Development and application of renormalised perturbation theory to models with strongly correlated electrons

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Declaration

I herewith certify that to the best of my knowledge all material in this dissertation which is not my own work has been properly acknowledged.

Vasileios Pandis

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Abstract

The subject of this thesis is the application of the Renormalised Perturbation Theory (RPT) to models of magnetic impurities embedded in a non-magnetic host metal. The theoretical description of such models is particularly challenging, for they present strong correlations that render the usual perturbation theory around the non-interacting limit inapplicable. The RPT addresses this difficulty by incorporating the concept of a quasi-particle into a perturbative framework, and organising the expansion in terms of the quasi-particle parameters of the model rather than the bare parameters; it can thus be carried out regardless of the strength of the interactions.

In the present work we present an introduction to the theory and discuss in detail the calculation of the renormalised self-energy expansions for the Anderson impurity model. To cope with the complexity of high-order calculations we develop and implement a computer algorithm to automatically compute the diagrammatic expansion in the renormalised theory to any order. As a demonstration of the usefulness of the theory, we use it to calculate the conductance of a single quantum dot, and of two quantum dots with an inter-dot coupling, to leading order in the quasi-particle interaction.

To perform calculations in the renormalised theory it is essential that the values of the renormalised parameters describing the quasi-particles are known. Here we develop a general method for determining them entirely within the RPT framework, which relies on constructing renormalisation flow equations relating the renormalised parameters of two models whose bare parameters differ infinitesimally. By determining the renormalised parameters for a model with bare parameters that render it amenable to ordinary perturbation theory, and solving the flow equations to relate them to the renormalised parameters of models with progressively stronger correlations, we succeed in deducing the renormalised parameters for models with strong correlations.
Publications

To satisfy the College’s requirements for clear attribution of credit in multi-author publications, I declare the following regarding work that appears in this thesis:


  I implemented the work described in Sec. III and contributed the corresponding plots, which are included in Sec. 4.3 of the present thesis. The work is cited as Ref. [34].

- **Numerical integration of discontinuous functions in many dimensions.** V. Pandis. Accepted for publication in Transactions on Mathematical Software

  This work was my own research initiative; the work and authoring of the paper were carried out by myself. A pre-print of the work is cited as Ref. [101] and is included here as Appendix D.


  This work was my own research initiative; the work and authoring of the paper were carried out by myself. The work is cited as Ref. [102] and is included here as Sec. 4.4.


  This work was based on my own research initiative and was carried out by myself. I authored the latter half of the paper, which forms the bulk of Sec. 4.5. A pre-print of the work, under a different title, is cited as Ref. [103] and has been written entirely by myself.
High-order terms in the renormalized perturbation theory for the Anderson impurity model. V. Pandis and A. C. Hewson. Submitted to Phys. Rev. B

This work was my own research initiative; the work and authoring of the paper were carried out by myself. A pre-print of the work is cited as Ref. [104]. An extension of this paper constitutes Chapter 3.
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Introduction

A core principle that has guided the development of physics in the past centuries is that of reductionism, the belief that a physical system can be understood by studying its individual constituents. To understand a system, one must break it down into smaller, simpler entities, which can be studied in isolation. The reductionist argument asserts that these units will be governed by simpler laws than apply to their collective behaviour, and thus a scientific theory for them will be easier to construct; the properties of the original system can then be understood as the sum of the properties of its components. This approach has so far been rather successful, and has led to the Standard Model of particle physics which is currently thought to describe nature at least down to scales of $10^{-20}$ m. Despite this success, in the course of the 20th century it became clear that some systems exhibit behaviour that cannot be understood in this manner and which is a result of the interactions of the particles rather than a naive sum of the individual behaviours. Explaining such emergent behaviour is one of the central challenges in modern physics.

In material science, the physics of a large class of materials, known as strongly correlated materials, stems from the interactions of their constituent electrons. This class includes high-temperature superconductors, heavy-fermion compounds, Mott insulators, mesoscopic quantum dots and other systems. Strongly correlated materials frequently exhibit highly unusual behaviour, such as a transition from a metallic to an insulating state, and have been a focal point for condensed matter physics for over eighty years.

The subject of this thesis is a class of strongly correlated systems, namely metallic systems containing a magnetic impurity. Metallic systems owe many of their characteristic properties to the periodicity of the underlying ion lattice. A striking prediction of quantum theory is that the electrons in such a crystalline environment can delocalise and form a conduction band that allows them to spatially dissociate from their parent ion. These conduction, or Bloch, bands lie at the very centre of our modern understanding of crystalline solids and lie at the core of the explanations of fundamental metallic properties, such as their
good electrical and thermal conductivity.

In systems with magnetic impurities this periodicity is spoiled. Far from the impurity we can expect its effects to be negligible, and electron wavefunctions to assume their Bloch form. But the impurity itself will present a scattering site to electrons in the conduction band, with which it may interact through a magnetic moment or Coulomb potential. Due to the large number of electrons in the conduction band (of order $10^{23}$) one must treat this as a many-body problem; one cannot simply ignore the electron-electron repulsion.

Historically, the study of magnetic impurities began with experimental observation that the resistivity of Au [30] had a minimum as a function of temperature. This contradicted the band theory of metals at the time, which required the resistivity to be a strictly increasing function of temperature as a result of non-magnetic impurity and phonon scattering [13]. This remained a puzzling observation for about three decades and a number of experiments [86, 8, 85] conducted over this period confirmed the presence of the resistance minimum in several dilute transition metal alloys. Furthermore, these experiments suggested a connection between the resistance minimum and the presence of a local magnetic moment on the impurity.

An explanation came in 1964 when Jun Kondo calculated [70] the resistivity of the $s$-$d$ model [140, 66, 136], a simple model involving a conduction electron bath interacting with a localised magnetic moment due to the impurity. He showed that the effect of the impurity scattering was to contribute a term to the resistivity with a logarithmic dependence on the temperature. As $T$ is decreased, the $\ln T$ contribution increases rapidly in magnitude and eventually dominates the non-magnetic and phonon scattering mechanisms, giving rise to a local minimum in the resistivity. As $T$ is further decreased the logarithmic term diverges, signalling the failure of Kondo’s solution. The problem of extending Kondo’s solution to lower temperatures became known as the Kondo problem.

Kondo’s original approach relied on the use of perturbation theory, a standard method for approaching problems in quantum physics. In Kondo’s perturbation theory begins by ignoring the exchange coupling and solving the non-interacting problem. This solution is assumed to be reasonably close to the solution of the interacting problem, and that the effect of the interactions is to merely introduce small corrections. For strongly correlated systems, such an approach is, by definition, inadequate. Extending Kondo’s solution to lower temperatures required the development of non-perturbative methods and was eventually accomplished by Kenneth Wilson in 1975 [131] and his Numerical Renormalisation Group,
ultimately earning him the 1982 Nobel Prize in Physics.

Though Kondo’s work was successful in explaining the resistance minimum in terms of a local moment, the existence of a local moment in metals was a puzzle in itself. The presence of such localised moments also seemed to coincide with a locally-suppressed superconducting temperature, putting more pressure on theorists to provide an explanation. A breakthrough was achieved in 1961 when P.W. Anderson introduced what is today known\(^1\) as the Anderson impurity model [9]. This will be extensively discussed in this thesis — we briefly mention here that it consists of a conduction band, an electronic level contributed by the impurity and which is connected to the conduction band via a hybridisation matrix element, and a term to account for Coulomb repulsion on the impurity site.

Early attempts to solve the Anderson model proved hard to extend to the regime of strong electron-electron interactions, with perturbation theory around the non-interacting limit proving again insufficient to describe the strong electron-electron interactions. Significant progress was achieved in the 1980, when exact solutions of an important special case of the model, the particle-hole symmetric model, were obtained using the Bethe Ansatz [127, 129, 11]. In the same year, the Numerical Renormalisation Group [72, 73] method was applied successfully to the model in its general case.

The limitations of perturbation theory had become apparent very early in the development of quantum field theory, where several calculations were observed to exhibit logarithmic divergences similar to the one present in Kondo’s solution. Following a period of controversy, a technique known as renormalised perturbation theory was developed to interpret the seemingly spurious infinities and extract predictions from the theory. This restored the legitimacy of quantum electrodynamics and was instrumental to the subsequent development of quantum chromodynamics.

Despite the well-understood analogy between quantum-field and many-body theory, the renormalised perturbation theory had not, until relatively recently, found applications to strongly correlated systems, except for the important influence it had on the development of the Numerical Renormalisation Group. In the past decades, however, it has been used to study the Anderson, s-d and Hubbard models in a number of scenarios. The approach is similar to perturbation theory, in that there is a perturbative expansion to be carried out, but differs from it

\(^1\)Not to be confused with the Anderson localisation model.
in how the series is organised. Though systems in condensed matter are not plagued by the infinities of particle physics, the idea of carrying out the expansion in a new set of parameters is useful in this context too, allowing meaningful perturbation expansions to be carried out.

The ideas of renormalised perturbation theory have many similarities to the conceptual underpinnings of Fermi liquid theory: the strong correlations between the electrons close to the Fermi surface force them to coalesce into quasi-particles, which behave somewhat like independent entities. However, this picture does not capture all the correlation effects; the residual effects manifest themselves as interactions between the quasi-particles. Crucially, the quasi-particle correlations are weak and permit us to carry a perturbation theory in powers of the quasiparticle–quasiparticle interaction. In a sense, a reductionist approach is still at work, with the ‘simple’ entities being the quasi-particles. The quasiparticle itself however must taken to be the building block of this picture. This is more useful framework to a condensed matter physicist than to think of a quasi-particle in terms of electrons and holes, similar to how the abstraction of a proton is more useful to an atomic physicist than its description in terms of quarks and gluons.

This thesis is structured as follows: In Chapter 1 a summary of relevant background material is given. We introduce the Anderson impurity model and discuss a number of different approaches to its solution, namely Anderson’s original mean-field approach, the ordinary perturbation theory, the Bethe Ansatz and the Numerical Renormalisation Group. We highlight some important properties of the Anderson impurity model, and define quantities such as the spin and charge susceptibilities which we refer to throughout the thesis.

In Chapter 2 we present a comprehensive introduction to the renormalised perturbation theory. We discuss some key results in the renormalised theory and illustrate how quantities such as the renormalised self-energy can be calculated in terms of the renormalised parameters, up to third order inclusive. We demonstrate the effectiveness of the theory by using it to calculate the conductance of a quantum dot under a small bias voltage. This calculation is then extended to the case of two coupled quantum dots.

In Chapter 3 we discuss how calculations in the renormalised perturbation theory can be automated and carried out entirely algorithmically. We discuss the implementation of this method as a computer program, which generates the diagrams, translates them to integrals and carries out the numerical integration, without any user intervention. To improve the efficiency of our calculation we
introduce a factorisation algorithm to simplify the resultant numerical integrals, in analogy to common practice in manual calculations. We present results for the self-energy, the spectral density to fifth order inclusive.

In Chapter 4 we address the question of determining the renormalised parameters without the use of the Numerical Renormalisation Group, which constitutes an inherent challenge in the renormalised theory. We develop the flow equation method, a general framework for constructing flow equations that relies on identifying a flow variable and constructing a system of differential equations to describe the renormalisation flow. We first discuss the case where the flow variable is provided by the impurity level and use it to obtain the renormalised parameters for asymmetric models. We then focus on the particle-hole symmetric model and, by implementing the flow scheme in the hybridisation, obtain numerical results for the renormalised parameters. Finally, we discuss the symmetric model and the scaling of the interaction, and deduce particularly simple flow equations that we solve exactly, obtaining closed-form expressions for the renormalised parameters.

The main text is followed by five appendices. In Appendix A the leading temperature dependence of the renormalised self-energy is determined; this is pertinent to the calculation of the quantum dot conductance in Chapter 2. This is followed by Appendix B, where a finite-temperature generalisation of the renormalised perturbation theory is considered. In Appendix C we discuss the calculation of the \( n \)-particle/hole propagators, introduced in Chapter 3, which was not included in the main text due to its technical nature. In Appendix D a geometric approach to the numerical integration of functions with planar discontinuities, such as self-energy amplitudes at zero external frequency, is entertained. Finally, Appendix E contains the Feynman diagrams generated during the calculations of Chapter 3.

**Notation**

Throughout the thesis we work in ‘natural’ units where \( \hbar = k_B = 1 \). For aesthetic reasons we occasionally use the notation \( \sigma = -\sigma \). Similarly, in the interests of legibility we employ the notation \( d\tilde{\omega} = d\omega/2\pi \) to denote the integration measure.
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I would like to thank Alex Hewson for his continuous help and advice during the course of my studies. I would like to thank Nina, for her unbounded support and patience when these were most needed. Τέλος, θα ήθελα να ευχαριστήσω τους γονείς μου, Αλέξανδρα και Αλέξανδρο, για την αμέριστη αγάπη τους, την υποστήριξη τους, και για όλα όσα έχουν κάνει για μένα.
1. Overview of the model

1.1. Overview of the Anderson impurity model

In the late 1950s the effects of magnetic impurities\(^1\) on the superconductivity of their non-magnetic host metals were the subject of extensive experimental investigations [86, 8, 85]. Such impurities were found to lead to the formation of regions of localised magnetic moments and seemed to suppress the superconducting transition temperature \(T_c\). Efforts to explain the origin of the magnetic moment led to the formulation of the Anderson impurity model (AIM) [9]. This model incorporates a localised atomic orbital contributed by the impurity, and a conduction band of free electrons. Electrons from the conduction band are allowed to transition to the impurity orbital through a hybridisation amplitude. Far from the impurity the conduction electron wavefunctions tend to Bloch states, but the potential of the impurity will tend to localise them in its vicinity. In the limit of an infinitely attractive impurity potential, the \textit{atomic} limit, this will lead to the formation of a bound state, whereas weaker potentials will merely induce a resonance in the conduction electron density of states; such states are known as \textit{virtual bound states} [37], [48, p. 9]. Double occupancy of the impurity orbital is energetically penalised through an on-site interaction \(U > 0\) which encodes the Coulomb energy cost of two localised electrons. The impurity is generally a transition metal or a lanthanide where the incomplete \(d\) or \(f\) shells correspond to the impurity orbital. The interaction constant \(U\) can be calculated from first principles as a matrix element involving the Coulomb interaction and the impurity states. In doing so, screening effects which act to reduce \(U\) must be taken into account; typical values for the constant thus lie in the range \(1 - 7\) eV [50].

---

\(^1\)Impurities are classified as magnetic if their contribution to the host susceptibility is of the Curie-Weiss type, \(\chi \propto \frac{1}{T+\theta}\).
Figure 1.1.: Impurity contribution to the non-interacting density of states \( \pi \Delta \rho(\omega) \), where \( \Delta \) denotes the hybridisation, in the limit of a wide (left) and a narrow (right) conduction band.

The Hamiltonian for the AIM is

\[
\hat{H} = \sum_{\sigma} \epsilon_d \sigma \hat{c}^\dagger_{d,\sigma} \hat{c}_{d,\sigma} + \sum_{\sigma, k} \epsilon_k \sigma \hat{c}^\dagger_{k,\sigma} \hat{c}_{k,\sigma} + \sum_{\sigma, k} \left( V_{k, d} \sigma \hat{c}^\dagger_{k,\sigma} \hat{c}_{d,\sigma} + V_{k, d}^* \sigma \hat{c}^\dagger_{d,\sigma} \hat{c}_{k,\sigma} \right) + U \sigma \hat{c}^\dagger_{d,\uparrow} \hat{c}^\dagger_{d,\downarrow} \hat{c}_{d,\downarrow} \hat{c}_{d,\uparrow} \quad (1.1)
\]

In Eq. (1.1) the variable \( \epsilon_d \) denotes the impurity level, \( \epsilon_k \) denotes the energy of a conduction electron with momentum \( k \) and \( V_{k, d} \) is the hybridisation matrix element. It is understood that energies are measured with respect to the Fermi level, which we have set to zero and omitted from Eq. (1.1). The creation and annihilation operators \( \hat{c}^\dagger_{d,\sigma}, \hat{c}_{d,\sigma} \) and \( \hat{c}^\dagger_{k,\sigma}, \hat{c}_{k,\sigma} \) correspond to the impurity site and conduction band respectively, and satisfy the usual fermionic canonical anti-commutation relations \( \{ \hat{c}_{d,\sigma}, \hat{c}^\dagger_{d,\sigma'} \} = \delta_{\sigma,\sigma'} \), \( \{ \hat{c}_{k,\sigma}, \hat{c}^\dagger_{k',\sigma'} \} = \delta_{\sigma,\sigma'} \delta_{k,k'} \). The occupancy of the impurity depends on the parameters \( \epsilon_d, V_{k, d} \) and \( U \), and takes the values 2 and 0 in the limits \( \epsilon_d \to -\infty \) and \( \epsilon_d \to +\infty \) respectively. When \( \epsilon_d = -U/2 \) the impurity occupation is equal to 1, with each spin species contributing 1/2 to it, and the model is said to be at half-filling, or to possess particle-hole symmetry. An external magnetic field \( h \) will shift the impurity levels from the zero-field values and can be absorbed in the definition of the impurity levels \( \epsilon_{d,\sigma} = \epsilon_d - \sigma h \).

1.1.1. The non-interacting limit

In the limit \( U \to 0 \) the physics of the AIM is attributed to the virtual bound state resonance induced by the local impurity potential. In this limit the model can be solved exactly and the solution will form the starting point for the perturbation
theory in $U$, which will be discussed later in this chapter. We define the advanced and retarded Green’s function operators, $\hat{G}^+$ and $\hat{G}^-$, through the Lippmann-Schwinger equation

$$(\omega \pm i\eta - \hat{H})\hat{G}^\pm = \hat{I},$$

where $\hat{I}$ is the identity operator and $\eta \to 0^+$. We now introduce impurity and conduction electron eigenstates $|d\sigma\rangle = c_{d,\sigma}^\dagger |0\rangle$ and $|k\sigma\rangle = c_{k,\sigma}^\dagger |0\rangle$, where $|0\rangle$ is the vacuum defined as $c_{d,\sigma} |0\rangle = c_{k,\sigma} |0\rangle = 0$. To simplify the analysis we will assume that these are orthogonal, $\langle d\sigma | k\sigma \rangle = 0$, but this is not essential and the assumption can be lifted if desired [48]. Furthermore, we will assume the absence of a magnetic field. By taking matrix elements of $\hat{H}$ in Eq. (1.2) with $U = 0$ and solving the resultant system of equations, we can deduce an expression for the impurity Green’s function

$$G^+_{\sigma}(\omega) = \langle d\sigma | \hat{G}^+ | d\sigma \rangle = \frac{1}{\omega + i\eta - \epsilon_d - K(\omega)},$$

where

$$K(\omega) = \sum_{k} \frac{|V_k|^2}{\omega + i\eta - \epsilon_k}.$$  

Using the Sokhotsky identity

$$\lim_{\eta \to 0^+} \frac{1}{x \pm i\eta} = P \left(\frac{1}{x}\right) \mp i\pi \delta(x),$$

where $P$ denotes a principal value integration, we write $K(\omega) = \Lambda(\omega) - i\Delta(\omega)$ where

$$\Lambda(\omega) = P \sum_{k} \frac{|V_k|^2}{\omega - \epsilon_k}, \quad \Delta(\omega) = \pi \sum_{k} |V_k|^2 \delta(\omega - \epsilon_k).$$

Since the number of states in a conduction band is of the order of the Avogadro constant, we can replace the sums over discrete states with integrals over a conduction density of states $\rho_c(\omega)$. In general, the underlying band structure is very complicated, material-specific and not always fully known, so it is standard to simplify the theoretical treatment by assuming a flat (i.e. dispersionless) band of width $2D$ with density of states

$$\rho_c(\omega) = \begin{cases} 
\rho_{c,0}, & \text{if } |\omega| \leq D \\
0, & \text{if } |\omega| > D 
\end{cases}$$
and ignoring the wavevector dependence of the hybridisation matrix elements $V_k = V$. We then find that

$$\Lambda(\omega) = \frac{\Delta}{\pi} \ln \left| \frac{D + \omega}{D - \omega} \right|, \quad \Delta(\omega) = \Delta \theta(D - |\omega|), \quad (1.8)$$

where

$$\Delta = \pi \rho_{c,0} |V|^2 \quad (1.9)$$

and $\theta(x)$ is the usual Heaviside step function. At this point two limiting cases naturally present themselves:

- **The wide-band limit** $D \gg \Delta$: In this limit the half-bandwidth $D$ is assumed to be the dominant scale of the problem. The expressions in Eq. (1.8) simply become

  $$\Lambda(\omega) = 0, \quad \Delta(\omega) = \Delta, \quad (1.10)$$

  and we arrive at the non-interacting (retarded) Green’s function

  $$G^{(0,+)}(\omega) = \frac{1}{\omega - \epsilon_{d,\sigma} + i\Delta}. \quad (1.11)$$

  This limit is adopted in the vast majority of published work on the Anderson model and will be assumed throughout this thesis.

- **The narrow-band limit** $D \ll \Delta$: In this limit the half-bandwidth is taken to be much smaller than all the other scales that appear in the problem. While this is not a useful simplification for ordinary host metals, it has been pointed out that it is relevant to the Dynamical Mean Field Theory [42] of the Mott insulator transition in the Hubbard model, in the infinite-dimensional limit. The physics of this limit has been explored in Refs. [56, 111, 110].

  In either case we can deduce the non-interacting contribution to the density of states using

  $$\rho_\sigma^{(0)}(\omega) = -\frac{1}{\pi} \text{Im} G^{(0,+)}(\omega). \quad (1.12)$$

  The results are shown in Fig. 1.1.

### 1.1.2. Parameter regimes

Based on the relative values of the parameters in Eq. (1.1) we can broadly distinguish two parameter regimes, the **magnetic** and **non-magnetic**. The former can
be further sub-divided into the local moment and intermediate valence regimes, and the latter into the empty orbital and doubly occupied regimes. These are defined as follows [50]:

- The local moment regime: This corresponds to the case where the two states lie on either side of the Fermi level and are well separated from it, i.e. \( \epsilon_d + U \gg \Delta, \epsilon_d \ll -\Delta \). Experimentally this regime is identified through the observation of a Curie contribution to the impurity spin susceptibility. In this regime the Anderson model can be well approximated by the \( s-d \) or Kondo model [140]

\[
\hat{H}_{sd} = \sum_{k,k'} J_{k,k'} \left[ \hat{S}^+ c_{k\uparrow}^\dagger c_{k'\uparrow}^\dagger + \hat{S}^- c_{k\downarrow}^\dagger c_{k'\downarrow}^\dagger + \hat{S}_z (c_{k\uparrow}^\dagger c_{k'\uparrow}^\dagger - c_{k\downarrow}^\dagger c_{k'\downarrow}^\dagger) \right],
\]

(1.13)

where \( \hat{S}_z \) and \( \hat{S}^\pm = \hat{S}_x \pm i\hat{S}_y \) are the standard spin operators. By means of a canonical transformation one can show that \( \hat{H}_{sd} \) and Eq. (1.1) are equal in the limit \( \Delta \to 0 \) [114].

- The intermediate valence regime corresponds to the situation where either the lower level \( \epsilon_d \) or the upper level \( \epsilon_d + U \) are within \( \Delta \) of the Fermi level and it is particularly relevant to lattice models of impurities. This regime is dominated by charge fluctuations.

- The non-magnetic regime, which can be further sub-divided into the empty orbital regime \( \epsilon_d - \epsilon_f \gg \Delta \) and the doubly occupied regime \( \epsilon_d + U \ll \Delta \). Since in either case the level is far from the Fermi energy, charge fluctuations are not important in this regime.
1.1.3. The \( n \)-channel Anderson model

So far we have considered only systems with spin \( S = 1/2 \) and a single impurity orbital — this is known as the non-degenerate or SU(2) Anderson model. A more realistic model ought to take into account the fact that in real systems the magnetic impurity is a transition or a rare-earth metal, and such systems do not typically donate an \( s \) orbital to the host metal. Instead, a more elaborate description is needed. Consequently, the model of Eq. (1.1) can be modified to accommodate \( N \) impurity states:

\[
\hat{H} = \sum_{\sigma} \epsilon_{d,\sigma} \hat{c}^{\dagger}_{d,\sigma} \hat{c}_{d,\sigma} + \sum_{\sigma,k} \epsilon_k \hat{c}^{\dagger}_{k,\sigma} \hat{c}_{k,\sigma} + \sum_{\sigma,k} \left( V_{k,d} \hat{c}^{\dagger}_{k,\sigma} \hat{c}_{d,\sigma} + V_{k,d}^{*} \hat{c}^{\dagger}_{d,\sigma} \hat{c}_{k,\sigma} \right) + \sum_{\sigma \neq \sigma'} U \hat{c}^{\dagger}_{d,\sigma} \hat{c}_{d,\sigma'} \hat{c}_{d,\sigma'} \hat{c}^{\dagger}_{d,\sigma},
\]

(1.14)

where \( \sigma = 1, \ldots, N \). The introduction of an additional variable \( N \) also opens up the possibility of carrying out a perturbation expansion around the atomic limit and performing a partial diagrammatic resummation of the leading terms in \( 1/N \). This is known as the \( 1/N \)-expansion (see Refs. [50, p. 171], [19]) and has been found in some cases to be reasonably accurate even for \( N = 2 \). In recent years SU(N) models have proven useful in modelling the behaviour of semiconductor [43, 28, 100, 78, 125] and carbon nanotube [23, 82, 21, 7] quantum dots.

In Eq. (1.14) the Coulomb term affects all spin species equally. This can be seen as a special case of the two-channel model [27]

\[
\hat{H} = \hat{H}_1 + \hat{H}_2 + U_{12}(n_{1,\uparrow} + n_{1,\downarrow})(n_{2,\uparrow} + n_{2,\downarrow}),
\]

(1.15)

where \( \hat{H}_i \) is the interacting SU(2) Anderson Hamiltonian of the \( i \)'th species

\[
\hat{H}_i = \sum_{\sigma} \epsilon_{d,i,\sigma} \hat{c}^{\dagger}_{d,i,\sigma} \hat{c}_{d,i,\sigma} + \sum_{k,\sigma} \epsilon_k \hat{c}^{\dagger}_{k,i,\sigma} \hat{c}_{k,i,\sigma} + \sum_{k,k'} (V_{\sigma} \hat{c}^{\dagger}_{k,i,\sigma} \hat{c}_{k',i,\sigma} + H.c) + U n_{i,\uparrow} n_{i,\downarrow}.
\]

(1.16)

In this model the Coulomb repulsion between electrons on different bands is not necessarily equal to the Coulomb repulsion experienced by electrons occupying the same band. By assuming that \( U_{12} \sim U \) we can use Eq. (1.15) to model impurities that contribute more than a single orbital, since both orbitals are localised around the same nucleus and will give rise to wavefunctions with similar overlap integrals. Furthermore, when \( U_{12} \ll U \), we can interpret Eq. (1.15)
as a model of two impurities. The $U_{12}$ term then describes the inter-impurity repulsion, and is weaker than $U$ due to the spatial separation of the impurity sites.

**1.2. Mean field theory**

Having tackled the non-interacting case, we now seek to take into account the Coulomb term. The mean-field theory (MFT), or Hartree-Fock theory, developed by Anderson in his original work [9] is the simplest way to accomplish this but, as we shall see, is far from the final word on the matter. In the MFT we attempt to simplify the Hamiltonian by assuming that the fluctuations of the orbital occupations from their mean-field values are small. Specifically, we aim to rewrite the interaction term so that it is linear in the fluctuations. The expectation values of the number operators $\langle n_\sigma \rangle$ are at present unknown and will be calculated self-consistently. Substituting $\delta n_\sigma = n_\sigma - \langle n_\sigma \rangle$ into Eq. (1.1), and ignoring the term $U\delta n_\uparrow \delta n_\downarrow$, as well as an overall additive constant which does not affect the physics of the model, we find that the Hamiltonian is formally identical to that of a non-interacting model with a renormalised level $\tilde{\epsilon}_{d,\sigma}^{(\text{hf})} = \tilde{\epsilon}_{d,\sigma} + U\langle n_{-\sigma} \rangle$. This is characteristic of mean-field methods; the complicated many-particle interactions are replaced with a much simpler one-particle interaction with an effective field, in this case $\langle n_{-\sigma} \rangle$, which is calculated self-consistently.

From our previous discussion of the non-interacting model it follows that

$$G^{(+,\text{hf})}_\sigma(\omega) = \frac{1}{\omega - \tilde{\epsilon}_{d,\sigma}^{(\text{hf})} + i\Delta}. \quad (1.17)$$

To formulate the self-consistency requirement we note that the mean-field impurity occupation $\langle n_{-\sigma} \rangle$ can be obtained by integrating the density of states obtained from $G^{(+,\text{hf})}_\sigma$. We thus find that

$$\langle n_\sigma \rangle = \frac{1}{\pi} \cot^{-1} \left( \frac{\epsilon_d + U\langle n_{-\sigma} \rangle}{\Delta} \right). \quad (1.18)$$

This equation admits a single root if $u = U/\pi\Delta < 1$ and three roots if $u > 1$. In the case of a unique root we have $n_{\uparrow} = n_{\downarrow}$, implying a non-magnetic ground state since the magnetisation is zero in the absence of an external magnetic field. Otherwise, Eq. (1.18) develops three possible roots, allowing for the possibility that $n_{\uparrow} \neq n_{\downarrow}$ (see Fig. 1.3). The SU(2) symmetry of the system is thus spontaneously broken and the system becomes magnetic.
Figure 1.3.: The solutions to the Hartree-Fock equations as a function of $\eta = \epsilon_d + U/2$ for $U/\pi \Delta = 0.8$ (left) and $U/\pi \Delta = 1.2$ (right). We see that in the latter case three solutions appear; two of them correspond to broken symmetry states and the third to the Restricted Hartree-Fock solution.

The mechanism outlined above was indeed put forward in Ref. [9] as an explanation for the existence of localised magnetic moments in metals. It later became apparent that the predicted broken symmetry states must be in fact be unphysical. This is largely due to Elitzur’s theorem which precludes the spontaneous breaking of local gauge symmetries [35]. As one progresses towards the magnetic solutions the fluctuations ignored by mean-field theory become increasingly important and act to preserve the gauge symmetry.

The simplest way to overcome the problem of the spontaneously broken states is to enforce a non-magnetic ground-state by imposing the condition $n^\uparrow = n^\downarrow$ in Eq. (1.18). This eliminates the magnetic state when $u > 1$ and only the central branch of in the right panel of Fig. 1.3 remains. This approximation is also known as the Restricted Hartree-Fock approximation.

1.3. Linear response functions

Physics is an experimental science, and it is therefore of crucial importance to ultimately be able to relate theoretical predictions to measurable quantities. Typically one aims to disturb the system in some manner and measure its response to the disturbance. In condensed matter physics this disturbance is typically a modification of the environment of the system: for instance, we can apply a magnetic field and measure the magnetisation, apply an electric field and measure the polarisation, or change the temperature of the system and measure the thermal capacity. The calculation of response functions is therefore a matter of
great importance.

For the Anderson model we can define two types of spin and charge susceptibilities, referred to as *longitudinal* and *transverse*

\[
\chi_s^t(t) = -i \langle T \{ c_{d\uparrow}^\dagger(t) c_{d\downarrow}^\dagger(0) c_{d\downarrow}(0) \} \rangle U, \\
\chi_c^t(t) = -i \langle T \{ c_{d\uparrow}^\dagger(t) c_{d\downarrow}(0) c_{d\uparrow}(0) \} \rangle U, \\
\chi_s^l(t) = -i \langle T \{ [n_\uparrow(t) - n_\downarrow(t)] [n_\uparrow(0) - n_\downarrow(0)] \} \rangle U, \\
\chi_c^l(t) = -i \langle T \{ [n_\uparrow(t) + n_\downarrow(t) - 1] [n_\uparrow(0) + n_\downarrow(0) - 1] \} \rangle U.
\]

In Eq. (1.19)-(1.22) it is understood that expectation values are to be calculated with respect to the interacting ground state and \( T \) is the time-ordering operator defined for fermionic fields \( A_1, A_2, \ldots, A_n \) as

\[
T \{ A_1(t_1) A_2(t_2) \ldots A_n(t_n) \} = \sum_p \text{sign}(p) \theta(t_{p_1} - t_{p_2}) \theta(t_{p_2} - t_{p_3}) \cdots \theta(t_{p_{n-1}} - t_{p_n}) \times A_{p_1}(\tau_{p_1}) A_{p_2}(\tau_{p_2}) \ldots A_{p_n}(\tau_{p_n}),
\]

where the sum runs over all permutations of \((1, 2, \ldots, n)\) and \( \text{sign}(p) = \pm 1 \) denotes the sign of the permutation\(^2\). In this thesis we will be concerned with the static susceptibilities, for which we have

\[
\chi_s^l(0) = \frac{m}{2h}, \\
\chi_c^l(0) = \frac{n - 1}{2e_d + U}, \\
\chi_s^l(0) = \frac{\partial m}{\partial h}, \\
\chi_c^l(0) = \frac{\partial n}{\partial e_d},
\]

in terms of the total occupation \( n = n_\uparrow + n_\downarrow \) and the magnetisation \( m = n_\uparrow - n_\downarrow \). The charge and spin susceptibilities are not unrelated quantities — they can be mapped into each other via the spin-isospin transformation which we will discuss in the Section 1.4. In the limit \( h \to 0, m \to 0 \) so it follows that

\[
\chi_s^t = \frac{m(h)}{2h} + \frac{1}{2} \frac{\partial m(h)}{\partial h} = \frac{1}{2} \chi_c^l,
\]

for a model which is not necessarily symmetric. A similar relation can be deduced\(^2\)

\(^2\)If \( P = (p_1, p_2, \ldots, p_n) \) can be obtained from \((1, 2, \ldots, n)\) by swapping an even number of elements then \( \text{sign} P = 1 \), otherwise \( \text{sign} P = -1 \).
for $\chi_c^f$ for the symmetric model, potentially in a non-zero magnetic field:

$$\chi_c^f = \frac{n - 1}{2\epsilon_d + U} \rightarrow \frac{1}{2} \frac{\partial n}{\partial \epsilon_d} = \frac{1}{2} \chi_c^f. \quad (1.29)$$

Another quantity of interest is the impurity contribution to the specific heat $C_d$, which is defined in terms of the impurity’s contribution $\delta F_G$ to the free energy $F_G$

$$C_d = -T \frac{\partial^2 \delta F_G}{\partial T^2}. \quad (1.30)$$

At low temperatures $C_d(T) \approx \gamma T$; we will see later that the linear coefficient $\gamma$ can be related to the derivative of the self-energy, and is consequently a quantity of considerable theoretical interest. We define the Wilson (or Sommerfeld) ratio $R$ defined as the ratio

$$R = \frac{4\pi^2 \Delta \chi_c^f}{3 \gamma}, \quad (1.31)$$

which can be loosely interpreted as a measure of the strength of the correlation effects. In the case of the non-interacting model model we find that $R = 1$. The Wilson ratio increases monotonically with $U$, with an asymptotic value of 2 as $U \rightarrow \infty$.

As defined, the quantities in Eq. (1.19)-(1.22) are dimensionful. We will find it convenient to define the corresponding dimensionless quantities

$$\bar{\chi}_s^f = 2\pi \Delta \chi_s^f, \quad \bar{\chi}_c^f = \frac{\pi \Delta}{2} \chi_c^f, \quad \text{and} \quad \bar{\gamma} = \frac{3\Delta}{2\pi \gamma}. \quad (1.32)$$

### 1.4. Spin-isospin transformation

The spin-isospin transformation [61, 53] is a symmetry transformation that relates a model with an interaction constant $U$ to a model with an opposite interaction constant $-U$. To demonstrate this we introduce the (unitary) spin-isospin operator $\mathcal{T}$ which effects a particle-hole transformation on one spin species whilst leaving the other spin invariant:

$$\mathcal{T} c_{d,\uparrow}^\dagger \mathcal{T}^{-1} = c_{d,\uparrow}^\dagger, \quad \mathcal{T} c_{d,\downarrow}^\dagger \mathcal{T}^{-1} = c_{d,\downarrow}, \quad \mathcal{T} c_{k,\uparrow}^\dagger \mathcal{T}^{-1} = c_{k,\uparrow}^\dagger, \quad \mathcal{T} c_{k,\downarrow}^\dagger \mathcal{T}^{-1} = c_{-k,\downarrow}. \quad (1.33)$$
By applying this transformation to the Hamiltonian in Eq. (1.1) we find that a model with parameters \((\epsilon_d, U, h)\) maps into a model with \((\epsilon'_d, U', h')\) with

\[
\begin{align*}
\epsilon'_d &= -h + U/2, \\
h' &= -\epsilon_d - U/2, \\
U' &= -U. \\
\end{align*}
\] (1.34)

This can be used, for instance, to map a symmetric AIM with interaction constant \(U\) in a magnetic field \(h\) to an asymmetric model with an interaction \(-U\), \(h' = 0\) and \(\epsilon'_d = -h + U/2\). Under the spin-isospin transformation the charge and spin susceptibilities map into one another

\[
\chi^{l,l}_s \rightarrow \chi^{l,l}_c, \quad \chi^{l,l}_c \rightarrow \chi^{l,l}_s.
\] (1.35)

This reflects the mapping of the particle-hole and particle-particle channels into each other. More generally, we can apply \(T\) to the expectation value with respect to the interacting vacuum of any operator in the Heisenberg picture. By expressing the expectation value as a trace, substituting the equations of motion, and repeatedly inserting \(T\), we find that [61]

\[
\langle A_1(t_1)A_2(t_2)\ldots \rangle_U = \langle A_1(t_1)A_2(t_2)\ldots \rangle_{-U}. 
\] (1.36)

From this we can deduce that the self-energy\(^3\) in the symmetric model must be an even function of \(U\).

### 1.5. The SIAM in the Lagrangian formalism

Historically, many-body field theory was developed in the framework of second quantisation. One begins with a classical Hamiltonian density, which is then quantised by introducing creation and annihilation operators, in analogy to the raising and lowering operators of the simple harmonic oscillator. In the case of bosons the commutation rules for the operators are prescribed, whereas in the case of fermions one imposes an anti-commutation relation to reflect the Fermi statistics of the particles. Subsequently, the canonical framework was supplemented by a functional approach based on the ideas by Feynman and Dirac.

\(\footnote{That is, if it is calculated with respect to the Hartree-Fock vacuum. If the Hartree-Fock term is not absorbed into the Green’s function then \(\Sigma(\omega) = U/2 + (a \text{ term even in } U)\).} \)
Whilst the Anderson model is usually discussed in the context of second quan-
tisation, we will find it useful in later chapters to discuss it within the functional
framework, which we will proceed to briefly outline. Our starting point is the
Hamiltonian density of Eq. (1.1) which can be converted to a suitable Lagrangian
density using a Legendre transformation (see Ref. [4, p. 167] for a thorough dis-
cussion). One finds that
\[
L_{\text{AIM}}(\tau) = \sum_\sigma d_\sigma(\tau)(\partial_\tau - \epsilon_{d,\sigma})d_\sigma(\tau) + \sum_{k,\sigma} \bar{c}_{k,\sigma}(\tau)(\partial_\tau - \epsilon_k)c_{k,\sigma}(\tau)
+ \sum_k (V_k \bar{d}_\tau(\tau)c_{k,\sigma}(\tau) + V_k^* \bar{c}_{k,\sigma}(\tau)d_\sigma(\tau)) + U \bar{d}_\uparrow(\tau)d_\downarrow(\tau)d_\downarrow(\tau).
\]
(1.37)

Note that we have re-written \( L \) in terms of a fictitious ‘imaginary time’ [83]
variable \( \tau = it \) that is defined only on the interval \([0, i/T]\). We now introduce
the Grassman fields \( c(\tau), \bar{c}(\tau) \) for the conduction electrons and \( d(\tau), \bar{d}(\tau) \) for the
impurity electrons. We adopt the notation \( \psi_\sigma(\tau) = (c_\sigma(\tau), d_\sigma(\tau)) \) for brevity,
and impose anti-periodic boundary conditions on the fields
\[
\psi_\sigma(0) = -\psi_\sigma(\beta), \quad \bar{\psi}_\sigma(0) = -\bar{\psi}_\sigma(\beta),
\]
(1.38)
where \( \beta = 1/T \). These boundary conditions enable us to transform to frequency-
space through a Fourier sum
\[
\psi_\sigma(\tau) = \frac{1}{\beta} \sum_n \psi_{\sigma,n}(\omega)e^{-i\omega_n \tau}, \quad \psi_{\sigma,n}(\omega) = \int_0^\beta d\tau \psi_\sigma(\tau)e^{i\omega_n \tau},
\]
(1.39)
where the \( \omega_n = (2n + 1)\pi/\beta \) denote the fermionic Matsubara frequencies. For
brevity let \( \bar{d} = (\bar{d}_\uparrow, \bar{d}_\downarrow) \), \( d = (d_\uparrow, d_\downarrow) \) and similarly \( \bar{c}_k = (\bar{c}_{k,\uparrow}, \bar{c}_{k,\downarrow}) \), \( c_k = (c_{k,\uparrow}, c_{k,\downarrow}) \). From Eq. (1.37) we can compute the action \( S_{\text{AIM}}[\bar{d}, d; \bar{c}_k, c_k] \) di-
rectly
\[
S_{\text{AIM}}[\bar{d}, d; \bar{c}_k, c_k] = \int_0^\beta d\tau L_{\text{AIM}}(\bar{d}, d; \bar{c}_k, c_k).
\]
(1.40)
In turn, this expression can be used to calculate the partition function as a
functional integral
\[
Z = \int D[\bar{d}_\sigma, d_\sigma] \prod_k D[\bar{c}_{k,\sigma}, c_{k,\sigma}] \exp(-S_{\text{AIM}}[\bar{d}, d; \bar{c}_k, c_k]).
\]
(1.41)
Assuming a flat conduction band and neglecting the wavevector dependence of \( V_k \)
we integrate out the conduction electron component. We now define an effective action

$$S_{\text{eff}}[\overline{d},d] = \int_0^\beta d\tau L_{\text{eff}}(\overline{d},d),$$  \hspace{1cm} (1.42)

where in the wide-band limit

$$L_{\text{eff}}(\overline{d},d) = \sum_\sigma \overline{d}_\sigma(\tau) \left( \partial_\tau + \epsilon_{d,\sigma} - i\Delta \right) d_\sigma(\tau) + U n_\uparrow(\tau)n_\downarrow(\tau),$$  \hspace{1cm} (1.43)

with $\Delta$ given by Eq. (1.9), which by construction allows us to rewrite the partition function of Eq. (1.41) as an integral over the impurity variables alone

$$Z = \int D[\overline{d},d] \exp(-S_{\text{eff}}[\overline{d},d]),$$  \hspace{1cm} (1.44)

where the abbreviation

$$D[\overline{d},d] = \prod_\sigma D[\overline{d}_\sigma,d_\sigma]$$  \hspace{1cm} (1.45)

has been introduced for clarity. The partition function can be used to define the expectation value of any operator with respect to the interacting vacuum as

$$\langle \ldots \rangle = Z^{-1} \int D[\overline{d},d] \ldots \exp(-S_{\text{eff}}[\overline{d},d]).$$  \hspace{1cm} (1.46)

At this point it is not clear how to handle the functional integral of Eq. (1.46). It is helpful to introduce a partition function with source terms and define expectation values of operators as moments with respect to the source. Using the notation $\mathbf{J}(\tau) = (J_\uparrow(\tau), J_\downarrow(\tau))$, $\overline{\mathbf{J}}(\tau) = (\overline{J}_\uparrow(\tau), \overline{J}_\downarrow(\tau))$ we define

$$Z[\mathbf{J},\overline{\mathbf{J}}] = \int D[d,d] \exp(-S_{\text{eff}}[\overline{d},d] - S[\mathbf{J},\overline{\mathbf{J}},d]),$$

where $S[\mathbf{J},\overline{\mathbf{J}},d] = \sum \int_0^\beta d\tau (\mathbf{J}(\tau) \cdot d(\tau) + \overline{d}(\tau) \cdot \mathbf{J}(\tau))$,  \hspace{1cm} (1.47)

which enables us to rewrite the expectation value of arbitrary string of impurity operators as functional integrals

$$\langle d_{\sigma_1}(\tau_1) \ldots d_{\sigma_k}(\tau_k)\overline{d}_{\sigma'_1}(\tau'_1) \ldots \overline{d}_{\sigma'k}(\tau'_k) \rangle = \delta \frac{\delta}{\delta J_{\sigma_1}(\tau_1)} \ldots \frac{\delta}{\delta J_{\sigma_k}(\tau_k)} \times \delta \frac{\delta}{\delta \overline{J}_{\sigma'_1}(\tau'_1)} \ldots \frac{\delta}{\delta \overline{J}_{\sigma'k}(\tau'_k)} \ln Z[\mathbf{J},\overline{\mathbf{J}}] \bigg|_{\mathbf{J}=\overline{\mathbf{J}}=0}.$$  \hspace{1cm} (1.48)
We will be primarily interested in calculating pair correlation functions. In the functional formalism the thermal Green’s function is defined as

$$G_\sigma(\tau_1, \tau_2) = G_\sigma(\tau_1 - \tau_2) = \langle d_\sigma(\tau_1) \bar{d}_\sigma(\tau_2) \rangle. \tag{1.49}$$

Similarly, we can define the two-particle correlation function

$$G'_{\sigma_1, \sigma_2}(\tau_1, \tau_2; \tau_3, \tau_4) = \langle d_{\sigma_1}(\tau_1) d_{\sigma_2}(\tau_2) \bar{d}_{\sigma_3}(\tau_3) \bar{d}_{\sigma_4}(\tau_4) \rangle. \tag{1.50}$$

Both Eq. (1.49) and Eq. (1.50) are special cases of the $2n$-point correlation function

$$C^{(2n)}_{\sigma_1, \ldots, \sigma_n; \sigma'_1, \ldots, \sigma'_n}(\tau_1, \ldots, \tau_n; \tau'_1, \ldots, \tau'_n) = \langle d_{\sigma_1}(\tau_1) \ldots d_{\sigma_n}(\tau_n) \bar{d}_{\sigma'_1}(\tau'_1) \ldots \bar{d}_{\sigma'_n}(\tau'_n) \rangle. \tag{1.51}$$

Physically, such correlations describe the simultaneous scattering of $n$ particles.

### 1.5.1. Frequency-space formulation

The boundary conditions in Eq. (1.38) also imply that the Greens functions admit a Fourier representation in the Matsubara basis

$$G_\sigma(\tau) = \frac{1}{\beta} \sum_n G_\sigma(i\omega_n) e^{i\omega_n \tau}, \tag{1.52}$$

where

$$G_\sigma(\omega_n) = \int_0^\beta d\tau G_\sigma(\tau) e^{-i\omega_n \tau}. \tag{1.53}$$

This periodicity applies to any $n$-point correlation function of the form of Eq. (1.51)

$$C^{(2n)}_{\sigma_1, \ldots, \sigma_n; \sigma'_1, \ldots, \sigma'_n}(\tau_1, \ldots, \tau_n; \tau'_1, \ldots, \tau'_n) = \frac{1}{\beta^n} \sum_{k_1, \ldots, k_n} C^{(2n)}_{\sigma_1, \ldots, \sigma_n; \sigma'_1, \ldots, \sigma'_n}(\omega_{k_1}, \ldots, \omega_{k_n}) \times \exp \left(i \sum_{i=0}^n (\tau_i - \tau'_i) \omega_{k_i} \right), \tag{1.54}$$
where
\[ C_{\sigma_1...\sigma_n,\sigma'_1...\sigma'_n}(\omega_{k_1},...,\omega_{k_n}) = \int_{[0,\beta]^n} d\tau_1 ... d\tau_n C_{\sigma_1...\sigma_n,\sigma'_1...\sigma'_n}(\tau_1, ..., \tau_n; 0, ..., 0) \times \exp \left( -i \sum_{i=0}^{n} (\tau_i - \tau'_i) \omega_{k_i} \right). \] (1.55)

Physically, the 2n-point correlation function describes the scattering of n \( \rightarrow \) n particles. The physically relevant quantities are the connected correlation functions, which comprise diagrams that are not trivially separable into two or more parts. It can be shown that the connected 4-point correlation function can be represented diagrammatically with interacting Green’s functions and in terms of a four-vertex which contains the genuine two-body interactions. This is achieved through the introduction of a generating functional \( \Gamma[\bar{d},d] \) defined by means of a Legendre transform as [71]
\[ \Gamma[\bar{d},d] = \int d\omega \left( \bar{J}(\omega)d(\omega) + \bar{d}(\omega)J(\omega) \right) - \ln Z[J,\bar{J}]. \] (1.56)

Note that the point of the Legendre transform is to trade the free variables J, \( \bar{J} \) for \( \bar{d},d \) (see Ref. [109, p. 260] for a more detailed discussion). Thus, in Eq. (1.56) the fields J, \( \bar{J} \) are defined as the solution to
\[ d = -\frac{\delta \ln Z[J,\bar{J}]}{\delta J}, \quad \bar{d} = -\frac{\delta \ln Z[J,\bar{J}]}{\delta \bar{J}}, \] (1.57)
and \( \bar{d}(\omega),d(\omega) \) can be defined from the Fourier expansion of their imaginary-time counter-parts. We thus arrive at the four-vertex \( \Gamma_{\sigma_1,\sigma_2,\sigma_3,\sigma_4}(\omega_1,\omega_2;\omega_3,\omega_4), \) which is the two-body analogue of the self-energy.

For notational brevity, the four-vertex \( \Gamma_{\sigma,\sigma',\sigma',\sigma}(\omega_1,\omega_2;\omega_3,\omega_4) \) will be, where convenient, denoted as \( \Gamma_{\sigma,\sigma'}(\omega_1,\omega_2;\omega_3) \) with the understanding that \( \omega_4 = \omega_1 + \omega_2 - \omega_3 \) and \( \sigma' = -\sigma \). Furthermore, we adopt the short-hand \( \Gamma_{\sigma,\sigma}(\omega_1,\omega_2) = \Gamma_{\sigma,\sigma,\sigma,\sigma}(\omega_1,\omega_2;\omega_1,\omega_2) \).

1.5.2. Analytic continuation

A complication that occurs in the Matsubara formalism outlined above arises due to the use of the imaginary time \( \tau \) rather than the usual \( t \). Through the Fourier transform, this carries over to the frequency-space formulation, with the use of \( i\omega_n \) rather than \( \omega \). Quantities defined on the imaginary axis are
not directly observable, so to extract meaningful results one must analytically continue these quantities to the real-axis. Given an analytic expression for a quantity defined on the Matsubara frequencies $i\omega_n$, an analytic continuation can be achieved by performing the substitution $i\omega_n \rightarrow \omega - i\delta$, where $\delta \rightarrow 0^+$. If the analytic form of the function in question is not known, and only the value of the function are, the analytic continuation has to be performed numerically. In most cases, this is very difficult to do; analytic continuation is an ill-conditioned problem [2] and is very sensitive to noise in the numerical data. Consequently, a number of sophisticated approaches have been developed to effect it, such as the use of Padé approximants [126], least-square fitting [117] and the Maximum Entropy Method [119], to mention a few.

### 1.6. Perturbation theory in $U$

When $U = 0$, the functional integration implicit in Eq. (1.44) can be carried out exactly, in analogy to the infinite-dimensional limit of a Gaussian integral, giving

$$\mathcal{Z} \sim \sum_{\sigma} \left( \det \hat{G}^{-1} \right)^{-1/2},$$

where a divergent numerical prefactor has been ignored, and we recover Eq. (1.11) (modulo a Wick rotation). It follows from Eq. (1.38) that $G(\tau)$ is a periodic function. It thus admits a Fourier decomposition in the Matsubara basis

$$G^{(0)}_{\sigma i}(\omega_n) = \frac{1}{i\omega_n - \epsilon_{d,\sigma} + i\Delta \text{sign}(\omega_n)}.$$  \hspace{1cm} (1.59)

The challenge, of course, is to take the effects of the Coulomb repulsion into account. Its effects will be to modify the Green’s function, which will now read

$$G_{\sigma i}(\omega_n) = \frac{1}{[G^{(0)}_{\sigma i}(\omega_n)]^{-1} - \Sigma^M_{\sigma}(i\omega_n)},$$

where the quantity $\Sigma^M_{\sigma}(i\omega_n)$ is the Matsubara self-energy. We will accomplish this by using the $U = 0$ as a starting point for a perturbation expansion in powers of $U$.

To compute the imaginary-axis self-energy $\Sigma^M_{\sigma}(i\omega_n)$ one may apply the following rules [84, p. 246]

---

Given a function $f : A \rightarrow \mathbb{C}$ where $A \subset \mathbb{C}$, we define its analytic continuation as an analytic function $f' : \mathbb{C} \rightarrow \mathbb{C}$ such that $f(x) = f'(x) \forall x \in A$. 

---
• Internal lines with a Matsubara frequency $\omega_n$ and spin $\sigma_i$ receive a factor of $G_{\sigma_i}(\omega_i)$.

• Interaction vertices are associated with a factor $-U$.

• Impose frequency conservation at all vertices and sum over the remaining undetermined Matsubara variables with measure $\frac{1}{\beta} \sum \omega_n$.

• If the diagram has an odd number of fermion loops multiply its amplitude by $-1$.

Physical quantities will generally depend not on the Matsubara self-energy, but its analytic continuation to the real axis; one can obtain this using the methods discussed in Sec. 1.5.2.

1.6.1. $T = 0$ formalism

The previous section detailed the rules for the calculation of $\Sigma_{\sigma}(\omega)$ for arbitrary temperatures. If we are only interested in the $T = 0$ behaviour of the system we may prefer to avoid the complications of the discrete Matsubara frequencies and the final analytic continuation. In this case we may resort to the $T = 0$ formalism in which the calculation is carried out directly on the real axis. The Feynman rules are then the following [84, p. 167]:

• Internal lines with frequency $\omega_i$ and spin $\sigma_i$ receive a factor of $iG_{\sigma_i}(\omega_i)$.

• Interaction vertices are associated with a factor $-iU$.

• Impose frequency conservation at all vertices and integrate over the undetermined frequencies with measure $\int_{-\infty}^{\infty} \frac{d\omega}{2\pi}$.

• If the diagram has an odd number of fermion loops multiply its amplitude by $-1$.

• Multiply the overall amplitude with $-i$.

1.6.2. Causal and retarded quantities

The result of perturbative calculations, in either the Matsubara or $T = 0$ formalism, is a causal quantity. In general, such quantities are continuous but not
differentiable at the origin. Given a causal quantity \( X^c(\omega) \) one can deduce the corresponding retarded quantity \( X^+(\omega) \) using the relation

\[
\text{Re} \ X^c(\omega) + i \text{Im} \ X^c(\omega) = \text{Re} \ X^+(\omega) + i \text{sign}(\omega) \text{Im} \ X^+(\omega). \tag{1.61}
\]

In this thesis the role of \( X \) is played either by a self-energy or a Green’s function.

\[1.7. \] Properties of the self-energy

In this section we summarise some important exact results for the Anderson model.

\[1.7.1. \] Ward identity

One of the key concepts in field theory is the concept of a symmetry, which is defined as a transformation that leaves the action of the system invariant. Symmetries are particularly important in light of Emmy Noether’s famous theorem, which asserts that there is a conserved quantity for each differential symmetry (or generator) of the system [139]. For example, many systems are invariant under a coordinate shift; this reflects the homogeneity of space and gives rise to the law of conservation of momentum. Similarly, invariance under a translation in the time coordinate leads to the concept of conservation of energy. Noether’s theorem thus links a fundamental assumption of physics — that its laws do not change with time and are the same anywhere — to the seemingly unrelated laws of energy and momentum conservation.

Noether’s theorem was originally derived in the context of classical field theory. Like classical theories, quantum field theories can possess the usual symmetries, such as invariance under a translation in the time coordinate, but can additionally exhibit an internal symmetry under a (potentially local) phase transformation of the fields. Such transformation are known as gauge transformations, which give rise to gauge symmetries which lie at the heart of the Standard Model of particle physics. Each symmetry will again give rise to a conserved quantity, i.e. an exact relation between quantities, which in the quantum context is termed a Ward identity.

The action of the Anderson model is invariant under the SU(2) rotation of the impurity fields

\[
\begin{pmatrix}
  d^\uparrow(\tau) \\
  d^\downarrow(\tau)
\end{pmatrix}
= M(\tau)
\begin{pmatrix}
  d'^\uparrow(\tau) \\
  d'^\downarrow(\tau)
\end{pmatrix}, \tag{1.62}
\]

35
where $M(\tau)$ is a $2 \times 2$ matrix defined as $M(\tau) = \exp(-i\sigma \cdot \alpha(\tau))$ in terms of a vector of the three Pauli matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ and a real differentiable function $\alpha(\tau)$. In the limit of a flat wide conduction band it can be shown that the invariance of the Hamiltonian under Eq. (1.62) implies that

$$\frac{\partial \Sigma_{\sigma}(\omega)}{\partial \omega} \bigg|_{\omega=0} + \frac{\partial \Sigma_{\sigma}(0)}{\partial \epsilon_d} = -\rho_{-\sigma}(0)\Gamma_{\sigma,\pi}(0,0),$$  

$$\frac{\partial \Sigma_{\sigma}(\omega)}{\partial \omega} \bigg|_{\omega=0} - \sigma \frac{\partial \Sigma_{\sigma}(0)}{\partial h} = \rho_{-\sigma}(0)\Gamma_{\sigma,\pi}(0,0).$$  

This result can be restated in a number of different ways, all of which are referred to as ‘the Ward identity’ in the literature. For instance, in the limit $\omega \to 0$ we can relate the self-energy to the reduced susceptibilities through

$$\text{Re } \Sigma_{\sigma}(\omega) = Un_{-\sigma} + \left(1 - \frac{\overline{\chi}_s + \overline{\chi}_c}{2}\right)\omega + O(\omega^2),$$  

$$\text{Im } \Sigma_{\sigma}(\omega) = -\left(\frac{\overline{\chi}_s - \overline{\chi}_c}{2}\right)^2 \frac{\omega^2}{2\Delta} + O(\omega^3).$$  

Finally, we can use Eq. (1.66) to show that

$$\overline{\chi}_s + \overline{\chi} = 2\gamma.$$  

The existence of the Ward identity for the AIM was originally derived from perturbation theory by Yamada and Yosida [134, 138, 135] and subsequently generalised by Oguri [96] to the AIM out of equilibrium. Recently Kopietz et al. presented a proof based on functional methods [71].

### 1.7.2. Results from Fermi liquid theory

Fermi liquid theory is a general phenomenological theory applicable to many interacting fermionic systems, and is particularly useful in describing the low temperature behaviour of many ‘ordinary’ metals. It was originally developed by Lev D. Landau in 1956 [76, 75] to explain why, at low temperatures, the specific heat of liquid $^3$He increases linearly with temperature as one would expect from a Fermi gas. Though the observed slope was larger than the theoretical prediction, such linear behaviour was thought to be characteristic of a non-interacting system, which a liquid ostensibly is not. Fermi liquid theory succeeded in ex-
plaining why an interacting system can behave qualitatively as a non-interacting
and has since been a central topic in condensed matter and particle physics.

Consider a non-interacting system in an a state \( \psi = |n_{p_1,\sigma_1}n_{p_2,\sigma_2} \ldots \rangle \), where
\( n_{p_i,\sigma_i} \) denotes the number of electrons with momentum \( p_i \) and spin \( \sigma_i \). In its
ground state, for instance, \( n_{p,\sigma} = \theta(p_F - p) \), where \( p_F \) is the Fermi momentum.
As we turn on the interactions, Fermi liquid theory argues that the resultant
state of the interacting system can again be labelled in the same way, and will
thus be in a one-to-one correspondence with the non-interacting ground-state.
Furthermore, it also asserts that this is true even for the excited states. To see
why, one must realise that the excited states of the non-interacting system can
again solely by labelled in terms of \( n_{p_i,\sigma_i} \) and that turning on interactions will,
in either case, not affect quantum numbers such as spin and momentum.

We thus arrive at the notion of a quasi-particle — an excited state, a com-
plicated mess of interactions and virtual processes that nonetheless behaves just
like a particle with modified dynamical properties (such as the effective mass).
Remarkably, the quasi-particles themselves are weakly interacting, since the ma-
ajority of the interaction effects have been already accounted for by the quasi-
particle picture.

Another key concept in Fermi liquid theory is thus the notion of the adiabatic
switching on of interactions, necessary to ensure that the system remains in
equilibrium throughout. Note that the quasi-particle excitations away from the
Fermi sphere have a finite lifetime \( \tau_q \) proportional to the inverse of the excitation
energy \( (\tau_q \varepsilon_{p,\sigma}^{-1}) \) before they decay in electron-hole pairs. The adiabatic switching
on of the interactions must therefore take place on time-scales smaller than \( \tau_q \).

A remarkable feature of the Fermi liquid quasi-particle pictures is that the
quasi-particles are weakly interacting. In Ref. [95] Nozières applied the principles
of Fermi liquid theory to the Kondo model and achieved an expansion in terms
of phenomenological Fermi liquid parameters. He conjectured that the Anderson
impurity model can be similarly described, though this was not actually pursued
until much later [89].

The self-energy \( \Sigma(\omega) \) of a Fermi liquid must satisfy certain properties. First,
\( \Sigma(0) \) and \( \Sigma'(0) \) must be real at zero frequency; this implies that in the limit
\( \omega \to 0 \), \( \text{Im } \Sigma(\omega) \sim \omega^2 \). This is confirmed by the explicit result in Eq. (1.66)
and will prove useful in formulating the renormalised perturbation theory.
1.7.3. Friedel-Langreth sum rule

The Friedel-Langreth \[77\] sum rule is another exact result for the Anderson model that we will make extensive use of. Given the (exact) self-energy at zero frequency, it allows us to calculate the impurity occupation from

\[
n_\sigma = \frac{1}{2} - \frac{1}{\pi} \tan^{-1}\left(\frac{\epsilon_d + \sigma h + \Sigma_{-\sigma}(0)}{\Delta}\right).
\]  

(1.68)

If the frequency dependence of the self-energy is known, then \(n_\sigma\) can also be found by directly integrating the spectral density up to the Fermi level

\[
n_\sigma = \int_{-\infty}^{0} d\omega \rho_\sigma(\omega).
\]  

(1.69)

If the self-energy is known exactly, the two expressions for the occupation will agree. Typically, however, the self-energy is only known to an approximation. We expect then that the two estimates will differ, and it is not \textit{a priori} clear whether Eq. (1.68) or Eq. (1.69) will provide a more accurate estimate for \(n_\sigma\).

1.8. The Bethe ansatz

The \textit{Bethe ansatz} is a method introduced by Hans Bethe in 1931 \[18\] in the context of the Heisenberg model, where he showed that it can be used for the exact calculation of the eigenvectors and eigenvalues of one-dimensional quantum systems. Nevertheless, it was not until the 1980s that it was applied to quantum impurity problems, starting from the Kondo model of Eq. (1.13) \[127, 129, 11\]. Solutions to the non-degenerate AIM appeared shortly thereafter \[130, 12, 67\].

In summary, the following exact equations were derived

\[
\chi^l_s = \sqrt{\frac{\pi}{2u}} \exp\left(\frac{\pi^2 u}{8} - \frac{1}{2u}\right) + \frac{1}{\sqrt{2\pi u}} \int_{-\infty}^{\infty} dx \frac{e^{-x^2/2u}}{1 + (\pi u/2 + ix)^2},
\]

(1.70)

\[
\chi^l_c = \frac{1}{\sqrt{2\pi u}} \int_{-\infty}^{\infty} dx \frac{e^{-x^2/2u}}{1 + (\pi u/2 + x)^2},
\]

(1.71)

\[
\gamma = \frac{1}{2} (\chi^l_s + \chi^l_c), \text{ where } u = \frac{U}{\pi \Delta}.
\]

(1.72)

Note that Eq. (1.72) is just an explicit statement of the Ward identity. We highlight the appearance of the exponential functions, which contain \(u\) to all powers. Important insight into the connection between these results and the perturbation theory was provided by Zlatić and Horvatić \[142, 60\] who expressed
Figure 1.4.: Exact results for the reduced spin and charge susceptibilities (Eq. 1.70, 1.71 for the particle-hole symmetric model.

Eq. (1.70)-(1.72) as a power series in $u$ by introducing a set of coefficients $C_n$ which can be calculated through a recurrence relation. They found that at $T = 0$

$$\chi^s_l = \sum_{n=0}^{\infty} C_n u^n, \quad \chi^c_l = \sum_{n=0}^{\infty} (-1)^n C_n u^n,$$

where the coefficients $C_n$ satisfy

$$C_n = (2n - 1)C_{n-1} - \frac{\pi^2}{4} C_{n-2},$$

with $C_0 = C_1 = 1$. The first terms in this expansion are none other than those calculated by Yamada and Yosida [137, 134, 138, 135]. The similarity in the two expressions of Eq. (1.73) is not coincidental and is a reflection of the spin-isospin symmetry discussed in Section 1.4. By iterating Eq. (1.74) we can calculate the susceptibilities to any order in $U$. An important property of the coefficients $C_n$ is that they decrease very rapidly with $n$ [142], allowing certainly quantities, such as the Wilson ratio (Eq. (1.31)), to be reliably calculated even in the strong correlation regime.

1.9. The Numerical Renormalisation Group

The renormalisation group is a framework developed largely by Kenneth Wilson for solving classes of problems in high-energy and condensed matter physics. In its early formulations it built on earlier work on scaling by Kadanoff, Widom and Fisher and succeeded in explaining the universal nature of critical exponents in second order transitions. It marked a significant improvement over Landau’s
mean-field approach to scaling relations, which, while successful in providing an effective description of universality, was incapable of deducing exponents in dimensions fewer than the upper critical dimension and could not be used to calculate non-universal properties, such as the transition temperature. Reviews of the application of the renormalisation group to statistical physics can be found in Ref. [133, 36].

The question of phase transitions aside, Wilson was one of the first to exploit the analogy between statistical mechanics and quantum field theory and apply the renormalisation group to impurity problems, with enormous success. The Numerical Renormalisation Group (NRG) is now one of the most reliable ways of calculating many properties of strongly correlated systems, having been applied to the usual and degenerate variations of the s-d model, the Anderson model, in or out of equilibrium; for a comprehensive review see Ref. [20]. A brief summary of the key points in the NRG will be presented in this section — the complexity of the method and subtleties associated with it prevent a more comprehensive exposition; more information can be found in Ref. [131, 132, 72, 73, 50, 20].

In Eq. (1.1) the Hamiltonian of the AIM is written in terms of the parameters $\epsilon_d, \Delta, U$. In general, any Hamiltonian can be written as $\mathcal{H}(K)$, where $K \in \mathcal{K}$ is a set of parameters in the manifold $\mathcal{K}$ of all possible Hamiltonian configurations. The Numerical Renormalisation Group is a mapping $R : \mathcal{K} \to \mathcal{K}$. The mapping is not necessarily linear or invertible, and is typically characterised by a parameter $\alpha$, which, for simplicity, we take to be a real number.

We also define an associative binary operation $\circ : \mathcal{K} \times \mathcal{K} \to \mathcal{K}$ that and assume that there is an identity element $I \in \mathcal{K}$. We require that

$$R_{\alpha \alpha'} = R_{\alpha} \circ R_{\alpha'}, \quad \forall \alpha, \alpha'. \quad (1.75)$$

To avoid confusion, we clarify that the word ‘group’ is somewhat of a misnomer, as ($R$ only constitutes a semi-group in the mathematical sense [132]). An important concept in the theory of the NRG is that of a fixed point $K^* \in \mathcal{K}$ under a transformation $R_\alpha$, defined such that

$$K^* = R_\alpha K^*. \quad (1.76)$$

Our starting point now is the Hamiltonian of Eq. (1.1) with a flat conduction band of width $2D$. We place the impurity at $\mathbf{r} = 0$ and assume an isotropic

---

It can also be seen as a mapping $R : \mathcal{H} \to \mathcal{H}$, where $\mathcal{H}$ is the manifold of possible Hamiltonians.
conduction band (i.e. that the conduction operators and hybridisation elements depend only on $k$, not $\mathbf{k}$). We then expand the operators in spherical harmonics, and, since by symmetry only $s$-states need to be considered, discard all states with $l \neq 0$.

We introduce a real number $\Lambda > 1$, known as the discretisation factor, and use it to partition the formerly-continuous conduction band into an infinity of logarithmically spaced discrete intervals i.e. the wavevector $k$ of the $n$‘th interval falls in the interval $(\Lambda^{-(n+1)}, \Lambda^{-n})$. Carrying out the discretisation in this manner introduces a hierarchy of clearly-separated energy scales. We thus arrive at the linear-chain Hamiltonian [72]

$$
\hat{H}^{(N)} = \Lambda^{N-1/2} \left[ \Lambda^{-n/2} \xi_n \sum_{\sigma} (f_{n,\sigma}^\dagger f_{n+1,\sigma} + f_{n+1,\sigma}^\dagger f_{n,\sigma}) \right],
$$

(1.77)

$$
\hat{H}^{(0)} = \hat{H}^{(0)}_0 + \hat{H}^{(0)}_c,
$$

(1.78)

$$
\hat{H}^{(0)}_0 = \sum_{\sigma} \varepsilon_{d,\Lambda} c_{d,\sigma}^\dagger c_{d,\sigma} + U_{\Lambda} (\sum_{\sigma} c_{d,\sigma}^\dagger c_{d,\sigma} - 1)^2,
$$

(1.79)

$$
\hat{H}^{(0)}_c = V_{d,\Lambda} \sum_{\sigma} \left( f_{0,\sigma}^\dagger c_{d,\sigma} + c_{d,\sigma}^\dagger f_{0,\sigma} \right),
$$

(1.80)

where the operators $f_{n,\sigma}$ define a basis which is related to the original basis through a unitary transformation, $\varepsilon_{d,\Lambda}, V_{d,\Lambda}, U_{\Lambda}$ are functions of the corresponding variable and $\Lambda$, and $\xi_n$ are exponentially decreasing functions of $n$. In the limit $N \to \infty$ we recover the original Hamiltonian of Eq. (1.1) up to a scale factor involving $\Lambda$ (this can also be achieved by setting $\Lambda = 1$).

This satisfies the recurrence relation

$$
\hat{H}^{(N+1)} = \Lambda^{1/2} \hat{H}^{(N)} + \xi_N \sum_{\sigma} (f_{N,\sigma}^\dagger f_{N+1,\sigma} + f_{N+1,\sigma}^\dagger f_{N,\sigma}),
$$

(1.81)

which also constitutes the definition of the renormalisation group mapping $R_{\Lambda}$. The significance of rewriting the Hamiltonian in this manner is that it permits its iterative diagonalisation. We begin with $\hat{H}^{(0)}$, which comprises a Hamiltonian $\hat{H}_0$ that involves only the impurity and a term $\hat{H}_c$ that couples the impurity to the 0th site. The eigenstates of Eq. (1.79) can be determined analytically. Given this basis one can then numerically obtain an eigenbasis $| \psi \rangle_0$ for the combined $\hat{H}^{(0)}$; the elements of this are labelled by the ‘good’ quantum numbers appropriate for the problem (for example, in the absence of a magnetic field spin and charge constitute ‘good’ quantum numbers). To determine the eigen-
basis of $H_{N+1}$, given the eigenbasis of $H_N$, we form the outer product of $|\rangle_N$ with a 1-particle eigenbasis for the additional site. The resultant spectrum increases quickly in size and practical computational considerations necessitate its truncation. Typically at each step one retains only the $10^4$ or so lowest-lying states and consequently, due to the loss of information, renders the transformation non-invertible. Another complication arises due to the discrete nature of the linear chain Hamiltonian, which results in a spectral density consisting of a series of delta functions. To obtain a smooth spectrum one must convolve these peaks with a broadening kernel; this is typically accomplished using log-Gaussian function, or another function with long tails.

Despite its power, the NRG has a number of drawbacks. First, the discretisation and broadening of the conduction band introduces an element of uncertainty to the calculation. In practice this itself as a spurious oscillation of the self-energy — or any operator expectation value — at low frequencies, making it sometimes difficult to extract precise results, particularly for large values of $\Lambda$. Consequently, schemes for combining calculations performed with different values of the discretisation have been developed [98, 128]. A more serious limitation to the method is the exponential increase in the number of states that have to be retained as further impurity sites are added to the problem. For computational reasons this greatly restricts the application of the NRG to highly degenerate models and multiple-impurity scenarios.
2. Renormalised perturbation theory

2.1. The Renormalised Perturbation Theory

In Sec. 1.6 we saw how a systematic perturbation expansion in powers of $U$ can be constructed around the non-interacting limit. The disadvantage of this approach is that in practice one can only calculate the first few terms of the series. For small values of $U$, the truncated series for the self-energy will, by construction, constitute a good approximation to the self-energy. As $U$ is increased this will progressively cease to be the case, and our approximation will not even be qualitatively correct. This is precisely the challenge posed by strong correlation physics.

The Renormalised Perturbation Theory (RPT) is an attempt to rectify this inapplicability of ordinary (or bare) perturbation theory to the strong correlation regime [48, 49, 47, 51, 55, 52, 53, 17]. In very broad terms, the reason the bare perturbation expansion fails when $U$ is large is that the non-interacting model is not a suitable starting point and, as a result, the perturbation corrections are quite large. The effect of the interactions is particularly important at low energies, and depending on their strength may result in very significant renormalisations of the parameters of the system. Rather than try to account for these in a perturbative manner, in the RPT these effects are automatically taken into account from the outset by working with the renormalised values directly. A penalty one has to pay is that the renormalised expansion is more cumbersome to carry out, as in addition to the interaction vertices, one must also include counter-terms, to ensure that effects included in the renormalised parameters are not over-counted.

In high-energy physics the renormalised perturbation theory has been used to extract physically significant predictions from quantum field theory [105, 109, 31]. In that context, the renormalisation effects were divergent, prompting the famous analogy to ‘sweeping infinities under the rug’. By absorbing these infinite renormalisations into the bare parameters of the model, one can make predictions in terms of the renormalised parameters, eliminating the dependence of the theory
on their unobservable bare values. The additional complication in this scenario is of course the divergence itself which has to be controlled through some regularisation scheme. In condensed matter physics such divergences do not occur in neither the high-energy limit, where the lattice spacing provides a high-frequency cut-off, nor the in low-energy limit where the system size sets a minimum scale. The principle is thus the same, but the technical details differ considerably.

We will set up the RPT of the Anderson model by adopting two different, but complementary, viewpoints. In the first case we will start with the interacting Green’s function and show how a Taylor expansion of the self-energy can be used to define a renormalised pair propagator. In the second point of view we will consider the renormalisation of the Lagrangian density directly.

2.1.1. Renormalisation of the correlation functions

Our starting point is the interacting Green’s function of the AIM in the zero-temperature formalism. The argument we will put forward is presented in Ref. [49], and is similar for the advanced and causal incarnations of the Green’s function. For concreteness we will use the retarded propagator

\[ G^+_\sigma(\omega) = \frac{1}{\omega - \epsilon_{d,\sigma} + i\Delta - \Sigma^+_\sigma(\omega)}, \]  

(2.1)

where a potentially non-zero magnetic field has been absorbed in \( \epsilon_{d,\sigma} = \epsilon_d - \sigma h \). Since we are interested in incorporating the low-energy interaction effects in the parameters, we perform a Taylor expansion of the self-energy around \( \omega = 0 \)

\[ \Sigma^+_\sigma(\omega) = \Sigma^+_\sigma(0) + \Sigma^+_\sigma'(0)\omega + \Sigma^{\text{rem,}+}_\sigma(\omega), \]  

(2.2)

where \( \Sigma^{\text{rem,}+}_\sigma(\omega) = O(\omega^2) \). To carry out the Taylor expansion we have to assume that \( \Sigma^+_\sigma(\omega) \) is an analytic function of frequency. Since the single-impurity model is a Fermi liquid in all parameter regimes (Sec. 1.7.2), this is justified assumption. Furthermore, it ensures that \( \Sigma^+_\sigma(0) \) and \( \Sigma^+_\sigma'(0) \) are real at zero temperature\(^1\). By inserting Eq. (2.2) into Eq. (2.1) we deduce that

\[ G^+_\sigma(\omega) = z_\sigma \tilde{G}^+_\sigma(\omega), \]  

(2.3)

\(^1\)We note in passing that the formulation of RPT is presently tied to models with Fermi-liquid behaviour. Furthermore, the renormalised parameters are only defined at zero temperature; in Appendix A we explore the possibility of formulating the theory for \( T \neq 0 \).
where \( \tilde{G}_\sigma^+(\omega) \) is the retarded renormalised (or quasi-particle) propagator given by
\[
\tilde{G}_\sigma^+(\omega) = \frac{1}{\omega - \tilde{\epsilon}_{d,\sigma} + i\tilde{\Delta}_\sigma - \tilde{\Sigma}_\sigma^+(\omega)}.
\] (2.4)

The renormalised quantities are defined with respect to their bare counter-parts as follows
\[
\tilde{\Delta}_\sigma = z_\sigma \Delta,
\] (2.5)
\[
\tilde{\epsilon}_{d,\sigma} = z_\sigma (\epsilon_{d,\sigma} + \Sigma_\sigma^+(0)),
\] (2.6)
\[
\tilde{\Sigma}_\sigma^+(\omega) = z_\sigma \Sigma_{\sigma}^{\text{rem},+}(\omega),
\] (2.7)

where the quasi-particle weight is given by
\[
z_\sigma = \frac{1}{1 - \Sigma_{\sigma}^{\text{rem}}(0)}.
\] (2.8)

Note that in Eq. (2.6) and (2.8) the retarded self-energy \( \tilde{\Sigma}_\sigma^+(\omega) \) can be replaced with the causal self-energy \( \tilde{\Sigma}_\sigma(\omega) \), since \( \tilde{\Sigma}_\sigma(0) \) and \( \tilde{\Sigma}_\sigma^+(0) \) are real. By studying the two-point correlation function we have shown how the low-energy effects can be absorbed into the two model parameters, \( \tilde{\epsilon}_d \) and \( \tilde{\Delta} \), with a one-particle nature.

To complete our treatment we have to consider the effects of two-particle interactions, which cannot be studied from the Green’s function alone. We therefore turn our attention to higher correlation functions and introduce a renormalised interaction constant \( \tilde{U} \), which we define in terms of the four-vertex at zero frequency as
\[
\tilde{U} = z_\sigma z_{-\sigma} \Gamma_{\sigma,-\sigma}(0,0).
\] (2.9)

For brevity we will henceforth adopt the shorthand notation \( \mu = (\epsilon_{d,\downarrow}, \Delta, U) \) and \( \tilde{\mu} = (\tilde{\epsilon}_{d,\downarrow}, \tilde{\Delta}, \tilde{U}) \) in the absence of a magnetic field. In non-zero magnetic fields the bare and renormalised levels are spin-dependent while in the renormalised theory the hybridisation is also spin-dependent (Eq. (2.5)). It is understood then that \( \mu = (\epsilon_{d,\downarrow}, \epsilon_{d,\uparrow}, \Delta, U) \) and \( \tilde{\mu} = (\tilde{\epsilon}_{d,\downarrow}, \tilde{\epsilon}_{d,\uparrow}, \tilde{\Delta}_\downarrow, \tilde{\Delta}_\uparrow, \tilde{U}) \).

### 2.1.2. Renormalisation of the Lagrangian density

In this section we consider the Lagrangian formulation of the renormalised theory presented in Ref. [51]. Consider Eq. (2.3), which relates the renormalised and bare Green’s function. From the observation that they only differ by a factor of \( z \), and with the operator definition of Eq. (1.49) in mind, we can conclude
that the renormalised fields must similarly only differ from the bare fields by a multiplicative factor. In either the $\tau$ or $\omega$ bases we have

\[
\tilde{d}_\sigma = z_{\sigma}^{-1/2} d_\sigma,
\]
\[
\tilde{\tilde{d}}_\sigma = z_{\sigma}^{-1/2} \tilde{d}_\sigma.
\] (2.10)

Furthermore, a 'number operator' can be defined as $\tilde{n}_\sigma = \tilde{d}_\sigma \tilde{\tilde{d}}_\sigma$ and will satisfy $\tilde{n}_\sigma = \tilde{z}_\sigma n_\sigma$.

We are now in a position to examine the renormalisation of the Lagrangian. We start by separating the bare Lagrangian density into a renormalised Lagrangian (in terms of renormalised parameters) and a counter-term Lagrangian of the same form

\[
\mathcal{L}(\mu) = \tilde{\mathcal{L}}(\tilde{\mu}) + \tilde{\mathcal{L}}_{ct}(\lambda(\tilde{\mu})),
\] (2.11)

where

\[
\tilde{\mathcal{L}}_{ct}(\lambda) = \sum_{\sigma=\uparrow,\downarrow} \tilde{d}_\sigma(\tau)(\lambda_{2,\sigma}\partial_\tau + \lambda_{1,\sigma})\tilde{d}_\sigma(\tau) + \lambda_3 \tilde{n}_\uparrow(\tau)\tilde{n}_\downarrow(\tau).
\] (2.12)

This counter-term Lagrangian will depend on $\tilde{\mu}$ only implicitly, through the counter-terms $\lambda = (\lambda_{1,\sigma}, \lambda_{2,\sigma}, \lambda_3)$ — we will discuss this shortly. To set up the RPT we separate the Lagrangian $\mathcal{L}$ into renormalised non-interacting and interacting components

\[
\tilde{\mathcal{L}}_0 = \sum_{\sigma} \tilde{d}_\sigma(\tau)\left(\partial_\tau - \tilde{\varepsilon}_{d,\sigma} + i\Delta_\sigma\right)\tilde{d}_\sigma(\tau),
\]
\[
\tilde{\mathcal{L}}_I = \tilde{U} \tilde{n}_\uparrow(\tau)\tilde{n}_\downarrow(\tau) + \tilde{\mathcal{L}}_{ct}(\mu).
\] (2.13)

The non-interacting component now gives rise to a renormalised non-interacting thermal Green’s function defined, on the imaginary time axis, in analogy to Eq. (1.49)

\[
\tilde{\tilde{G}}_\sigma(\tau_1, \tau_2) = \tilde{\tilde{G}}_\sigma(\tau_1 - \tau_2) = \langle \tilde{d}_\sigma(\tau_1)\tilde{\tilde{d}}_\sigma(\tau_2) \rangle.
\] (2.14)

Of particular practical importance for diagrammatic calculations is its frequency-space non-interacting version, which is equal to

\[
\tilde{\tilde{G}}_\sigma^{(0)}(\omega_n) = \frac{1}{i \omega_n - \tilde{\varepsilon}_{d,\sigma} + i\Delta_\sigma \text{sign}(\omega_n)},
\] (2.15)

and can be related to causal variant of the retarded $T = 0$ propagator of Eq. (2.1)
by an analytic continuation, as discussed in Sec. 1.5.2. Note that in contrast to
the bare perturbation theory, the structure of the interacting Lagrangian in the
renormalised theory is more complicated due to the presence of the counter-
terms. In particular, the $\lambda_{1,\sigma}$ and $\lambda_{2,\sigma}$ counter-terms will contribute one-particle
vertices to the diagrammatics of the RPT. Similarly, $\lambda_3$ constitutes a two-particle
interaction vertex, somewhat similar to the renormalised four-vertex but which
is a polynomial in $\tilde{U}$. Along with the renormalised Coulomb term, the counter-
terms will give rise to a renormalised self-energy $\tilde{\Sigma}(\omega)$ and an interacting Green’s
function $\tilde{G}_\sigma(\omega)$, defined through the Dyson equation 
\[ \tilde{G}_{\sigma}(\omega)\] 
\[ \frac{1}{\tilde{G}_{\sigma}(\omega)} = \left( \tilde{G}_{\sigma}^{(0)}(\omega) \right)^{-1} - \tilde{\Sigma}_{\sigma}(\omega; \tilde{\mu}). \]

To determine the counter-terms as functions of the renormalised par ameters
we impose the renormalisation conditions
\[ \tilde{\Sigma}_{\sigma}(0) = 0, \]
\[ \tilde{\Sigma}_\sigma'(0) = 0, \]
\[ \tilde{\Gamma}_{\sigma, -\sigma}(0, 0) = \tilde{U}. \] (2.16)

Note that the first two renormalisation conditions are equivalent to the definition
of $\tilde{\Sigma}_{\sigma}(\omega)$ in terms of the Taylor remainder of Eq. (2.7), though they do not
make explicit reference to the bare self-energy. To impose these conditions one
is forced to adopt some approximation for $\tilde{\Sigma}_{\sigma}(\omega)$; the counter-terms will thus
clearly depend on the chosen approximation, in contrast to the renormalised
parameters which depend only on the model.

In generalising our treatment to non-zero magnetic fields, two ways of defining
the renormalised parameters naturally present themselves:

1. **Field-independent counter-terms**: We apply the conditions of Eq. (2.16)
at zero-field. Turning the field on then renders the cancellation of the counter-term with the self-loop diagram incomplete, necessitating the explicit inclusion of the counter-term in any calculation (also see Sec. 2.3.1).

2. **Field-dependent counter-terms**: Following Refs. [53, 17], we define the renormalised parameters as

   \[ z_{\sigma}(h) = [1 - \partial_\omega \Sigma_{\sigma}(\omega, h)|_{\omega=0}]^{-1}, \] (2.17)

   \[ \tilde{\epsilon}_{d,\sigma}(h) = z_{\sigma}(h)(\epsilon_{d,\sigma} + \Sigma_{\sigma}(0, h)), \] (2.18)

   \[ \tilde{\Delta}_{\sigma}(h) = z_{\sigma}(h)\Delta, \] (2.19)
and the renormalised self-energy as
\[ \tilde{\Sigma}_\sigma(\omega, h) = z_\sigma(h) \left[ \Sigma_\sigma(\omega, h) - \omega \partial_\omega \Sigma_\sigma(\omega, h) \bigg|_{\omega=0} - \Sigma_\sigma(0, h) \right]. \] (2.20)

The renormalisation conditions in Eq. (2.16) are imposed at finite-field, yielding field-dependent counter-terms \( \lambda_{1,\sigma}(h) \), \( \lambda_{2,\sigma}(h) \) and \( \lambda_{3}(h) \). Using these definitions, we can rewrite the bare Green’s function in a magnetic field (Eq. (2.1)) as
\[ G_\sigma(\omega) = \frac{z_\sigma(h)}{\omega - \tilde{\epsilon}_d(h) + z_\sigma(h)\sigma h + i\tilde{\Delta}_\sigma(h) - \tilde{\Sigma}_\sigma(\omega, h)}. \] (2.21)

### 2.1.3. The renormalised parameters

In the previous section, we saw how the renormalised parameters \( \tilde{\mu} \) can be determined from the bare self-energy and four-vertex. However, these quantities are not generally known; after all, determining them is essentially the challenge of many-body physics. Crucially, the definitions of the parameters in terms of the bare self-energy and four-vertex involve only \( \Sigma_\sigma(0), \Sigma'_\sigma(0) \) and \( \Gamma(0) \). This opens up the possibility of determining the parameters from the NRG introduced in Sec. 1.9. Since the NRG can determine the self-energy itself, the definitions in Eq. (2.5), (2.6) (2.9) can in principle be used directly. In practice, the accuracy of this approach is vitiated by oscillatory artefacts in the NRG caused by the broadening and discretisation [63]) procedure, and which are particularly pronounced at low energies. To overcome this, Ref. [55] describes a method by which the renormalised parameters can be extracted from the NRG fixed point directly.

In the special case of particle-hole symmetry, the exact results of the Bethe Ansatz (see Sec. 1.8) can also be used to deduce the renormalised parameters. From the definitions of the susceptibilities, we can infer the relations
\[ \tilde{U} = 2\pi \Delta \frac{\tilde{\chi}_s - \tilde{\chi}_c}{(\tilde{\chi}_s \tilde{\chi}_c)^2}, \] (2.22)
\[ \tilde{\Delta} = 2\Delta \frac{1}{\tilde{\chi}_s \tilde{\chi}_c}, \] (2.23)
which allow us to numerically compute \( \tilde{U} \) and \( \tilde{\Delta} \) from Eq. (1.70), (1.71). By carefully evaluating these expressions numerically, we can calculate the stationary
Figure 2.1.: The renormalised parameters $\tilde{U}, \tilde{\Delta}$ for (2.1a) a symmetric and an
(2.1b) asymmetric (right) model as a function of $U/\pi \Delta$.

point of $\tilde{U}(U)$

$$\frac{U_s}{\pi \Delta} = 0.856122.$$  \hfill (2.24)

In Fig. 2.1 we show how the renormalised parameters $\tilde{U}, \tilde{\Delta}$ (determined from
the NRG) depend on $U$. We see that in the case of Kondo limit ($U \to \infty$) of
the symmetric model, a single energy scale emerges as $U$ is increased. We can
write $\tilde{U} \to 4T_K$ and $\pi \tilde{\Delta} \to 4T_K$, where $T_K$ is known as the Kondo temperature,
as $U \to \infty$ [49]. Note furthermore that in this limit, $\tilde{U}\tilde{\rho}(0) = \tilde{U}/\pi \tilde{\Delta} \to 1$.

One might object that the RPT will be of limited use so long as it depends on
external methods for the determination of the renormalised parameters. This is
indeed a legitimate concern and we will address it in Chapter 4, where we will
discuss how they can be determined exclusively within the framework of RPT.

2.2. The Feynman rules in the renormalised theory

We proceed to discuss the rules in the renormalised theory (a more comprehensive
discussion is included in Ref. [15, p. 30]. In the Lagrangian formalism it is easy
to repeat the steps described in Sec. 1.5, but with the renormalised fields as
integration variables. The Green’s function can then be computed from the
explicit form of the functional definition of $\tilde{G}_\sigma(\tau_1, \tau_2)$ in Eq. (2.14)

$$\tilde{G}_\sigma(\tau_1, \tau_2) = \frac{\int D[\tilde{d}]D[\tilde{d}]d_\sigma(\tau_1)\tilde{d}_\sigma(\tau_2) \exp \left(-S[\tilde{d}, \tilde{d}]\right)}{\int D[\tilde{d}]D[\tilde{d}] \exp \left(-S[\tilde{d}, \tilde{d}]\right)}, \hfill (2.25)$$
where the action is computed in the renormalised theory as

\[ S[\tilde{\sigma}, \tilde{d}] = \int d\tau \left( \tilde{\mathcal{L}}(\tilde{\sigma}, \tilde{d}, \tilde{\mu}; \partial_\tau) + \tilde{\mathcal{L}}_{ct}(\tilde{\sigma}, \tilde{d}, \tilde{\lambda}(\tilde{\mu}); \partial_\tau) \right), \tag{2.26} \]

and is equal to action in the bare theory. We thus arrive at the following rules:

- Internal lines of frequency \( \omega_i \) and spin \( \sigma \) receive a factor \( i\tilde{G}_{\sigma}^{(0)}(\omega_i) \).
- Vertices are assigned a factor \( -i\tilde{U} \).
- Impose frequency conservation at each vertex and integrate over the remaining free variables with measure \( \int_{-\infty}^{\infty} d\omega \frac{d^2}{2\pi} \).
- Diagonals with an odd number of fermion loops receive a factor of \( -1 \).
- Multiply the overall amplitude by \( i \), to obtain \( \tilde{\Sigma}_{\sigma}(\omega) \), rather than \( -i\tilde{\Sigma}_{\sigma}(\omega) \).

Note that in the Lagrangian formalism the re-scaling of the Grassmann fields does not enter the derivation of the rules at all. By contrast, in the canonical formalism\(^2\) the re-scaled fields will satisfy the non-standard anti-commutation relation \( \{\tilde{c}_{d,\sigma}(\tau_1), \tilde{c}^\dagger_{d,\sigma'}(\tau_2)\} = z_\sigma \delta_{\sigma,\sigma'} \delta(\tau_1 - \tau_2) \). As a result, Wick’s theorem [1, p. 66], which the canonical formalism is usually based on, will have to be modified. These complexities can be avoided by re-introducing the bare operators in the renormalised theory. We can then make use of the usual rules of the bare perturbation theory (Sec. 1.6) with the substitutions \( \epsilon_d \to z_\sigma^{-1}\tilde{\epsilon}_d, \Delta \to z_\sigma^{-1}\tilde{\Delta}_\sigma \) and \( U \to z_\uparrow z_\downarrow \tilde{U} \) leading to peculiar form for the propagator

\[ \tilde{G}_{\sigma}^{(0)}(\omega) = \frac{1}{\omega - z_\sigma \tilde{\epsilon}_{d,\sigma} + iz_\sigma \tilde{\Delta}_\sigma \text{sign}(\omega)}. \tag{2.27} \]

After writing down the expression corresponding to a diagram we can perform the substitution \( \omega \to z\omega' \) — each diagram will be thus expressed as a product of a power of \( z \) and an expression involving renormalised variables. For an \( n \)th order diagram there are \( n-1 \) free integration variables, each contributing a factor of \( z \) from the Jacobian, \( n \) vertices contributing in total \( 2n \) factors of \( z^{-1} \) and \( 2n - 1 \) instances of Eq. (2.27) from which, when expressed in \( \omega' \), we can isolate a \( z^{-n} \) term. Altogether, the overall power of the factor of \( z \) is then \( -1 \). We thus conclude that we can effectively ignore the unusual commutation relation of the renormalised operators and deduce the same rules as given above.

\(^2\)In the interests of brevity, a discussion of perturbation theory in the canonical formalism has been omitted from Chapter 1; the interested reader is referred to Ref. [1, 84].
2.3. Perturbation expansions in $\tilde{U}$

In this section we discuss the perturbation theory in powers of $\tilde{U}$ and calculate the self-energy and four-vertex to order $\tilde{U}^3$ inclusive (this calculation was first carried out in Refs. [49, 51] in the special case of particle-hole symmetry, and also appears in Ref. [32]). The counter-terms represent a complication not present in the bare theory, and are best dealt by organising the calculation order-by-order. To simplify the notation we introduce an effective interaction $\tilde{U}_{\text{eff}} = \tilde{U} + \lambda_3$, which will also serve as a tentative expansion variable before we impose the renormalisation group equations. We will use the notation $X^{[n]}$ to denote the (strictly) $n$th order term in the power series expansion of $X$. We have the choice of using the $T = 0$ formalism (Sec. 2.1.1) or the Matsubara formalism in the zero temperature limit (Sec. 2.1.2). For simplicity we choose the former, to avoid the need for an analytic continuation. In our diagrams the internal lines will thus correspond to

$$\tilde{G}^{(0)}(\omega) = \frac{1}{\omega - \tilde{\epsilon}_d + i\tilde{\Delta} \text{sign}(\omega)}. \quad (2.28)$$

To simplify the calculation we will assume that any magnetic field is zero, i.e. $\tilde{\epsilon}_{d,\uparrow} = \tilde{\epsilon}_{d,\downarrow}$.

2.3.1. Mean-field

We begin by calculating the amplitude of the simplest possible diagram, the tadpole of Fig. 2.2 (see Ref. [49]). As this is frequency-independent it will be always cancelled by the counter-term. Similarly, the four-vertex trivially consists of a single instance of the effective interaction vertex. We thus have $\lambda_{1,\sigma} = -\tilde{U}\tilde{n}_{-\sigma} + \mathcal{O}(\tilde{U}), \lambda_{2,\sigma} = \lambda_3 = \mathcal{O}(\tilde{U}^2)$. Trivially, $\tilde{\Sigma}_{\sigma}^{[1]}(\Omega) = 0$ and $\tilde{\Gamma}_{\uparrow\downarrow}^{[1]} = \tilde{U}$. Note that — as remarked at the end of Sec. 2.1.2 — the counter-term will no longer cancel the self-loop if we turn on a magnetic field.
2.3.2. Second-order calculation

The second-order self-energy can be deduced [49] by calculating the diagram in Fig. 2.2b. The $\lambda_{1,\sigma}$ counter-term will only make a static contribution and therefore can be entirely ignored for our purposes. Similarly, the $O(\tilde{U}^2)$ cannot form part of a second-order diagram and is similarly ignored. By applying the Feynman rules as usual and defining the renormalised particle/hole-pair propagators

$$\tilde{\Pi}_{\sigma,-\sigma}^{pp}(\Omega) = i \int d\omega \tilde{G}^{(0)}_\sigma(\omega) \tilde{G}^{(0)}_{-\sigma}(\Omega - \omega),$$

$$\tilde{\Pi}_{\sigma,-\sigma}^{ph}(\Omega) = i \int d\omega \tilde{G}^{(0)}_\sigma(\omega) \tilde{G}^{(0)}_{-\sigma}(\Omega + \omega).$$

(2.29)

we arrive at two equivalent expressions for the self-energy

$$\tilde{\Sigma}^{[2]}_\sigma(\Omega) = -i \tilde{U}^2 \int d\omega \tilde{G}^{(0)}_\sigma(\omega - \Omega) \tilde{\Pi}_{\sigma,-\sigma}^{ph}(\omega) + \Omega \lambda^{[2]}_{2,\sigma} + \lambda^{[2]}_{1,\sigma}$$

$$= -i \tilde{U}^2 \int d\omega \tilde{G}^{(0)}_\sigma(\omega - \Omega) \tilde{\Pi}_{\sigma,-\sigma}^{pp}(\omega) + \Omega \lambda^{[2]}_{2,\sigma} + \lambda^{[2]}_{1,\sigma},$$

(2.30)

Note that the interaction vertex in the diagrams of Fig. (2.2) is really $\tilde{U}_{\text{eff}}$, not $\tilde{U}$. However, from the first-order calculation of the four-vertex we have that $\tilde{U}_{\text{eff}}^2 = \tilde{U}^2 + O(\tilde{U}^3)$, allowing us to ignore the influence of the $\lambda_3$ counter-term.

To find $\lambda^{[2]}_{2,\sigma}$ and $\lambda^{[2]}_{1,\sigma}$ we impose the renormalisation conditions of Eq. (2.16).

This can be done numerically using a finite-difference estimate of the derivative of the first term on the right-hand side of Eq. (2.30). From a numerical point of view, however, it is usually preferable to analytically differentiate Eq. (2.30) and only then to resort to numerics. From Eq. (2.28) we find\(^8\) that

$$\frac{d\tilde{G}^{(0)}_\sigma(\omega)}{d\omega} = \left[\tilde{G}^{(0)}_\sigma(\omega)\right]^2 - \frac{2i\Delta_\sigma}{\epsilon^2_{d,\sigma} + \Delta^2_\sigma} \delta(\omega) = \left[\tilde{G}^{(0)}_\sigma(\omega)\right]^2 - 2i\pi \rho^{(0)}_\sigma(0) \delta(\omega).$$

(2.31)

\(^8\)It is helpful to note that $\text{sign}(x) = 2\theta(x) - 1$ so $d\text{sign}(x)/dx = 2\delta(x)$. 

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Figure 2.3.: The two diagrams that contribute to the renormalised four-vertex to second order in $\tilde{U}$. 

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Figure 2.4.: The quantity $\pi\Delta\alpha_2$ (Eq. (2.35) plotted as a function of $\epsilon_d + U/2$ for a model with $U = 3\pi\Delta$.

We thus deduce an expression for the derivative of the self-energy:

$$
\partial_\omega \tilde{\Sigma}[2]_{\sigma}(\Omega) = -i \tilde{U}^2 \int d\omega \left[ \tilde{G}_{\sigma-\sigma}^{(0)}(\Omega - \omega) \right]^2 \tilde{\Pi}^{\text{ph}}_{\sigma-\sigma}(\omega) - \tilde{\rho}_{-\sigma}(0) \tilde{\Pi}^{\text{ph}}_{\sigma-\sigma}(\Omega) + \lambda[^2]_{2,\sigma}.
$$

(2.32)

We now turn our attention to the two particle four-vertex. The diagrams that contribute to it are shown in Fig. 2.3 and give

$$
\tilde{\Gamma}[2]_{\uparrow\downarrow}(\Omega_1, \Omega_2) = \tilde{U}^2_{\text{eff}} \left[ \tilde{\Pi}^{\text{ph}}_{\uparrow\downarrow}(0) + \tilde{\Pi}^{\text{pp}}_{\uparrow\downarrow}(0) \right].
$$

(2.33)

Applying the renormalisation condition we thus obtain

$$
\tilde{U} = \tilde{U}_{\text{eff}} + \tilde{U}^2_{\text{eff}} \alpha_2 + O(\tilde{U}^3) \quad \Rightarrow \quad \tilde{U}_{\text{eff}} = \tilde{U} - \tilde{U}^2 \alpha_2 + O(\tilde{U}^3),
$$

(2.34)

where

$$
\alpha_2 = \tilde{\Pi}^{\text{ph}}_{\uparrow\downarrow}(0) + \tilde{\Pi}^{\text{pp}}_{\uparrow\downarrow}(0) = \tilde{\rho}_{\sigma}(0) - \frac{1}{\pi\epsilon_d} \tan^{-1} \left( \frac{\epsilon_d}{\Delta} \right).
$$

(2.35)

Note that in the limit of particle-hole symmetry ($\epsilon_d = 0$) the two diagrams of Fig. 2.3 cancel and $\alpha_2 = 0$. This is true for all even-order terms of the $\tilde{U}$. Away from particle-hole symmetry we thus have that

$$
\lambda_3 = -\tilde{U}^2 \alpha_2 + O(\tilde{U}^3).
$$

(2.36)
2.3.3. Third-order calculation

The third-order skeleton diagrams that contribute to the self-energy [51] are shown in Fig. 2.5, which are equal to

\[
\tilde{\Sigma}_a^{[3]}(\Omega) = -\tilde{U}_\text{eff}^3 \int d\tilde{\omega} \tilde{G}^{(0)}(\omega - \Omega) \left[ \tilde{\Pi}_{\pi\sigma,\sigma}(\omega) \right]^2, \quad (2.37)
\]

\[
\tilde{\Sigma}_b^{[3]}(\Omega) = -\tilde{U}_\text{eff}^3 \int d\tilde{\omega} \tilde{G}^{(0)}(\Omega - \omega) \left[ \tilde{\Pi}_{\pi\sigma,\sigma}(\omega) \right]^2. \quad (2.38)
\]

At lower orders, the counter-term \(\lambda_3\) has not played an important role in our calculation. However, from Eq. (2.34) we find that \(\tilde{U}_\text{eff}^2 = \tilde{U}^2 - 2\alpha_2 \tilde{U}^3 + \mathcal{O}(\tilde{U}^4)\) and \(\tilde{U}_\text{eff}^3 = \tilde{U}^3 + \mathcal{O}(\tilde{U}^4)\). So, in addition to the contributions of the diagrams in Fig. 2.5, we have to consider the two diagrams obtained by replacing each of the interaction vertices in Fig. 2.2b with the \(\lambda_3\) counter-term given by Eq. (2.36).

We thus simply have

\[
\tilde{\Sigma}_c^{[3]}(\Omega) = -2i\tilde{U}_\text{eff}^3 \alpha_2 \int d\tilde{\omega} \tilde{G}^{(0)}(\Omega - \omega) \tilde{\Pi}_{\pi\sigma,\sigma}(\omega), \quad (2.39)
\]

where \(\alpha_2\) is given by Eq. (2.35). The third-order self-energy is thus

\[
\tilde{\Sigma}_\sigma^{[3]}(\Omega) = \tilde{\Sigma}_a^{[3]}(\Omega) + \tilde{\Sigma}_b^{[3]}(\Omega) + \tilde{\Sigma}_c^{[3]}(\Omega) + \Omega \lambda_2^{[3]} + \lambda_1^{[3]}. \quad (2.40)
\]

Again it is preferable to use Eq. (2.31) to analytically perform the differentiation needed to determine the \(\lambda_2\) counter-term, rather than a numerical derivative based on finite differences.

Note that a very considerable simplification of the calculation has been afforded by the assumption of a zero magnetic field. In a finite magnetic field one would have to account for the partial cancellation between the tadpole of Fig. 2.2a and the \(\lambda_1,\sigma\) counter-term defined at zero temperature. Thus we would have to consider insertions of the self-loop (and counter-term) in the second-order diagrams, and staggered tadpole diagrams, if we aim to calculate \(\tilde{\Sigma}_{\sigma}(\omega = 0, h)\).
In order to compare the results of the calculations above to the NRG results for the self-energy we set \( \pi \Delta = 0.01 \), \( \epsilon_d = -1.5\pi \Delta \) and \( U = 4\pi \Delta \), for which we find that \( \ddot{\epsilon}_d = 7.422 \times 10^{-6} \), \( \ddot{\Delta} = 1.113 \times 10^{-4} \) and \( \ddot{U} = 3.505 \times 10^{-4} \). Our results are shown in Fig. 2.6. We see that the corrections from the third-order term to the second-order self-energy are small, and, as is evident in the plot of the imaginary part, improve the agreement of the results with those obtained from the NRG.

### 2.4. Properties of the renormalised self-energy

#### 2.4.1. The Ward identities

In Sec. 1.7.1 we discussed how the theory’s gauge invariance leads to the identities of Eq. (1.63), (1.64). In this section we focus on Eq. (1.63) and derive the corresponding identity in the renormalised theory following Ref. [49]. Consider a model with the impurity orbital at \( \epsilon_d \). In the renormalised theory, the counter-terms are introduced so that Eq. (2.16) are satisfied, that is, the terms subtracted in Eq. (2.7) cancel \( \Sigma(\omega, \epsilon_d, \lambda(\epsilon_d)) \) at \( \omega = 0 \). When the orbital is shifted to \( \epsilon_d + \delta \epsilon_d \) with the counter-terms held constant, the cancellation is incomplete, resulting in a non-zero \( \partial \epsilon_d \Sigma(0, \epsilon_d, \lambda(\epsilon_d)) \). We thus have

\[
\frac{\partial}{\partial \epsilon_d} \Sigma(0, \epsilon_d, \lambda(\epsilon_d)) = \frac{\partial}{\partial \epsilon_d} (z(\epsilon_d)\Sigma(0, \epsilon_d) + \omega\lambda_2(\epsilon_d) + \lambda_1(\epsilon_d)) = \frac{\partial}{\partial \epsilon_d} (\ln z(\epsilon_d)\Sigma(0, \epsilon_d, \lambda(\epsilon_d)) + z(\epsilon_d)\frac{\partial}{\partial \epsilon_d} \Sigma(0, \epsilon_d))
\]  

(2.41)
Figure 2.7.: Diagrammatic representation of (2.7a) transverse spin susceptibilities and (2.7b) transverse charge susceptibilities in terms of the four-vertex in the particle-hole channel.

Noting the renormalisation conditions (Eq. (2.16)), the Ward identity in Eq. (1.63), and Eq. (2.3) we find that

\[
\frac{\partial \tilde{\Sigma}_\sigma(0, \epsilon_d)}{\partial \epsilon_d} = -\tilde{\rho}_\sigma(0) \tilde{U}. \tag{2.42}
\]

We can exploit the spin-isospin transformation to deduce the corresponding identity with respect to the magnetic field

\[
\frac{\partial \tilde{\Sigma}_\sigma(0, h)}{\partial \sigma_h} = \tilde{\rho}_\sigma(0) \tilde{U}. \tag{2.43}
\]

### 2.4.2. The Friedel-Langreth sum rule in RPT

The renormalised perturbation theory accommodates the Friedel-Langreth sum rule in a very natural way [49]. Starting with the statement of the rule in terms of the bare quantities, and invoking Eq. (2.5), (2.6)

\[
n_\sigma = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_{d,\sigma} + \Sigma_{\sigma}(0)}{\Delta} = \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \frac{\epsilon_{d,\sigma}}{\Delta_\sigma}. \tag{2.44}
\]

We see that the occupation in the renormalised theory can be determined from the renormalised parameters alone, without involving the renormalised self-energy.

### 2.4.3. Susceptibilities

By applying the definitions of the susceptibilities (Eqs. (1.21), (1.22)) to the statement of the Friedel-Langreth sum rule (Eq. (2.44)) we can derive concise expressions for the longitudinal susceptibilities in terms of the renormalised parameters [48, 49]. Expressions for the dynamic transverse susceptibilities in terms
of the renormalised parameters can be derived by considering their diagrammatic representation in Figs. 2.7a and 2.7b

\[ \chi_L^t(0) = \tilde{\Pi}_{\updownarrow \downarrow}^{ph}(0) \left[ 1 + \tilde{U} \tilde{\Pi}_{\updownarrow \downarrow}^{ph}(0) \right], \]  
\[ \chi_L^c(0) = \tilde{\Pi}_{\updownarrow \downarrow}^{pp}(0) \left[ 1 + \tilde{U} \tilde{\Pi}_{\updownarrow \downarrow}^{pp}(0) \right], \]  

where the renormalised pair propagators are defined in Eq. (2.29). Furthermore, we find that the longitudinal susceptibilities satisfy [52, 53, 17]

\[ \chi_L^t = -\left[ \tilde{\rho}_\uparrow(h) + \tilde{\rho}_\downarrow(h) + 2\tilde{U} \tilde{\rho}_\uparrow(h)\tilde{\rho}_\downarrow(h) \right], \]  
\[ \chi_L^c = \tilde{\rho}_\uparrow(h) + \tilde{\rho}_\downarrow(h) - 2\tilde{U} \tilde{\rho}_\uparrow(h)\tilde{\rho}_\downarrow(h). \]  

### 2.5. The second derivative

Of particular importance is the second frequency derivative of the self-energy. This will become evident in Sec. 2.6, where we will see that it plays a crucial role in the determination of the impurity conductance at low temperatures. In the RPT the leading contribution to \( \partial^2 \Omega \tilde{\Sigma}(\Omega) \bigg|_{\Omega=0} \) is of order \( \tilde{U}^2 \) [49]. To calculate this we follow the steps outlined in [49, 15] and differentiate Eq. (2.31) to find the operator equation

\[ \frac{d^2}{d\omega^2} \tilde{G}^{(0)}(\omega) = 2 \left[ \tilde{G}^{(0)}(\omega) \right]^3 - \frac{4i\tilde{\epsilon}_{d,\sigma}^2}{\Delta_{\sigma}} \tilde{\rho}_\sigma^2 \delta(\omega) + 2i\pi \tilde{\rho}_\sigma(0) \delta(\omega) \frac{d}{d\omega}. \]  

Inserting this in Eq.(2.30), we find

\[ \tilde{\Sigma}''(\Omega) = -2i \int d\tilde{\omega} \left[ \tilde{G}^{(0)}(\omega + \Omega) \right]^3 \tilde{\Pi}_{\sigma,-\sigma}^{ph}(\omega) \]
\[ - \frac{2\pi i \tilde{\epsilon}_{d,\sigma}^2}{\Delta_{\sigma}} \tilde{\rho}_\sigma^2 \tilde{\Pi}_{\sigma,-\sigma}^{ph}(-\Omega) + \tilde{\rho}_\sigma(0) \partial_\Omega \tilde{\Pi}_{\sigma,-\sigma}^{ph}(-\Omega), \]

where the derivative of the propagator is given by

\[ \partial_\Omega \tilde{\Pi}_{\sigma_1,\sigma_2}^{ph}(\Omega) = -i \int d\tilde{\omega} \tilde{G}^{(0)}(\omega) \left[ \tilde{G}^{(0)}(\omega + \Omega) \right]^2 + \tilde{\rho}_\sigma(0) \tilde{G}^{(0)}(\omega) \tilde{\Pi}_{\sigma_1}^{ph}(\Omega). \]  

At particle-hole symmetry the integral in Eq.(2.50) vanishes due to parity, and
we find\(^4\) that
\[
\lim_{\Omega \to 0} \text{Im} \tilde{\Sigma}^\sigma_\sigma(\Omega) = \frac{-\pi \tilde{U}^2}{2(\pi \Delta)^3} \Omega^2 + \mathcal{O}(\Omega^4).
\] (2.52)

In the case of the one-orbital AIM at particle-hole symmetry Eq. (2.52) gives an exact result for the imaginary part of the curvature (note that the real part vanishes). This follows by re-writing the exact relation [134, 135]
\[
\lim_{\omega \to 0} \text{Im} \Sigma^\sigma_\sigma(\omega) = -i\pi \Gamma^{\sigma\sigma}_{\uparrow\downarrow}(0,0) \frac{\tilde{\rho} \tilde{U}^2}{2(\pi \Delta)^3} \Omega^2 + \mathcal{O}(\omega^4)
\] (2.53)
in terms of the renormalised parameters \(\tilde{\Delta} = z \Delta, \tilde{U} = z^2 \Gamma^{\sigma\sigma}_{\uparrow\downarrow}(0,0)\), to recover precisely Eq. (2.52) (see also Ref. [49]). Due to the parity of the Green’s function, it is easy to show for a symmetric model that \(\text{Re} \Sigma_\sigma''(0) = \text{Re} \tilde{\Sigma}_\sigma''(0) = 0\). Consequently, we conclude that at particle-hole symmetry the renormalised theory yields an exact result for the second derivative of \(\Sigma_\sigma(\omega)\) [49].

It is interesting to investigate whether these results hold for asymmetric models. The proof of Eq. (2.53) relies on the assumption of particle-hole symmetry, and consequently cannot be used to justify the renormalised theory away from the symmetric point. Nevertheless, by writing Eq. (2.52) in terms of the renormalised density of states as
\[
\lim_{\Omega \to 0} \text{Im} \tilde{\Sigma}^\sigma_\sigma(\Omega) = \frac{-\pi \tilde{U}^2}{2(\pi \Delta)^3} \Omega^2 + \mathcal{O}(\Omega^4)
\] (2.54)
we obtain an expression that we conjecture holds even away from particle-hole symmetry \(^5\). That the second derivative does not involve powers of \(\tilde{U}^3\) can be explicitly confirmed by differentiating the analytic result and showing that the contribution of the diagrams with a \(\lambda_3\) to the second derivative cancels that of the diagrams containing three \(\tilde{U}\) vertices. Of course, this does not preclude the appearance of \(\omega^2\) terms in the imaginary part of \(\tilde{\Sigma}_\sigma(\omega)\) at higher-orders in \(\tilde{U}\).

However, we can numerically check Eq. (2.54) away from particle-hole symmetry by using the NRG to calculate \(\Sigma_\sigma(\omega)\).

To calculate \(\Sigma_\sigma(\omega)\) we will use the NRG LJUBLJANA [62] framework, which implements a \(z\)-averaging procedure [63] that reduces the severity of the spurious oscillations in \(\Sigma_\sigma(\omega)\) at low frequencies. We then perform a least-squares fit of \(\Sigma(\omega)\) to a quadratic polynomial \(\zeta_0 + \zeta_1 \omega + \zeta_2 \omega^2\) over the frequency range \([-R, R]\).

\(^4\)It is helpful to pick a one-sided limit such as \(\Omega \to 0^+\).

\(^5\)One can obtain the same result by calculating the second derivative explicitly. This is particularly convenient to do in the Matsubara formalism, as in Ref. [51].
where $R$ is chosen so that the fitting errors $|\delta \text{Re} \zeta_2 / \text{Re} \zeta_2|$ and $|\delta \text{Im} \zeta_2 / \text{Im} \zeta_2|$ are separately minimised. We perform such a fit as a function $\epsilon_d$, keeping $\Delta$ and $U$ fixed, and determining an ‘optimal’ $R$ for each $\epsilon_d$. We clarify that the real and imaginary parts are fitted independently with different values of $R$.

Our results for the real part of $\tilde{\Sigma}''_\sigma(\omega)$ are shown in Fig. 2.8a, where we plot $\text{Re} \zeta_2$ as obtained from the fitting procedure described above, against the corresponding results in the renormalised theory. To relate the latter to the bare self-energy we make use of the identity

$$\Sigma''_\sigma(\omega) = z_\sigma \tilde{\Sigma}''_\sigma(\omega), \quad (2.55)$$

and Eq. (2.50). Clearly, the second-order result for $\text{Re} \tilde{\Sigma}''_\sigma(\omega)$ is only approximate — except for the trivial case of particle-hole symmetry where it vanishes, in exact agreement with the analytic result — and will receive potentially significant corrections from higher order terms. Our results for the imaginary part are shown in Fig. 2.8b, where the points labelled ‘RPT’ are obtained by combining Eq. (2.55) and Eq. (2.54), and the ‘NRG’ line corresponds to $\text{Im} \zeta_2$. We see that the two curves are in excellent agreement for all values of the asymmetry. We draw the conclusion that Eq. (2.54) is an excellent approximation to imaginary part of $\Sigma''_\sigma(\omega)$; this is compatible with the conjecture that it is an exact result.
2.6. Quantum dot conductance

The Anderson impurity model, originally used to model magnetic impurities, has in recent years found important applications in modelling semi-conductor quantum dot systems [43, 28]. Due to their materials’ chemical properties, such devices trap an integer number of electrons in a localised potential well, which due to its small size is responsible for the plethora of interesting quantum mechanical properties exhibited by the dot. A typical set-up consists of a AlGaAs/GaAs heterostructure, traps a two-dimensional electron gas. Using optical lithography, metallic leads are placed on the (insulating) surface of the device and which can be used to manipulated the underlying electron gas by the application of a negative voltage [43, 68]. The quantum dot is also coupled to a metallic reservoir, with which it can exchange electrons. The multi-channel generalisations of the Anderson model can be used to model more elaborate experimental setups, in which two dots are present and potentially coupled (e.g. capacitively). When used to model semi-conductor quantum dots, the appropriate values of the parameters $\epsilon_d, \Delta$ and $U$ of the Anderson model differ considerably from those encountered in the impurity case [43], with typical values lying in the range $0.1 - 1 \text{ meV}$. The associated Kondo scale is typically of the order of $1 \mu\text{eV}$, and sets an upper temperature scale at which one can observe the relevant Kondo physics.

We now turn to the question of determining the leading temperature dependence of the electrical conductance $g_d$ of a single quantum dot in the limit of zero bias voltage. This calculation has appeared in Ref. [49] and Ref. [15, p.49 ] for a particle-hole symmetric model; we aim to extend this treatment to general models. Extensions of the calculation to non-zero small bias voltages have been considered in Refs. [96, 97, 54]. Our starting point is the general expression for $\sigma_d$ in terms of the density of states [138, 50]

$$g_d(T) = \Delta e^2 \sum \sigma \int \frac{d\omega}{2\pi} \Im G_{\sigma}(\omega, T) \frac{\partial F(\omega, T)}{\partial \omega},$$  \hspace{1cm} (2.56)

e is the electron charge and $F(\omega, T)$ is the Fermi-Dirac distribution. This can be trivially rewritten [15, p.49 ] in terms of renormalised quantities as

$$g_d(T) = e^2 \sum \sigma \tilde{\Delta}_\sigma \int \frac{d\omega}{2\pi} \Im \tilde{G}_{\sigma}^+(\omega, T) \frac{\partial F(\omega, T)}{\partial \omega}$$

$$= -e^2 \sum \sigma \tilde{\Delta}_\sigma \int \frac{d\omega}{2\pi} \frac{\partial \Im \tilde{G}_{\sigma}^+(\omega, T)}{\partial \omega} F(\omega, T),$$ \hspace{1cm} (2.57)
where the surface term has been set to zero, since \( \tilde{G}_+^{\sigma}(\omega, T) \to 0 \) as \( \omega \to -\infty \) by assumption. In the limit \( T \to 0 \) we have that \( F(\omega, T) \to \theta(-x) \), where \( \theta(x) \) is the Heaviside step function. Consequently, in this limit we find

\[
g_d(0) = \frac{e^2}{2} \sum_{\sigma} \Delta_\sigma \tilde{p}_\sigma(0). \tag{2.58}
\]

We can derive a formula for the leading temperature dependence of \( g_d(T) \) by applying Sommerfeld’s expansion (see Appendix A) to obtain

\[
g_d(T) - g_d(0) = \frac{e^2}{2\pi} \sum_{\sigma} \Delta_\sigma \left[ -\text{Im} \tilde{G}_+^{\sigma}(0, T) + \text{Im} \tilde{G}_+^{\sigma}(0, 0) \right. \\
- \frac{\pi^2}{6} T^2 \frac{\partial^2 \text{Im} \tilde{G}_+^{\sigma}(\omega, 0)}{\partial \omega^2} \bigg|_{\omega=0} + \mathcal{O}(T^4) \bigg]. \tag{2.59}
\]

We can write

\[
\tilde{G}_+^{\sigma}(\omega, T) = \left( -\tilde{\epsilon}_{d, \sigma} + i\tilde{\Delta}_\sigma \right)^{-1} \left[ 1 + \frac{\omega - \tilde{\Sigma}_+^{\sigma}(\omega, T)}{\tilde{\Sigma}_d^{\sigma}} \right] \tag{2.60}
= \tilde{G}_+^{\sigma}(0)^{(0, +)}(0) \left[ 1 - \left( \omega - \tilde{\Sigma}_+^{\sigma}(\omega, T) \right) \tilde{G}_+^{\sigma}(0)^{(0, +)}(0) \right.
+ \left( \omega - \tilde{\Sigma}_+^{\sigma}(\omega, T) \right) \left( \tilde{G}_+^{\sigma}(0)^{(0, +)}(0) \right)^2 + \ldots \right]. \tag{2.61}
\]

In Eq. (2.61) the terms involving \( \tilde{\Sigma}_\sigma(\omega) \) are sometimes known as the inelastic component of the Green’s function, while the contributions from \( \tilde{G}_+^{\sigma}(0)^{(0, +)}(\omega) \) constitute the elastic component. We thus have to leading order in \( \tilde{\Sigma}_\sigma(\omega) \)

\[
\tilde{G}_+^{\sigma}(0, T) - \tilde{G}_+^{\sigma}(0, 0) = \left[ \tilde{G}_+^{\sigma}(0)^{(0, +)}(0) \right]^2 \tilde{\Sigma}_+^{\sigma}(0, T) + \ldots, \tag{2.62}
\]

and furthermore

\[
\left. \frac{\partial^2 \text{Im} \tilde{G}_+^{\sigma}(\omega, 0)}{\partial \omega^2} \right|_{\omega=0} = \left[ \tilde{G}_+^{\sigma}(0)^{(0, +)}(0) \right]^2 \left( \tilde{\Sigma}_+^{\sigma}(0, 0) + 2 \tilde{\Sigma}_+^{\sigma}(0, 0) \right). \tag{2.63}
\]

\(^6\) Note that the notation \( \tilde{G}_+^{\sigma}(0)(\omega) \) is unambiguous, for we have not defined a non-interacting propagator at non-zero temperatures.
Inserting these expression in Eq. (2.59) we find that

\[ g_d(T) - g_d(0) = -\frac{e^2}{2\pi} \sum_\sigma \tilde{\Delta}_\sigma \text{Im} \left\{ [\tilde{G}^{(0,+)}_\sigma(0)]^2 \right. \]

\[ \times \left. \left[ \tilde{\Sigma}^+(0, T) + \frac{\pi^2}{6} T^2 \left( \tilde{\Sigma}^{++}(0, 0) + 2\tilde{G}^{(0,+)}_\sigma(0) \right) \right] \right\} + \ldots \]

(2.64)

We discuss the cases of a symmetric and an asymmetric model separately.

**Symmetric model**

For a symmetric Anderson model in the absence of a magnetic field we have \( \tilde{G}^{(0,+)}_\sigma(0) = \frac{i}{\tilde{\Delta}} \) and Eq. (2.59) reduces to

\[ \frac{g_d(T) - g_d(0)}{g_d(0)} = -\frac{1}{\tilde{\Delta}} \left[ \text{Im} \tilde{\Sigma}^+(0, T) + \frac{\pi^2}{6} T^2 \left( \text{Im} \tilde{\Sigma}^{++}(0, 0) - \frac{2}{\tilde{\Delta}} \right) \right] + \ldots \]

(2.65)

Recall from Sec. 2.5 that at particle-hole symmetry \( \tilde{\Sigma}^{++}(0, 0) \) is purely imaginary and given by Eq. (2.52). Additionally, we can use the results of our calculations, which so far have been carried out only at \( T = 0 \), to deduce \( \text{Im} \tilde{\Sigma}^+_\sigma(0, T) \)

7. It can be shown [50, p. 121] that, to leading order in \( T \) and \( \Omega \), Eq. (2.54) generalises to

\[ \text{Im} \Sigma^+_\sigma(\Omega, T) = \frac{1}{2} \text{Im} \Sigma^{++}_\sigma(0, 0)(\Omega^2 + \pi^2 T^2 + \ldots). \]

(2.66)

We remark that the proof in Ref. [50] assumes a symmetric model, though the result holds for models with arbitrary asymmetry. We can verify this explicitly in the weak-coupling regime from the results of Ref. [57, 58] reproduced in the Appendix (Eq. (B.4)). More generally, that the imaginary part of the self-energy is proportional to \( \omega^2 + \pi^2 T^2 \) can be seen as a consequence of the Fermi liquid theory for the model [49]. By invoking Eq. (2.52) we finally find

\[ \frac{g_d(T) - g_d(0)}{g_d(0)} = \frac{\pi^2 T^2}{3\tilde{\Delta}^2} \left[ 1 + 2 \left( \frac{\tilde{U}}{\pi\tilde{\Delta}} \right)^2 \right]. \]

(2.67)

Incidentally, we note that at particle-hole symmetry, \( \text{Re} \tilde{\Sigma}_\sigma(0, T) = 0 \). This follows from the fact that the tadpole diagram involving the interacting renormalised Green’s function will evaluate to \( \tilde{U}^2 \) at any temperature, and thus cancel with the \( \lambda_1 \) counter-term (which is defined at \( T = 0 \)).
Asymmetric model

Turning our attention to the asymmetric model, we note that the effects of the asymmetry will be to introduce a real component to \( \tilde{G}^{(0,+)}(0) \), which is now equal to \((\tilde{\epsilon}_d + i\Delta)^{-1}\), and \( \tilde{\Sigma}^+(0, T) \). The latter quantity can be calculated, approximately, using the renormalised theory — the details of the calculation are discussed in Appendix A. In brief, to calculate \( \tilde{\Sigma}^+(0, T) \) for an asymmetric model one deduces its imaginary component in the same way as in the symmetric case, that is, by taking into account the second-order diagram of Fig. 2.2b. Additionally, one must calculate the contribution to the real part, which comprises the real component of the second-order and the tadpole diagrams. We arrive at the expression

\[
\frac{g_d(T) - g_d(0)}{g_d(0)} = -\frac{1}{\pi \sum_{\sigma} \Delta_\sigma \tilde{\rho}_\sigma(0, 0)} \sum_{\sigma} \text{Im} \left\{ \left[ \tilde{G}^{(0,+)}(0) \right]^2 \times \left[ \tilde{\Sigma}^+(0, T) + \frac{\pi^2}{6} T^2 \left( \tilde{\Sigma}^{++}(0, 0) + 2 \tilde{G}^{(0,+)}(0) \right) \right] \right\} + \ldots .
\]

Note that the right hand side of the above equation is proportional to \( T^2 \) since, as per the analysis of Appendix A, we plot the dimensionless quantity

\[
\bar{g}_d = \lim_{T \to 0} \frac{\pi^2 \tilde{\rho}^2(0) g_d(T) - g_d(0)}{T^2 g_d(0)}
\]

in Fig. (2.9). We see that the conductance is even around the point of particle-hole symmetry, where it is also maximum. As the asymmetry is increased \( \bar{g}_d \) decreases and eventually becomes negative, with the sign change occurring at \(|\tilde{\epsilon}_d + U/2| \approx 1.2\pi \Delta \).

2.7. Partial series resummation

In Secs. 2.3 we organised the calculation by including all contributions up to some power of \( \tilde{U} \) and truncating the higher-order components; we refer to such calculations as fixed-order expansions. Sometimes, particularly when \( \tilde{U} \) is large and repeated scattering is important, it is preferable to isolate a sub-set of diagrams and resum them to all orders in \( \tilde{U} \). We will focus here on two cases, the Renormalised Random Phase Approximation (RRPA-PH), in which repeated particle-hole scattering is taken into account, and the RRPA-PP which involves
Figure 2.9.: The coefficient of the $T^2$ term in the conductance of a quantum dot in the linear response limit.

Figure 2.10.: The RRPA in the particle-hole channel.

a ladder of repeated particle-particle scattering. Infinite series such as these were introduced in Ref. [52] and were shown to be especially useful in describing magnetic field effects [53, 17, 16, 15]. Furthermore, they play a crucial role in the determination of the renormalisation parameter flow in a magnetic field [32, 33]; we will return to this point in Chapter 4.

2.7.1. RRPA-PH

The RRPA-PH [52, 53, 17, 16, 15] corresponds to the diagrams in Fig. (2.10). The infinite series of diagrams for the four-vertex can be resummed by means of the Bethe Salpeter equation:

$$\tilde{\Gamma}_{\uparrow\downarrow}(\Omega_1, \Omega_2; \Omega_3, \Omega_4) = \tilde{U}_{\text{eff}} + i \int \frac{d\omega}{2\pi} \tilde{G}^{(0)}_\uparrow(-\omega) \tilde{G}^{(0)}_\downarrow(\omega) \tilde{\Gamma}_{\uparrow\downarrow}(\omega, -\omega; \Omega_3, \Omega_4).$$

(2.70)
Figure 2.11.: Comparison of the second-order, RRPA-PH and RRPA-PP approximations to $\text{Im} \tilde{\Sigma}((\omega))$ to the NRG results for $\text{Im} \tilde{\Sigma}((\omega))$. In both figures the comparison is carried out for a model with $\Delta/D = 0.01$ and $U = 3\pi \Delta$; furthermore on the left $\epsilon_d = -0.01$, corresponding to $\tilde{\Delta} = 3.75 \times 10^{-4}$, $\tilde{\epsilon}_d = 5.00 \times 10^{-5}$ and $\tilde{U} = 1.18 \times 10^{-3}$, while on the right $\epsilon_d = -0.035$, corresponding to $\tilde{\Delta} = 2.99 \times 10^{-3}$, $\tilde{\epsilon}_d = -6.81 \times 10^{-3}$ and $\tilde{U} = 1.27 \times 10^{-2}$.

Noting that the particle-hole propagator, and thus the four-vertex, depends only on the difference of the incoming frequencies, we have

$$
\tilde{\Gamma}_{\uparrow \downarrow}(\Omega_1, \Omega_2; \Omega_3, \Omega_4) = \frac{\tilde{U}_{\text{eff}}}{1 - \tilde{U}_{\text{eff}} \tilde{\Pi}^{\text{ph}}_{\uparrow \downarrow}(\Omega_2 - \Omega_1)} \equiv \tilde{\Gamma}_{\uparrow \downarrow}(\Omega_2 - \Omega_1).
$$

We can relate the effective interaction $\tilde{U}_{\text{eff}}$ to $\tilde{U}$ as per Eq. (2.16)

$$
\tilde{U} = \frac{\tilde{U}_{\text{eff}}}{1 - \tilde{U}_{\text{eff}} \tilde{\Pi}^{\text{ph}}_{\uparrow \downarrow}(0)}.
$$

Note that in the absence of a magnetic field $\tilde{\Pi}^{\text{ph}}_{\sigma, -\sigma}(0) = \rho_{\sigma}(0)$ (see Appendix C). Turning to the self-energy we find

$$
\tilde{\Sigma}_{\sigma}(\Omega) = \tilde{U} \tilde{n}_{\sigma} - i \tilde{U}_{\text{eff}} \int d\omega \tilde{G}^{(0)}_{\sigma, -\sigma}(\omega - \Omega) \tilde{\Pi}^{\text{ph}}_{\sigma, -\sigma}(\omega) \tilde{\Gamma}_{\sigma, -\sigma}(\Omega_2 - \Omega_1) + \Omega \lambda_{2,\sigma} + \lambda_{1,\sigma}.
$$

To implement the RPA for given renormalised parameters we start with Eq. (2.72) which allows us to deduce $\tilde{U}_{\text{eff}}$ and allows the counter-terms to be deduced from Eq. (2.73). Our treatment here is general and valid even in the presence of a magnetic field, since the loop diagram has been explicitly accounted for in Eq. (2.73).
Figure 2.12.: Left: The magnitude of the effective interaction constant $\tilde{U}_{ph}$ in the particle-hole channel, compared to $\tilde{U}$, as a function of the model’s asymmetry. Right: The magnitude of the expansion constant in the denominator of Eq. (2.72). In both cases $U = 3\pi\Delta$.

In Figs. 2.11a and 2.11b we plot the imaginary parts of Eq. (2.73) for the model with $U = 3\pi\Delta$ and $\epsilon_d = -\pi\Delta/2$ and $\epsilon_d = -U/2$ respectively. We see that the RRPA-PH can reproduce the low-frequency behaviour of the self-energy. We conclude therefore that for the symmetric model it is principally these ‘spin-flip’ processes captured by the RRPA-PH that are responsible for the strong correlation effects.

We remark that the application of the RPA to the AIM is not a new idea; its application was the subject of much of the early literature on the model [122, 79, 22, 108, 81, 112]. These were ultimately unsuccessful, and suffered from a divergence of the RPA sum due to a root in the denominator in the bare version of Eq. (2.71)

$$\Gamma_{\uparrow\downarrow}(\Omega_2 - \Omega_1) = \frac{U}{1 - U\Pi_{\uparrow\downarrow}^{ph}(\Omega_2 - \Omega_1)}.$$  (2.74)

Physically this corresponds to a divergence in the transverse spin susceptibility and the appearance of a local magnetic moment. This is unphysical but is indicative of the importance of spin-flip processes. In contrast, the RRPA-PH does not suffer from such a divergence as the renormalisation of the parameters prevent such a pole from occurring. This is shown explicitly in Fig. 2.13, where $\tilde{U}\tilde{\rho}(0)$ is shown to always remain less than 1.
Figure 2.13.: The RPA denominator $\tilde{U}\tilde{\rho}(0)$, plotted as a function of $\epsilon_d$ for various values of $U/\pi\Delta$. Note how $\tilde{U}\tilde{\rho}(0) < 1$ for any $\epsilon_d$, with $\tilde{U}\tilde{\rho} \to 1$ in the Kondo limit.

Figure 2.14.: The RRPA in the particle-particle channel.

2.7.2. RRPA-PP

In the RRPA-PP [52, 53, 17, 16, 15] one considers the effect of repeated particle-particle scattering (Fig. 2.14), very much in analogy to the treatment of particle-hole scattering in the RRPA-PH. The dependence of the ladder on just the sum of the incoming frequencies allows us to reduce the its calculation to a geometric series summation, finding

$$\tilde{\Sigma}_\sigma(\Omega) = \Omega \lambda_{2,\sigma} + \lambda_{1,\sigma} + \tilde{U}_\sigma - i\tilde{U}_\text{eff} \int d\bar{\omega} \tilde{G}^{(0)}_{\sigma}(\omega - \Omega) \tilde{\Pi}^{pp}_{\sigma,-\sigma}(\omega) \tilde{\Gamma}_{\sigma,-\sigma}(\Omega_1 + \Omega_1). \quad (2.76)$$

In the context of the bare perturbation theory, the particle-particle ladder is known as the low-density approximation and is expected to provide an reliable
description for the self-energy for sufficiently asymmetric models. We will return to this discussion in Sec. 4.3. The convergence of Eq. (2.75) depends on the magnitude of \( \tilde{U}_{pp} \), and is reliant on \( \tilde{U}_{pp} \tilde{\Pi}_{pp} \uparrow\downarrow \). From the plots of Fig. 2.15 we see that \( \tilde{U}_{pp} \) is small for very asymmetric models but increases rapidly in size in the vicinity of \( |\epsilon_d + U/2| \approx \pi \Delta \), where it apparently diverges. The uncontrolled increase in magnitude is a clear sign of the failure of theory, and we expect the RRPA-PP approximation to be poor for \( \epsilon_d + U/2 \ll \pi \Delta \). The sign change in Fig. 2.15 is unphysical and provides further evidence of the unsuitability of the approximation in this regime.

2.8. Extensions to the two-channel model

The discussion of the renormalised theory can be extended to the case of the two-channel model introduced in Sec. 1.1.3. The renormalised Hamiltonian is given by [92, 91, 94, 93]

\[
\tilde{H} = \tilde{H}_1 + \tilde{H}_2 + \tilde{U}_{12}(\tilde{n}_{1,\uparrow} + \tilde{n}_{1,\downarrow})(\tilde{n}_{2,\uparrow} + \tilde{n}_{2,\downarrow})
\]

(2.77)

where \( \tilde{H}_i \) is the usual interacting SU(2) Anderson Hamiltonian of the \( i \)th species

\[
\tilde{H}_i = \sum_{\sigma} \tilde{c}^\dagger_{i,d,\sigma} \tilde{c}_{i,d,\sigma} + \sum_{k,\sigma} \tilde{\epsilon}_{k,\sigma} \tilde{c}^\dagger_{i,k,\sigma} \tilde{c}_{i,k,\sigma} + \sum_{k,k'} (\tilde{V}_{\sigma} \tilde{c}^\dagger_{i,k,\sigma} \tilde{c}_{i,k',\sigma} + \text{H.c}) + \Delta \tilde{n}_{i,\uparrow} \tilde{n}_{i,\downarrow},
\]

(2.78)
where $\sigma = \{\uparrow, \downarrow\}$. Given the interpretation of the two-channel model as a model for quantum dots, we are interested in calculating its conductance in the linear response regime. In particular, we are interested in the leading finite-temperature corrections at zero temperature, which will be of order $T^2$.

We proceed in analogy to the one-channel model and the calculation outlined in Sec. 2.5, 2.6. The diagrammatic calculation of the self-energy is very similar to the case of the one-channel model, only that one is faced with more diagrams as a result of the term involving $\tilde{U}_{12}$, that allows propagators of the same spin but corresponding to different channels to interact. To second order in the couplings the self-energy is simply

$$\tilde{\Sigma}_\sigma(\Omega) = -i \int \frac{d\omega}{2\pi} \tilde{G}_\sigma^{(0)}(\omega + \Omega) \tilde{F}_\sigma(\omega) + \lambda_2 \omega + \lambda_1,$$  \hspace{1cm} (2.79)

with the counter-terms set by Eq. (2.16) and where now

$$F_\sigma(\omega) = \tilde{U}_2^2 \tilde{\Pi}_{-\sigma,-\sigma}^{ph}(\omega) + \tilde{U}_{12}^2 \left[ \tilde{\Pi}_{-\sigma,-\sigma}^{ph}(\omega) + \tilde{\Pi}_{\sigma,\sigma}^{ph}(\omega) \right].$$  \hspace{1cm} (2.80)

Following the steps of Sec. 2.5 we find that

$$\tilde{\Sigma}_\sigma''(\Omega) = -2i \int d\tilde{\omega} [\tilde{G}_\sigma^{(0)}(\omega + \Omega)]^3 \tilde{F}_\sigma(\omega) - \frac{2\pi \tilde{\epsilon}_d \sigma}{\Delta_\sigma} \tilde{\rho}_\sigma^2 \tilde{F}_\sigma(-\Omega) + \tilde{\rho}_\sigma^{(0)}(0) \partial_\Omega \tilde{F}_\sigma(-\Omega),$$  \hspace{1cm} (2.81)

where the derivative of $\tilde{F}_\sigma(-\Omega)$ can be computed using Eq. (2.51) and

$$\partial_\Omega \tilde{\Pi}_{\sigma_1,\sigma_2}^{pp}(\Omega) = -i \int d\tilde{\omega} \tilde{G}_\sigma^{(0)}(\omega) \left[ \tilde{G}_\sigma^{(0)}(\Omega - \omega) \right]^2 + \tilde{\rho}_\sigma^{(0)}(0) \tilde{G}_\sigma^{(0)}(\Omega).$$  \hspace{1cm} (2.82)

Given the renormalised parameters for the two-channel, the conductance can now be computed from Eq. 2.68; our results are shown in Fig. 2.16.
Figure 2.16.: The coefficient of the $T^2$ term in the conductance of a double quantum dot with $U = 20\pi\Delta$ and $U_{12} = 5\pi\Delta$ in the linear response limit.
3. Automatic perturbation expansions

A recurrent theme throughout this thesis has been the calculation of the self-energy by drawing Feynman diagrams and translating them to integrals via a simple set of rules\(^1\). Working order-by-order one can, in principle, determine an arbitrary number of corrections to the ‘non-interacting’ term\(^2\) of the perturbation series. Though this process is not difficult \textit{per se}, it is tedious and time-consuming; the effort required increases exponentially with the order, limiting the feasibility of this approach to only the lowest orders. This presents a problem when the interaction constant (in the bare perturbation theory \(U\); in the renormalised theory \(\tilde{U}\)) is large, for then the truncation of the series after only a few terms constitutes a poor approximation to the self-energy.

In this chapter we demonstrate how such perturbative expansions can be completely automated. A process is outlined whereby all diagrams of order greater than or equal to two are automatically generated and translated into integrals. These are then evaluated numerically and summed, yielding results for the impurity self-energy and its frequency derivative. The largest order accessible is limited only by the computational power available. In the interests of efficiency we develop an optimisation algorithm to identify the cases where the resultant multi-dimensional integral can be factorised into a product of a term that can be integrated analytically, and a residual integral of reduced dimensionality which is evaluated numerically. We present results for the self-energy and four vertex, though the method can be generalised to the calculation of any \(n\)-point function.

Automated perturbative calculations are, of course, far from new, and have been employed in computer-assisted calculations of cross-sections in high-energy physics for several decades \([121]\). Off-the-shelf, very advanced and configurable

\(^1\)Too simple for Julian Schwinger, who famously lamented that Feynman’s graph representation of terms in perturbation theory ‘brought quantum field theory to the masses’ \([118]\).

\(^2\)The quotes are to highlight the fact that the division of the Lagrangian into a ‘non-interacting’ and an ‘interacting’ component is arbitrary; it is common for the ‘non-interacting’ component to include some interactions, so long as a closed-form solution for the corresponding Green’s function can be found.
packages [74, 5, 107] exist to aid calculations within and beyond the Standard Model (see Ref. [45] for a review) The approach outlined here is condensed-matter-specific and differs from such approaches in several important aspects:

- The loop integrals encountered are finite, non-divergent quantities and therefore the spectacularly complex affair of automating multi-loop regularisation and subtraction methods is entirely side-stepped. Our method can therefore seamlessly handle diagrams with any number of loops.

- Relativistic considerations such as four-momenta and traces over Dirac gamma matrices do not enter the discussion at all. The impurity Green’s function is local, that is, it depends only on frequency.

- To the best of the author’s knowledge the analytic simplification method is entirely novel.

Our method can be used to compute either the bare or the renormalised perturbation expansion. Here we focus only the latter, since the former has been discussed extensively in the literature [57, 58, 141, 59]. Our approach will be based our the concept of skeleton diagrams, which we define as diagrams that do not contain any lower-order self-energy insertions. We will start by calculating the bare theory order-by-order and then explicitly re-ordering it to obtain the renormalised expansion. The advantage of organising our calculation in this manner is that the counter-terms do not have to considered as separate interaction vertices when generating the diagrams.

Conceptually, the process can be divided into three distinct stages: the diagram generation, the translation into an integral by applying the Feynman rules and the numerical integration. This chapter will deal with each one in order. First we describe a simple combinatorial algorithm to generate all possible diagrams to given order. Then, by regarding Feynman diagrams as directed graphs, we appeal to standard algorithms from graph theory to identify and retain only the subset of skeleton diagrams. Subsequently, we discuss how the Feynman rules can be applied algorithmically to each diagram, and describe the factorisation procedure used to reduce the dimensionality of the numerical integration. To aid the explanation of the factorisation algorithm we discuss a particular example in detail. We then proceed to discuss how the numerical integration can be carried out efficiently. Finally, we present results for the renormalised self-energy to fifth-order in $\tilde{U}$ and for the four-vertex to fourth order.
Figure 3.1.: To generate all Feynman diagrams of a given order $n$ (here $n = 3$) one must connect $n$ vertices in all possible ways. A line can only be connected to other lines of the same spin, which is denoted by the arrows.

3.1. Diagram generation

3.1.1. Drawing graphs

The problem at hand is to generate all $n$th order diagrams for the impurity self-energy. By definition, an $n$th order diagram will involve $n$ interaction vertices. Without loss of generality we take the external legs to have spin $\uparrow$. We classify the diagrams into two types: dynamic diagrams, which have the incoming and outgoing legs on different vertices, and consequently are functions of the external frequency, while static diagrams have both legs on the same vertex and are frequency-independent. In calculations in the bare theory that are strictly ordered\(^3\) in $U$, and away from particle-hole symmetry, static diagrams should be taken into account explicitly up to the appropriate order of $U$. However, in the renormalised theory, in the absence of a magnetic field, they can always be ignored, since they will be cancelled by the $\lambda_{1,\sigma}$ counter-term. Henceforth our discussion will focus primarily on the generation of dynamic diagrams.

To order $n$, we begin by considering all the possible ways that $n$ vertices, as shown in Fig. 3.1, can be linked to each other. It is helpful to think of the orientation of the arrows as immutable. Internal lines carry spin and we must ensure we only connect lines of equal spin.

Each diagram can be completely characterised by specifying which incoming and outgoing lines are to be joined together. In the SU(2) case we are considering, we use two arrays to describe the diagrams — one array for each spin flavour. Let $A$ be the array corresponding to the spin-$\uparrow$ lines and $B$ the array corresponding to the spin-$\downarrow$ lines. The $k$th element in the $A$ [$B$] array denotes the index of the

\(^3\)In other words, calculations where $\Sigma_\sigma(0)$ is calculated from first principles and not determined self-consistently or from the impurity occupation.
interaction vertex from which the incoming line to the \((k+1)\)th interaction vertex originates. For example, when we write for a fourth-order diagram \(A = [1, 3, 2]\) we mean that the spin-\(\uparrow\) line entering the second vertex is the outgoing line from vertex 1, the line entering the third vertex is the outgoing line from vertex 3 and the line entering the fourth vertex originates from vertex number 2. Similarly, if for a fourth-order diagram \(B = [2, 1, 2, 4]\) then the interpretation is that the first vertex receives a spin \(\downarrow\) from vertex 2 \textit{et cetera}. By specifying the \(A\) and \(B\) arrays (for spin \(\uparrow\) and \(\downarrow\) respectively) we have completely specified the diagram.

We clarify that for both static and dynamic diagrams the \(B\) array contains \(n\) elements, a permutation of the numbers 1 to \(n\). In dynamic diagrams, the last \((n)\)th vertex is not available to contribute an outgoing line, as this is external. Consequently the \(A\) array will consist of only \(n - 1\) elements, a permutation of the numbers 1 to \(n - 1\). By considering all possible permutations in the above notation we can see that to order \(n\) there are \(2 \times n! \times (n-1)!\) diagrams in total.

3.1.2. Diagrams with a self-loop

A special case of diagrams is those that contain at least one \textit{self-loop}, that is, a line which starts and ends on the same vertex. As discussed in Chapter 2, such diagrams do not contribute to the renormalised self-energy in the absence of a magnetic field, since they are always cancelled by the counter-term. It is thus best to avoid generating them altogether. We thus reject any graph whose \(A\) array is such that \(A_i = i + 1\), or for which \(B_i = i\) (where \(i = 1, \ldots, N\)).

3.1.3. Irreducibility

Through the above method we generate all possible diagrams to a given order. Recalling that we have set out to calculate the \textit{irreducible} self-energy, we now seek a way of identifying the reducible diagrams and discarding them. This is a challenging problem in its own right, and we turn to graph theory for a solution. It is very useful to regard Feynman diagrams as directed, multi-edge graphs. To determine whether a given diagram \(D\) is reducible we create a diagram \(D'\) by deleting all internal lines (\textit{edges}) in \(D\) with edge connectivity strictly less than two. We then analyse the number of weakly connected components in the graph; if there is more than one then \(D\) is reducible and is discarded.
3.1.4. Equivalent diagrams

Having discarded reducible diagrams, we have to ensure that we are not over-counting some of the remaining diagrams, i.e. that we are not including topologically equivalent diagrams more than once. Such equivalent diagrams are certain to arise due to the arbitrariness in the labelling of the vertices: all vertices not attached to external legs are equivalent, so the numeric label we have assigned to them cannot matter. In graph-theoretic terms, this equivalence is known as an isomorphism and this is essentially just the graph isomorphism problem; informally, two graphs are isomorphic if there is a bijective mapping between their vertices (or equally informally, they are identically up to a permutation of the internal vertices). Such a mapping must of course involve only vertices not directly attached to external legs. To identify pairs of isomorphic diagrams we use the the VF2 [65, 26] algorithm.

3.1.5. Skeleton graphs

The next step is to select the skeleton diagrams, defined as those diagrams that cannot be generated from a self-energy insertion in a lower-order diagram (see also Fig. 3.2). We thus aim to identify non-skeleton diagrams and discard them. We accomplish this by generating all diagrams, order-by-order up to order \( n \), rather than just the diagrams of the desired order. By storing the lower-order graphs, and realising that the problem of identifying a non-skeleton diagram is equivalent to identifying a subgraph isomorphism, we can discard all non-skeleton graphs. In checking whether a graph \( D_m \) of order \( m < n \) is a subisomorphism of a higher-order graph we must be careful to distinguish lines of different spins. For every graph \( D_m \) we must thus also check whether the graph \( D'_m \), generated by reversing the spins on \( D_m \), is an isomorphism too.

3.1.6. Graph properties

To associate each diagram with the correct numerical sign we must know how many fermion loops it contains. A diagram contains a fermion loop if there exists a sequence of adjacent internal lines, with the same spin, which connects this vertex \( V \) with itself. Of these fermion loops we distinguish self-loops, which start and end on the same vertex without linking to other vertices, and cycles which must involve at least two vertices. In graph-theory parlance, our cycles are simple cycles.
Figure 3.2.: Examples of a fourth-order skeleton diagram (left) and a non-
skeleton diagram (right) which comprises a second-order skeleton
diagram with a second-order insertion.

<table>
<thead>
<tr>
<th>Order</th>
<th>dynamic</th>
<th>static</th>
<th>Total</th>
<th>RPT</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>5</td>
<td>3</td>
<td>8</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>31</td>
<td>13</td>
<td>44</td>
<td>12</td>
</tr>
<tr>
<td>5</td>
<td>225</td>
<td>71</td>
<td>296</td>
<td>73</td>
</tr>
</tbody>
</table>

Table 3.1.: Number of self-energy diagrams to given order in $\tilde{U}$. The fifth column lists the number of diagrams that actually contribute to the renormalised self-energy, i.e. dynamic diagrams with no self-loops.

To determine the number of cycles algorithmically, we take the original diagram $D$ and create derivatives of it $D_i$, where $i = 1, \ldots, 2k$ for the $k$-channel model, which are structured like $D$ but contain only lines of spin $i$. For each $D_i$ we count the number $c_i$ of strongly connected components. Each strongly connected component is really a cycle, so the total number of cycles $c = \sum c_i$. We note in passing that self-loops are easier to count, for one must only count the number $s$ of lines that start and end on the same vertex — we stress however that for the purposes of our calculation we can disregard diagrams with a self-loop entirely. The number of fermion loops is thus $c + s$.

3.1.7. Generating the self-energy graphs

In summary, this section described the process of generating all possible diagrams, discarding the reducible ones and then ensuring we count equivalent diagrams only once. The number of self-energy diagrams generated to each order is reported in Table 3.1.
3.1.8. Generating the four-vertex

The approach outlined in the previous section can be extended to the case of the four-vertex $\Gamma_{\sigma,-\rho}(\omega_1,\omega_2;\omega_3,\omega_4)$ (or any $n$-point vertex, but we will not consider the general problem here). For simplicity we consider here the particle-particle channel (this is not an approximation but merely a way of organising the calculation). Diagrams now feature two incoming lines of particles of different spin, and two outgoing lines.

We begin the generation process again by considering a sequence of vertices as in Fig. 3.1. We can again classify the diagrams depending on whether the incoming and outgoing spin-$\uparrow$ particles attach to the same vertex or not. To generate all diagrams, both cases need to be explicitly taken into account. Unlike the case of the self-energy however, the latter diagrams cannot be ignored. After fixing the placement of the external spin-$\uparrow$ lines we need to assign the external spin-$\downarrow$ lines to vertices. We adopt the simple brute-force strategy of considering all possible ways of choosing two vertices out of $n$.  

As in the case of the self-energy, we have to ensure that isomorphic graphs are only included only once and that one-particle-reducible graphs are discarded. At any given order it is evident that the number of possible four-vertex diagrams is much greater than the number of self-energy diagrams, due to the extra external legs which restrict the number of isomorphic diagrams. Though greater in number, the four-vertex diagrams involve one integration fewer compared to the self-energy diagrams and are thus easier to evaluate. The number of diagrams appearing to given order is given in Table 3.2.

3.1.9. Implementation details

The code to generate the diagrams was written in PYTHON using the library igraph [29] library for the graph-theoretic aspects. An important point to note

\footnote{This can be optimised significantly to reduce the number of potentially equivalent diagrams, but the bottleneck of the calculation is the numerical integration, not the diagram generation.}

<table>
<thead>
<tr>
<th>Order</th>
<th>Total (ex. self loops)</th>
<th>Total (inc. self-loops)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>3</td>
<td>9</td>
<td>13</td>
</tr>
<tr>
<td>4</td>
<td>58</td>
<td>104</td>
</tr>
<tr>
<td>5</td>
<td>438</td>
<td>940</td>
</tr>
</tbody>
</table>

Table 3.2.: Number of four-vertex diagrams to given order in $\bar{U}$. 

77
is that the igraph implementation of the VF2 [65, 26] algorithm used to determine graph (Sec. 3.1.4) and subgraph isomorphisms (Sec. 3.1.5) is only directly applicable to directed graphs without self-loops and without multiple edges. Nevertheless it does allow each line \( l \) to carry a scalar attribute \( p_l \). To apply the algorithm we thus employ an ‘edge colouring’ trick: for a given graph \( \mathcal{D} \) we make a copy \( \mathcal{D}' \) of \( \mathcal{D} \), and collapse the edges in \( \mathcal{D}' \) that have the same start and end points into a single edge, with \( p_l = 100n'_\sigma + n'_\uparrow \), where \( n'_\sigma \) denotes the number of lines of spin \( \sigma \) connecting this pair of vertices\(^5\). For each multi-edge graph \( \mathcal{D} \) we thus obtain a simple graph \( \mathcal{D}' \) whose edges \( p_l \) attribute encodes the spin information. The one-to-one correspondence can therefore be used to conclude that \( \mathcal{D}_1 \) and \( \mathcal{D}_2 \) will be isomorphic if \( \mathcal{D}'_1 \) and \( \mathcal{D}'_2 \) are isomorphic.

3.2. Diagram evaluation

3.2.1. The rules

As discussed in the introduction, we will tentatively set up the calculation in a ‘mixed’ perturbation theory, which is to be carried out using the renormalised Green’s function and in powers of an effective interaction constant \( \tilde{U}_{\text{eff}} \) (which equal to \( \tilde{U} + \lambda_3 \), though this has no bearing on the Feynman rules). At this point we are free to ignore the \( \lambda_{1,\sigma}, \lambda_{2,\sigma} \) counter-terms; these will be reintroduced in Sec. 3.3 by virtue of the skeleton formalism. We use the \( T = 0 \) formalism, in which the Feynman rules read

- Each vertex receives a factor \(-i\tilde{U}_{\text{eff}}\).
- Each internal free quasi-particle line with frequency \( \omega_i \) and spin \( \sigma \) is associated with a factor \( i\tilde{G}^{(0)}_{\sigma}(\omega_i) \), where \( \tilde{G}^{(0)}_{\sigma}(\omega) = \left[ \omega - \tilde{\epsilon}_{d,\sigma} + i\tilde{\Delta}_\sigma \text{sign}(\omega) \right]^{-1} \).
- Each free variable \( \epsilon \) should be integrated over using measure \( \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \).
- If a diagram has an odd number of fermion loops its amplitude receives a factor of \(-1\).
- The overall amplitude of each diagram is multiplied with a factor of \(-i\).

3.2.2. Frequency conservation

In this section we describe how frequency conservation for the self-energy can be enforced at each vertex; the following discussion carries over to the four-vertex

\(^5\)The factor of 100 can be replaced with any other sufficiently large number.
with the substitution $2n - 1 \rightarrow 2n - 2$, to account for the fact that the four-vertex contains one fewer internal line. We begin by enumerating all internal lines — for an $n$th-order calculation we have $4n$ lines in total, two of which are external and thus do not receive a label. These are connected in pairs, giving us a total of $(4n - 2)/2 = 2n - 1$ internal lines; to each one we assign an index from 1 to $2n - 1$. We then proceed to impose an algebraic condition to ensure frequency conservation on each vertex, namely that the sum of the incoming frequencies at each vertex is equal to the sum of outgoing frequencies.

For each vertex, we have thus $\omega_{\text{in},1} + \omega_{\text{in},2} - \omega_{\text{out},1} - \omega_{\text{out},2} = 0$. The first and last vertices deserve special attention, for they involve the external line, which we take to have frequency $\Omega$. The frequency conservation rule on the first vertex is therefore $\Omega + \omega_{\text{in}} - \omega_{\text{out},1} - \omega_{\text{out},2} = 0$, whilst similarly on the last vertex we have $\omega_{\text{in},1} + \omega_{\text{in},2} - \omega_{\text{out}} - \Omega = 0$. In summary, the frequency conservation is imposed through a system of $n$ linear equations, one for each vertex, in $2n - 1$ variables for the self-energy and $2n - 2$ variables for the four-vertex. We can write this as

$$C\omega = \Omega_{\text{ext}},$$  \hfill (3.1)

where $\omega = (\omega_1, \ldots, \omega_{2n-1})$ denotes the internal line frequencies and $C$ is an $n \times (2n - 1)$ matrix with integer entries 0 or ±1 encoding the constraints. The vector $\Omega_{\text{ext}} = (-\Omega, 0, 0, \ldots, \Omega)$ has $2n - 1$ entries and the graph’s external frequency dependence. It is important to note that not all $n$ equations are independent — one is certainly dependent as a consequence of overall frequency conservation, which we have already implicitly imposed by taking the external outgoing frequency to be equal to the incoming frequency$^6$.

To summarise, we have to solve Eq. (3.1). We have $2n - 1$ variables and $n - 1$ independent constraints. We thus expect to find $n$ free variables — these will be our integration variables. It is not possible to know at this stage which of the $\omega_i$ will be the independent variables, and no clever enumeration scheme seems to exist to guarantee that, say, the first $n$ $\omega$-variables will be independent. Instead, we have to solve the undetermined, linear, and, in general, inhomogeneous, system of equations. We can write the solution to Eq. (3.1) as

$$\omega = f\epsilon + \Omega^{(p)},$$  \hfill (3.2)

$^6$Note that in the case of self-loops, which we are ignoring here, some of the $2n - 1$ frequencies $\omega_i$ will not appear in the system. Such frequencies are free variables and have to be integrated over.
where \( \epsilon = (\epsilon_1, \ldots, \epsilon_n) \) are the free variables, and \( \Omega^{(p)} \) is a particular solution to Eq. (3.1). The matrix \( f \) has dimensions \((2n - 1) \times n\) known as the null space matrix or kernel; we will refer to it as the \( f \)-matrix.

The null space of a matrix is usually numerically determined using the Singular Value Decomposition of a matrix [106, p. 39]. This involves a significant number of floating-point operations which will inevitably introduce numerical round-off errors. To prevent this, we note that the matrix \( C \) is not an arbitrary matrix but one with integer entries, since at every vertex an internal line will appear with either a + or a −, or not at all. This can be exploited by applying the Lenstra-Lenstra-Lovász lattice basis reduction algorithm [80] through which the kernel can be determined exactly. This is implemented in the number-theory library pari/gp [124] which was accessed through the PYTHON interface python-pari [87]. Furthermore, inverting the matrix in this way results in an \( f \)-matrix that resembles what one would obtain when solving the problem by hand, that is, all elements of \( f \) are equal to −1, 0 or 1. We clarify that we use the Singular Value Decomposition to determine the particular solution.

### 3.2.3. Analytic simplifications

It is possible, though very inefficient, to apply the Feynman rules at this point, to obtain for each diagram an expression proportional to

\[
P_D \int d\epsilon \tilde{G}^{(0)}_{\sigma_1}(\omega_1) \cdots \tilde{G}^{(0)}_{\sigma_{2n-1}}(\omega_{2n-1}),
\]

where \( \omega \) is given by Eq. (3.2), and proceed with the numerical integration. However, in calculations by hand, such as those in Sec. 2.3 where the renormalised self-energy was calculated to third order in \( \tilde{U} \), it is common to analytically factorise out terms that correspond to pair propagators. This has the advantage of reducing the dimension of the numerical integration, and consequently reducing the number of integrand evaluations needed to achieve a given precision. This idea can be generalised to accommodate the propagation of \( k > 1 \) free quasi-particles, or quasi-holes, with arbitrary spins \( \sigma_1, \ldots, \sigma_k \) and frequencies.
\( \Omega_1, \ldots, \Omega_k \). An example is shown in Fig. 3.3. We define the \( k \)-particle/hole propagator as

\[
\tilde{\Pi}^{(k)}_{\sigma, s}(\Omega_1, \ldots, \Omega_k) = i^k \int \frac{d\omega}{2\pi} \tilde{G}^{(0)}_{\sigma_1}(s_1 \omega + \Omega_1) \tilde{G}^{(0)}_{\sigma_2}(s_2 \omega + \Omega_2) \cdots \tilde{G}^{(0)}_{\sigma_k}(s_k \omega + \Omega_k),
\]

(3.4)

where \( s_i \in \{-1, 1\} \) (terms with \( s_i = 1 \) correspond to particles and \( s_i = -1 \) to holes). Through a change of variables we can show that \( \tilde{\Pi}^{(k)}_{\sigma, s} \) is really a function of only \( k-1 \) variables but the form of Eq. (3.4) is more convenient for our purposes. The details of the evaluation of Eq. (3.4) are described in Appendix C; we find that the answer involves logarithms of complex quantities.

Evaluating these complex logarithms is a computationally expensive operation, so we seek to further optimise our setup by implementing interpolation tables. For the particle-particle and particle-hole pair-propagators introduced in Eq. (2.29) (which correspond to Eq. (3.4) for \( k = 2 \)) this can be achieved by tabulating the values of \( \tilde{\Pi}^{ph}_{\sigma,-\sigma}(\Omega) \) and \( \tilde{\Pi}^{pp}_{\sigma,-\sigma}(\Omega) \) for different values of \( \Omega \). To achieve the optimal compromise between precision and performance we used a un-evenly spaced grid with points distributed like \( x^2 \), and carried out the interpolation using a cubic Lagrange polynomial \([106, p. 118]\).

For higher \( k \), tabulating \( \tilde{\Pi}^{(k)}_{\sigma, s}(\Omega_1, \ldots, \Omega_k) \) is not as straightforward. We discuss only the \( k = 3 \) case, noting that the curse of dimensionality will impose prohibitive memory requirements for higher \( k \). We remark that, while the \( k = 3 \) version of the propagator in Eq. (3.4) seems to be a function of three variables, we can perform a substitution and reduce it to a function of two variables. This allows us to set up a two-dimensional grid on which we will tabulate the values of the propagator. To achieve this, we need to consider the cases \( s_1 = 1 \) and \( s_1 = -1 \) separately, whilst allowing \( s_2 \) and \( s_3 \) to be arbitrary. We write

\[
\begin{align*}
\tilde{\Pi}^{(3)}_{\sigma,(1,s_2,s_3)}(\Omega) &= i^3 \int \frac{d\omega}{2\pi} \tilde{G}^{(0)}_{\sigma_1}(\omega) \tilde{G}^{(0)}_{\sigma_2}(s_2 \omega + \Omega_2 - s_2 \Omega_1) \tilde{G}^{(0)}_{\sigma_3}(s_3 \omega + \Omega_3 - s_3 \Omega_1), \\
\tilde{\Pi}^{(3)}_{\sigma,(-1,s_2,s_3)}(\Omega) &= i^3 \int \frac{d\omega}{2\pi} \tilde{G}^{(0)}_{\sigma_1}(-\omega) \tilde{G}^{(0)}_{\sigma_2}(s_2 \omega + \Omega_2 + s_2 \Omega_1) \tilde{G}^{(0)}_{\sigma_3}(s_3 \omega + \Omega_3 + s_3 \Omega_1).
\end{align*}
\]

(3.5)

The different possible configurations of the signs \( s \) have now to be considered separately and a separate interpolation table constructed for each configuration. Additionally, in a magnetic field one would have to account for all possible values of \( \sigma \). For the interpolation we used a two-dimensional cubic Lagrange polynomial, which is discussed in Appendix C.
Having defined the $k$-particle/hole propagator we now describe an algorithm to identify instances of it from the information encoded in the $f$-matrix. Our strategy will be to first inspect the $f$-matrix and identify groups of Green’s functions that can be combined to form a product of the form of Eq. (3.4). We accomplish this by traversing the $f$-matrix column-by-column — since each column corresponds to an integration variable — and examining each column’s non-zero entries. Ultimately, our goal is to delete from the $f$-matrix the columns which correspond to integration variables that have been absorbed in $\tilde{\Pi}^{(k)}_{\sigma,s}$, and to delete the rows that correspond to Green’s functions that comprise $\tilde{\Pi}^{(k)}_{\sigma,s}$. To avoid modifying the $f$-matrix while we are traversing it we will maintain a list $L_c$ of columns and a list $L_r$ of rows which are to be removed, both of which are empty at the start of the search, and we will only delete the rows and columns after all possible simplifications have been identified. We will refer to the resultant simplified matrix as the $g$-matrix, to distinguish it from the original $f$-matrix.

To identify instances of $\tilde{\Pi}^{(k)}_{\sigma,s}$ we scan each column $m$ of the $f$-matrix and identify the columns with exactly $k$ non-zero entries $\mu_1, \ldots, \mu_k$ on the rows $r_1, \ldots, r_k$. If $m \notin L_c$ and $r_1, \ldots, r_k \notin L_R$ then column $m$ indeed corresponds to a $k$-particle/hole propagator; if not, and either $m \in L_c$ or at least one of $r_1, \ldots, r_k \in L_R$, it means that the corresponding Green’s function has already been absorbed into another propagator, and we proceed to the next column. With the $j$th $k$-particle/hole propagator we will associate a matrix $q_j$, which encodes its dependence on the remaining integration variables, and vectors $\sigma_j$, $s_j$ describing the spin and sign configuration respectively. The $k$ frequency arguments of $\tilde{\Pi}^{(k)}_{\sigma,s}$ will therefore be given by the rows of $q_j$. Furthermore, we construct a $k$-dimensional vector $\Omega_{q_j}$ that contains the external frequency dependence of the rows $r_1, \ldots, r_k$, i.e. $\Omega_{q_j} = (\Omega^{(p)}_{r_1}, \ldots, \Omega^{(p)}_{r_k})$. In other words, the $\omega_i$ that appear in Eq. (3.4) can be obtained from the $i$th component of

$$q_j \epsilon' + \Omega_{q_j},$$

where $\epsilon'$ denotes the free variables that remain after all propagator simplifications. After constructing the $q$-matrix we add $m$ to $L_c$ and all of $r_1, \ldots, r_k$ to $L_r$ and examine the next column. When the columns of the matrix have been exhausted we delete all columns in $L_c$ and rows in $L_r$ from the original $f$-matrix.

---

7Since we are using the LLL algorithm to find $f$ we also know that $|\mu_1| = \ldots = |\mu_k| = 1$, since any non-zero entry will be $\pm 1$.

8The variable $j$ here is merely a label; the first $k$-particle/hole propagator we identify is labelled $j = 1$, the second is $j = 2$ and so on.
Figure 3.4.: One of the two diagrams that contribute to the self-energy to third order in $\tilde{U}_{\text{eff}}$.

to obtain its final form $g$. Furthermore, to account for the fact that components of the original $\Omega^{(p)}$ have been absorbed into the various $\Omega_{q}$ we delete all the rows in $L_{r}$ from $\Omega^{(p)}$ to obtain its final form, which we denote $\Omega^{(g)}$. Finally, we eliminate the columns in $L_{c}$ from the provisional $q$ matrices.

For each diagram we thus arrive at an expression for the amplitude of the form

$$I_{D} = P_{D} \int d\epsilon \tilde{G}_{\sigma_{1}}^{(l_{1})} \tilde{G}_{\sigma_{2}}^{(l_{2})} \ldots \tilde{\Pi}_{\sigma_{1};\epsilon_{1}}^{(k_{1})} \tilde{\Pi}_{\sigma_{2};\epsilon_{2}}^{(k_{2})} \ldots ,$$

where $P_{D}$ is a complex prefactor containing powers of $\tilde{U}_{\text{eff}}$, $i$ and $2\pi$. In Eq. (3.7) it is understood that the argument of $\tilde{G}_{\sigma_{i}}^{(l_{i})}$ corresponds to the $i$th row of

$$\omega = g\epsilon + \Omega^{(g)} ,$$

which is similar to Eq. (3.2) but involves $g$, the simplified form of the $f$-matrix, and that the (vector) argument of the $j$th $\tilde{\Pi}_{\sigma_{j};\epsilon_{j}}^{(k_{j})}$ is given by Eq. (3.6). We remark that while the final integral of Eq. (3.7) is at least one-dimensional for all self-energy diagrams, some four-vertex diagrams factorise completely.

**An example**

To illustrate this with an example consider the diagram of Fig. 3.4. We find that the amplitude is proportional to

$$\int d\epsilon \tilde{G}_{\sigma}^{(0)}(\epsilon_{1} - \epsilon_{3} + \Omega) \tilde{G}_{\sigma}^{(0)}(\epsilon_{2} - \epsilon_{3} + \Omega) \tilde{G}_{-\sigma}^{(0)}(\epsilon_{1}) \tilde{G}_{-\sigma}^{(0)}(\epsilon_{2}) \tilde{G}_{-\sigma}^{(0)}(\epsilon_{3}) ,$$

or in matrix notation,

$$f = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Omega^{(p)} = \begin{bmatrix} \Omega \\ \Omega \\ 0 \\ 0 \\ 0 \end{bmatrix}. \quad (3.10)$$
We begin with the first column and identify the first particle-particle pair propagator by the first and third row entries. The propagator is $\tilde{\Pi}^{(2)}_{\sigma, \bar{\sigma}}$, where $\sigma = (\sigma, -\sigma)$, because the first and third Green’s functions have spin $\sigma$ and $-\sigma$ respectively, and $s = (1, 1)$ because $f_{11} = f_{31} = 1$. Having ‘used’ the Green’s functions in question, we mask their corresponding entries in $f$ by appending ‘1’ to $L_c$ and ‘1,3’ to $L_r$ so that $L_c = \{1\}$ and $L_r = \{1,3\}$. We temporarily associate this propagator with the matrices

$$q_1 = \begin{bmatrix} 1 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}, \quad \Omega_{q_1} = \begin{bmatrix} \Omega \\ 0 \end{bmatrix},$$

constructed from the first and third rows of $f$ and $\Omega^{(p)}$ in Eq. (3.10). We now examine the second column of $f$ in Eq. (3.10) and note that the two non-zero entries are contained in the second and fourth rows, neither of which is in $L_r$. This is thus another instance of $\Pi^{(2)}_{(\sigma, -\sigma);(1,1)}$, and after updating $L_c = \{1,2\}$, and $L_r = \{1,3,2,4\}$. We associate this propagator with a $q_2$ matrix equal to Eq. (3.11). We proceed to the third column and examine the possibility that it corresponds to a triple propagator. We conclude that it does not, since its non-zero elements appear on rows 1, 2, 5, the first two of which are already in $L_r$. Having exhausted the columns of $f$, the final step is to remove all columns in $L_c$ and all rows in $L_r$ from $f$ to obtain $g$, and all column in $L_c$ from $q_1$, $q_2$ to obtain their final simplified form and remove the references to the variables of integration that have been eliminated. To conclude the procedure we also delete all rows in $L_r$ from $\Omega^{(p)}$, to obtain $\Omega^{(g)}$. We thus have $f = [1]$, $\Omega^{(g)} = [0]$ and

$$q_1 = q_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \Omega_{q_2} = \Omega_{q_1} = \begin{bmatrix} \Omega \\ 0 \end{bmatrix},$$

and the amplitude in Eq. (3.9) simplifies to

$$\int d\epsilon_1 \tilde{G}^{(0)}_\sigma(\epsilon_1) \left[ \Pi^{(2)}_{(\sigma, -\sigma);(1,1)}(\epsilon_1 + \Omega, 0) \right]^2.$$

### 3.2.4. Reducing the number of diagrams

In the absence of a magnetic field it is possible for diagrams to be topologically distinct, yet numerically equal. For example, if we consider the diagrams arising from insertions of the second-order self-energy to the second-order skeleton diagrams (Fig. 3.5), we find that both have the same numerical value when the
magnetic field is zero. To prove this, one can appeal to their $f$-matrices before any simplifications take place, and show that they are equal up to permutations of the rows and columns.

In practice, implementing this approach is unnecessarily complicated from a computational viewpoint. Instead, a more straightforward technique was adopted: a quick integration is carried out over all the diagrams individually, at a randomly chosen non-zero frequency of order $\tilde{\Delta}$. If two diagrams are found to have real and imaginary parts equal to within a prescribed tolerance level, they are assumed to be numerically equal. Thus, the correct result can be obtained by removing one diagram from the list of the diagrams to be integrated and doubling the prefactor of the other.

At particle-hole symmetry, an additional potential simplification arises, namely that two diagrams may precisely cancel each other due to parity of the Green’s function. Eliminating pairs that cancel is very advantageous from a computational point of view since the cancellation acts to increase the error in the integration stage (and is the limiting factor in the calculation of the high-frequency sector of the spectrum). We deal with this in a similar manner to the case of equal diagrams, by examining whether diagrams are numerically opposite at a random frequency.

### 3.2.5. Numerical integration

The final step of the calculation is the numerical evaluation of integrals of the form of Eq. (3.7). From a numerical point of view, this is a particularly challenging integral. Each Green’s function is discontinuous at zero frequency; for an $n$-dimensional integral with $2n - 1$ terms this implies that each Green’s function is discontinuous on $2n - 1$ infinite ($n - 1$)-dimensional hyperplanes defined by the
roots of the \( \text{sign}(\ldots) \) terms. At zero frequencies, these discontinuities contain a common point, the origin, and one can exploit properties of convex polytopes to devise a geometric integration algorithm. This idea is explored in Appendix D but cannot be generalised to non-zero frequencies. The discontinuities present a difficulty for most numerical integration algorithms, particularly adaptive ones which rely on interval bisection. Around the origin, the integrand is sharply peaked in both directions, which leads to loss of precision and is a manifestation of the \textit{sign problem} commonly encountered in condensed matter physics.

Finally, the integrand of Eq. (3.7) also decays like \( 1/x \) in \( n-1 \) directions defined by the roots of the off-diagonal \( \text{sign}(\ldots) \) terms. This results in long ‘tails’ in \( n \)-dimensional space, along which quadrature converges only logarithmically.

Generally speaking, there are three ways of handling such integrals: repeated quadrature, cubature and Monte Carlo methods [106, p. 196]. Algorithms belonging to the first class constitute the oldest and most developed methods of determining the area under a curve. However, the computational complexity of applying them recursively restricts their application only to two-dimensional, or maybe three-dimensional integrals. On the other hand, Monte Carlo methods perform poorly in ‘few’ dimensions, particularly for integrals with the pathologies described above. We thus chose to use the adaptive methods found in the \textsc{cubature} [64] library.

For completeness, we note that integration algorithms such as those of Ref. [64] cannot be readily applied to \( \mathbb{R}^n \) and one must construct a mapping \( h : \mathbb{R}^n \to [0,1]^n \). This can be done in a number of ways [106] and one must generally determine the optimal choice of \( f \) on a case-by-case basis. We achieved best performance with the \( n \)-dimensional generalisation of the 1-dimensional rule

\[
\int_{\mathbb{R}} d\epsilon h(\epsilon) = \int_{[0,1]} dt \frac{(1 + t^2)}{(1-t^2)^2} (h(\epsilon) + h(-\epsilon)).
\]  

which led to faster convergence than the mappings \( \epsilon = \tilde{\epsilon}d + \tilde{\Delta}\tan(y) \) and \( \epsilon = \sinh(y) \). Though the latter factorise part of the integrand’s denominator, this did not seem to compensate the additional computational effort required to compute the trigonometric functions. We note that we made use of \textsc{cubature}’s vector interface in combination with \textsc{OpenMP} [99] to parallelise the numerical integration. Further parallelisation can be trivially achieved by adopting a hybrid \textsc{OpenMP}+\textsc{MPI} paradigm — when a plot of the self-energy against frequency is required, each node can be assigned a different value of the external...
Figure 3.6.: An illustration of the discontinuities exhibited by the integrand of the second-order diagram. We plot the real (top) and imaginary (bottom) parts of $\tilde{G}^{(0)}(\omega_1)\tilde{G}^{(0)}(\omega_2)\tilde{G}^{(0)}(\omega_1+\omega_2-\Omega)$, the integrand of the second-order diagram, for an asymmetric model with $\epsilon_d = -1.2\Delta$ and $\Omega = 0.4\Delta$. 
frequency for which to carry out the calculation.

3.3. Assembling the RPT

3.3.1. Systematics

So far we have been working order-by-order in the effective interaction \(\tilde{U}_{\text{eff}} = \tilde{U} + \lambda_3\), expressing the self-energy as

\[
\tilde{\Sigma}(\omega) = \sum_{n=2}^{\infty} \gamma_n(\omega)\tilde{U}_{\text{eff}}^n.
\] (3.15)

Ultimately, we aim to obtain \(\tilde{\Sigma}(\omega)\) as a power series in \(\tilde{U}\) rather than \(\tilde{U}_{\text{eff}}\). To accomplish this, we note that the counter-term \(\lambda_3\) is defined as in Eq. (2.16). By calculating the renormalised four-vertex at zero frequency we can thus obtain \(\tilde{U}\) as a power series in \(\tilde{U}_{\text{eff}}\),

\[
\tilde{U} = \tilde{\Gamma}_{\uparrow\downarrow}(0, 0; 0, 0) = \tilde{U}_{\text{eff}} + \sum_{n=2}^{\infty} \alpha_n\tilde{U}_{\text{eff}}^n.
\] (3.16)

Working order-by-order we can invert this equation:

\[
\tilde{U}_{\text{eff}} = \tilde{U} + \sum_{n=2}^{\infty} \beta_n\tilde{U}^n.
\] (3.17)

Working to \(O(\tilde{U}_{\text{eff}}^7)\) we find that

\[
\begin{align*}
\beta_2 &= -\alpha_2, \\
\beta_3 &= 2\alpha_2^2 - \alpha_3, \\
\beta_4 &= -5\alpha_2^3 + 5\alpha_2\alpha_3 - \alpha_4, \\
\beta_5 &= 14\alpha_2^4 - 21\alpha_2^2\alpha_3 + 6\alpha_2\alpha_4 + 3\alpha_3^2 - \alpha_5, \\
\beta_6 &= -42\alpha_2^5 + 84\alpha_2^3\alpha_3 - 28\alpha_2^2\alpha_4 - 28\alpha_2\alpha_3^2 + 7\alpha_2\alpha_5 + 7\alpha_3\alpha_4 - \alpha_6.
\end{align*}
\] (3.18)

Thus, the calculation of the self-energy in terms of \(\tilde{U}_{\text{eff}}\) can be rewritten as a series in \(\tilde{U}\)

\[
\tilde{\Sigma}(\omega) = \sum_{n=2}^{\infty} \gamma_n(\omega)\tilde{U}_{\text{eff}}^n \quad \Rightarrow \quad \tilde{\Sigma}(\omega) = \sum_{n=2}^{\infty} \delta_n(\omega)\tilde{U}^n,
\] (3.19)
where

\[
\begin{align*}
\delta_2(\omega) &= \gamma_2(\omega), \\
\delta_3(\omega) &= -2\alpha_2\gamma_2(\omega) + \gamma_3(\omega), \\
\delta_4(\omega) &= [5\alpha_2^2 - 2\alpha_3]\gamma_2(\omega) - 3\alpha_2\gamma_3(\omega) + \gamma_4(\omega), \\
\delta_5(\omega) &= -14\alpha_2^3\gamma_2(\omega) + 9\alpha_2^2\gamma_3(\omega) + [12\alpha_3\gamma_2(\omega) - 4\gamma_4(\omega)]\alpha_2 \\
&\quad - 3\alpha_3\gamma_3(\omega) - 2\alpha_4\gamma_2(\omega) + \gamma_5(\omega), \\
\delta_6(\omega) &= 42\alpha_2^4\gamma_2(\omega) - 28\alpha_2^3\gamma_3(\omega) + [-56\alpha_3\gamma_2(\omega) + 14\gamma_4(\omega)]\alpha_2^2 \\
&\quad + [21\alpha_3\gamma_3(\omega) + 14\alpha_4\gamma_2(\omega) - 5\gamma_5(\omega)]\alpha_2 + [7\alpha_2^3 - 2\alpha_3]\gamma_2(\omega) \\
&\quad - 4\alpha_3\gamma_4(\omega) - 3\alpha_4\gamma_3(\omega) + \gamma_6(\omega).
\end{align*}
\]

These relations enable us to deduce the renormalised expansion from the bare one and show explicitly how the inclusion of counter-terms results in the reorganisation of the series.

### 3.3.2. Checks

To check our calculation for the self-energy we can relate the renormalised perturbation expansion to the perturbation theory of Yamada and Yosida [137, 134, 138, 135] by replacing \(\tilde{U}_{\text{eff}}\) in Eq. (3.19) with the bare \(U\) and the parameters \(\tilde{\epsilon}_d, \tilde{\Delta}\) with their bare counter-parts and setting all the counter-terms equal to zero. Similarly, we can check the four-vertex against the calculation of Ref. [51].

We find that the analytic results

\[
\begin{align*}
\partial_\omega \Sigma(\omega)|_{\omega=0} &= -\left(3 - \frac{\pi^2}{4}\right) u^2 - \left(105 - \frac{45\pi^2}{4} + \frac{\pi^4}{16}\right) u^4 + \ldots, \\
\Gamma_{\uparrow\downarrow}(0, 0) &= U \left[1 + \left(15 - \frac{3\pi^2}{2}\right) u^2 + \ldots\right],
\end{align*}
\]

where \(u = U/\pi\Delta\), are reproduced by our calculation.

### 3.4. Results

In this section we present numerical results for the irreducible self-energy and resultant spectral density. For all the calculations we fix \(\pi\Delta = D/100\), where \(D\) is the conduction band width, and \(U = 3\pi\Delta\). In our discussion we consider the following parameter configurations: (i) a symmetric model with \(\epsilon_d = -U/2\); (ii) a
model with weak asymmetry $\epsilon_d = -1.2\pi \Delta$; and (iii) a model with pronounced asymmetry and $\epsilon_d = -3\pi \Delta$.

### 3.4.1. Self-energy

For comparison purposes we will juxtapose the renormalised self-energy obtained from RPT with the corresponding result obtained from the NRG. Since NRG calculations are set up with the bare self-energy in mind, we have to use Eq. (2.7) to relate the two quantities. We find that

$$\text{Im} \tilde{\Sigma}_{\sigma}(\omega) = z_{\sigma} \text{Im} \Sigma_{\sigma}(\omega).$$  \hspace{1cm} (3.22)

A similar equation can be derived for the real part,

$$\tilde{\epsilon}_{d,\sigma} + \tilde{\Sigma}_{\sigma}(\omega) = z_{\sigma} (\Sigma_{\sigma}(\omega) + \epsilon_{d,\sigma}) - (1 - z_{\sigma})\omega.$$  \hspace{1cm} (3.23)

In practice however, it is of limited use; this is due to the fact that the renormalised parameters $\tilde{\epsilon}_d$ and $\tilde{\Delta}$ are not determined from the NRG using the definitions in Eq. (2.5), (2.6) but from the effective linear chain Hamiltonian (for more information see the Appendix of Ref. [55]). Since the low-energy limit of Eq. (3.23) relies crucially on the numerical cancellation between $\Sigma(\omega)$ and $(z - 1)\omega$, it is difficult to obtain a result for $\text{Re} \tilde{\Sigma}(\omega)$ with a vanishing derivative at zero frequency. It is for this reason that we only show NRG results for $\text{Im} \tilde{\Sigma}(\omega)$. Note that due to the NRG’s successive elimination of higher energy scales we expect that its estimate for $\tilde{\Sigma}(\omega)$ will only be accurate in the low frequency sector.

We begin by discussing the symmetric model (case (i)). As we have already
Figure 3.8.: The real (left) and imaginary (right) parts of the renormalised self-energy for a weakly correlated asymmetric model.

Figure 3.9.: The real (left) and imaginary (right) parts of the renormalised self-energy for a strongly correlated asymmetric model.
remarked, in the presence of particle-hole symmetry $\tilde{\epsilon}_d = 0$ and the propagator is an odd function of frequency. The parity of the Green's function also results in the cancellation of the particle-hole and particle-particle propagators

$$\tilde{\Pi}^{(2)}_{\uparrow\downarrow(1,1)}(\Omega_1, \Omega_2) = \tilde{\Pi}^{(2)}_{\uparrow\downarrow(1,-1)}(\Omega_1, \Omega_2)$$

and consequently the odd-order terms of the self-energy vanish for all frequencies. Using the method described in Ref. [55] we find that $\tilde{\Delta} = 2.54 \times 10^{-4}$ and $\tilde{U} = 7.95 \times 10^{-4}$, giving $\tilde{U}/\pi \tilde{\Delta} = 0.994$. That this ratio is almost 1 is no coincidence; in the Kondo limit a universal scale, the Kondo temperature $T_K$ emerges and $\tilde{U} \to 4T_K, \pi \tilde{\Delta} \to 4T_K$ [49].

In all cases, the RPT estimate of the renormalised self-energy will always be exact in the limit $\omega \to 0$, in the sense of Eq. (2.16). At particle-hole symmetry, and for small but finite frequencies $|\omega \tilde{\rho}_0| < 1$, the $\omega^2$ coefficient of $\tilde{\Sigma}(\omega)$ is reproduced exactly [49] by the second-order calculation; the fourth order term does not contribute terms of order $\omega^2$. As we increase $|\omega|$ the dominant term is the $\omega^4$ term, which is not exactly given by the second-order calculation; this is corrected by the fourth-order contribution, extending the domain of validity of the RPT. At higher frequencies the disparity between the two RPT curves suggests the breakdown of the expansion; to obtain reliable results one must calculate the higher-order terms. We thus expect more elaborate approximations within RPT to continually extend the domain of validity of the resultant $\tilde{\Sigma}(\omega)$.

Were we to somehow have the ability to take into account all Feynman diagrams to all orders we would recover a $\tilde{\Sigma}(\omega)$ exact for all frequencies, though clearly then we would also be able to calculate the $\Sigma(\omega)$ in the first place.

Next, we discuss a slightly asymmetric model with $\epsilon_d = -1.2\pi \Delta$, for which we find that $\tilde{\epsilon}_d = 2.14 \times 10^{-5}$, $\tilde{\Delta} = 2.93 \times 10^{-4}$ and $\tilde{U} = 9.18 \times 10^{-4}$. The non-zero but small in magnitude $\tilde{\epsilon}_d$ now gives rise to odd-order terms in $\tilde{\Sigma}(\omega)$. In Fig. 3.8 we see that the third and fifth order terms are small in value and essentially only slightly modify the second and fourth order curves respectively. To determine the stability of the series to order $n$ we see that to simply look at the $n+1$ term is not sufficient.

Finally, we turn our attention to Fig. (3.9) and case (iii). a very asymmetric model with $\epsilon_d = -3\pi \Delta$. For small $|\omega|$ we find again that the RPT is in good agreement with the NRG and that the lower order contributions dominate the result. A dramatic breakdown of the expansion, in both the real and imaginary components, is evident for small negative value of $\omega$ in contrast to cases (i) and
Figure 3.10.: The spectral density for the particle-hole symmetric model.

(ii) where it is reasonably well-behaved even around $\omega \tilde{\rho}_0 \approx 0.5$.

3.4.2. Spectral density

Recall the definition in Eq. (2.1) of the renormalised retarded interacting Green’s function

$$\tilde{G}^{(+)}_g(\omega) = \frac{1}{\omega - \tilde{\epsilon}_d + i\Delta - \tilde{\Sigma}^+(\omega)}, \quad (3.25)$$

where the \textit{retarded} self-energy $\tilde{\Sigma}^+(\omega)$ differs from the causal $\tilde{\Sigma}(\omega)$ one obtains from the diagrammatics only by a sign($\omega$) term in the imaginary part. We now turn our attention to the quasi-particle spectral density, defined as

$$\tilde{\rho}(\omega) = -\frac{1}{\pi} \text{Im} \tilde{G}(\omega)$$

and express it in terms of the renormalised parameters as

$$\tilde{\rho}(\omega) = -\frac{1}{\pi} \frac{\text{Im} \tilde{\Sigma}^+(\omega) - \tilde{\Delta}}{(\omega - \tilde{\epsilon}_d - \text{Re} \tilde{\Sigma}^+(\omega))^2 + (\tilde{\Delta} - \text{Im} \tilde{\Sigma}^+(\omega))^2}, \quad (3.26)$$

Note that the spectral density is sensitive to the \textit{reducible} self-energy. The low-frequency properties of the $n$th order spectral density are thus the result of competition between higher-order irreducible self-energies and powers of $\tilde{G}^{(0)}(\omega)$ combined with powers of lower-order irreducible self-energies.

Results for cases (i), (ii) and (iii) are shown in Figs. 3.10, 3.11a and 3.11b respectively. To avoid the instability in the real part of $\tilde{\Sigma}(\omega)$ we do not use Eq. (3.26) directly to extract the result from the NRG; instead we use the NRG result for $\rho(\omega)$ and, from Eq. (2.3), $\tilde{\rho}(\omega) = z\rho(\omega)$.

For the particle-hole symmetric model of case (i) we find again that the second and fourth order terms coincide for small $\omega$ and start deviating from each other and the NRG result as $|\omega|$ is increased, with the RPT4 curve being in closer
Figure 3.11.: The spectral density for model (ii), with some asymmetry (left) and model (iii), with pronounced asymmetry (right).
agreement with the latter. This picture persists in Fig. (3.11a) where, as in the case of the self-energy, two two pairs of similar curves emerge. We remark that at particle-hole symmetry $\tilde{\rho}(\omega = 0) = (\pi \Delta)^{-1}$; away from particle-hole symmetry $\tilde{\rho}(\omega = 0)$ is given exactly by $\tilde{\rho}(\omega = 0) = \tilde{\rho}(0)(\omega = 0) = 0$. 
4. Renormalised parameters without the NRG

In our discussion of RPT so far we have assumed that the renormalised parameters are always known, and we have used values obtained from the NRG to obtain numerical results where needed. We return now to the difficulty noted in Sec. 2.1.3, namely that of determining the renormalised parameters in the first place. To apply the definitions of Eq. (2.5), (2.6), (2.9) one must know the self-energy and four-vertex at zero frequency. But most quantities of interest, for instance the susceptibilities, depend on precisely these quantities. Generally speaking, one must have already ‘solved’ the model to obtain the renormalised parameters, and in such cases the RPT provides little additional information to what can already be deduced from the NRG.

Up to now, we have temporarily circumvented this problem by using the NRG to determine the parameters. This however renders RPT a technique complementary to the NRG, rather than an alternative to it, and restricts the application of RPT to problems that have already been solved with the NRG. Hence, if we seek to obtain new insight into the model that does not follow from the NRG, we must find another way of determining the renormalised parameters.

The flow equation method (FEM) seeks to address this problem. In this approach one first identifies the parameter $\alpha$ of the original model that will be varied. Then, one has to determine a limit $\alpha \to \alpha_0$ in which $\tilde{\mu}(\alpha)$ can be analytically determined. The value of $\alpha_0$ does not need to be physically realisable or experimentally relevant; this is a mathematical trick to obtain a solvable model. Finally, RPT is used to derive a differential equation for $d\tilde{\mu}/d\alpha$, with $\tilde{\mu}(\alpha_0)$ constituting the boundary condition to the differential equation at $\alpha = \alpha_0$. By integrating the system from $\alpha_0$ to more realistic values of $\alpha$ one can thus determine the renormalised parameters for a physically relevant model.

The FEM was introduced in Refs. [32, 33] where it was applied to the one-channel Anderson model at half-filling by introducing a magnetic field $h$, which played the role of the parameter $\alpha$. The magnetic field breaks the SU(2) sym-
metry of the model, and consequently suppresses the spin fluctuations which are responsible for the bulk of the renormalisation effects. As a result, the $h \to \infty$ limit of the model can be tackled using (bare) mean-field theory\(^\dagger\) and the renormalised parameters can be deduced directly from their definitions. The RRPA and a Ward identity were then used to construct a flow equation for $\tilde{\Delta}(h)$. These were solved numerically and the renormalised parameters thus obtained were found to be in very good agreement with the NRG over several orders of magnitude of $h$. Furthermore, the exponential dependence of $T_K$ on $U$ predicted by the Bethe Ansatz (see Sec. 1.8) was reproduced.

An approach similar to the introduction of a magnetic field was pursued in Ref. [34], where the parameter $\alpha$ was taken to be the impurity level $\epsilon_d$. The convergence of the bare perturbation theory is, generally speaking, controlled by the dimensionless product $U \rho_0$. In the limit of an infinite asymmetric model this can be made arbitrarily small, eventually rendering mean field theory valid. Flow equations are then constructed for $\tilde{\mu}(\epsilon_d)$ and solved numerically. Note again the recurring theme of symmetry breaking; the introduction of an asymmetry breaks the particle-hole symmetry of the model, which is eventually restored by the flow equations. We discuss this approach in more detail in Sec. 4.3.

In Sec. 4.4 we consider the possibility of varying $\Delta$ for a symmetric model without a magnetic field [102]. In this case the constraint of particle-hole symmetry and the absence of a magnetic field eliminate the need for calculating $\tilde{\epsilon}_d$, which is zero. By taking $\Delta \to \infty$ we put the model in the weakly-correlated regime, where perturbation theory can be used to deduce the boundary condition. By slowly decreasing the hybridisation we slowly increase the correlation effects and, by incorporating them into the renormalised parameters, we deduce $\tilde{\Delta}(\Delta)$ and $\tilde{U}(\Delta)$.

Finally, in Sec. 4.5 we show how the scaling of the interaction can be controlled by varying $U$ directly [103]. For simplicity, our study is confined to the particle-hole symmetric model where the scaling theory assumes a particularly simple form. By construction, the bare perturbation is accurate as $U \to 0$; we use it to impose a boundary condition and adiabatically increase $U$ to access the strong correlation regime. This effectively constitutes a direct implementation of the fundamental idea of Fermi liquid theory. Interestingly, the results we obtain

\(^\dagger\)In fact, Ref. [33], following Ref. [113], used the RPA-enhanced mean-field theory to determine $\tilde{U}$ in the high-field regime. Though this allows one to account for the renormalisation of $\tilde{U}$ at weak couplings, it breaks down and develops a pole when $U \geq \pi \Delta$ (see Sec. 2.7). I have found that this step is unnecessary and by taking large enough $h$ one can neglect the renormalisation of $\tilde{U}$.
using this technique are analytic and reliable even for strong correlations.

4.1. General formalism

We introduce the notation $\tilde{\mu}(\mu)$ to denote the renormalised parameters $\tilde{\mu} = (\tilde{\epsilon}_d, \tilde{\Delta}, \tilde{U})$ corresponding to a model with bare parameters $\mu = (\epsilon_d, \Delta, U)$; in the presence of a magnetic field the notation generalises to $\tilde{\mu} = (\tilde{\epsilon}_d, \tilde{\epsilon}_{d,\uparrow}, \tilde{\Delta}_{\uparrow}, \tilde{\Delta}_{\downarrow}, \tilde{U})$. We consider two models whose bare parameters differ infinitesimally by $\delta\mu$, and seek a relation between the corresponding renormalised parameters $\tilde{\mu}(\mu)$ and $\tilde{\mu}(\mu + \delta\mu)$. Our strategy is to start with the Lagrangian of a model with parameters $\mu + \delta\mu$ and rewrite it in two different ways, once in terms of $\tilde{\mu}(\mu + \delta\mu)$ and once in terms of $\tilde{\mu}(\mu)$. The two ways of expressing the bare Lagrangian in the renormalised theory lead to two different expressions for the (same) bare Green’s function. These, and their derivatives, can then be equated to deduce the flow equations for the parameters.

Recall the standard way of re-expressing the Lagrangian in terms of renormalised parameters as per Eq. (2.11)

$$L(\mu + \delta\mu) = \tilde{L}(\tilde{\mu}(\mu + \delta\mu)) + \tilde{L}_{ct}(\lambda(\tilde{\mu}(\mu + \delta\mu))).$$

(4.1)

We can expand around $L(\mu)$ by writing

$$L(\mu + \delta\mu) = \tilde{L}(\tilde{\mu}(\mu)) + \delta\mu \cdot \frac{\partial L}{\partial \mu} = L(\mu) + \mathcal{L}_r(\delta\mu),$$

(4.2)

where the notation $\mathcal{L}_r(\mu)$ has been introduced for clarity. Note that in the case of the Anderson model the Lagrangian is linear in the parameters, so Eq. (4.2) is exact and furthermore $\mathcal{L}_r$ depends only on $\delta\mu$. Recalling the partitioning of the renormalised Lagrangian into an interacting and non-interacting component, Eq. (2.13), we can rewrite the RHS of Eq. (4.1) as

$$L(\mu + \delta\mu) = \tilde{L}_0(\tilde{\mu}(\mu + \delta\mu)) + \left[\tilde{L}_I(\tilde{\mu}(\mu + \delta\mu)) + \tilde{L}_{ct}(\lambda(\tilde{\mu}(\mu + \delta\mu)))\right].$$

(4.3)

Similarly, by expressing $L(\mu)$ in Eq. (4.2) in terms of renormalised quantities we have

$$L(\mu + \delta\mu) = \tilde{L}_0(\tilde{\mu}(\mu)) + \left[\tilde{L}_I(\tilde{\mu}(\mu)) + \tilde{L}_{ct}(\lambda(\tilde{\mu}(\mu))) + \mathcal{L}_r(\delta\mu)\right].$$

(4.4)

In Eqs. (4.3) and (4.4) we have two different ways of rewriting the same bare
Lagrangian in terms of renormalised quantities. The set-up of Eq. (4.2) is standard, along the lines of Sec. 2.1.2; the Lagrangian \( \tilde{\mathcal{L}}_0(\tilde{\mu}(\mu + \delta \mu)) \) describes the non-interacting quasi-particles which interact through the term in square brackets (the perturbation) and which gives rise to the renormalised self-energy \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu + \delta \mu)) \). By contrast, in the set-up of Eq. (4.4) the free quasi-particles are described in terms of \( \tilde{\mu}(\mu) \). This results in an additional interaction term, \( \mathcal{L}_r(\mu) \) which generates a corresponding interaction vertex. This must be appropriately included in the diagrammatic expansions which now give rise to a self-energy \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu) \). In the trivial case of \( \delta \mu = 0 \) this does not contribute at all and we see that \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), 0) = \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu + \delta \mu)) \).

We emphasise that \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu) \) implicitly involves the counter-terms as functions of \( \tilde{\mu}(\mu + \delta \mu) \) determined by the usual renormalisation conditions of Eq. (2.16). By contrast, \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu) \) is assembled using the counter-terms determined by imposing the renormalisation conditions to \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), 0) \), and will only satisfy them when \( \delta \mu = 0 \). Nevertheless, \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu) \) is structurally similar to \( \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu)) \) and so shares the same Fermi liquid properties

\[
\text{Im} \tilde{\Sigma}_\sigma^+(0; \tilde{\mu}(\mu), \delta \mu) = \frac{\partial \text{Im} \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu)}{\partial \omega} \bigg|_{\omega=0} = 0. \tag{4.5}
\]

To relate the two self-energies we express the bare propagator in two different ways:

\[
G_\sigma^+(\omega) = \frac{z_\sigma(\mu + \delta \mu)}{\omega - \tilde{\epsilon}_{d,\sigma}(\mu + \delta \mu) + i\tilde{\Delta}_\sigma(\mu + \delta \mu) - \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu + \delta \mu))} = \frac{z_\sigma(\mu)}{\omega - \tilde{\epsilon}_{d,\sigma}(\mu) + i\tilde{\Delta}_\sigma(\mu) - \tilde{\Sigma}_\sigma^+(\omega; \tilde{\mu}(\mu), \delta \mu)}. \tag{4.6}
\]

By equating the real parts of the two expressions for \( \omega = 0 \) and we deduce that

\[
\tilde{\epsilon}_{d,\sigma}(\mu + \delta \mu) = z_\sigma(\mu; \delta \mu) \left[ \tilde{\epsilon}_{d,\sigma}(\mu) + \tilde{\Sigma}_\sigma(0; \tilde{\mu}(\mu), \delta \mu) \right], \tag{4.8}
\]

where \( z_\sigma(\mu; \delta \mu) = z_\sigma(\mu + \delta \mu)/z_\sigma(\mu) \); equating the imaginary parts does not yield additional information. Furthermore, by taking the reciprocal of Eq. (4.7), equating the derivatives at zero and taking the real part we find

\[
z_\sigma(\mu; \delta \mu) = \left[ 1 - \frac{\partial \text{Re} \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), \delta \mu)}{\partial \omega} \bigg|_{\omega=0} \right]^{-1}. \tag{4.9}
\]
Further differentiation yields
\[ \frac{\partial^2}{\partial \omega^2} \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu + \delta \mu)) = z_\sigma(\mu; \delta \mu) \frac{\partial^2}{\partial \omega^2} \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), \delta \mu)). \] (4.10)

By expanding the denominator of Eq. (4.9) in \( \delta \mu \) and retaining the leading term we find that
\[ z_\sigma(\mu; \delta \mu) = 1 + q_\sigma(\tilde{\mu}(\mu)) \cdot \delta \mu, \] (4.11)
where
\[ q_\sigma(\tilde{\mu}(\mu)) = \frac{\partial}{\partial \mu} \left. \Re \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), \delta \mu) \right|_{\omega=0, \delta \mu=0}. \] (4.12)

From the definition of \( z_\sigma(\mu; \delta \mu) \) and Eq. (4.11) we find that
\[ \frac{\partial \ln z_\sigma(\mu)}{\partial \mu} = q_\sigma(\tilde{\mu}(\mu)), \] (4.13)
or equivalently
\[ \frac{\partial \ln \Delta_\sigma(\mu)}{\partial \mu} = q_\sigma(\tilde{\mu}(\mu)). \] (4.14)

This constitutes the flow equation for \( \Delta(\mu) \). To derive a flow equation for \( \tilde{\epsilon}_{d,\sigma}(\mu) \) we define
\[ p_\sigma(\tilde{\mu}(\mu)) = \left. \frac{\partial}{\partial \mu} \Re \tilde{\Sigma}_\sigma(0; \tilde{\mu}(\mu), \delta \mu) \right|_{\delta \mu=0}. \] (4.15)
and find
\[ \frac{\partial \tilde{\epsilon}_{d,\sigma}(\mu)}{\partial \mu} = p_\sigma(\tilde{\mu}(\mu)) + \tilde{\epsilon}_{d,\sigma}(\mu)q_\sigma(\tilde{\mu}(\mu)). \] (4.16)

4.2. Calculating \( \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), \delta \mu) \)

We see that the flow equations are determined by the quantity \( \tilde{\Sigma}_\sigma(0; \tilde{\mu}(\mu), \delta \mu) \). The previous section discussed how this can be deduced diagrammatically from the Lagrangian. Alternatively, we can also deduce this directly from the bare self-energy through a Taylor expansion
\[
\Sigma_\sigma(\omega, \mu + \delta \mu) = \Sigma_\sigma(0, \mu) + \omega \frac{\partial \Sigma_\sigma(\omega, \mu)}{\partial \omega} \bigg|_{\omega=0} \\
+ \left( \frac{\partial \Sigma_\sigma(0, \mu)}{\partial \mu} + \omega \frac{\partial^2 \Sigma_\sigma(0, \mu)}{\partial \omega \partial \mu} \bigg|_{\omega=0} \right) \cdot \delta \mu \\
+ \Sigma^{\text{rem}}_\sigma(\omega, \mu + \delta \mu) \] (4.17)
Figure 4.1.: The possible ways in which an infinitesimal one-particle vertex can enter the calculation of the bare self-energy. In Fig. 4.1b and 4.1c we see how the diagrams representing the corrections from $\delta \epsilon_{-\sigma}$ and $\delta \epsilon_{\sigma}$ respectively can be expressed exactly in terms of the bare interacting Green’s function and four vertex. The dotted line in 4.1a denotes the bare interaction $U$.

which we use to rewrite the bare propagator at $\mu + \delta \mu$ in the form of Eq. (4.7). We thus find

$$\tilde{\Sigma}_\sigma(\omega; \bar{\mu}(\mu), \delta \mu) = z_\sigma(\mu) \left( \frac{\partial \Sigma_\sigma(0, \mu)}{\partial \mu} + \omega \frac{\partial^2 \Sigma_\sigma(0, \mu)}{\partial \omega \partial \mu} \right)$$

$$+ z_\sigma(\mu; \delta \mu) \tilde{\Sigma}_\sigma(\omega, \bar{\mu}(\mu + \delta \mu))$$

(4.18)

We thus deduce the following equations

$$p_\sigma(\bar{\mu}(\mu)) = z_\sigma(\mu) \frac{\partial \Sigma_\sigma(0, \mu)}{\partial \mu}$$

(4.19)

$$q_\sigma(\bar{\mu}(\mu)) = z_\sigma(\mu) \frac{\partial^2 \Sigma_\sigma(\omega, \mu)}{\partial \omega \partial \mu} \bigg|_{\omega=0}$$

(4.20)

Our problem is effectively the following: Given exact knowledge of $\Sigma(\omega, \mu)$ and $\Gamma(\omega, \mu)$, how can one obtain $\Sigma(\omega, \mu + \delta \mu)$? To answer this question we have to separately consider the cases of a one-particle vertex, as occurs during flows in $\epsilon_d$, $\Delta$ and $h$, and the case of a two-body interaction implied by a scaling in $U$. The ways in which one-particle vertices and two-particle vertices can enter the calculation are shown in Fig. (4.1) and Fig. 4.2 respectively. We will only discuss the latter in detail; the former can be treated in a similar manner.

Let $\Sigma(\omega)$, $G(\omega)$ and $\Gamma(\omega_1, \omega_2; \omega_3)$ be the self-energy, interacting Green’s function and four-vertex for a model with interaction constant $U$. Consider now the effects of introducing an additional $\delta U$ term into the Hamiltonian (or Lagrangian), and the two-fold effect it will have on the diagrammatics of the calculation. First, it will obviously introduce an infinitesimal two-particle vertex similar to the interaction. More subtly, the infinitesimal vertex will generate an
Figure 4.2.: The three possible ways in which a single instance of an infinitesimal two-body vertex can enter the calculation of the bare self-energy. The lines represent the interacting bare propagator and the shaded square represents the four-vertex in the bare theory. For models away from particle-hole symmetry the tadpole diagram discussed in the main text will also have to be taken into account.

infinitesimal tadpole diagram, which is of a one-particle nature. If we do not simultaneously vary $\epsilon_d$ as we vary $U$, we will have to explicitly take this into account in our diagrammatic treatment. To eliminate the tadpole diagrams and simplify the discussion we will assume particle-hole symmetry for the rest of this section. Our discussion thus applies to the transformation $U \rightarrow U + \delta U$ and $\epsilon_d \rightarrow \epsilon_d - \delta U/2$. The extension to asymmetric models is therefore straightforward, if a bit tedious, and requires that we simultaneously take into account the genuine two-body term, in the manner that will be described in this section, and the implicit one-body term as per Fig. 4.1.

We now turn our attention to the infinitesimal two-body vertex. In the bare theory this can be taken into account exactly by calculating the three diagrams of Fig. 4.2, with the lines corresponding to the exact propagator $G(\omega)$, which represent all possible ways a two-particle interaction can enter the calculation. We consider first the diagram of Fig. 4.2a, from which we have

$$\delta \Sigma_\sigma(\Omega) = \delta U \int d\bar{\omega}' d\bar{\omega}'' G_\sigma(\Omega + \omega'') G_{-\sigma}(\omega') G_{-\sigma}(\omega' + \omega'') \Gamma_{\sigma,-\sigma}(\Omega, \omega' + \omega''; \omega'), \tag{4.21}$$

where $d\bar{\omega}' = d\omega'/2\pi$. At zero frequency this becomes

$$\frac{\partial \Sigma_\sigma(0)}{\partial U} = \int d\bar{\omega}' d\bar{\omega}'' G_\sigma(\omega'') G_{-\sigma}(\omega') G_{-\sigma}(\omega' + \omega'') \Gamma_{\sigma,-\sigma}(0, \omega' + \omega''; \omega'). \tag{4.22}$$
To express this in terms of renormalised quantities we write \( G_\sigma(\omega) = z_\sigma \tilde{G}_\sigma(\omega) \) and \( \Gamma_{\sigma,-\sigma}(\omega_1, \omega_2; \omega_3, \omega_4) = z_\sigma z_{-\sigma} \tilde{\Gamma}_{\sigma,-\sigma}(\omega_1, \omega_2; \omega_3, \omega_4) \). Using Eq. (4.19), we obtain an expression for \( p_\sigma(\tilde{\mu}(\mu)) \) containing factors of \( z \), which is exact

\[
\frac{\partial \Sigma_\sigma(0)}{\partial U} = z_{-\sigma} \int d\omega' d\omega'' \tilde{G}_\sigma(\omega'') \tilde{G}_{-\sigma}(\omega') \tilde{G}_{-\sigma}(0, \omega' + \omega''; \omega').
\]  

(4.23)

We will now perform similar manipulations on the frequency derivative of \( \Sigma_\sigma(\omega) \). Differentiating with respect to the external frequency \( \Omega \), we find that

\[
\frac{\partial \Sigma_\sigma(\Omega)}{\partial U} = \int d\omega' d\omega'' \partial \Omega G_\sigma(\Omega + \omega'') G_{-\sigma}(\omega' + \omega''; \omega') + \int d\omega' d\omega'' G_\sigma(\Omega + \omega'') G_{-\sigma}(\omega' + \omega''; \omega') \partial \Omega \Sigma_{-\sigma}(\Omega, \omega' + \omega''; \omega').
\]  

(4.24)

Note that the derivative\(^2\) of the propagator can be expressed as [50, p. 119]

\[
\partial_\omega G_\sigma(\omega) = -G_\sigma^2(\omega) \left( 1 - \partial_\omega \Sigma_\sigma(\omega) \right) - 2i \rho_\sigma(0) \delta(\omega).
\]  

(4.25)

Furthermore, the derivative of the self-energy can be expressed as \[50, p. 119\]

\[
\partial_\omega \Sigma_\sigma(\omega) = -\int d\omega' \Gamma_{\sigma,-\sigma}(\omega, \omega') G_{-\sigma}^2(\omega') - i \rho_\sigma(0) \Gamma_{\sigma,-\sigma}(\omega, 0; \omega).
\]  

(4.26)

Combining Eqs. (4.24), (4.25), (4.26) and setting \( \Omega = 0 \) we find that

\[
\frac{\partial \Sigma_\sigma'(0)}{\partial U} = -\int d\omega' d\omega'' G_\sigma^2(\omega'') G_{-\sigma}(\omega') G_{-\sigma}(0, \omega' + \omega''; \omega') - \int d\omega'' i \rho_\sigma(0) G_\sigma^2(\omega'') \Gamma_{\sigma,-\sigma}(\omega'', 0; \omega') G_{-\sigma}(\omega') \times G_{\sigma}(\omega' + \omega''; \omega') \Gamma_{\sigma,-\sigma}(0, \omega' + \omega''; \omega') + \int d\omega' d\omega'' d\omega''' G_\sigma^2(\omega''') \Gamma_{\sigma,-\sigma}(\omega'', \omega'''; \omega''') G_{\sigma}(\omega') \times G_{\sigma}(\omega' + \omega''; \omega') \Gamma_{\sigma,-\sigma}(0, \omega' + \omega''; \omega') - \int d\omega' G_\sigma(0) G_{\sigma}^2(\omega') \Gamma_{\sigma,-\sigma}(0, \omega'; \omega') + \int d\omega' d\omega'' G_\sigma(\omega'') G_{-\sigma}(\omega') G_{-\sigma}(\omega' + \omega''; \omega') \partial \Omega \Gamma(0, \omega' + \omega''; \omega').
\]  

(4.27)

\(^2\)Note that the causal self-energy is differentiable just like the retarded self-energy. Though their imaginary parts differ by a \( \text{sign}(\omega) \) term, this is only relevant to \( \mathcal{O}(\omega^2) \) and thus does not complicate the discussion.
As before, we express this in terms of renormalised quantities to find the exact equation

\[
\frac{\partial \Sigma'(0)}{\partial U} = -z_\sigma z_{-\sigma} \int d\omega' d\omega'' \tilde{G}^2(\omega'') \tilde{G}_{-\sigma}(\omega') \tilde{G}_{-\sigma}(\omega' + \omega'') \tilde{\Gamma}_{-\sigma}(0, \omega' + \omega''; \omega') \\
- z_\sigma \tilde{U} \int d\omega' d\omega'' i \tilde{\rho}_\sigma(0) \tilde{G}_{\sigma}(\omega') \tilde{G}_{-\sigma}(\omega', 0; \omega') \tilde{G}_{-\sigma}(\omega') \\
\times \tilde{G}_{-\sigma}(\omega' + \omega'') \tilde{\Gamma}_{-\sigma}(0, \omega' + \omega''; \omega') \\
+ z_3^2 \frac{z_\sigma}{z_{-\sigma}} \tilde{U} \int d\omega' d\omega'' d\omega''' \tilde{G}_{\sigma}(\omega') \tilde{G}_{-\sigma}(\omega', \omega''; \omega''') \tilde{G}_{-\sigma}(\omega') \\
\tilde{G}_{-\sigma}(\omega' + \omega'') \tilde{\Gamma}_{-\sigma}(0, \omega' + \omega''; \omega') \\
- z_{-\sigma} \tilde{U} \int d\omega' 2 \tilde{\rho}_\sigma(0) \tilde{G}_{\sigma}(\omega') \tilde{\Gamma}_{-\sigma}(0, \omega' + \omega'') \\
+ z_{-\sigma} \frac{z_\sigma}{z_{-\sigma}} \tilde{U} \int d\omega' d\omega'' \tilde{G}_{\sigma}(\omega') \tilde{G}_{-\sigma}(\omega' + \omega'', 0; \omega') \partial_3 \tilde{\Gamma}_{-\sigma}(0, \omega' + \omega''; \omega'),
\]

(4.28)

where \( \rho_\sigma(0) = z_\sigma \tilde{\rho}_\sigma(0) \). The obvious difficulty in working with the above equation is that we only have an approximation to the renormalised self-energy and the four-vertex. To leading order in \( \tilde{U} \), however, we can replace \( \tilde{G}(\omega) \rightarrow \tilde{G}^{(0)}(\omega) \), and \( \tilde{\Gamma} \rightarrow \tilde{\Gamma} \).

Furthermore, noting that \( z = 1 + \mathcal{O}(\tilde{U}^2) \), we can ignore the factors of \( z \) if we only seek to calculate the leading term. Retaining only the terms of order \( \tilde{U} \) we find that

\[
\frac{\partial \Sigma'(0)}{\partial U} = \tilde{U} \int d\omega' d\omega'' [\tilde{G}^{(0)}(\omega'')^2 \tilde{G}(\omega') \tilde{G}(\omega' + \omega'')] - \tilde{U} \tilde{\rho}(0) \int \frac{d\omega'}{2\pi} [\tilde{G}^{(0)}(\omega')]^2.
\]

(4.30)

Note that in the RHS we have recovered the analytic expression for the derivative of the second-order renormalised self-energy. From our discussion it follows that
to calculate the leading term, we need not consider diagrams of the form of Fig. 4.2 which involves two instances of $\Gamma$ will therefore be at least of order $\tilde{U}^2$. Furthermore, the treatment presented here can be applied without modification to the class of diagrams in Fig. 4.2b, simply introducing a factor of two into our calculations. The full derivative of $\Sigma(\omega)$ at $U + \delta U$ includes a term that does not involve the infinitesimal interaction at all:

$$\Sigma'(0, U + \delta U) = \Sigma'(0, U) + \delta U \frac{\partial \Sigma'(0)}{\partial U} + O(\delta U^2).$$

(4.31)

We now straightforwardly find that

$$z(U + \delta U) = \frac{1}{1 - \Sigma'(0, U + \delta U)} = \frac{1}{z^{-1}(U) - \delta U \frac{\partial \Sigma'(0)}{\partial U}}$$

(4.32)

and deduce that $\tilde{\Delta}(U)$ must satisfy Eq. (4.14) with

$$q(U) = z \frac{\partial \Sigma'(0)}{\partial U},$$

(4.33)

with $\frac{\partial \Sigma'(0)}{\partial U}$ given by Eq. (4.30).

4.3. Flow equations in $\epsilon_d$

We first consider the possibility of varying $\epsilon_d$ relative to the Fermi level. We will take the limit $\epsilon_d \to -\infty$ to put the model into the tractable double-occupancy regime. Another possibility, which leads to equivalent results, is to use the opposite limit $\epsilon_d \to \infty$. In either regime mean-field theory [9] is applicable and, assuming the absence of a magnetic field, gives

$$\tilde{\epsilon}_\sigma^{\text{MFT}} = \epsilon_d + \Sigma^{\text{MFT}}_\sigma,$$

(4.34)

$$\tilde{\Delta}^{\text{MFT}}_\sigma = \Delta,$$

(4.35)

$$\tilde{U}^{\text{MFT}} = U,$$

(4.36)

where following Sec. 1.2

$$\Sigma^{\text{MFT}}_\sigma = U \left[ \frac{1}{2} - \frac{1}{\pi} \tan^{-1} \left( \frac{\epsilon_{d,-\sigma} + \Sigma^{\text{MFT}}_{-\sigma}}{\Delta} \right) \right].$$

(4.37)

Our aim is to incrementally increase $\epsilon_d$ from $-\infty$ to obtain the renormalised parameters as a function of $\epsilon_d$. Note that the renormalised parameters have a
symmetry with respect to the point of half-filling, \( \epsilon_d = -U/2 \), with \( \bar{\Delta} \) and \( \bar{U} \) being even with respect to it and \( \bar{\epsilon}_d \) being odd. In presenting our results it is thus not necessary to increase \( \epsilon_d \) to values larger than \( \epsilon_d = -U/2 \). Furthermore, note that this provides a check for an implementation of the flow equations, for they too must exhibit the same symmetry. We remark that, as \( \epsilon_d \) is increased, \( \bar{U} \) renormalises before the other parameters, and can differ appreciably from its unrenormalised value even though \( \bar{\Delta} \approx \Delta \) and \( \bar{\epsilon}_d \approx \epsilon_d \). To use the boundary Eq. (4.36) we must therefore ensure we start with a sufficiently large value of \( |\epsilon_d| \). We found \( \epsilon_d = -10\pi\Delta \) to be adequate (the sensitivity to the initial value of \( |\epsilon_d| \) can be controlled by increasing it until it no longer bears on the final results).

As we move out of the mean-field regime — that is, for slightly less asymmetric models, but whose occupation is still close to 0 or 2 — we are forced to go beyond the mean-field approximation in order to account for the renormalisation of \( \bar{U} \). In this regime the problem can be treated as a Fermi gas with short-range forces and the low-density approximation [39, 40, 113] is applicable. Consequently, we expect particle-particle correlations to be responsible for the bulk of the strong correlation effects. By resumming the bare particle-particle ladder [113, 32] using mean-field propagators, it is possible to extend the range of validity Eq. (4.36). The modified expression reads [113]

\[
\bar{U}^{\text{MFT+RPAPP}} = \frac{U}{1 + \frac{\bar{U}}{\pi \epsilon_{\text{MFT}}} \tan^{-1} \left( \frac{\epsilon_{\text{MFT}}}{\Delta} \right)}.
\]

(4.38)

We clarify that, for the purposes of imposing a boundary condition on the flow equations, we found it sufficient to work with Eq. (4.36).

As \( \epsilon_d \) is increased yet more, the frequency-dependence of the self-energy will start to play an important role and will have to be incorporated in a more sophisticated approximation to \( \bar{\Sigma}_\sigma(\omega) \). For values of \( \epsilon_d \) for which the dynamic nature of the self-energy cannot be disregarded, but still far from the particle-hole symmetric point, the low-density approximation can be used to describe the dynamic effects when the correlations are not too strong. However, it is expected to break down for sufficiently symmetric models and predict a local moment. A more suitable description is provided by RPA-PP approximation, which is the analogous to the low-density approximation, but formulated in terms of renormalised quantities, and, as discussed in Sec. 2.7, retains its validity even in the strong correlation regime.

With this in mind, we seek to formulate flow equations based on the RPA-PP
approximation. The infinitesimal Lagrangian that generates the flow is

$$\mathcal{L}_r(\delta \epsilon_d) = \sum_{\sigma} \mathcal{L}_\sigma(\epsilon_d) \delta \epsilon_d d_{\sigma}(\tau).$$

(4.39)

Given the renormalised parameters, we construct the RPA-PP as per Eq. (2.76) and find \( q_\sigma(\tilde{\mu}(\epsilon_d)) \) as per Eq. (4.12), where the derivative with respect to \( \mu \rightarrow \epsilon_d \) is evaluated numerically by substituting

$$\tilde{\epsilon}_d \rightarrow \tilde{\epsilon}_d + \delta \epsilon_d$$

(4.40)
in Eq. (2.76). We thus obtain the first equation

$$\frac{\partial \ln \tilde{\Delta}_\sigma(\epsilon_d)}{\partial \epsilon_d} = q_\sigma(\tilde{\mu}(\epsilon_d)).$$

(4.41)

To deduce the second flow equation, we appeal to the Ward identity of Eq. (1.63), (2.42), from which we obtain

$$p(\tilde{\mu}(\epsilon_d)) = 1 - \tilde{U} \tilde{\rho}_{-\sigma'}.$$ 

(4.42)

We emphasise that this is an \textit{exact} relation. It is only to determine \( q \), which depends on \( \partial_\omega \Sigma(\omega)|_{\omega=0} \), that we have to resort to the RRPA-PP; the renormalised parameters alone suffice to determine \( p(\tilde{\mu}(\epsilon_d)) \). Finally, to derive a flow equation for \( \tilde{U} \) recall Eq. (2.46), an \textit{exact} expression for the transverse charge susceptibility in terms of \( \tilde{\rho} \) and \( \tilde{U} \). Through a re-arrangement we obtain

$$\tilde{U} = \frac{1}{\tilde{\rho}(0)} \left[ 1 - \frac{\chi_{\Sigma}(0)}{\tilde{\rho}(0)} \right],$$

(4.43)
i.e. an expression for \( \tilde{U} \) involving \( \tilde{\rho}(\omega) \) and \( \chi_{\Sigma}(0) \), which can be calculated from

$$\chi_{\Sigma}(0) = \frac{n - 1}{2\epsilon_d + U},$$

(4.44)

where \( n = n_\uparrow + n_\downarrow \) can be deduced in the renormalised theory from the Friedel sum rule in Eq. (2.44). We can therefore use Eq. (4.43) to deduce \( \tilde{U} \) from \( \tilde{\epsilon}_d \) and

\footnote{Mysteriously, the RRPA-PP estimate for \( p(\tilde{\mu}(\epsilon_d)) \) does not agree with Eq. (4.42) and does not correctly describe the renormalisation of \( \tilde{\epsilon}_d \). A similar discrepancy was observed in Ref. [32, p. 98], where it was attributed to a ‘numerical instability’, though no supporting evidence is offered. The author of the present thesis does not agree with this conclusion and attributes the discrepancy to a material deficiency in the RRPA, at least in its present formulation.}
\( \Delta \) at every step of the flow process, and the flow is described by a \( 2 \times 2 \) system of differential equations.

Our results for \( \tilde{\epsilon}_d \), \( \tilde{\Delta} \) and \( \tilde{U} \) for \( U = 3\pi \Delta \) are shown in Fig. 4.3a, 4.4a and 4.5a respectively, where they are referred to as ‘RPT1’. The values of \( \tilde{\Delta} \) are very well reproduced in the weakly correlated region, where they are in close agreement with the NRG result. As \( \epsilon_d \) is increased, this agreement progressively deteriorates, and starts to differ appreciably from the NRG values at \( \epsilon_d + U/2 \approx -1.8\pi\Delta \). Since the determination of \( \tilde{U} \) is sensitive to the value of \( \tilde{\Delta} \), the error in \( \tilde{\Delta} \) is also reflected in the results in Fig. 4.4a\(^4\); we also note in passing that the relative renormalisation of \( \tilde{U} \) is stronger than \( \tilde{\Delta} \) for \( \epsilon_d + U/2 < -\pi\Delta \).

**An improvement**

In the previous section the flow equations were deduced by performing the substitution \( \tilde{\epsilon}_d \to \tilde{\epsilon}_d + \delta \epsilon_d \) in the RPA, which spoils the cancellation with the counterterms and results in a non-trivial flow. To improve on our results, we remark that the non-interacting propagator in the renormalised theory can be interpreted as a mean-field propagator

\[
\tilde{G}^{(0)}(\omega) = \frac{1}{\omega - \tilde{\epsilon}_d + i\tilde{\Delta} \text{sign}(\omega) - \tilde{\Sigma}_\text{MFT}^{\sigma}},
\]

where \( \tilde{\Sigma}_\text{MFT}^{\sigma} \) consists of a static component determined self-consistently following Sec. 1.2 and a \( \lambda_1 \) counter-term that precisely cancels this so that \( \tilde{\Sigma}_\text{MFT}^{\sigma} = 0 \).

When the impurity level is shifted infinitesimally the component of \( \tilde{\Sigma}_\text{MFT}^{\sigma} \) determined self-consistently will change value, giving a residual \( \tilde{\Sigma}_\text{MFT}^{\sigma} \neq 0 \) equal to

\[
\tilde{\Sigma}_\text{MFT}^{\sigma} \to -\frac{\tilde{U} \tilde{\rho}_{-\sigma}}{1 - U^2 \tilde{\rho}_\sigma \tilde{\rho}_{-\sigma}} \delta \epsilon_d \quad (4.45)
\]

Adding this to the original \( \delta \epsilon_d \) we obtain the effective substitution

\[
\tilde{\epsilon}_d \to \tilde{\epsilon}_d + \frac{\delta \epsilon_d}{1 - \tilde{\rho} \tilde{U}} \quad (4.46)
\]

which reduces to Eq. (4.40) in the weak correlation limit. To include self-loops originating from the \( \lambda_3 \) counter-term we can work in terms of the effective inter-
The renormalised parameter \( \tilde{\epsilon}_d \) obtained from the flow equations in \( \epsilon_d \) for the (a) \( U = 3\pi\Delta \) model and (b) \( U = -3\pi\Delta \).

The results obtained using Eq. (4.46) and Eq. (4.47) are shown in Fig. 4.3a, 4.4a and 4.5a, where they are labelled ‘RPT2’ and ‘RPT3’ respectively. In all cases, ‘RPT2’ constitutes an improvement over the ‘RPT1’ approach, though it is again unable to describe models with \( |\epsilon_d + U/2| < 1.5\pi\Delta \), a region where the parameters deviate considerably from the NRG values. In this region, ‘RPT2’ fails to even capture the general behaviour of the parameters and the parameters \( \tilde{\Delta} \) and \( \tilde{U} \) diverge when \( |\epsilon_d + U/2| < \pi\Delta \). In this respect, ‘RPT3’ marks a considerable improvement on the previous approximations. It gives an \( \tilde{\epsilon}_d \to 0 \) as \( \epsilon_d \to 0 \), and finite values for \( \tilde{\epsilon}_d \) and \( \tilde{\Delta} \) in the strong correlation regime which are in qualitative agreement with the NRG. However even this approximation fails to reproduce the parameters close to particle-hole symmetry with any degree of accuracy.

Despite these limitations, we note the very good agreement between the ‘RPT3’ results for the charge susceptibility and the NRG calculation, where the approximation remarkably succeeds in capturing the local maximum at \( \epsilon_d + U/2 \approx -1.5\pi\Delta \), and only starts to depart considerably from the NRG values at \( |\epsilon_d + U/2| < -0.6\pi\Delta \). Furthermore, we see that ‘RPT3’ also reproduces the general shape of the spin susceptibility. However, this depends on \( 1 - \tilde{U}\tilde{\rho} \), which is sensitive to the value of \( \tilde{U}\tilde{\rho} \) whereas \( \chi^s_c \), which depends on \( 1 + \tilde{U}\tilde{\rho} \), is not. As a result, \( \chi_s \) is not as well described.
Figure 4.4.: The renormalised parameter $\tilde{U}$ obtained from the flow equations in $\epsilon_d$ for (a) $U = 3\pi\Delta$ model and (b) $U = -3\pi\Delta$.

Figure 4.5.: The renormalised parameter $\Delta$ obtained from the flow equations in $\epsilon_d$ for (a) $U = 3\pi\Delta$ and (b) $U = -3\pi\Delta$.

Figure 4.6.: The charge (left) and spin (right) susceptibilities for a model with $U = 3\pi\Delta$. 

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Extension to a magnetic field

In this section we discuss the implementation of the flow equations in $\epsilon_d$ for a model in a non-zero magnetic field. When $h \neq 0$, the self-energy and its derivatives become spin-dependent; consequently $\epsilon_d, \uparrow \neq \epsilon_d, \downarrow$ and $\Delta \uparrow \neq \Delta \downarrow$. Despite these apparent complications, one can still carry out the flow approach described in this section by taking the spin dependence of $p(\mu(\epsilon_d))_\sigma$ and $q(\mu(\epsilon_d))_\sigma$ and solving a $4 \times 4$, rather than $2 \times 2$ system of equations.

Negative-$U$ models

The Anderson impurity model is typically discussed in the context of a positive Coulomb constant $U$. This is reasonable, since it reflects the energy cost in localising two test charges of the same sign, which of course repel each other. Nevertheless, the model remains mathematically consistent and, despite its apparent unphysical character, has been useful in describing the physics of impurities in semi-conductor glasses [10, 90], the properties of heavy-fermion systems [123], superconductivity [88] and the transport properties of molecular quantum dots [3, 69, 6], where it can arise as a result of potential inversion due to the coupling of the orbital to the molecular vibrational modes.

The flow equation method described in this section makes no assumptions on the sign of the interaction. To probe this parameter regime we carry out the previous comparison to the NRG, this time setting $U = -3\pi \Delta$. From Fig. 4.3b, 4.4b, 4.5b we see that the results of the method are in much closer agreement with the NRG than they were for a positive-$U$ model. In particular, we see that both ‘RPT1’ and ‘RPT3’ are both very close to the correct values, with ‘RPT2’ now constituting the least accurate approximation.

Recall from Sec. 1.4 that a negative-$U$, asymmetric, Anderson impurity model, in the absence of a magnetic field, can be mapped onto a positive-$U$, symmetric model with a non-zero field. This mapping allows us to relate the method outlined here to the flow equation method outlined in Ref. [32], where a symmetric Anderson model was studied by considering the scaling in the magnetic field. In fact, it shows that the two approaches are equivalent, since under the spin-isospin transformation the particle-hole ladder of Ref. [32] maps onto the particle-particle ladder used here. Consequently, the faithful reproduction of the renormalised parameters for the negative-$U$ model in Fig. 4.3b, 4.4b, 4.5b) is hardly surprising, a merely a re-statement of results already obtained in Ref. [32]. This confirms that the comparatively inferior results obtained here for the positive-$U$ model
are not due to an oversight in implementing the method, but are indicative of a genuine weakness in the theory. Furthermore, we can infer that the method of Ref. [32] will not perform as well for symmetric negative-$U$ models in a magnetic field.

4.4. Flow equations in $\Delta$

In this section we focus on the symmetric model and construct flow equations by varying $\Delta$ [102]. Since the convergence of the perturbation theory depends on the ratio $U/\pi \Delta$, taking $\Delta \to \infty$ allows us to use ordinary perturbation theory to deduce the boundary conditions for the renormalised parameters$^5$. We thus have, from the results of Yamada and Yosida [137, 134, 138, 135] that when $\Delta \to \infty$

$$\hat{\Delta} = \Delta \left[ 1 - \left( 3 - \frac{\pi^2}{4} \right) \left( \frac{U}{\pi \Delta} \right)^2 \ldots \right],$$

$$\hat{U} = U \left[ 1 - (\pi^2 - 9) \left( \frac{U}{\pi \Delta} \right)^2 \ldots \right].$$

(4.48)

(4.49)

We highlight that $\tilde{\epsilon}_{d} = 0$ in the particle-hole symmetric limit. We thus need to derive only two flow equations, for $\hat{\Delta}$ and $\hat{U}$. To determine $q(\tilde{\mu}(\Delta))$ we note that the particle-hole symmetry of the model must be reflected in the diagrammatic expansion, which should treat particles and holes similarly. In this limit, previous work [32] employed the RRPA-PH expansion (Sec. 2.7), which additionally has the advantage of featuring terms to all orders in $\tilde{U}$. We thus adopt the RRPA-PH to calculate $q(\tilde{\mu}(\Delta))$. To calculate the flow equation for $\hat{U}$ we consider the effects of the infinitesimal vertex on the pair propagator alone, and find that

$$\frac{\partial \hat{U}}{\partial \Delta} = \frac{\hat{U}_{\text{eff}}^2/2\pi \Delta^2}{\left( 1 - \Pi_{1+}^{\text{ph}}(0) \hat{U}_{\text{eff}} \right)^2}.$$  

(4.50)

Our results are shown in Fig. 4.7; for comparison, the results from bare perturbation theory in Eq. (4.49) are also shown. We see that $\hat{\Delta}(\Delta)$ is reproduced very well for weak and intermediate couplings but begins to depart from the NRG results for $U/\pi \Delta > 1.5$. By contrast, the results for $\hat{U}(\Delta)$ start to depart from the NRG results at $U/\pi \Delta \approx 0.5$, approximately the same coupling strength

$^5$Note that this limit should be taken so that the conduction band width remains the dominant scale.
at which the bare perturbation theory becomes unreliable. Nevertheless, some qualitative agreement is maintained even into the strong correlation regime.

To improve the results, a more sophisticated treatment of the infinitesimal one-body vertex is needed. It is likely that better results can be obtained by deducing $q(\tilde{\mu}(\Delta))$ with the method outlined in Sec. 4.2 coupled to either the second-order renormalised theory or the RRPA-PH considered here. To obtain a flow equation for $\tilde{U}(\Delta)$ one could then use Eq. (4.10) (this method is used in the next section).

4.5. Flow equations in $U$

A final possibility is to carry out the flow in the interaction constant. We remark that this constitutes a direct implementation of the Fermi liquid theory framework, where, starting from a non-interacting system, one considers the effects of ‘adiabatically’ turning on the interactions. In Fermi liquid theory, the system is described in terms of effective Fermi liquid parameters, which can be directly related to the parameters of the renormalised perturbation theory. Thus, by carrying out the flow in $U$ one can also deduce the flows of the Fermi parameters.

4.5.1. Particle-hole symmetry

To derive a flow equation for $\tilde{U}(U)$ we make use of Eq. (4.10), evaluated at $\omega = 0$, and exploit the fact that $\tilde{U}(U + \delta U)$ will inevitably appear on the LHS. We can then solve for $\tilde{U}$ to obtain a flow equation. In the special case of particle-
hole symmetry we can exploit the analytic result of Eq. (2.52) for the second derivative of the renormalised self-energy to obtain the LHS. Equation (2.52) can also be used to deduce the RHS of Eq. (4.10). Following the recipe for \( \tilde{\Sigma}_\sigma(\omega; \mu(U), \delta U) \) which dictates the substitution \( \tilde{U}(U) \rightarrow \tilde{U}(U) + z(U)\tilde{U}(U) \), we can deduce the leading-order relation

\[
\frac{\tilde{U}^2(U + \delta U)}{\Delta^3(U + \delta U)} = z(U; \delta U) \frac{\tilde{U}(U) + z\delta U}{\Delta^3(U)}. \tag{4.51}
\]

By retaining only terms linear in \( \delta U \) we derive the flow equation for \( \tilde{U}(U) \)

\[
\frac{\partial \tilde{U}(U)}{\partial U} = 2q(U)\tilde{U}(U) + z(U). \tag{4.52}
\]

To determine \( q(U) \) we appeal to the discussion of Sec. 4.2. By evaluating the expression in Eq. (4.30) at particle-hole symmetry we deduce that

\[
q(U) = -z \times (6 - \pi^2/2) \frac{\tilde{U}}{(\pi \Delta)^2}, \tag{4.53}
\]

to leading order in \( \tilde{U} \). We can now combine Eq. (4.52) and Eq. (4.14) to derive the complete system of differential flow equations

\[
\frac{\partial \bar{\Delta}}{\partial U} = \xi \tilde{U},
\]

\[
\frac{\partial \tilde{U}}{\partial U} = 2\xi \frac{\tilde{U}^2}{\Delta} + \frac{\bar{\Delta}}{\Delta}, \tag{4.54}
\]

where

\[
\xi = -(6 - \pi^2/2) \frac{1}{\pi^2 \Delta} < 0. \tag{4.55}
\]

We proceed by eliminate \( \tilde{U} \), finding

\[
\bar{\Delta} \frac{d^2 \tilde{U}}{d\tilde{U}^2} = 2 \left( \frac{d\tilde{U}}{d\tilde{U}} \right)^2 - \kappa^2 \Delta^2,
\]

where \( \kappa = \sqrt{|\xi|/\Delta} \). We thus obtain a simple closed form expression for \( \bar{\Delta}(U) \)

\[
\bar{\Delta}(U) = c_2 \frac{1}{e^{-\kappa U} + e^{\kappa U + \epsilon_1}} \tag{4.56}
\]

\(^6\)Note that, as discussed in Sec. 2.5, this relation is conjectured to be exact even away from particle-hole symmetry, though we have not rigorously proven this claim. This opens up the possibility of using this equation to determine \( \tilde{U} \) even away from particle-hole symmetry.
Figure 4.8.: The renormalised parameters obtained from the flow equations for the symmetric model (Eq. (4.58)) plotted against the NRG results.

where \( c_0, c_1 \) are arbitrary constants. We fix these by requiring that \( \hat{\Delta}(0) = \Delta \) and that \( \hat{\Delta}(U) \) be quadratic in \( U \) for \( U \to 0 \). The result is

\[
\hat{\Delta}(U) = \Delta \text{sech}(\kappa U),
\]

\[
\hat{U}(U) = \frac{\sinh(\kappa U)}{\kappa \cosh^2(\kappa U)}. \tag{4.58}
\]

These equations are compared to data from the NRG in Fig. 4.8. We find that at small values of \( U/\pi \Delta \) both renormalised parameters are in excellent agreement with the NRG. From the plots we also confirm that the maximum of \( \hat{U}(U) \) is faithfully reproduced by Eq. (4.58) — from Eq. (4.58) we find that the stationary point of \( \hat{U}(U) \) occurs at

\[
U_s = \frac{\text{atanh} \left( \frac{1}{\sqrt{2}} \right)}{\sqrt{6 - \pi^2/2}}, \tag{4.59}
\]

which is indicated by the vertical line in Fig. 4.8. As \( U \) increases further a small discrepancy arises and becomes more severe with \( U \). We attribute this to the fact that \( \hat{U}/\pi \Delta \) is approaching one so higher-order terms in the renormalised series start to contribute. The ratio \( \hat{U}/\pi \Delta \) is plotted alongside data from the NRG in Fig. 4.9. In the Kondo limit we obtain that

\[
\lim_{U \to \infty} \frac{\hat{U}(U)}{\pi \Delta(U)} = \frac{1}{\sqrt{6 - \pi^2/2}} \approx 0.9689, \tag{4.60}
\]

which is close to 1, the exact result.

Given the renormalised parameters, the spin and charge susceptibilities can be computed from Eq. (2.47), (2.48); the results are shown in Fig. 4.10. Both quantities are reproduced very well at weak coupling, where they are in excel-
lent agreement with the NRG results. When $U > \pi \Delta$ we observe that the RPT result for the spin susceptibility becomes less accurate, eventually predicting an entirely erroneous dependence on $U$ when $U > 2\pi \Delta$. By contrast, the charge susceptibility is in excellent quantitative agreement with the NRG values even well into the strong correlation regime. The reason for this difference in behaviour can be traced to Eq. (2.47), (2.48), from which we see that the charge susceptibility is rather sensitive to the precise value of $\tilde{U}\tilde{\rho}$, which tends to one, whereas the spin susceptibility is not.

Given the renormalised parameters, we can write the impurity conductance as [49]

$$\sigma(T)/\sigma(0) = 1 + (k_B T)^2 \phi,$$

where

$$\phi = \frac{\pi^2}{3\Delta^2} \left[ 1 + 2 \left( \frac{\tilde{U}}{\pi \Delta} \right)^2 \right].$$

This is shown in Fig. 4.11, where we find that RPT and NRG results are in very good agreement even for large values of $U$.

**Extensions**

In the previous section we discussed the scaling behaviour in $U$, for the symmetric model to leading order in $\tilde{U}$. Two natural extensions of this work present themselves: the extension to asymmetric models, and the inclusion of terms involving higher powers in $\tilde{U}$.

In considering asymmetric models, a $2 \times 2$ system will not suffice — one must also consider $\tilde{\epsilon}_d$, which will be non-zero and exhibit a non-trivial flow. To study
Figure 4.10.: The spin (left) and charge (right) susceptibilities as a function of $u/\pi\Delta$.

Figure 4.11.: The $\phi$ coefficient of the conductance, defined through $\sigma(T)/\sigma(0) = 1 + (k_B T)^2 \phi$. 

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such model, one can choose whether the original model is to be specified in terms of $\epsilon_d$, or the impurity occupation $n$. In this case, it seems that the latter choice lends itself, for if $n$ is fixed one can determine $\tilde{\epsilon}_d$ exactly from the Friedel sum rule (2.44), and deduce the exact flow equation

$$ \frac{d\tilde{\epsilon}_d}{dU} = \frac{\epsilon_d}{\Delta} \frac{d\tilde{\Delta}}{dU}. $$

As discussed in Sec. 4.2, away from particle-hole symmetry one must also consider the one-particle tadpole terms that the infinitesimal vertex will give rise to. Finally, we note that Eq. (4.51) assumes that the RPT estimate of the imaginary part of the second frequency-derivative of the self-energy is exact; as discussed in Sec. 2.5, this is only been proven at particle-hole symmetry, but is likely to hold away from it too.

To extend the calculation to include terms of higher powers in $U$, we must return to Eq. (4.28) and truncate the resultant series to the appropriate power. In principle, one must also calculate the higher-order terms on the RHS of Eq. (4.52), which for $\delta U \neq 0$ will not be precisely cancelled by the counter-terms. We remark, however, that Eq. (4.52) seems accurate even for $U$ as large as $12\pi\Delta$, suggesting that higher-order terms are not very important. We substantiate this claim by interpolating $\tilde{\Delta}(U)$ from the NRG results, and using Eq. (4.52) to deduce $\tilde{U}(U)$. Our results are shown in Fig. 4.12, where we see that the resultant $\tilde{U}(U)$ is in virtually exact agreement with the correct values.

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7These two are not independent, but determining $n$ given $\epsilon_d$, or vice-versa, requires knowledge of $\Sigma(0)$, which we cannot compute for large values of $U$. 

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Finally, we note the possibility of further extending this approach to other impurity models. One could, for instance, consider the effects of a finite band-size, or study the model in the narrow band limit. It is also likely that minimal modifications would be needed to apply this treatment to the pseudo-gap Anderson model, or to the calculation of the susceptibility of the Mattis model. More ambitiously, one could conceivably use this method to study models of more than one impurity, for example by combining our approach with the DMFT, to study lattice models, or implementing the scaling in $U_{12}$ to study the two-channel model.
5. Conclusion

This chapter concludes the discussion on renormalised perturbation theory. We have shown how the ideas of quasi-particles and renormalised parameters can be used to construct a useful perturbation expansion, even when the interactions are too strong to be handled within ordinary perturbation theory. The static properties of the resulting theory are largely exact, and can be used to calculate experimentally measurable properties of the Anderson impurity model such as the conductance. As a practical application, we calculated the conductance of a single quantum dot, and of a double quantum dot. Next, we discussed the automation of high-order self-energy and four-vertex calculations in the renormalised theory and presented a calculation of the $\tilde{U}^5$ term in the self-energy expansion. Finally, we considered the question of determining the renormalised parameters by tracing the flow in one of the model’s parameters and using the parameters of a weakly correlated model to deduce those of models with increasingly stronger correlations.

The renormalised perturbation theory is undoubtedly a powerful method with which to study systems in condensed matter. At present, the most reliable way of computing the parameters is through the Numerical Renormalisation Group. This constitutes, in the author’s opinion, the central limitation of the theory, for it requires the model to be tractable through the NRG and a method of determining the parameters from Numerical Renormalisation Group results. The development of a general, reliable method of determining the renormalised parameters without such external methods must thus be a priority for the future.

In the course of this thesis we have applied the flow equation method to the single impurity Anderson model, where we explored all different ways of transitioning from a weakly correlated model to a strongly correlated model. Future effort could focus towards refining and implementing the systematic framework presented in Sec. 4.2. This general method of deducing the flow equations in any parameter ought to be, in principle, applicable to any model. When carried out to fixed order in $\tilde{U}$, flow equation schemes are not expected to generally yield

\footnote{We did not however consider simultaneous changes to more than one parameter.}
results accurate for very large values of $U$. However, the possibility of combining such an approach with all-orders resummations based on the RPA, or an elaborated form of it, opens up the possibility of developing a reliable method for calculating the renormalised parameters in all regimes, regardless of the strength of the correlations.
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A. Leading temperature dependence of the self-energy

In this Appendix we use the Matsubara formalism of Sec. 1.5 to calculate the temperature dependence of $\tilde{\Sigma}_\sigma(\omega)$ for a general, potentially asymmetric, Anderson model. Some parts of this calculation have appeared in Ref. [51], where furthermore identity Eq. (2.66) was exploited to isolate the $T^2$ term of the temperature dependence. We will begin by discussing the single-channel case and then proceed to discuss the two-channel model.

A.1. Calculation in the Matsubara formalism

A.1.1. Single channel model

Consider the second-order diagram of Fig. A.1, with the internal lines representing the non-interacting renormalised thermal Green’s function of Eq. (1.59). In addition to this diagram, away from particle-hole symmetry one must also take into account the tadpole diagrams that contribute due to the incomplete cancellation at finite temperatures with the $\lambda_1$ counter-term, which is defined at zero temperature.

After an application of the Feynman rules we find that

$$\tilde{\Sigma}^{[2a]}_\sigma(\Omega_m, T) = -\tilde{U}^2 T^2 \sum_{n_1 \text{ even}} \sum_{n_2 \text{ odd}}(\tilde{G}_\sigma^{(0)}(\omega_{n_1} + \Omega_m)\tilde{G}_\sigma^{(0)}(\omega_{n_2}) - \tilde{G}_\sigma^{(0)}(\omega_{n_1} + \omega_{n_2})). \quad (A.1)$$

Figure A.1.: The sole dynamic self-energy diagram of order $\tilde{U}^2$. 

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We can express $\tilde{G}_\sigma(\omega_n, T)$ in terms of a spectral density as follows

$$\tilde{G}_\sigma^{(0)}(\omega_n, T) = \int \frac{d\epsilon}{\epsilon - i\omega_n},$$

(A.2)

where $\tilde{\rho}_\sigma^{(0)}(\omega) = -\text{Im} \tilde{G}_\sigma^{(0,+)}(\omega, 0)/\pi$ is the usual spectral density at $T = 0$.

We substitute Eq. (A.2) into Eq. (A.1) and carry out the summations over the Matsubara frequencies using the useful identity [24]

$$T \sum_n F(i\omega_n) = \oint_C \frac{dz}{2\pi i} F(z) f(z),$$

(A.3)

where $f(z) = (e^{\beta z} + 1)^{-1}$ is the analytic continuation of the Fermi function and $C$ is a contour that encloses the poles of $F(z)$ and has a counter-clockwise sense.

We then find that the imaginary part of the self-energy is given by [51]

$$\text{Im} \tilde{\Sigma}_\sigma^{[2a]}(\omega, T) = -\pi \tilde{U} \int d\epsilon_1 d\epsilon_2 \tilde{\rho}_\sigma^{(0)}(\epsilon_1) \tilde{\rho}_\sigma^{(0)}(\epsilon_2) \tilde{\rho}_\sigma^{(0)}(\omega - \epsilon_1 - \epsilon_2) D(\omega, \epsilon_1, \epsilon_2, T),$$

(A.4)

where $D(\omega, \epsilon_1, \epsilon_2, T) = (1 - f(\epsilon_1, T) - f(\epsilon_2, T)) f(\epsilon_1 + \epsilon_2 - \omega, T) + f(\epsilon_1, T) f(\epsilon_2, T) - f(\epsilon_2, T) f(\epsilon_1, T) f(\epsilon_2, T)$.

Since $\tilde{\Sigma}_\sigma(\omega)$ is an analytic function which vanishes at least as fast as $1/|x|$ as $x \to \pm \infty$, we can deduce its real part from the Kramers-Kronig relation

$$\text{Re} \tilde{\Sigma}_\sigma^{[2a]}(\omega) = \mathcal{P} \int \frac{d\omega'}{\pi} \frac{\text{Im} \tilde{\Sigma}_\sigma^{[2a]}(\omega')}{\omega - \omega'},$$

(A.5)

where the second relation is less susceptible to numerical instabilities when implemented on a computer. We now consider the tadpole diagram of Fig. A.2. Starting with Fig. (A.2a), and tacitly including a counter-term subject to the usual renormalisation conditions of Eq. (2.16) at $T = 0$, we find that

$$\tilde{\Sigma}_\sigma^{[1]}(T) = \tilde{U} \int_{-\infty}^{\infty} d\epsilon \tilde{\rho}_\sigma^{(0)}(\epsilon) u(\epsilon, T),$$

(A.6)

$$u(\epsilon, T) = f(\epsilon, T) - f(\epsilon, 0),$$

(A.7)

where $f(\epsilon, 0) = \theta(-\epsilon)$, where $\theta(x)$ denotes the Heaviside step function. Turning

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1 We can verify this identity by substituting $i\omega_n \to \omega + i0^+$ and applying the Sokhotsky identity. It is easy to see then that the imaginary parts are equal, and the real part follows from the Kramers-Kronig relation.
Figure A.2.: First (a) and second (b) order tadpole diagrams that contribute to \( \text{Re} \tilde{\Sigma}_\sigma(\omega, T) \) for \( T \neq 0 \) away from particle-hole symmetry.

now our attention to Fig. A.2b we find that

\[
\tilde{\Sigma}^{[2b]}_\sigma(T) = \tilde{U} \tilde{\Sigma}^{[1]}_\sigma(T) \int d\epsilon_1 d\epsilon_2 \tilde{\rho}^{(0)} - \sigma_\sigma(\epsilon_1) \tilde{\rho}(0) - \sigma_\sigma(\epsilon_2) Q(\epsilon_1, \epsilon_2, T),
\]

where again we have included the counter-term by subtracting the amplitude of the diagram at \( T = 0 \). We remark that the static diagram of Fig. A.2a factorises entirely. The total self-energy to order \( \tilde{U}^2 \) is thus

\[
\tilde{\Sigma}_\sigma(\omega, T) = \tilde{\Sigma}^{[1]}_\sigma(T) + \tilde{\Sigma}^{[2]}_\sigma(T) + \tilde{\Sigma}^{[2a]}_\sigma(\omega, T) + \omega \lambda_2 + \lambda_1,
\]

where the counter-terms \( \lambda_2, \lambda_1 \) are set as per Eq. (2.16) at \( T = 0 \) (note that we are only interested in \( \tilde{\Sigma}_\sigma(0, T) \) and can therefore ignore the \( \lambda_2 \) counter-term).

A.1.2. Two channel model

In the case of the two-channel model, we have to consider, in addition to the on-site impurity interaction \( \tilde{U} \), the effects of the intra-impurity repulsion \( \tilde{U}_{12} \). This generates additional diagrams that contribute to \( \tilde{\Sigma}_\sigma(\omega, T) \) and which can be trivially calculated in analogy to the \( SU(2) \) case. To leading order in \( \tilde{U} \) and \( \tilde{U}_{12} \) we find

\[
\tilde{\Sigma}^{[1]}_\sigma(T) = \int_{-\infty}^{\infty} d\epsilon \left[ (\tilde{U} + \tilde{U}_{12}) \tilde{\rho}^{(0)}(\epsilon) + \tilde{U}_{12} \tilde{\rho}^{(0)}(\epsilon) \right] u(\epsilon, T).
\]
To second order in $\tilde{U}$ and $\tilde{U}_{12}$ we have

$$\tilde{\Sigma}_\sigma^{[2a]}(T) = \int d\epsilon_1 d\epsilon_2 \left[ (\tilde{U} + \tilde{U}_{12})\tilde{\rho}^{(0)}_{\sigma}(\epsilon_1)\tilde{\Sigma}_\sigma^{[1]}(T)\tilde{\rho}^{(0)}_{\sigma}(\epsilon_2) + \tilde{U}_{12}\tilde{\rho}^{(0)}_{\sigma}(\epsilon_1)\tilde{\Sigma}_\sigma^{[1]}(T)\tilde{\rho}^{(0)}_{\sigma}(\epsilon_2) \right] Q(\epsilon_1, \epsilon_2, T). \quad (A.12)$$

Finally we generalise Eq. (A.4), which will also contribute to $\tilde{\Sigma}_\sigma(0)$ away from particle-hole symmetry, finding

$$\text{Im} \tilde{\Sigma}_\sigma^{[2a]}(\omega, T) = -\pi \int d\epsilon_1 d\epsilon_2 \tilde{\rho}^{(0)}_{\sigma}(\omega - \epsilon_1 - \epsilon_2) D(\omega, \epsilon_1, \epsilon_2, T) \times \left[ (\tilde{U}^2 + \tilde{U}_{12}^2)\tilde{\rho}^{(0)}_{\sigma}(\epsilon_1)\tilde{\rho}^{(0)}_{\sigma}(\epsilon_2) + \tilde{U}_{12}^2\tilde{\rho}^{(0)}_{\sigma}(\epsilon_1)\tilde{\rho}^{(0)}_{\sigma}(\epsilon_2) \right], \quad (A.13)$$

with the real part following from Eq. (A.5).

### A.2. Extracting the temperature dependence

In this section we discuss the extraction of the $T^2$ term from the full temperature dependence of the results of the previous section. First, we consider the one-dimensional integrals arising from the tadpole diagrams and then proceed to discuss the temperature-dependence of the second-order diagram. For simplicity we begin by discussing the single-channel model and then transfer our results by analogy to the two-channel model.

#### A.2.1. Single-channel model

##### One-dimensional integrals

Consider the expression in Eq. (A.7); it is clear that the $T$ dependence is solely due to $u(\epsilon, T)$, which tends to zero when $T \rightarrow 0$. The naive approach of constructing a Taylor expansion by differentiating $f(\epsilon, T)$ around $T = 0$ is not possible, since $f(\epsilon, T)$ is not differentiable at $T = 0$ and so another approach is needed\(^2\). Fortunately, the structure of Eq. (A.7) is particularly simple, and we

\(^2\)In extracting the temperature dependence from integrals like Eq. (A.15) one must be careful using the substitution $x = (\epsilon - \mu)/T$. A direct substitution yields

$$\int_{-\infty}^{\infty} d\epsilon H(\epsilon) f(\epsilon) = T \int_{-\infty}^{\infty} dx H(xT) f(\epsilon T). \quad (A.14)$$

Here the Fermi function involves $xT$, so it does not depend on $T$, and one may be tempted to Taylor-expand $H(xT)$ to obtain an expression involving powers of $T$. This is however an
can use the following lemma known as the *Sommerfeld expansion* [120].

**Lemma**: Let $H(\epsilon)$ be a smooth function that vanishes as $\epsilon \to -\infty$, and which diverges at worst polynomially as $\epsilon \to \infty$. In the limit $T \to 0$ it can be approximated as

$$\int_{-\infty}^{\infty} d\epsilon H(\epsilon) f(\epsilon, T) \approx \int_{-\infty}^{\infty} d\epsilon H(\epsilon) + \frac{\pi^2 T^2}{6} H'(\mu) + \mathcal{O}(T^4). \quad (A.15)$$

**Proof**: Let $K(\epsilon) = \int_{-\infty}^{\epsilon} d\epsilon' H(\epsilon')$. We can then integrate the LHS by parts to find

$$\int_{-\infty}^{\infty} d\epsilon H(\epsilon) f(\epsilon, T) = \left[ H(\epsilon) f(\epsilon) \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} d\epsilon K(\epsilon) f'(\epsilon, T). \quad (A.16)$$

where

$$f'(\epsilon, T) = -\frac{1}{T} \frac{e^{(\epsilon - \mu)/T}}{(e^{(\epsilon - \mu)/T} + 1)^2}. \quad (A.17)$$

From our assumptions on $H(\epsilon)$ as $\epsilon \to \pm \infty$ we conclude that the surface term in Eq. (A.16) vanishes. Note furthermore that at zero temperature $f(x, 0) = \theta(\mu - x)$, and that raising the temperature will only have a significant effect on $f(x, T)$ in the vicinity of $x = \mu$. We can therefore expand $K(\epsilon)$ around this point

$$K(\epsilon) = \sum_{n=0} \frac{(\epsilon - \mu)^n}{n!} \frac{d^n K(\epsilon)}{d\epsilon^n} \bigg|_{\epsilon = \mu},$$

and, upon substituting this in Eq. (A.16) and performing the substitution $x = (\epsilon - \mu)/T$, obtain

$$\int_{-\infty}^{\infty} d\epsilon H(\epsilon) f(\epsilon, T) = -K(\mu) \int_{-\infty}^{\infty} d\epsilon f'(\epsilon) + TK'(\mu) \int_{-\infty}^{\infty} dx \frac{x e^x}{(e^x + 1)^2}$$

$$+ \frac{1}{2} T^2 \int_{-\infty}^{\infty} dx \frac{x^2 e^x}{(e^x + 1)^2} + \ldots. \quad (A.18)$$

The lemma then follows by noting that the first integral is trivial, that the second integral vanishes due to its integrand being odd, and that the third integral can be carried out with magic and is equal to $\frac{\pi^2}{6}$. □

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Using the lemma we find that
\[ \tilde{\Sigma}_\sigma^{[1]}(T) = \tilde{U} \frac{\pi^3 T^2}{3 \Delta_{-\sigma}} \tilde{\epsilon}_{d,-\sigma}^2(0). \]  
(A.19)

Additionally, since \( \tilde{\Sigma}_\sigma^{[1]}(T) \sim T^2 \) we see that the integral of Eq. (A.8) will contribute a leading term of order \( T^4 \), and can thus be ignored entirely — this follows from the fact that \( u(\epsilon, 0) = 0 \), from which we automatically have that \( Q(\epsilon_1, \epsilon_2, 0) = 0 \) and that therefore \( Q(\epsilon_1, \epsilon_2, T) = O(T) \).

Note that the statement of the Sommerfeld expansion is general and does not assume that \( \mu = 0 \). In the nearly-free electron theory [13, p. 30] this is crucial in establishing the correct temperature dependence of various quantities, since \( \mu - \mu_0 \sim (T/E_F)^2 \).

Technically, one must take this effect into account in the impurity case too; note however that in Eq. (A.19) the scale is set by \( \tilde{\rho}(0) \ll E_F \), and the temperature dependence involves powers of \( T/\tilde{\rho} \). Consequently we can, to an excellent approximation, ignore the chemical potential entirely.

### Multi-dimensional integrals

We now turn our attention to the dynamic diagram, considering first the contribution from \( \text{Im} \tilde{\Sigma}_\sigma^{[2h]}(0, T) \). This was studied in the particle-hole symmetric case in Ref. [51], where an expression for the \( T^2 \) coefficient of \( \text{Im} \tilde{\Sigma}_\sigma(\omega, 0) \) was deduced\(^3\). Strictly speaking, one does not need to explicitly calculate this, for we can invoke the Fermi liquid property that

\[ \left. \frac{\partial^2 \text{Im} \tilde{\Sigma}_\sigma(\omega, 0)}{\partial \omega^2} \right|_{\omega=0} = \left. \frac{\partial^2 \text{Im} \tilde{\Sigma}_\sigma(0, T)}{\partial (\pi T)^2} \right|_{T=0} \]  
(A.20)

to reduce the question of finding the \( T^2 \) coefficient to that of finding the \( \omega^2 \) coefficient (see Sec. 2.5). In the presence of particle-hole symmetry this is sufficient to determine the temperature dependence of \( \tilde{\Sigma}_\sigma(0, T) \) at low \( T \), since \( \text{Re} \tilde{\Sigma}_\sigma(0, T) = 0 \) [137, 134]. (see also Eq. (B.4).

Away-from particle-hole symmetry \( \text{Re} \tilde{\Sigma}_\sigma(0, T) \) is non-trivial and temperature-dependent (the general form at finite temperatures is given by Eq. (B.4)). Since \( \text{Re} \tilde{\Sigma}_\sigma(\omega, T) \) is deduced from the imaginary part using Eq. (A.5), we seek an expression for the \( T^2 \) coefficient of \( \text{Im} \tilde{\Sigma}_\sigma(\omega, T) \) at finite frequencies. This cannot be deduced as in Ref. [51] or through Eq. (A.20), which is only valid at \( \omega = 0 \). We will therefore organise the calculation in a manner that permits the application

\(^3\)Note that Eq. (34) in Ref. [51] has the wrong sign.
of the Sommerfeld expansion. To proceed we rewrite \( D(\omega, \epsilon_1, \epsilon_2, T) \) as

\[
D(\omega, \epsilon_1, \epsilon_2, T) = f(\epsilon_1 + \epsilon_2 - \omega, T) - f(\epsilon_1, T)f(\epsilon_1 + \epsilon_2 - \omega, T) - f(\epsilon_2, T)f(\epsilon_1 + \epsilon_2 - \omega, T) + f(\epsilon_1, T)f(\epsilon_2, T)
\]  
(A.21)

and Eq. (A.4) as

\[
\text{Im} \tilde{\Sigma}_\sigma^{[2a]}(\omega, T) = -\pi U^2 (I_1(\omega, T) + I_2(\omega, T) + I_3(\omega, T) + I_4(\omega, T)),
\]

where

\[
I_1(\omega, T) = \int d\epsilon_1 \tilde{\rho}_{\sigma}(\epsilon_1) \int d\epsilon_2 \tilde{\rho}_{\sigma}(\epsilon_2) \tilde{\rho}_{\sigma}(\omega - \epsilon_1 - \epsilon_2)f(\epsilon_1 + \epsilon_2 - \omega, T),
\]  
(A.22)

\[
I_2(\omega, T) = \int d\epsilon_1 \tilde{\rho}_{\sigma}(\epsilon_1) f(\epsilon_1, T) \int d\epsilon_2 \tilde{\rho}_{\sigma}(\epsilon_2) \tilde{\rho}_{\sigma}(\omega - \epsilon_1 - \epsilon_2)f(\epsilon_1 + \epsilon_2 - \omega, T),
\]  
(A.23)

\[
I_3(\omega, T) = \int d\epsilon_1 \tilde{\rho}_{\sigma}(\epsilon_1) \int d\epsilon_2 \tilde{\rho}_{\sigma}(\epsilon_2) \tilde{\rho}_{\sigma}(\omega - \epsilon_1 - \epsilon_2)f(\epsilon_2, T)f(\epsilon_2 + \epsilon_1 - \omega, T),
\]  
(A.24)

\[
I_4(\omega, T) = \int d\epsilon_1 \tilde{\rho}_{\sigma}(\epsilon_1) f(\epsilon_1, T) \int d\epsilon_2 \tilde{\rho}_{\sigma}(\epsilon_2) \tilde{\rho}_{\sigma}(\omega - \epsilon_1 - \epsilon_2)f(\epsilon_2, T).
\]  
(A.25)

In fact, it is easy to see by swapping the labels on the integration variables that \( I_2(\omega, T) = I_3(\omega, T) \), and so only three cases have to be examined. All three can be dealt with in a similar manner: apply Sommerfeld’s expansion to the inner integral and retain only the \( T^2 \) term; then perform the outer integral, and in the case of \( I_2(\omega, T) \) and \( I_4(\omega, T) \) apply Sommerfeld’s expansion to the outer integration too. We thus obtain

\[
I_1(\omega, T) - I_1(\omega, 0) = \frac{\pi^2 T^2}{6} \sigma_{\omega}(\omega),
\]  
(A.26)

\[
I_2(\omega, T) - I_2(\omega, 0) = I_3(\omega, T) - I_3(\omega, 0) = \frac{\pi^2 T^2}{6} \sigma_{\omega}(\omega),
\]  
(A.27)

\[
I_4(\omega, T) - I_4(\omega, 0) = \frac{\pi^2 T^2}{3} \sigma_{\omega}(\omega),
\]  
(A.28)

giving in total

\[
\text{Im} \tilde{\Sigma}_\sigma^{[2a]}(\omega, T) - \text{Im} \tilde{\Sigma}_\sigma^{[2a]}(0, 0) = -\frac{\pi^3 U^2 T^2}{6} Q_{\omega}(\omega),
\]  
(A.29)
where

\[
Q_{\sigma_1,\sigma_2}(\omega) = g_{\sigma_1,\sigma_2}^{(1)}(\omega) - 2g_{\sigma_1,\sigma_2}^{(2)}(\omega) + 2g_{\sigma_1,\sigma_2}^{(3)}(\omega), \tag{A.30}
\]

\[
g_{\sigma_1,\sigma_2}^{(1)}(\omega) = \tilde{\rho}_{\sigma_1}^{(0)}(0) \int_{-\infty}^{\infty} d\epsilon \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \partial_\omega \tilde{\rho}_{\sigma_2}^{(0)}(\omega - \epsilon)
- \partial_\omega \tilde{\rho}_{\sigma_1}^{(0)}(\omega)|_{\omega=0} \int_{-\infty}^{\infty} d\epsilon \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \tilde{\rho}_{\sigma_2}^{(0)}(\omega - \epsilon), \tag{A.31}
\]

\[
g_{\sigma_1,\sigma_2}^{(2)}(\omega) = \tilde{\rho}_{\sigma_1}^{(0)}(0) \int_{-\infty}^{0} d\epsilon \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \partial_\omega \tilde{\rho}_{\sigma_2}^{(0)}(\omega - \epsilon)
- \partial_\omega \tilde{\rho}_{\sigma_1}^{(0)}(\omega)|_{\omega=0} \int_{0}^{\infty} d\epsilon \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \tilde{\rho}_{\sigma_2}^{(0)}(\omega - \epsilon)
+ \partial_\omega \tilde{\rho}_{\sigma_2}^{(0)}(\omega)|_{\omega=0} \int_{0}^{\infty} d\epsilon \tilde{\rho}_{\sigma_1}^{(0)}(\epsilon) \tilde{\rho}_{\sigma_2}^{(0)}(\omega - \epsilon), \tag{A.32}
\]

\[
g_{\sigma_1,\sigma_2}^{(3)}(\omega) = \partial_\omega \tilde{\rho}_{\sigma_2}^{(0)}(\omega)|_{\omega=0} \int_{-\infty}^{0} d\epsilon \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \tilde{\rho}_{\sigma_1}^{(0)}(\omega - \epsilon)
- \tilde{\rho}_{\sigma_2}^{(0)}(0) \int_{-\infty}^{0} \tilde{\rho}_{\sigma_2}^{(0)}(\epsilon) \partial_\omega \tilde{\rho}_{\sigma_1}^{(0)}(\omega - \epsilon) \tag{A.33}
\]

These integrals can be evaluated analytically but the result is rather lengthy and is not reproduced here. At particle-hole symmetry, and assuming the absence of a magnetic field the spectral density is an even function of \(\omega\). Exploiting this, we find when \(\omega = 0\) that

\[
g^{(1)}(0) = 0, \quad g^{(2)}(0) = -\tilde{\rho}^{3}(0), \quad g^{(3)}(0) = \tilde{\rho}^{3}(0)/2, \tag{A.34}
\]

where \(\tilde{\rho}(0) = 1/\pi \Delta\), and conclude that

\[
\text{Im} \hat{\Sigma}^{[2a]}[0, T] - \text{Im} \hat{\Sigma}^{[2a]}[0, 0] = -\frac{\pi^3 \tilde{U}^2 T^2}{2(\pi \Delta)^3} \tag{A.35}
\]

which agrees with Ref. [51], except for a sign as we have already noted, and with Eq. (A.20). Finally, we return to the evaluation of the real part for a general model, and find from Eq. (A.5) that

\[
\text{Re} \hat{\Sigma}^{[2a]}[\omega] = \frac{\pi^3 \tilde{U}^2 T^2}{6} \mathcal{P} \int \frac{d\omega'}{\pi} \frac{Q_{\sigma,-\sigma}(\omega) - Q_{\sigma,-\sigma}(\omega')}{\omega - \omega'}. \tag{A.36}
\]
A.2.2. Two channel model

The results of the previous section trivially generalise to the two channel model. One finds for the static contribution

$$\tilde{\Sigma}^{[1]}_\sigma(T) = \frac{\pi^3 T^2}{3} \left[ (\tilde{\mathcal{U}} + \tilde{\mathcal{U}}_{12}) \frac{\tilde{\epsilon}_{d,-\sigma} \rho_{\sigma}^2(0)}{\Delta_{-\sigma}} + \tilde{\mathcal{U}}_{12} \frac{\tilde{\epsilon}_{d,\sigma} \rho_{\sigma}^2(0)}{\Delta_{\sigma}} \right]$$,

(A.37)

while $$\tilde{\Sigma}^{[2b]}_\sigma(T) = \mathcal{O}(T^4)$$. The imaginary part of the dynamic contribution is given by

$$\text{Im} \tilde{\Sigma}^{[2a]}_\sigma(\omega,T) = \frac{\pi^3 T^2}{6} \left[ (\tilde{\mathcal{U}}^2 + \tilde{\mathcal{U}}_{12}^2) Q_{\sigma,-\sigma}(\omega) + \tilde{\mathcal{U}}_{12}^2 Q_{\sigma,\sigma}(\omega) \right]$$,

(A.38)

and the real part can be evaluated with the help of Eq. (A.5)

$$\text{Re} \tilde{\Sigma}^{[2a]}_\sigma(\omega) = \frac{\pi^3 T^2}{6} \mathcal{P} \int \frac{d\omega'}{\pi} \frac{(\tilde{\mathcal{U}}^2 + \tilde{\mathcal{U}}_{12}^2) W_{\sigma,-\sigma}(\omega,\omega') + \tilde{\mathcal{U}}_{12}^2 W_{\sigma,\sigma}(\omega,\omega')}{\omega - \omega'}$$,

(A.39)

where

$$W_{\sigma_1,\sigma_2}(\omega,\omega') = Q_{\sigma_1,\sigma_2}(\omega) - Q_{\sigma_1,\sigma_2}(\omega')$$.

(A.40)
B. Renormalised perturbation theory at finite temperatures

B.1. Renormalisation of the Green’s function

This section generalises the formulation of Renormalised Perturbation Theory to the case of finite temperature. Our starting point is the Matsubara formalism and the (interacting) thermal propagator

\[ G_{\sigma}(\omega_n) = \frac{1}{[G_{\sigma}^{(0)}(\omega_n)]^{-1} - \Sigma_{M\sigma}(i\omega_n; T)}, \quad \text{(B.1)} \]

where

\[ G_{\sigma}^{(0)}(\omega_n) = \frac{1}{i\omega_n - \tilde{\epsilon}_d + i\Delta \text{sign}(\omega_n)}. \quad \text{(B.2)} \]

and \( \Sigma_{M\sigma}(i\omega_n; T) \) denotes the self-energy, defined on the imaginary frequency axis. Before considering the effects of non-zero temperature, it is instructive to construct the RPT in the Matsubara formalism at \( T = 0 \). We emphasise that the self-energy that appears in Eq. (B.1) is the quantity one calculates diagrammatically in the Matsubara formalism, and it is technically defined only at the discrete Matsubara frequencies. Ultimately, we are interested in the retarded self-energy \( \Sigma_{R\sigma}(\omega, T) \) which can be deduced from \( \Sigma_{M\sigma}(i\omega_n; T) \) using the transformation \( i\omega_n \rightarrow i\omega + \delta \), where \( \delta \rightarrow 0^+ \) [1, p. 147-149].

We are now interested in generalising this treatment to finite temperatures. Contrary to the zero-temperature case, at finite temperatures the imaginary part of \( \Sigma_{R\sigma}(\omega; T) \) and its derivative do not vanish at zero frequency\(^1\). This is generally true in Fermi Liquid theory; here we can see a particular manifestation of this behaviour by inspecting the leading-order perturbative results for the

\(^1\)Equivalently, the real part of \( \frac{\partial \Sigma_{M\sigma}(\omega; T)}{\partial \omega} \) does not vanish.
asymmetric model at finite temperatures [57, 58].

\[
\text{Re } \Sigma^R_\sigma(\omega; T) \sim (\psi_0(\theta) + \psi_1(\theta)\omega + \ldots) + T^2 (\psi^T_0(\theta) + \psi^T_1(\theta)\omega + \ldots) \tag{B.3}
\]

\[
\text{Im } \Sigma^R_\sigma(\omega; T) \sim \phi_0(\theta)\omega^2 + T^2 (\pi^2\phi_0(\theta) + \phi_1(\theta)\omega + \ldots) \tag{B.4}
\]

where \(\psi_i(\theta), \psi^T_i(\theta)\) and \(\phi_i(\theta)\) are real functions of the asymmetry factor \(\theta = (\epsilon_d + U\langle n \rangle_{HF})/\Delta\) defined in terms of the Hartree-Fock occupation.

To proceed in analogy to the \(T = 0\) case we perform a Taylor expansion similar to Eq. (2.2)

\[
\Sigma^R_\sigma(\omega; T) = \Sigma^R_\sigma(0; T) + \left. \frac{\partial \Sigma^R_\sigma(\omega; T)}{\partial \omega} \right|_{\omega=0} \omega + \Sigma^{(R,\text{rem})}_\sigma(\omega; T), \tag{B.5}
\]

where now the quantities \(\Sigma^R_\sigma(0; T)\) and \(\left. \frac{\partial \Sigma^R_\sigma(\omega; T)}{\partial \omega} \right|_{\omega=0}\) are complex valued, with both \(\text{Im } \Sigma^R_\sigma(0; T)\) and \(\text{Im } \partial_\omega \Sigma^R_\sigma(0; T)\) being of order \(T^2\). To accommodate them, we absorb them into the definition of the renormalised hybridisation. We thus define the temperature-dependent renormalised parameters

\[
z_\sigma(T) = \left[1 - \text{Re } \frac{\partial \Sigma^R_\sigma(\omega; T)}{\partial \omega} \right|_{\omega=0}\right]^{-1} \tag{B.6}
\]

\[
\tilde{\epsilon}_{d,\sigma}(T) = z_\sigma(T) \left[\epsilon_d + \text{Re } \Sigma^R_\sigma(0; T)\right] \tag{B.7}
\]

\[
\tilde{\Delta}_\sigma(T, \omega) = z_\sigma(T) \left[\Delta - \Sigma^R_\sigma(0; T) - \omega \text{Im } \frac{\partial \Sigma^R_\sigma(\omega; T)}{\partial \omega} \right|_{\omega=0}\right] \tag{B.8}
\]

\[
\tilde{U}(T) = \tilde{\Gamma}_{\sigma,\sigma,\sigma,\sigma}^{0,0,0}(0, 0; T), \tag{B.9}
\]

and obtain a temperature-dependent renormalised Green’s function

\[
\tilde{G}_\sigma(\omega) = \frac{z_\sigma(T)}{\omega - \tilde{\epsilon}_{d}(T) + i\tilde{\Delta}(T, \omega) - \Sigma^R_\sigma(\omega; T)}. \tag{B.10}
\]

From this, we can deduce the corresponding Matsubara Green’s function

\[
\tilde{G}_\sigma(\omega_n) = \frac{z_\sigma(T)}{i\omega_n - \tilde{\epsilon}_{d}(T) + i\tilde{\Delta}(T, \omega) \text{sign}(\omega_n) - \Sigma^M_\sigma(i\omega_n; T)}. \tag{B.11}
\]

We see that non-zero temperatures result in a linear frequency dependence of the hybridisation \(\tilde{\Delta}(\omega)\). Consequently, this can be written in the form

\[
\tilde{\Delta}(\omega) = \tilde{\Delta}_0 + \omega \tilde{\Delta}_1, \tag{B.12}
\]

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where $\tilde{\Delta}_0 = z_\sigma(T)(\Delta - \Sigma^R_\sigma(0; T))$ and $\tilde{\Delta}_1 = -\omega \text{Im} \frac{\partial}{\partial \omega} \Sigma^R_\sigma(\omega; T)\big|_{\omega=0}$. In other words, the Green’s function at finite temperatures (and in the absence of a magnetic field) depends on three parameters $\tilde{\epsilon}_d, \tilde{\Delta}_0, \tilde{\Delta}_1$, with $\tilde{\Delta} \to 0$ as $T \to 0$.

**B.1.1. Flow equations at finite temperatures**

In this Section we discuss the derivation of flow equations in the finite-temperature theory. As discussed in Chapter 4, for the RPT to be useful as a method for solving problems with strong correlations there must exist a way of determining the parameters independently of the NRG. This is particularly true in the finite-temperature case, where it is harder to extract the parameters from the NRG results.

This section is a straightforward generalisation of Sec. 4.1 for a hybridisation that is a linear function of frequency. We begin by expressing the retarded propagator in two different ways, using the renormalised parameters at $\mu$ and $\mu + \delta \mu$.

$$G_\sigma(\omega, T) = \frac{z_\sigma(\mu + \delta \mu, T)}{\omega - \tilde{\epsilon}_d, \sigma(\mu + \delta \mu, T) + i\tilde{\Delta}_\sigma(\omega, \mu + \delta \mu, T) - \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu + \delta \mu), T)}$$  \hspace{1cm} (B.13)

$$= \frac{z_\sigma(\mu, T)}{\omega - \tilde{\epsilon}_d, \sigma(\mu, T) + i\tilde{\Delta}_\sigma(\omega, \mu, T) - \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), T; \delta \mu)}. \hspace{1cm} (B.14)$$

We invert Eq. (B.14), differentiate with respect to $\omega$ and equate the real and imaginary parts of the resultant expression to find

$$z_\sigma(\mu, T; \delta \mu) = \left[1 - \frac{\partial}{\partial \omega} \tilde{\Sigma}_\sigma(\omega; \tilde{\mu}(\mu), \delta \mu)\big|_{\omega=0} \right]^{-1}$$  \hspace{1cm} (B.15)

$$\tilde{\Delta}_{1,\sigma}(\mu + \delta \mu, T) = z_\sigma(\mu, T; \delta \mu) \left(\tilde{\Delta}_{1,\sigma}(\mu, T) - \frac{\text{Im} \tilde{\Sigma}_\sigma(\omega, \tilde{\mu}(T); \delta \mu)\big|_{\omega=0}}{\partial \omega} \right), \hspace{1cm} (B.16)$$

where we have introduced the notation of Eq. (B.12) for the components of $\Delta_\sigma(\omega)$. By equating the two propagators in Eq. (B.14) at $\omega = 0$ we find

$$\tilde{\epsilon}_{d,\sigma}(\mu + \delta \mu, T) = z_\sigma(\mu, T; \delta \mu) \left[\tilde{\epsilon}_{d,\sigma}(\mu, T) + \text{Re} \tilde{\Sigma}_\sigma(0\tilde{\mu}(\mu), T; \delta \mu)\right], \hspace{1cm} (B.17)$$

$$\tilde{\Delta}_{0,\sigma}(\mu + \delta \mu, T) = z_\sigma(\mu, T; \delta \mu) \left[\tilde{\Delta}_{0,\sigma}(\mu + \delta \mu, T) - \text{Im} \tilde{\Sigma}_\sigma(0\tilde{\mu}(\mu), T; \delta \mu)\right]. \hspace{1cm} (B.18)$$
We introduce the notation
\[
q_{\sigma}(\tilde{\mu}(\mu), T) = \left. \frac{\partial \tilde{\Sigma}_{\sigma}(\omega; \tilde{\mu}(\mu), T, \delta \mu)}{\partial \omega} \right|_{\omega=0}, \tag{B.19}
\]
\[
p_{\sigma}(\tilde{\mu}(\mu), T) = \frac{\partial \tilde{\Sigma}_{\sigma}(0; \tilde{\mu}(\mu), T, \delta \mu)}{\partial \mu}, \tag{B.20}
\]
where now \(q_{\sigma}(\tilde{\mu}(\mu), T)\) and \(p_{\sigma}(\tilde{\mu}(\mu), T)\) are complex-valued quantities. We thus have the closed system
\[
\frac{\partial \ln \tilde{\Delta}_{0,\sigma}(\mu)}{\partial \mu} = \text{Re} q_{\sigma}(\tilde{\mu}(\mu)), \tag{B.21}
\]
\[
\frac{\partial \tilde{\epsilon}_{d,\sigma}(\mu)}{\partial \mu} = \text{Re} p_{\sigma}(\tilde{\mu}(\mu)) + \tilde{\epsilon}_{d,\sigma}(\mu) \text{Re} q_{\sigma}(\tilde{\mu}(\mu)). \tag{B.22}
\]
Note that the candidate flow variables now include the temperature itself; one could potentially take the \(T \to \infty\) regime as the boundary condition where mean-field theory is applicable, and consider the effects of adiabatically lowering \(T\). We do not pursue such an approach here, as it is not clear how to calculate the resultant \(\tilde{\Sigma}(\omega, \tilde{\mu}(T), \delta; \delta \mu)\).
C. Particle/hole propagators

C.1. Pair propagators

In Chapter 2 we defined the pair propagators (Eq. (2.29))

\[ \tilde{\Pi}^{pp}_{\sigma_1,\sigma_2}(\Omega) = i \int \frac{d\omega}{2\pi} \tilde{G}_{\sigma_1}^d(\omega) \tilde{G}_{\sigma_2}^d(\Omega - \omega). \]

\[ \tilde{\Pi}^{ph}_{\sigma_1,\sigma_2}(\Omega) = i \int \frac{d\omega}{2\pi} \tilde{G}_{\sigma_1}^d(\omega) \tilde{G}_{\sigma_2}^d(\Omega + \omega). \]

(C.1)

It is easy to show that \( \tilde{\Pi}^{ph}_{\sigma_1,\sigma_2}(\Omega) = \tilde{\Pi}^{ph}_{\sigma_2,\sigma_1}(-\Omega) \) for any \( \epsilon_d \) in the absence of a magnetic field. Furthermore, note that \( \tilde{\Pi}^{ph}_{\sigma_1,\sigma_2}(0) = \frac{1}{2} \).

The evaluation of the pair propagators is lengthy, but straightforward — one divides the region of integration into three intervals and carries out the integration in each region separately. Note that in the case of the particle-hole propagator one need only consider the case \( \Omega > 0 \), whereas for the particle-particle propagator the cases \( \Omega > 0 \) and \( \Omega < 0 \) have to be considered separately.

Assuming, in the interests of generality, that \( \tilde{\epsilon}_{d,\uparrow} \neq \tilde{\epsilon}_{d,\downarrow} \) and \( \tilde{\Delta} \neq \tilde{\Delta} \) we find for \( \Omega > 0 \)

\[ \tilde{\Pi}^{ph}_{\sigma_1,\sigma_2}(\Omega) = -\frac{i}{2\pi} \left\{ \ln(-\Omega - \tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1}) - \ln(-\tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2}) \right. \]

\[ + \frac{\ln(-\tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1}) - \ln(-\tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1})}{\tilde{\epsilon}_{d,\sigma_1} - \tilde{\epsilon}_{d,\sigma_2} + \Omega + i(\tilde{\Delta}_{\sigma_1} - \tilde{\Delta}_{\sigma_2})} \]

\[ + \frac{\ln(-\tilde{\epsilon}_{d,\sigma_2} + i\tilde{\Delta}_{\sigma_2}) - \ln(-\tilde{\epsilon}_{d,\sigma_2} + i\tilde{\Delta}_{\sigma_2})}{\tilde{\epsilon}_{d,\sigma_1} - \tilde{\epsilon}_{d,\sigma_2} + \Omega + i(\tilde{\Delta}_{\sigma_1} + \tilde{\Delta}_{\sigma_2})} \]

\[ + \frac{\ln(\Omega - \tilde{\epsilon}_{d,\sigma_1} + i\tilde{\Delta}_{\sigma_2}) - \ln(-\tilde{\epsilon}_{d,\sigma_1} + i\tilde{\Delta}_{\sigma_1})}{\tilde{\epsilon}_{d,\sigma_1} - \tilde{\epsilon}_{d,\sigma_2} + \Omega - i(\tilde{\Delta}_{\sigma_1} - \tilde{\Delta}_{\sigma_2})} \right\}. \]

(C.2)

where \( \ln(z) = |z| + i\arg(z) \), is the complex logarithm. The case \( \Omega < 0 \) can be
deduced from $\Pi_{\sigma_1,\sigma_2}^{ph}(\Omega) = \Pi_{\sigma_2,\sigma_1}^{ph}(-\Omega)$. Similarly, we find for $\Omega > 0$ that

$$\tilde{\Pi}_{\sigma_1,\sigma_2}^{pp}(\Omega) = -\frac{i}{2\pi} \left\{ \frac{\ln(\tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1}) - \ln(-\Omega + \tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2})}{\tilde{\epsilon}_{d,\sigma_1} + \tilde{\epsilon}_{d,\sigma_2} - \Omega + i(\tilde{\Delta}_{\sigma_1} - \tilde{\Delta}_{\sigma_2})} \right. $$

$$+ \frac{\ln(\Omega - \tilde{\epsilon}_{d,\sigma_1} + i\tilde{\Delta}_{\sigma_1}) - \ln(-\tilde{\epsilon}_{d,\sigma_1} + i\tilde{\Delta}_{\sigma_1})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega - i(\Delta_{\sigma_1} + \Delta_{\sigma_2})} $$

$$+ \frac{\ln(-\Omega + \tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2}) - \ln(\tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega - i(\Delta_{\sigma_1} + \Delta_{\sigma_2})} $$

$$+ \frac{\ln(\tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2}) - \ln(\Omega - \tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega + i(\Delta_{\sigma_1} - \Delta_{\sigma_2})} \right\} $$

(C.3)

and for $\Omega < 0$

$$\tilde{\Pi}_{\sigma_1,\sigma_2}^{pp}(\Omega) = -\frac{i}{2\pi} \left\{ \frac{\ln(\Omega - \tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1}) - \ln(\tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2})}{\tilde{\epsilon}_{d,\sigma_1} + \tilde{\epsilon}_{d,\sigma_2} - \Omega + i(\tilde{\Delta}_{\sigma_1} - \tilde{\Delta}_{\sigma_2})} \right. $$

$$+ \frac{\ln(-\tilde{\epsilon}_{d,\sigma_1} - i\tilde{\Delta}_{\sigma_1}) - \ln(\Omega - \tilde{\epsilon}_{d,\sigma_2} - i\tilde{\Delta}_{\sigma_2})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega + i(\Delta_{\sigma_1} + \Delta_{\sigma_2})} $$

$$+ \frac{\ln(\tilde{\epsilon}_{d,\sigma_2} + i\tilde{\Delta}_{\sigma_2}) - \ln(-\tilde{\epsilon}_{d,\sigma_2} + i\tilde{\Delta}_{\sigma_2})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega - i(\Delta_{\sigma_1} + \Delta_{\sigma_2})} $$

$$+ \frac{\ln(-\Omega + \tilde{\epsilon}_{d,\sigma_2} + i\tilde{\Delta}_{\sigma_2}) - \ln(-\tilde{\epsilon}_{d,\sigma_1} + i\tilde{\Delta}_{\sigma_1})}{\epsilon_{d,\sigma_1} + \epsilon_{d,\sigma_2} - \Omega - i(\Delta_{\sigma_1} - \Delta_{\sigma_2})} \right\} $$

(C.4)

**C.2. n-particle/hole propagators**

The concept of a pair propagator can be generalised to include more particles (or holes). In Eq. (3.4) we defined the n-particle/hole propagator as

$$\Pi_{\sigma_1,\ldots,\sigma_n}^{(n)}(\Omega_1, \ldots, \Omega_n) = i^n \int \frac{d\omega}{2\pi} G_{\sigma_1}(s_1\omega + \Omega_1)G_{\sigma_2}(s_2\omega + \Omega_2) \ldots G_{\sigma_n}(s_n\omega + \Omega_n), $$

(C.5)

where $s_i \in \{-1, 1\}$. Due to the sign term in the causal Green’s function, the integrand can be thought of as a piecewise function in $\omega$. We begin by identifying the branch points $\omega_i$, which we will call nodes where $s_i\omega + \Omega_i = 0$. We can ensure by appropriate labelling of the nodes that $-\infty \geq x_1 \geq x_2 \ldots \geq x_n$. For brevity, we write the $i$th Green’s function in the form

$$G_{\sigma_i}(\omega) = \frac{s_i}{\omega - \alpha_i(\omega)}, $$

(C.6)
where \( \alpha_i = s_i \left[ -\Omega_i + \epsilon_{d, \sigma_i} - i \Delta \text{sign}(s_i, \omega + \Omega_i) \right] \). We temporarily make the assumption, which will be lifted later, that all the \( \alpha_i \) are distinct. Thus written, the integrand depends on \( \omega \) explicitly but also implicitly through the dependence of the \( \alpha_i \). Having identified the nodes we can rewrite Eq. (C.5) as

\[
i^{-n} \Pi_{\sigma_i}^{(n)}(\Omega_1, \ldots, \Omega_n) = J(\omega_1, \omega_n) + \sum_{i=1}^{n-1} F(\omega_i, \omega_{i+1}), \tag{C.7}\]

where

\[
F(\omega_i, \omega_{i+1}) = \int_{\omega_i}^{\omega_{i+1}} d\omega G_{\sigma_1}(s_1 \omega + \Omega_1) \ldots G_{\sigma_n}(s_n \omega + \Omega_n) \]

\[
J(\omega_1, \omega_n) = \lim_{\Lambda \to \infty} \left\{ \int_{-\Lambda}^{\omega_1} d\omega G_{\sigma_1}(s_1 \omega + \Omega_1) \ldots G_{\sigma_n}(s_n \omega + \Omega_n) + \int_{\omega_n}^{\Lambda} d\omega G_{\sigma_1}(s_1 \omega + \Omega_1) \ldots G_{\sigma_n}(s_n \omega + \Omega_n) \right\}. \tag{C.8}\]

The decomposition of the real axis into intervals on which the integrand does not change form means that we can perform a partial fraction decomposition with coefficients specific to the region. Hence we can write

\[
\frac{1}{(\omega - \alpha_1)(\omega - \alpha_2) \ldots (\omega - \alpha_n)} = \sum_{i=1}^{n} \frac{\beta_i}{\omega_i - \alpha_i}, \tag{C.10}\]

where \( \beta_j = 1/f'(\alpha_j) \), \( f(\omega) = (\omega - \alpha_1) \ldots (\omega - \alpha_n) \). We can now simply integrate each partial fraction separately. Let \( \alpha^{(i)} \) and \( \beta^{(i)} \) denote the values of the relevant quantities in the region \((\omega_i, \omega_{i+1})\). Then

\[
F(\omega_i, \omega_{i+1}) = \sum_{j=1}^{n} \beta_j^{(i)} \ln \left( \frac{\omega_{i+1} - \alpha_j^{(i)}}{\omega_i - \alpha_j^{(i)}} \right) \]

\[
J(\omega_1, \omega_n) = \sum_{j=1}^{n} \left[ \beta_j^{(0)} \ln \left( \omega_1 - \alpha_j^{(0)} \right) - \beta_j^{(n+1)} \ln \left( \omega_n - \alpha_j^{(n+1)} \right) \right], \tag{C.11}\]

where \( \ln(z) \) denotes the principal branch of the complex logarithm defined as \( \ln |z| + i \text{Arg}(z) \), \( -\pi < \text{Arg}(z) < \pi \) and the labels \( 0, n+1 \) denote the values of the underlying quantities in the intervals \((-\infty, \omega_1)\) and \((\omega_n, \infty)\) respectively. The expressions given above are numerically stable under the assumptions made in the beginning, so long as one does not try to combine the logarithms into one logarithm.
In practical applications we may encounter numerical difficulties if the $\Omega$ are such that any two $\alpha_i$ in a particular region coincide, or nearly coincide. This will cause our partial fraction to break down. We deal with this in a crude yet effective manner: when any $\alpha_i, \alpha_j$ are too close to each other, we separate them by a very small, arbitrary constant. After separating the offending $\alpha_i, \alpha_j$ it is important to update the values of the corresponding $\Omega_i, \Omega_j$ to ensure the consistency of the calculation.

C.3. Interpolation formulae

In the main body we discussed how the pair propagator can be written as a univariate function and how the triple particle/hole propagator can be similarly written as a function of two variables. This is useful as it enables us to tabulate the function and use an interpolation scheme, a process that significantly speeds up our calculation.

For functions of one variable, the simplest method is to interpolate linearly from known function points $(x_1, y_1), (x_2, y_2)$ according to the formula

$$y(x) \approx y_1 \frac{x - x_2}{x_1 - x_2} + y_2 \frac{x - x_1}{x_2 - x_1}.$$  \hspace{1cm} (C.12)

Whilst trivial to implement, the obvious drawback of this method is that it does not take any curvature into account. There are many ways to improve on this but the simplest extension is to add a quadratic term. Given the points $(x_1, y_1), (x_2, y_2), (x_3, y_3)$ we must now construct a polynomial that passes through all three. Waring, Euler and Lagrange solved this problem in the general case and the result is known as the Lagrange interpolating polynomial. For three points, we have

$$y(x) \approx y_1 \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} + y_2 \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} + y_3 \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)}.$$  \hspace{1cm} (C.13)

One can keep adding more terms but it does not necessarily follow that the higher-order polynomial will be more accurate.

For functions of two variables, the simplest possible scheme is that of bilinear interpolation. Multi-dimensional interpolation formulae can be constructed by interpolating in each direction separately. The bilinear interpolation scheme just
does that, using Eq. (C.12) in each direction.

\[
f(x, y) \approx \frac{1}{(x_2 - x_1)(y_2 - y_1)} \left( f(x_1, y_1)(x_2 - x)(y_2 - y) + f(x, y_2)(x_2 - x)(y_2 - y_1) + f(x_2, y_2)(x - x_1)(y_2 - y) \right) + \left( f(x_1, y_1)(x_2 - x)(y_2 - y) + f(x, y_2)(x_2 - x)(y_2 - y_1) + f(x_2, y_2)(x - x_1)(y_2 - y) \right) \tag{C.14}
\]

Note that the qualification *bilinear* is somewhat misleading. As before, we would like to take curvature into account. This tedious but straightforward to do, by using Eq. (C.13) in each direction. Interpolating along \( x \) we have

\[
f(x, y_k) \approx f_{1k} \frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)} + f_{2k} \frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)} + f_{3k} \frac{(x - x_1)(x - x_2)}{(x_3 - x_1)(x_3 - x_2)} \tag{C.15}
\]

for \( k = 1, 2, 3 \) and with the shorthand notation \( f_{i,j} = f(x_i, y_j) \). We now interpolate along \( y \) to find

\[
f(x, y) \approx f(x, y_1) \frac{(y - y_2)(y - y_3)}{(y_1 - y_2)(y_1 - y_3)} + f(x, y_2) \frac{(y - y_1)(y - y_3)}{(y_2 - y_1)(y_2 - y_3)} + f(x, y_3) \frac{(y - y_1)(y - y_2)}{(y_3 - y_1)(y_3 - y_2)} \tag{C.16}
\]

The process of tabulating a function and then interpolating from known values absolves us from the burden of calculating complex logarithms. An undesirable effect is that it reduces the effectiveness of the CPU cache by filling it up with the interpolation table. Nevertheless this method drastically reduces the running time of our program.
D. Multi-dimensional integration of functions with planar discontinuities

(An expanded version of this section will appear in the journal ‘Transactions On Mathematical Software’ published by the Association for Computing Machinery.)

It relies on the observation that in the case of zero external frequency the hyperplanes on which the integrand of Eq. (3.3) is discontinuous all meet at the origin. These planes define open infinite regions in $\mathbb{R}^N$ on which the integrand is smooth. Through a rather involved process described in the Appendix we partition $\mathbb{R}^N$ in smaller regions on which the integrand in question is smooth. We then make use of HIntLib’s adaptive cubature routines to integrate over each region separately and sum the individual results to obtain an estimate for $I_D$. However, we have already remarked that the self-energy itself at zero frequency is not an interesting quantity. We expect our calculation to produce, at the very minimum, an estimate of the derivative of the self-energy. Interestingly, it is possible to reformulate the perturbation theory in such a way that it reproduces $\partial_0 \Sigma(\omega)|_{\omega=0}$ directly, rather than through a finite-difference on $\Sigma(\Omega)$. Nevertheless this approach was abandoned as it proved to be slow, complicated and could not produce the spectral density at finite frequencies.

In one dimension discontinuities are easily accommodated within an adaptive framework simply by dividing the region of integration into sub-regions on which the integrand is smooth. In this appendix we show how this process can be extended to higher dimensionalities. Our method is applicable to integrals which are discontinuous on any number of hyperplanes that contain the origin, and in any number of dimensions. We limit our attention to integrals over the entire $\mathbb{R}^N$ — this is not a material limitation as integrals over a proper hyperrectangle can be straightforwardly mapped onto $\mathbb{R}^N$. We assume that the discontinuities in question arise from terms of the form $\text{sign}(C_x)$ where $C_x$ is any linear combination of the coordinates. These is precisely the form of the discontinuities encountered
in the Green’s functions of fermionic systems.

D.0.1. The method

Let $S$ be the set of all $M \times M$ diagonal matrices with diagonal components $\pm 1$ ($|S| = 2^M$). To determine the regions on which the integrand is continuous we thus have to solve the homogeneous system of simultaneous inequalities

$$\mathbf{C}_i \mathbf{x} \geq 0,$$

for every $\mathbf{S}_i \in S$. Each inequality defines a closed-half space; the solution to the system is the intersection of these half-spaces which can be interpreted geometrically as a convex polytope in its half-space representation (see [44, p. 31]). In the case of a homogeneous system the resultant polytope is in fact a polyhedral (infinite) convex cone [143].

Let $P$ be the set of cones obtained by solving Eq. (D.1). A set of vectors $\mathbf{W}_K = \{\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_p\}$ is a skeleton of a cone $K$ if $\mathbf{x} = \sum_{i=1}^{p} \lambda_i \mathbf{w}_i$ belongs to $K$ for every $\lambda_i \geq 0$ [143]. The duality in the representation of a cone as either a system of linear inequalities or a conical combination of the skeleton is the essence of the well known Weyl-Minkowski theorem on cones. As we are only interested in subspaces of $\mathbb{R}^N$ with dimension $N$ — lower-dimensional subspaces correspond to polyhedral facets which do not contribute to the integral — we can assume that $p \geq N$. The skeleton of an acute cone is unique up to scalar multiplication of the vectors [143]. Once the normalisation of the skeleton is fixed, each point in $K$ can be specified through its $\lambda$ coefficients ($\lambda_1, \ldots, \lambda_p$).

Having achieved our goal of partitioning $\mathbb{R}^N$ into regions where the integrand is continuous we now have to consider how to perform the integration over a cone $K \in P$. When $p = N$ the polytope constitutes an $N$-simplex which can be readily mapped onto the positive orthant by exploiting the bijection between $\mathbf{x} \in K$ and $\mathbf{\lambda}$. When $p > N$ the situation is more complex, for the skeleton is linearly dependent and there is no bijection to be exploited. To overcome this problem, each cone $K$ is decomposed into $N$-simplices $\gamma^K_1, \gamma^K_2, \ldots$ which can then be individually mapped onto the positive orthant. The set of all simplices $\mathcal{F} = \{\gamma^K_1, \gamma^K_2, \ldots \mid K \in P\}$ evidently partitions $\mathbb{R}^N$; the original integration problem has thus been broken down into multiple, separate integrations, one over each simplex in $\mathcal{F}$. The method is inherently parallel — barring error control considerations each region of integration can be processed independently of the others.
To control the precision of the calculation we use an unsophisticated two-pass scheme. The first pass consists of a crude integration over every simplex $\gamma \in \Gamma$, with a relative precision of 10%, yielding a result $\mu^{(1)}_\gamma$ with an associated error $\sigma^{(1)}_\gamma$. From the $\mu^{(1)}_\gamma$ we determine the simplex which contributes the most; let $\mu_{\text{max}} = \max \{|\mu_\gamma|, \gamma \in \Gamma\}$. To achieve a requested relative precision $f$ on the entire integral $I$ we then repeat the integration, now evaluating each simplex to an absolute precision given by $\epsilon_{\text{abs}} = f \mu_{\text{max}} / \sqrt{\nu}$, where $\nu = |\Gamma|$ denotes the total number of simplices, ensuring obviously we do not re-evaluate the regions for which $\sigma^{(1)}_\gamma < \epsilon_{\text{abs}}$. The end result $I = \sum \mu^{(2)}_\gamma$ is then associated with an absolute error

$$\sigma_I = \sqrt{\sum_{\gamma \in \Gamma} (\sigma^{(2)}_\gamma)^2 / \nu}. \tag{D.2}$$

In practice small deviations of the resultant precision for the requested precision may occur when there are significant cancellations. This is not a particularly grave disadvantage as the actual error is always known.

Finally, we return to the question of the number of constraints. We have been assuming that the number of rows $M$ of the constraint matrix $C$ is larger than the dimension of the integral, ignoring the case of an integrand which has discontinuities on fewer than $N$ planes. This is dealt with by padding the rows of $C$ with arbitrary vectors (so long as they are not parallel to any other vectors) until $M \geq N$. This trick has the disadvantage of causing unnecessary divisions of the region of integration but is necessary to guarantee the existence of cones.

**D.0.2. Implementation**

The process outlined above is implemented in C++ with support for matrices provided by GSL [38]. The input is the integrand and the matrix $C$ construct as above specifying the discontinuities. The first step is the decomposition of $\mathbb{R}^N$ into the polyhedral cones $\mathcal{P}$. To this end we use skeleton [143] which implements a modified version of the Motzkin-Burger algorithm. This package is called from our code and returns the vectors comprising the skeleton of the polyhedral cones in $\mathcal{P}$.

To cut the polyhedral cones in $\mathcal{K}$ into $N$-simplices we first project the vectors in $W_K$ onto the cone’s $(N - 1)$-dimensional base. By ‘base’ here we mean the subspace obtained by subtracting from all $\mathbf{w} \in W_k$ their components along the axis of the cone and then expressing them as linear combinations of $(N - 1)$ orthonormal vectors. We can then construct the desired decomposition of $\mathcal{K}$.
into $N$-simplices by triangulating the points in the $(N - 1)$-dimensional base and then adding the origin to these $(N - 1)$-simplices. In general this triangulation is not unique. There are several algorithms to handle the triangulation of the base. We use the Quickhull algorithm implemented in Qhull [14].

Each point $x$ of the simplex can be written as a conical combination of the $(\lambda)$ and its skeleton vectors. To map the positive orthant onto the unit hypercube we use the rule $\lambda_i = 1/u_i - 1$. Depending on the integrand other rules may be more suitable but this was chosen for its simplicity.

The final step is the integration itself. We use HINTLib [115, 116], a sophisticated C++ library that among other things implements adaptive cubature with a variety of rules and a range of Monte Carlo methods. It would be perhaps more efficient to use an adaptive code that can directly handle the simplicial geometry, such as CUBPACK [25, 41] but for practical reasons this approach was not followed here. The integrations are performed in parallel using OpenMP (HINTLib’s native parallelisation is not used).

D.0.3. Note on floating point round-off

We return to the point made at the end of Section 3.2.2 regarding the round-off error in the determination of the null space of system Eq. (3.1) which we chose to determine using the Lenstra-Lenstra-Lovász lattice basis reduction algorithm rather than the more conventional Singular Value Decomposition in an effort to reduce floating point error.
E. Feynman diagrams

In Sec. 3.3 we described how the renormalised perturbation theory can be constructed by explicitly re-arranging the bare series expansions. This was achieved by taking advantage of properties of the skeleton diagrams, which were calculated order-by-order in $U$. This Appendix explicitly lists the skeleton diagrams of the bare perturbation theory, arranged in power of $U$. Note that to condense their presentation the interaction vertices have been contracted to a point, with the colour of the lines denoting their spin.

E.0.4. Fourth order
E.0.5. Fifth order