - E_n - i\eta} \\ &= \frac{1}{\omega + E_m - E_n} \end{aligned} \quad (\text{E.0.7})$$

The frequency-domain Green's function is thus

$$G_{dd}^\sigma(\omega) = \frac{1}{Z} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left(e^{-\beta E_m} + e^{-\beta E_n} \right) \frac{1}{\omega + E_m - E_n} \quad (\text{E.0.8})$$

The zero temperature Green's function is obtained by taking the limit of $\beta \rightarrow \infty$. In both the partition function as well as inside the summation, the only term that will survive is the exponential of the ground state energy E_0 .

$$Z \equiv \sum_m e^{-\beta E_m} \implies \lim_{\beta \rightarrow \infty} Z = d_0 e^{-\beta E_0}, \quad E_0 \equiv \min \{E_n\}$$

where d_0 is the degeneracy of the ground state. The Greens function then simplifies to

$$\begin{aligned} G_{dd}^\sigma(\omega, \beta \rightarrow \infty) &= \frac{1}{d_0 e^{-\beta E_0}} \sum_{m,n} \|\langle m | \mathcal{O}_\sigma | n \rangle\|^2 \left[e^{-\beta E_m} \delta_{E_m, E_0} + e^{-\beta E_n} \delta_{E_n, E_0} \right] \frac{1}{\omega + E_m - E_n} \\ &= \frac{1}{d_0} \sum_{n,0} \left[\|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \frac{1}{\omega + E_0 - E_n} + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \frac{1}{\omega - E_0 + E_n} \right] \end{aligned} \quad (\text{E.0.9})$$

The label 0 sums over all states $|0\rangle$ with energy E_0 . The spectral function is the imaginary part of this Green's function. To extract the imaginary part, we insert an infinitesimal imaginary part in the denominator:

$$G_{dd}^\sigma(\omega, \eta) = \frac{1}{d_0} \lim_{\eta \rightarrow 0^-} \sum_{n,0} \left[\|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \frac{1}{\omega + E_0 - E_n + i\eta} + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \frac{1}{\omega - E_0 + E_n + i\eta} \right] \quad (\text{E.0.10})$$

The spectral function at zero temperature can then be written as

$$\begin{aligned} \mathcal{A}(\omega) &= -\frac{1}{\pi} \text{Im} [G_{dd}^\sigma(\omega)] \\ &= \frac{1}{d_0} \frac{1}{\pi} \text{Im} \left[\lim_{\eta \rightarrow 0^-} \sum_{n,0} \left(\frac{-i\eta \|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2}{(\omega + E_0 - E_n)^2 + \eta^2} + \frac{-i\eta \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2}{(\omega - E_0 + E_n)^2 + \eta^2} \right) \right] \\ &= \frac{1}{d_0} \frac{1}{\pi} \sum_{n,0} \left[\|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \pi \delta(\omega + E_0 - E_n) + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \pi \delta(\omega - E_0 + E_n) \right] \\ &= \frac{1}{d_0} \sum_{n,0} \left[\|\langle 0 | \mathcal{O}_\sigma | n \rangle\|^2 \delta(\omega + E_0 - E_n) + \|\langle n | \mathcal{O}_\sigma | 0 \rangle\|^2 \delta(\omega - E_0 + E_n) \right] \end{aligned} \quad (\text{E.0.11})$$

Appendix F

Topological interpretation of the Wilson ratio

From the Friedel sum rule[12], we can relate the phase shift $\delta(0)$ due to scattering (at the Fermi surface) off a local impurity to the number of electrons bound in the potential well produced by that impurity:

$$\tilde{N} = \frac{1}{2\pi i} \text{Tr} \ln S(0) = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln S(0) \quad (\text{F.0.1})$$

From the optical theorem, we can write

$$S = 1 + TG_0 = \frac{G}{G_0} \quad [G = G_0 + G_0TG_0] \quad (\text{F.0.2})$$

This allows us to write [13]

$$\tilde{N} = \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \text{Tr} \ln \frac{G}{G_0} \quad (\text{F.0.3})$$

Since $\text{Tr} \ln \hat{O} = \sum_{\lambda} \ln O_{\lambda} = \ln \prod_{\lambda} O_{\lambda} = \ln \text{Det} \hat{O}$, we get

$$\begin{aligned} \tilde{N} &= \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \text{Det} \frac{G}{G_0} \\ &= - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln \frac{\text{Det} G_0}{\text{Det} G} \\ &\equiv - \int_{\Gamma} dz \partial_z \frac{1}{2\pi i} \ln D \\ &= - \int_{\Gamma(D)} \frac{dD}{D} \end{aligned} \quad (\text{F.0.4})$$

From the work of Seki and Yunoki [14], we know that this quantity is essentially the winding number of the curve $\Gamma(D)$ in the complex plane spanned by the real and imaginary parts of D , and is equal to the change in Luttinger's volume V_L at $T = 0$.

$$\tilde{N} = - \int_{\Gamma(D)} \frac{dD}{D} = -\Delta V_L \quad (\text{F.0.5})$$

The incoming electrons can have $\sigma = \uparrow, \downarrow$. Since the impurity singlet ground state is rotationally invariant, we have $\delta_{\uparrow} = \delta_{\downarrow} = \delta(0)$.

$$\begin{aligned} \tilde{N} &= \frac{1}{\pi} \sum_{\sigma} \delta_{\sigma}(0) \\ \implies \delta(0) &= \frac{\pi}{2} \tilde{N} = -\frac{\pi}{2} \Delta V_L \end{aligned} \quad (\text{F.0.6})$$

$$\begin{aligned} R &= 1 + \sin^2 \left(\frac{\pi}{2} \tilde{N} \right) \\ &= 1 + \sin^2 \left(\frac{\pi}{2} \Delta V_L \right) \end{aligned} \quad (\text{F.0.7})$$

We note that this connection between R and ΔV_L has not been obtained in the existing literature thus far. In the unitary limit, $\delta(0) = \frac{\pi}{2}$, giving $\Delta V_L = -1 = -\tilde{N}$ [11] (i.e., one electronic state from the impurity has been absorbed into the Luttinger volume of the conduction bath), such that $R = 2$ in this limit. In this way, we see that a change in the topological quantum number \tilde{N} causes the well known renormalisation of the Wilson ratio R from its non-interacting value (1) to the value (2) obtained for the local Fermi liquid [9].

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