Collective Excitations in Strongly Correlated Systems

Charge conservation in the dual boson approach

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Summary

Conservation laws play a crucial role in our understanding of physics. They are closely linked with the symmetries of a system. When conserved quantities are known, the dimensionality of the problem can be greatly reduced. An approximation can be tested by checking the conservation laws. In quantum theory, conservation laws apply to quantities that commute with the Hamiltonian. An example is charge conservation in electron systems. These electron systems can be too strongly interacting for a description using a weak coupling expansions. Mean field theories can be used to study these systems even at strong interactions. In a mean-field theory different lattice sites are approximated to be uncorrelated. Charge conservation means that if one location has more charge, then some other location has less. So there has to be correlation to get charge conservation. The dual boson method described in this thesis allows to take into account these correlations. This means it can give a charge conserving treatment of strongly interacting electron systems.
This thesis consists of several chapters. In the first chapter, some important concepts that are needed in the remainder of this thesis are introduced. First, the definition of the Hubbard model is given and some of the known features of this model are explained. Then the formalism of quantum field theory at finite temperature is introduced. It will be used throughout this thesis. Lastly, the Random Phase Approximation, which is an often used tool to calculate charge correlation (susceptibility), is explained and some results of this method are presented for future comparison.

The second chapter is devoted to Dual Boson theory, the main topic of this thesis. A derivation is given and some approximation schemes in the method are discussed. There is a focus on how charge conservation relates to the dual boson method. The dual boson formalism has been numerically implemented as part of this work. The structure of this implementation is also covered in chapter two, the more technical details of the implementation are covered in the third chapter.

In chapter four, the dual boson method is applied to several systems. An accurate calculation of the susceptibility is necessary in the proper understanding of these systems. The dual boson method is compared to other methods to calculate the susceptibility and is shown to solve the problems that exist with charge conservation in previous mean field based methods. The Mott and charge order transition are studied and their impact on the charge susceptibility is illustrated. The dual boson method gives accurate results even in these complicated strongly correlated systems.

A conclusion and outlook is given in chapter five.
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## Notation

- **Inverse temperature** \( \beta = \frac{1}{T} \)
- **Chemical potential** \( \mu \)
- **Fermionic matsubara frequency** \( \nu_n = (2n + 1)\pi T \)
- **Bosonic matsubara frequency** \( \omega_n = 2n\pi T \)
- **Momenta** \( \mathbf{K}, \mathbf{k} \)
- **Density fluctuation** \( \rho = n - \langle n \rangle \)
- **Number of lattice sites** \( N_k \)
- **Dual fermion bare propagator** \( \tilde{G}^0 \)
- **Dual boson bare propagator** \( \tilde{X}^0 \)
- **Dual fermion self-energy** \( \tilde{\Sigma} \)
- **Dual boson self-energy** \( \tilde{\Pi} \)
- **Dual fermion full propagator** \( \tilde{G} \)
- **Dual boson full propagator** \( \tilde{X} \)
- **Impurity vertex** \( \gamma \)
- **Impurity mixed vertex** \( \lambda \)

**Important points in the Brillouin zone**

- \( \Gamma = (0, 0, 0) \)
- \( \mathbf{X} = (\pi, 0, 0) \)
- \( \mathbf{M} = (\pi, \pi, 0) \)
- \( \mathbf{R} = (\pi, \pi, \pi) \)
Chapter 1

Introduction

This introductory chapter contains background information on the methods, techniques and models used in the remainder of this thesis. Important and useful results from the literature will be summarized. In the first part, the Hubbard model will be introduced. This model will be studied using various techniques in this thesis. The second part of the chapter will be about quantum field theory and how it can be used in finite temperature systems. The Matsubara formalism provides an important toolbox that will be used a lot in the remainder of this thesis. The last part of this chapter is devoted to the Random Phase Approximation, the most elementary approach to charge susceptibilities and plasmon physics.

1.1 Models

The microscopic laws that govern materials are well known. From particle physics, we know about fundamental particles and their behaviour. At the scale of materials, there are electrons and nuclei and they interact via the Coulomb potential. The system is governed by the Schrödinger equation, which looks very simple:

\[ i \frac{d}{dt} |\psi\rangle = H |\psi\rangle \tag{1.1} \]

The Hamiltonian contains the kinetic energies and interactions of all the nuclei and electrons. For one nucleus and one electron, this is just the hydrogen problem that is solved in elementary quantum mechanics. For a couple of particles, getting an exact solution has so far proved to be impossible, but reasonably good approximations exist. But materials do not consist of just a couple of particles, they contain on the order of \(10^{23}\) particles. Solving the Schrödinger equation for such an amount of particles is not feasible. Condensed matter physics concerns itself with finding ways to still make predictions about these systems with many particles.

One way to circumvent this issue is to study simpler model systems that contain the most relevant parts of the full problem and allow for a (partial) solution. One hopes that the investigation of these simpler models will lead to knowledge about the physics of real life materials. Finding an appropriate model is an art, it needs to be rich enough to contain interesting physics but simple.

\[^{1}\text{Throughout, units with } \hbar = 1, k_B = 1 \text{ are used.}\]
enough to allow theoretical predictions. Nowadays, optical lattices with ultracold atoms provide an opportunity to also study model systems experimentally, which gives another justification for studying simple models.

The Hubbard model is an example of a model system that was introduced to describe materials. This system and some of its extensions will be studied in this thesis. In this section, the model will be introduced, the connection to real systems will be explained and some of its properties will be derived.

1.1.1 Justification

Materials consist of nuclei and electrons. Since the electrons and the nuclei have a vastly different mass, they are associated with different time scales. This makes it possible to separate these two parts of the system and to solve them one by one. The nuclei are heavy and slow compared to the electrons. They are localized and can be described as point particles that form a lattice. When they move around their equilibrium position, they feel a repulsive force that drives them back. This force can be approximated by a quadratic potential, which leads to harmonic oscillations. When this harmonic system is quantized, it gives rise to the familiar physics of phonons [1].

For the treatment of the electronic system, the nuclei are then treated as a static background that causes an effective potential for the electrons. The phonons and their interaction with the electronic system can in principle be added perturbatively, but this will not be done here. Some of the electrons are tightly bound to the nuclei and effectively form ions. The valence electrons on the other hand are not associated with one of the sites on the lattice of nuclei. If one such an electron is considered in a periodic potential, it will form a delocalized Bloch wave. When several of these electrons are considered, the Coulomb interaction between them has to be considered on top of the Bloch waves. This interaction is minimized when two electrons are not near to each other. It is favourable for the interaction to have localized electrons that do not overlap. So the eigenstates of the interaction are localized electrons, while the eigenstates of the periodic potential caused by the lattice are delocalized Bloch waves. There is a competition between these effects that makes the electrons somewhat localized, somewhat delocalized. These systems are most interesting when the interaction can not be described as a small perturbation, but when it is comparable with the energies of the Bloch states. The goal is to have a model of such a strongly interacting system that contains the competition between localization and delocalization.

1.1.2 Hubbard Model

As was mentioned before, electrons are the main object of our study and the atomic lattice is treated as a fixed external condition. Studying lattices where the unit cell has only a single atom is simplest, since all atoms are identical in this case. Examples of such lattices are the two-dimensional triangular lattice and hypercubic lattices such as the two-dimensional square and the three-dimensional cubic lattice. In this thesis most attention will be given to two- and three-dimensional lattices. In higher dimensions, mean field theories, which will be introduced later, become more and more exact. This thesis is focussed on methods that go beyond mean field theory, so low dimensional systems are the most interesting. On the other hand, one-dimensional systems are very special and allow for many techniques that do not generalize well to higher dimension.
This thesis also only uses single-band models for calculational simplicity. This means that the electrons have spin and lattice site as their quantum numbers. By the Pauli principle, this means that there can only be a single spin up and a single spin down electron on every site. There are also models which give the electrons a band index, which is just another quantum number. This means that there can be a spin up electron per lattice site for every band.

In 1963, Hubbard introduced his famous model\cite{2,3}. It describes the previously mentioned competition between delocalization and localization. The Hubbard Hamiltonian consists of two parts that describe these two effects. It contains free electrons with a dispersion $t$ and a localizing interaction part given by $U$. The Coulomb interaction between the electrons would normally be a long-range repulsion. This is very complicated, since it leads to $\frac{1}{2}N_{\text{electrons}}(N_{\text{electrons}} - 1)$ interactions. The Coulomb interaction decays as a function of the distance, so it is largest for two electrons at the same site. The Hubbard model only contains this on-site interaction. This leads to the introduction of the Hamiltonian:

$$H_{\text{Hubbard}} = H_{\text{hopping}} + H_{\text{interaction}} + H_{\text{chemical potential}} \quad (1.2)$$

$$H_{\text{hopping}} = \sum_{\text{sites} \ i,j \ s=\uparrow,\downarrow} c_{i,s}^\dagger t_{ij} c_{j,s} \quad (1.3)$$

$$H_{\text{interaction}} = \sum_{\text{site} \ i} U n_{i,\uparrow} n_{i,\downarrow} \quad (1.4)$$

$$H_{\text{chemical potential}} = -\sum_{\text{site} \ i \ s=\uparrow,\downarrow} \mu c_{i,s}^\dagger c_{i,s} \quad (1.5)$$

The operators $c^\dagger$ and $c$ are fermionic creation and annihilation operators. The counting operator $n$ is given by $n = c^\dagger c$. The Hamiltonian contains the parameters $\mu$, $t_{ij}$ and $U$ which are real numbers. $\mu$ is the chemical potential that controls the number of particles. The term $t_{ij}$ describes the hopping amplitude from lattice site $i$ to lattice site $j$. To make a model that has translational symmetry, $t$ should only depend on the difference between $i$ and $j$. To make the Hamiltonian Hermitian, $t_{ij} = t_{ji}$ is required. The amplitude to hop from $i$ to $j$ should decrease when $i$ and $j$ are further apart, as it is more difficult to travel further. Since the aim is to get a model that is as simple as possible, only hopping to nearest-neighbours is allowed:

$$t_{ij} = \begin{cases} t_1 & \text{if } i \text{ and } j \text{ are nearest neighbours} \\ 0 & \text{otherwise} \end{cases} \quad (1.6)$$

Since there is only a single hopping parameter $t_1$, it will be noted simply by $t$. A graphical illustration of the model is given in figure 1.1.

The hopping was introduced to cover the delocalized part of the problem. This suggests that it is useful to study it in momentum space. Indeed, since $t_{ij}$ only depends on the difference between $i$ and $j$, the Fourier transform of $t$, assuming a periodic lattice, is especially simple. For a hypercubic lattice in $m$ dimensions it is given by:

$$t_k = -2t \sum_{j=1}^m \cos(k_j) \quad (1.7)$$

The momentum components $k_j$ are in the first Brillouin zone, either $k_j \in [0, 2\pi]$ or $k_j \in [-\pi, \pi]$ depending on the particular choice of the Brillouin zone. On a finite lattice, it is easiest to take $k_j = \frac{2\pi l}{N_j}$ with $N_j$ the number of lattice sites in the direction $j$ and $0 \leq l < N$ a natural number.
Figure 1.1: A graphical illustration of the Hubbard model. There is an on-site repulsion \( U \) and electrons can move from one site to another with a hopping amplitude \( t \).

For a hypercubic (e.g. square, cubic) lattice, \( t_k \) takes on values that are symmetric around zero. The chemical potential \( \mu \) in the grand-canonical ensemble controls the number of particles (per lattice site). The special case \( \mu = \frac{U}{2} \) generates a half-filled model. In this case, there is a symmetry between particles and holes. The replacement \( c \to c^\dagger, c^\dagger \to c, n \to 1 - n \) leaves the Hamiltonian the same. Instead of talking about electrons that have an interaction \( U \) and a dispersion \( t_k \), there is an equivalent picture of holes with the same interaction and dispersion. This additional symmetry often makes the half-filled model simpler to understand. The formal implications of particle-hole symmetry will be described in 1.2.9.

### 1.1.3 Extensions

The regular Hubbard model has only an on-site interaction between charges. The idea is that this contains the dominant part of the effective Coulomb interaction for the valence electrons. It is possible to add additional non-local interactions to the model, to describe the effects of the Coulomb interaction beyond the dominant contribution. Such an extension could improve the similarities between the model and physical systems, but it also increases the complexity of the model, so a trade-off has to be made which interactions will be included. The Hubbard model with additional off-site interactions is usually called an Extendend Hubbard Model.

\[
H_{\text{Extended}} = H_{\text{Hubbard}} + H_{\text{non-local}} \quad (1.8)
\]

\[
H_{\text{non-local}} = \frac{1}{2} \sum_{\text{sites } i,j} (n_{i,\uparrow} + n_{i,\downarrow})V_{ij}(n_{j,\uparrow} + n_{j,\downarrow}) \quad (1.9)
\]

This is an interaction between charges \( (n = n_{\uparrow} + n_{\downarrow}) \). More complicated models, which also include non-local interactions between spins, can also be treated in the formalism presented here. However, this thesis will not focus on them. In this text, only nearest-neighbour interactions are used:

\[
V_{ij} = \begin{cases} 
 v_l & \text{if } i \text{ and } j \text{ are nearest neighbours} \\
 0 & \text{otherwise}
\end{cases} \quad (1.10)
\]
This has the same shape as \( t_{ij} \), so it also has a similar Fourier transform.

### 1.1.4 Conserved quantities

When the Hamiltonian of a system is known, it is a good idea to look at the conserved quantities. There is a simple criterion to find conserved quantities. If a Hermitian operator \( A \) commutes with the Hamiltonian, then in the Heisenberg picture \( A(t) = A \) and the corresponding quantity is conserved. For Hamiltonians that contain raising and lowering operators, calculating the commutator is not always necessary. Such a Hamiltonian can be written as a sum of terms, with each term a product of raising and lowering operators.\(^2\) A quantity \( A \) which has quantum numbers \( a \) is conserved if every term in this sum has the same number of raising and lowering operators for this particular quantum number.\(^3\)

For the total charge, every raising and lowering operator has the quantum number 1. Since every term in the (Extended) Hubbard Hamiltonian contains the same number of creation and annihilation operators, the total charge is conserved. The total charge is given by:

\[
N_{\text{total}} = \sum_{\text{sites } i} \sum_{s=\uparrow,\downarrow} n_{i,s}
\]

(1.11)

For the total spin in the \( z \)-direction, the quantum number 1 is associated with \( \uparrow \) and -1 with \( \downarrow \). Every term in the Hubbard Hamiltonian has the same number of spin up creation and spin up annihilation operators, and similar for spin down, so the total amount of spin up and spin down are conserved, as is the total spin in the \( z \)-direction:

\[
S_{z,\text{total}} = \sum_{\text{sites } i} \sum_{s=\uparrow,\downarrow} sn_{i,s}
\]

(1.12)

These conservation laws can also be checked by calculating the commutators explicitly. Checking these conservation laws is a good test of numerical calculation schemes.

On the other hand, the charge on a single lattice site is not conserved. Looking at the Hamiltonian, there is a term \( c_i^\dagger c_j \), which changes the number of particles on the lattice site \( i \) (and \( j \) ). The hopping part of the Hamiltonian means that the charge on one site is not conserved. In terms of commutators, the interaction commutes with \( n_k \) since \([n_i, n_k] = 0\), but the non-interacting part of the Hamiltonian does not conserve the charge on a single site. To check this explicitly, first calculate the commutator:

\[
[c_i, c_j^\dagger, n_k] = c_i [c_j^\dagger, n_k] + [c_i, n_k] c_j^\dagger \\
= -c_i c_j^\dagger \delta_{ik} + c_i c_j^\dagger \delta_{ik}
\]

(1.13)

\[
= -c_i c_j^\dagger \delta_{ik} + c_i c_j^\dagger \delta_{ik}
\]

(1.14)

\(^2\)This is a power series in the operators. Most reasonable mathematical functions can be written in this way.

\(^3\)This description is sufficient for the quantities conserved here, but it is not a necessary condition. For example, if the Hamiltonian has a term which annihilates two particles with \( a = 1 \) and creates one particle with \( a = 2 \), then the quantity \( A \) is conserved.
Then sum over sites $i, j$ to give:

$$[H_{\text{hopping}}, n_k] = \sum_{i,j} t_{ij} [c_j^\dagger, n_k]$$

(1.15)

$$= \sum_{i,j} t_{ij} \left(-c_i c_j^\dagger \delta_{jk} + c_i c_j^\dagger \delta_{ik}\right)$$

(1.16)

$$= \sum_j t_{kj} c_k c_j^\dagger - \sum_i t_{ik} c_i c_k^\dagger$$

(1.17)

$$\neq 0$$

(1.18)

The total charge is $\sum_k n_k$, this does commute since summing both terms in (1.17) over $k$ gives zero, where it is used that $t_{ij} = t_{ji}$:

$$\sum_k [H_{\text{hopping}}, n_k] = \sum_{j,k} t_{kj} c_k c_j^\dagger - \sum_{i,k} t_{ik} c_i c_k^\dagger = 0$$

(1.19)

These conservation laws can be expressed in terms of the correlation function or susceptibility $X_{ij,t} = \langle n_i, n_j, t \rangle - \langle n_i \rangle \langle n_j \rangle$, or more conveniently, the Fourier transform $X_{K,\omega}$. For $K = 0$ this is the frequency-dependent correlation of the total charge. Since the total charge is time-independent, this correlator is zero for $\omega \neq 0$. This is a good test of charge conservation.

Since the Hubbard model is an approximation to electrodynamics, it is good to see that the conservation of total spin and charge that occur in electrodynamics still hold.

1.1.5 Example: Hubbard atom

Before studying more complicated systems, it can be useful to take a look at simple exactly solvable models that have similar physics. In case of the lattice Hubbard model, the simplest system is the Hubbard atom. It contains one site that has place for an up and a down electron. If there are two electrons on the atom, they have an interaction $U$. The Hamiltonian is given by:

$$H_{\text{atom}} = U n_\uparrow n_\downarrow - \mu (n_\uparrow + n_\downarrow)$$

(1.20)

This Hamiltonian has four eigenstates with eigenvalue $U - 2\mu, -\mu, -\mu, 0$. The correlation function can be calculated analytically.

$$Z = \exp(-U\beta + 2\mu\beta) + 2\exp(\mu\beta) + 1$$

(1.21)

$$\langle n \rangle = \frac{2\exp(-U\beta + 2\mu\beta) + 2\exp(\mu\beta)}{Z}$$

(1.22)

$$\langle nn \rangle = \frac{4\exp(-U\beta + 2\mu\beta) + 2\exp(\mu\beta)}{Z}$$

(1.23)

$$\langle nn \rangle - \langle n \rangle \langle n \rangle = \frac{4\exp(-U\beta + 2\mu\beta) + 2\exp(-U\beta + 3\mu\beta) + 2\exp(\mu\beta)}{Z^2}$$

(1.24)

Taking $2\mu - U = 0$ gives half-filling ($\langle n \rangle = 1$). In this case $\langle nn \rangle - \langle n \rangle \langle n \rangle = \frac{2}{2+2\exp(\mu\beta)}$. For $U \to -\infty$, the interaction is very attractive. Having two electrons on the site is very favourable compared to one. Due to half-filling, the empty and full state have a similar probability, which
goes to \( \frac{1}{2} \) for \( U \to -\infty \). The state with \( n = 2 \) has \( nn \langle n \rangle n = 4 - 1 = 3 \), the state with \( n = 0 \) has \( nn - \langle n \rangle \langle n \rangle = 0 - 1 = -1 \), so \( \langle nn \rangle \langle n \rangle = \frac{1}{2} (3 - 1) = 1 \), which can also be seen from the explicit formula. For \( U \) very positive, it is too expensive to add another electron to the atom, so the states with \( n = 1 \) both have probability \( \frac{1}{2} \). This gives \( \langle nn \rangle \langle n \rangle = 1 \) for them.

The \( U \to \infty \) case is very insulating, which shows in a low charge-charge susceptibility.

### 1.1.6 Example: Two Hubbard atoms

A slightly more complicated model is the Hubbard dimer. It consists of two Hubbard atoms coupled by a hopping parameter \( t \). The electrons now have two quantum numbers, namely site index and spin, which combine to four different possible states for a single electron. All of these can be either occupied or not occupied, leading to \( 2^4 = 16 \) states. The Hamiltonian is given by:

\[
H_{\text{dimer}} = \sum_{\text{spin } s = \uparrow, \downarrow} t \left( c_{s,2}^\dagger c_{s,1} + c_{s,1}^\dagger c_{s,2} \right) + U \left( n_{\uparrow,1} n_{\downarrow,1} + n_{\uparrow,2} n_{\downarrow,2} \right) - \mu \sum_{\text{site } i} n_{s,i}
\]  

(1.25)

Solving the Hubbard dimer means diagonalizing a 16x16 matrix. However, the total number of particles and the spin in the z-direction \( (n_{\uparrow} - n_{\downarrow}) \) are conserved quantities. This means the Hamiltonian is block diagonal in different blocks with (total charge, total \( S_z \)) equal to \((0,0), (1,1),(1,-1), (2,2), (2,0), (2,-2), (3,1),(3,-1), (4,0)\). These blocks can be solved one by one to find the partition function.

The Hamiltonians of the blocks are given by:

\[
H_{N=0,S_z=0} = 0
\]

(1.26)

\[
H_{N=1,S_z=1} = \begin{pmatrix} -\mu & t \\ t & -\mu \end{pmatrix}
\]

(1.27)

\[
H_{N=1,S_z=-1} = \begin{pmatrix} -\mu & t \\ t & -\mu \end{pmatrix}
\]

(1.28)

\[
H_{N=2,S_z=2} = -2\mu
\]

(1.29)

\[
H_{N=2,S_z=0} = \begin{pmatrix} -2\mu & 0 & t & t \\ 0 & -2\mu & t & t \\ t & t & U - 2\mu & 0 \\ t & t & 0 & U - 2\mu \end{pmatrix}
\]

(1.30)

\[
H_{N=2,S_z=-2} = -2\mu
\]

(1.31)

\[
H_{N=3,S_z=1} = \begin{pmatrix} -3\mu & t \\ t & -3\mu \end{pmatrix}
\]

(1.32)

\[
H_{N=3,S_z=-1} = \begin{pmatrix} -3\mu & t \\ t & -3\mu \end{pmatrix}
\]

(1.33)

\[
H_{N=4,S_z=0} = -4\mu
\]

(1.34)

As a simple example, one can look at the \( N = 1, S_z = 1 \) block for \( \mu = 0 \). A basis for this block is \(|\uparrow,0\rangle, |0,\uparrow\rangle\). The Hamiltonian in this basis is given by:

\[
H_{N=1,S_z=1} = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix}
\]

(1.35)
Which has eigenvectors and eigenvalues:
\[ H \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = t \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad (1.36) \]
\[ H \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -t \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad (1.37) \]
\[ (1.38) \]

The matrix \( V = V^{-1} \) diagonalizes the Hamiltonian:
\[ V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (1.39) \]

If an operator \( \hat{A} \) is represented by a matrix \( A \) in the original basis, then we can calculate its time evolution as (remember \( V = V^{-1} \) in this case):
\[ A(\tau) = V \begin{pmatrix} \exp(it\tau) & 0 \\ 0 & \exp(-it\tau) \end{pmatrix} VAV^{-1} \begin{pmatrix} \exp(-it\tau) & 0 \\ 0 & \exp(it\tau) \end{pmatrix} V \quad (1.40) \]

The operator \( N_{\text{total}} \) is given by:
\[ N_{\text{total}} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.41) \]
\[ N_{\text{total}}(\tau) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.42) \]

The total charge is conserved, since it commutes with the Hamiltonian.

The charge on site 1 is given by:
\[ n_1 = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad (1.43) \]
\[ n_1(\tau) = \frac{1}{4} \begin{pmatrix} 2 + \exp(2it\tau) + \exp(-2it\tau) \\ \exp(2it\tau) - \exp(-2it\tau) \end{pmatrix} \begin{pmatrix} \exp(2it\tau) - \exp(-2it\tau) \\ 2 - \exp(2it\tau) - \exp(-2it\tau) \end{pmatrix} \quad (1.44) \]

By symmetry reasons, within this sector the states \( \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \) and \( \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \) both have probability \( \frac{1}{4} \), so an expectation value can be calculated as:
\[ \langle A \rangle = \frac{1}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} A \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} A \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (1.45) \]
\[ = \frac{1}{2} \text{Tr} A \quad (1.46) \]

This allows the calculation of the correlator:
\[ n_1(\tau)n_1(\tau = 0) = \frac{1}{4} \begin{pmatrix} 2 + \exp(2it\tau) + \exp(-2it\tau) \\ \exp(2it\tau) - \exp(-2it\tau) \end{pmatrix} \begin{pmatrix} \exp(2it\tau) - \exp(-2it\tau) \\ 2 - \exp(2it\tau) - \exp(-2it\tau) \end{pmatrix} \quad (1.47) \]
\[ \langle n_1(\tau)n_1(\tau = 0) \rangle - \langle n_1 \rangle \langle n_1 \rangle = \frac{1}{2} \frac{1}{4} \begin{pmatrix} 2 + \exp(2it\tau) + \exp(-2it\tau) \\ \exp(2it\tau) - \exp(-2it\tau) \end{pmatrix} - \frac{1}{4} \quad (1.48) \]
\[ = \frac{1}{4} \cos(2t\tau) \quad (1.49) \]
The charge on one site is not conserved, since the electron can hop from one site to the other. This means there is a non-zero charge-charge correlator with a time-dependence. The other sectors of the Hamiltonian can be solved in a similar fashion. Expectation values over the entire Hamiltonian can then be calculated by weighing each sector with the probability of being in that sector.

\[ \langle A \rangle = \sum_{\text{sectors } i} P(\text{sector } = i) \langle A \rangle_{\text{sector } i} \]  

This will give similar results: \( N_{\text{total}} \) is conserved, so it has a time-independent correlator. The charge on one site \( n_1 \) is not conserved, the correlator has a time-dependence. In the full system, this time-dependence will be more complicated and a function of \( t, \mu \) and \( U \).

1.1.7 The Mott Transition

The half-filled Hubbard model describes the competition between the delocalization of electrons by their kinetic energy and the interaction that localizes them. As the ratio \( \frac{U}{t} \) increases, the system becomes more and more localized. This gives rise to the Mott transition\(^4\). At low \( U \), the Hubbard model is metallic and the electrons are itinerant. While at large \( U \) they are localized and the system is insulating. A good overview of the Mott transition can be found in Kotliar and Vollhardt\(^5\), where it is studied using Dynamical Mean Field Theory.

This transition between insulating and metallic is clearly visible in the local density of states (figure 1.2). For \( U = 0 \) the electrons are free and the density of states is given by their dispersion. It is a band with the Fermi level in the middle. When \( U \) increases, the electrons can be described as quasi-particles with a renormalized mass. As \( U \) increases further, two Hubbard bands start to appear at energies \( \pm \frac{U}{2} \). With increasing \( U \), more and more of the spectral weight is transferred to these bands and the weight of the quasi-particle peak at the Fermi level goes away. As the quasi-particle peak vanishes, the Mott transition occurs. There are no longer low energy modes around the Fermi level available, a gap appears and the system is now insulating.

The system in figure 1.2 comes from a calculation in an infinite dimensional study. In a two dimensional system the non-interacting density of states does not have this semi-elliptical shape, instead it has a divergence at \( E = 0 \). The non-interacting Hubbard model in two dimensions is studied in appendix A.
Figure 1.2: Evolution of the local density of states across the Mott transition in DMFT. Image from [5]. This is the behaviour in an infinite dimensional system, the non-interacting density of states looks differently in a finite dimension.
1.2 Quantum Field Theory at Finite Temperature

In this section, a short introduction into quantum field theory at finite temperature will be given along the lines of chapter 3 of Mahan\(^6\) and chapter 2 of Negele and Orland\(^7\). Alternatively, the book by Altland and Simons\(^8\) can be used. A pedagogical treatment can also be found in Sweep\(^9\). The focus in this section will be on summarizing the main results and formulas that will be used in this thesis. This theory was originally developed by and is named after Matsubara\(^10\).

1.2.1 General idea

The thermal expectation value of an operator in the (grand-)canonical\(^4\) ensemble is given by:

\[
\langle A \rangle = \text{Tr} \left[ \exp(-\beta H) A \right] \quad (1.51)
\]

On the other hand, the time evolution of an operator in regular quantum mechanics is given by:

\[
A(t) = \exp(itH) A \exp(-itH) \quad (1.52)
\]

The idea of the Matsubara formalism is to treat temperature and time as real and imaginary parts of a single complex variable. An imaginary time \( \tau \) is introduced as \( \tau = it \). This imaginary time runs in the domain \([-\beta, \beta]\) or \([0, \beta]\). In this way, the usual formalism of quantum field theory can simply be used to describe systems at a finite temperature.

1.2.2 Imaginary Time Path Integral

The approach to the derivation of the imaginary time path integral in Negele and Orland\(^7\) is to interpret the partition function as a time evolution operator over a time interval of length \( \beta \):

\[
Z = \text{Tr} \exp(-\beta H) \quad (1.53)
\]

\[
= \sum_\phi \langle \phi | \exp(-\beta H) | \phi \rangle \quad (1.54)
\]

\[
= \text{Tr} U(\tau = \beta) \quad (1.55)
\]

This time interval of length \( \beta \) is split up into \( M \) parts. The time evolution is then given by a product of time evolution operators over a time interval with length \( \frac{\beta}{M} \). As \( M \) tends to infinity, the Trotter formula can be used to apply a normal ordering to these infinitesimal time-evolution operators. The completeness relation has been used to insert a sum over all states at each time slice, which in the limit of \( M \) to infinity produces an integral over all possible paths.

In many particle physics, instead of using position and momentum operators, creation and annihilation operators are used. The path integral then becomes an integral over all possible field configurations. In the end, the expression that appears in the exponent is the action \( S \). In a very short notation we can write:

\[
Z = \int D[\phi, \phi^*] \exp(-S[\phi, \phi^*]) \quad (1.56)
\]

\(^4\)In this thesis, the grand-canonical ensemble is used unless otherwise noted. For convenience the \( H \) includes the chemical potential, \( H \to H - \mu N \)
where $\phi$ is used to denote all fields. In the case of a real field $\phi$, the integration over $\phi^*$ is redundant. The integration $D[\phi, \phi^*]$ is over all fields that satisfy the boundary conditions:

$$\phi(\beta) = \zeta \phi(0)$$  \hspace{1cm} (1.57)

with $\zeta = 1$ for bosons and $\zeta = -1$ for fermions.

The action contains the physical information about the system. It is given by:

$$S[\phi, \phi^*] = \int_0^\beta d\tau \phi^* \left( \frac{\partial}{\partial \tau} - \mu \right) \phi + H(\phi, \phi^*)$$  \hspace{1cm} (1.58)

### 1.2.3 Grassmann Variables

A new mathematical object called a Grassmann number is useful in the treatment of fermions. These numbers are thoroughly introduced in Section 1.5 of Negele and Orland[7]. Here we summarize the most important properties of Grassmann numbers. For Grassmann numbers $\xi_a, \xi_b$, the following properties hold:

$$\xi_a \xi_b = -\xi_b \xi_a$$  \hspace{1cm} (1.59)

$$\langle \lambda \xi_\alpha \rangle^* = \lambda^* \xi_\alpha$$  \hspace{1cm} (1.60)

$$\langle \xi_a \xi_b \rangle^* = \xi_b^* \xi_a^*$$  \hspace{1cm} (1.61)

$$\int d\xi \xi = 1$$  \hspace{1cm} (1.62)

$$\int d\xi 1 = 0$$  \hspace{1cm} (1.63)

$$\frac{d}{d\xi} \xi = 1$$  \hspace{1cm} (1.64)

$$\frac{d}{d\xi} 1 = 0$$  \hspace{1cm} (1.65)

Bosonic operators can be studied using complex fields, when the same is done for fermionic operators it is necessary to use Grassmann variables instead of complex numbers for the fields to correctly get the anticommutation relations. The field $\phi$ mentioned in the previous section will be a Grassmann field for fermions.

### 1.2.4 Green’s functions

Green’s functions are the fundamental objects of quantum field theory. They can be calculated within the theory and can be used to determine experimentally observable quantities. A Green’s function describes the propagation of particles. In the Matsubara formalism, the Green’s function for a field $\phi$ is defined as:

$$G_{ab} = -\langle T_\tau \phi_b \phi^*_a \rangle$$  \hspace{1cm} (1.66)

Here $T_\tau$ is a time ordering operator in imaginary time. It orders the field operators with their imaginary time decreasing from left to right. In the case of a real field $\phi$, one obviously has $\phi^* = \phi$.

The letters $a, b$ here were used to denote the various numbers, that are used to describe a field, like
position, imaginary time, spin, et cetera. In translationally invariant systems, only the difference in position between \(a\) and \(b\) is relevant, and a Fourier transform from real space to momentum space can be applied to get \(G(k)\). The Green’s function also depends only on the imaginary time difference between \(a\) and \(b\), so it is possible to write \(G(\tau)\) instead of \(G(\tau_1, \tau_2)\). When the field \(\phi\) describes the charge, the Green’s function will also be called (charge) susceptibility.

1.2.5 Fermions and bosons

Bosons and fermions are characterized by the fact that their imaginary time Green’s functions (which are both denoted by \(G\) here) are even and odd under a shift of \(\beta\).

\[ G(\tau) = +G(\tau + \beta) \quad \text{boson} \quad (1.67) \]
\[ G(\tau) = -G(\tau + \beta) \quad \text{fermion} \quad (1.68) \]

This means that a Fourier transform of \(G\) on the interval \([-\beta, \beta]\) will only contain the frequencies:

\[ \omega_n = \frac{2n\pi\beta^{-1}}{1} \quad \text{boson} \quad (1.69) \]
\[ \nu_n = (2n + 1)\pi\beta^{-1} \quad \text{fermion} \quad (1.70) \]

These frequencies are called Matsubara frequencies and the letters \(\omega\) and \(\nu\) will only be used for bosonic and fermionic Matsubara frequencies respectively throughout this thesis.

The Fourier transform is defined in the same way as in Mahan:

\[ G(\tau) = \frac{1}{\beta} \sum_n \exp(-i\omega_n \tau) G(i\omega_n) \quad (1.71) \]
\[ G(i\omega_n) = \int_0^\beta d\tau \exp(i\omega_n \tau) G(\tau) \quad (1.72) \]

The definition for the fermions is obtained by replacing \(\omega_n \rightarrow \nu_n\).

Observe that the fermionic and bosonic Matsubara frequencies are exactly the locations of the poles of the Fermi and Bose distribution function respectively.

1.2.6 Conserved quantities

Conserved quantities are very similar in the imaginary time formalism used here and the real time formalism that is familiar from introductory quantum mechanics. If an operator \(A\) commutes with the Hamiltonian \(H\) then the imaginary time evolution of this operator will be trivial:

\[ A(\tau) = \exp(\tau H)A \exp(-\tau H) \quad (1.73) \]
\[ = A \exp(\tau H) \exp(-\tau H) \quad (1.74) \]
\[ = A \quad (1.75) \]
\[ = A(\tau = 0) \quad (1.76) \]

This means that the Fourier transform of \(A\) will be simple, only the frequency zero can have a non-zero value.
1.2.7 Analytical continuation

In the Matsubara formalism, the Green’s functions are calculated as a function of Matsubara frequency. To relate these functions to experimental quantities, it is necessary to transform them to functions of energy $E$. These are the real and imaginary part of the same complex variable. Since the Green’s functions are analytical functions, once they have been determined exactly at all Matsubara frequencies, the function is known on the entire real axis. Given an analytical expression for $G(i\nu_n)$, to get the retarded Green’s function $G(E)$, one just needs to replace all occurrences of $i\nu_n$ by $E + i\delta$, where $\delta$ is some small parameter. The advanced Green’s function is obtained by using $E - i\delta$ instead.

However analytical expressions for $G(i\nu_n)$ are rare, usually one calculates $G(i\nu_n)$ using some numerical scheme. In that case, analytical continuation can be done using Padé approximants. In this thesis all analytical continuations are done using an implementation by Hartmut Hafermann of the algorithm in Vidberg and Serene\cite{11}.

The spectral function is one of the quantities that can be obtained from the analytically continued Green’s function. It is given by:

$$A(E, k) = -\frac{1}{\pi} \text{Im} G(E, k) \quad (1.77)$$

The electron spectral function can be interpreted as a probability distribution, since $A(E, k) \geq 0$ and $\int_{E,k} A(E,k) = 1$. For bosons, such an interpretation does not exist. For bosons, the Green’s function is defined with a minus sign $-\langle \phi_a \phi_b \rangle$, but the analytically continued spectral function will be given without this minus sign.

A good overview of analytical continuation and some of the problems associated with it can be found in\cite{12} and references therein.

1.2.8 Some useful results

The Green’s function of free non-interacting fermions can be calculated exactly. If they have a dispersion $t_k$, the action can be written as:

$$S = \int_0^\beta d\tau \sum_k c_k^* \left( \frac{\partial}{\partial \tau} - \mu \right) c_k + c_k^* t_k c_k \quad (1.78)$$

$$= -\sum_{\nu,k} c_{\nu,k}^* (i\nu - t_k + \mu) c_{\nu,k} \quad (1.79)$$

$$= -\sum_{\nu,k} c_{\nu,k}^* G(i\nu, k)^{-1} c_{\nu,k} \
\quad (1.80)$$

With the Green’s function:

$$G(i\nu_n, k) = \frac{1}{i\nu_n - t_k + \mu} \quad (1.81)$$

In the low temperature limit, the spectral function at $E = 0$ is related to the imaginary time Green’s function at $\tau = \frac{\beta}{2}$ in the following way.\footnote{A similar relation is given by Ayral\cite{13}, but this derivation is not very careful with taking limits and ends up with a wrong prefactor.} The first step in the derivation is to write how
\( G(\frac{\beta}{2}) \) depends on \( A(\omega) \) in a symmetric way.

\[
G(\tau) = -\int_{-\infty}^{\infty} dE' A(E') \frac{e^{-E' \tau}}{1 + e^{-E' \beta}} \tag{1.82}
\]

\[
G(\frac{\beta}{2}) = -\int_{-\infty}^{\infty} dE' A(E') \frac{e^{-E' \frac{\beta}{2}}}{1 + e^{-E' \beta}} \tag{1.83}
\]

\[
= -\int_{-\infty}^{\infty} dE' A(E') \frac{1}{e^{E' / \beta} + e^{-E' / \beta}} \tag{1.84}
\]

\[
= -\int_{-\infty}^{\infty} dE' A(E') \frac{1}{2 \cosh\left(\frac{E' \beta}{2}\right)} \tag{1.85}
\]

The function \( \frac{1}{\cosh(x)} \) has a maximum at \( x = 0 \) and decays quickly as \( x \) goes away from zero. In particular, 99% of the volume is concentrated in the interval \( x \in [-6, 6] \), so \( |\beta E| < 12 \). In the low temperature limit, \( \beta \) becomes large, and this means that only the part of the density of states close to zero energy contributes to \( G(\frac{\beta}{2}) \). In this small region, \( A(E) \approx A(0) \). So the fundamental assumption is that \( A(E) \) is approximately constant on some interval with a length which scales as \( \beta^{-1} \). This becomes true as \( \beta \to \infty \). Using this assumption gives:

\[
G(\frac{\beta}{2}) = -\int_{-\infty}^{\infty} dE' A(E') \frac{1}{2 \cosh\left(\frac{E' \beta}{2}\right)} \tag{1.86}
\]

\[
\approx -\frac{A(0)}{\beta} \int_{-\infty}^{\infty} dE' \frac{1}{\cosh\left(\frac{E' \beta}{2}\right)} \tag{1.87}
\]

\[
\approx -\frac{A(0)}{\beta} \frac{2}{\pi} \int_{-\infty}^{\infty} d\alpha \frac{1}{\cosh(\alpha)} \tag{1.88}
\]

\[
\approx -\frac{A(0)}{\beta} \frac{2}{\pi} \tag{1.89}
\]

\[
\approx -\frac{A(0)}{\beta} \frac{2}{\pi} \tag{1.90}
\]

\[
A(0) \approx -\frac{\beta}{\pi} G(\frac{\beta}{2}) \tag{1.91}
\]

This relation is useful since the spectral function at energy zero shows if the system is metallic or insulating.

### 1.2.9 Particle-hole symmetry

Some systems exhibit particle-hole symmetry. In this case, all observables stay the same under the exchange of fermion creation and annihilation operators \( c \leftrightarrow c^* \). This means that the fermionic Green’s function is symmetric around \( \frac{\beta}{2} \). To prove this, first use the particle-hole symmetry, then use the anti-commuting property of the Grassmann numbers and finally use that the Green’s function only depends on the time difference.

\[
G(-\tau) = -\langle c_{-\tau} c_0^* \rangle \tag{1.92}
\]

\[
= -\langle c_{-\tau} c_0^* \rangle \tag{1.93}
\]

\[
= \langle c_0 c_{-\tau} \rangle \tag{1.94}
\]

\[
= \langle c_\tau c_0^* \rangle \tag{1.95}
\]

\[
= -G(\tau) \tag{1.96}
\]
According to (1.68) $G(-\tau) = -G(\beta - \tau)$, so this results in $G(\beta - \tau) = G(\tau)$. This symmetry can be used in the Fourier transformation (1.72) to Matsubara frequencies. Split up the integral into two parts, change variables $\tau = \beta - \tau'$ in the second part and use $\exp(i\nu_n\beta) = -1$.

\[
G(i\nu_n) = \int_0^\beta d\tau \exp(i\nu_n\tau)G(\tau)
\]

\[
= \int_0^{\frac{\beta}{2}} d\tau \exp(i\nu_n\tau)G(\tau) + \int_{\frac{\beta}{2}}^\beta d\tau \exp(i\nu_n\tau)G(\tau)
\]

\[
= \int_0^{\frac{\beta}{2}} d\tau \exp(i\nu_n\tau)G(\tau) - \int_0^{\frac{\beta}{2}} d\tau' \exp(i\nu_n(\beta - \tau'))G(\beta - \tau')
\]

\[
= \int_0^{\frac{\beta}{2}} d\tau \exp(i\nu_n\tau)G(\tau) + \int_0^{\frac{\beta}{2}} d\tau' \exp(i\nu_n(\beta - \tau'))G(\tau')
\]

\[
= \int_0^\beta d\tau [\exp(i\nu_n\tau) - \exp(-i\nu_n\tau)] G(\tau)
\]

This shows that $\text{Re} G(i\nu_n) = 0$.

The relation (1.68) between the Green's function and the spectral function can be rewritten as:

\[
G(\tau) = \int_{-\infty}^{\infty} dE A(E) \frac{e^{(\beta-\tau)E}}{e^{-\frac{\beta}{2}E} + e^{\frac{\beta}{2}E}}
\]

In case of particle hole symmetry, the left hand side stays the same under the transformation $\tau \rightarrow \beta - \tau$. The fraction in the integral also stays the same, if at the same time the transformation $E \rightarrow -E$ is performed. So the requirement

\[
A(E) = A(-E)
\]

makes sure that the entire relation is satisfied in the particle-hole symmetric case.

### 1.2.10 Self-energy and Dyson's equation

One of the goals in quantum field theory is the calculation of full propagators. These are represented diagrammatically by all diagrams with two external lines.\(^6\) This set of diagrams can be reduced by summing certain infinite sets of diagrams. One such approach is done by considering all diagrams that can not be cut into two parts by removing one propagator. The diagrams are called irreducible. Every diagram for the full propagator consists of irreducible pieces, connected by single propagators. The full propagator can be recovered by summing over the number of irreducible parts. These irreducible diagrams, with the incoming and outgoing propagator amputated, are called self-energy diagrams and are denoted by $\Sigma$. More information on self-energies can be found in section 2.4 of Negele and Orland\(^7\) or section 3.4 of Mahan\(^6\).

Now, this classification of diagrams in terms of the number of irreducible parts can be written down. They form a geometric sum, which can be calculated once $\Sigma$ is known:

\[
\rightarrow = \rightarrow + \Sigma \rightarrow + \Sigma \rightarrow + \Sigma \rightarrow + \cdots
\]

\(^6\)As usual, only connected diagrams are used, since vacuum polarization diagrams are cancelled in the denominator.
(a) Not a skeleton diagram.  
(b) Corresponding skeleton diagram.

Figure 1.3: An expansion in skeleton diagrams with bold lines has the same diagrams as an expansion in irreducible diagrams with bare lines.

\[ G = G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \ldots \]  
\[ = G_0 \sum_{n=0, \infty} (\Sigma G_0)^n \]  
\[ = \frac{G_0}{1 - \Sigma G_0} \]

Thus it is only necessary to calculate irreducible diagrams and then Dyson’s equation can be used to get the full propagator.

A further simplification of the set of diagrams is possible. There are diagrams where replacing part of them by a single propagator still gives a valid diagram. Such a contribution can also be generated by only including the simpler diagram, but by using a renormalized Green’s function instead of the bare Green’s function. Diagrams which can not be simplified by replacing some part of them by a single propagator are called skeleton diagrams. An illustration of this concept is shown in figure 1.3. One can calculate the self-energy purely using skeleton diagrams with renormalized Green’s functions. But these renormalized Green’s function require knowledge of the self-energy. To calculate the self-energy, one would need the self-energy. So the calculation should be solved self-consistently. In practice, one starts with the bare Green’s function as a guess, calculates \( \Sigma \), uses (1.106) to get the renormalized Green’s function, then calculates the skeleton diagrams again using the new Green’s function. This process is repeated until it converges to the fixed point of the equation:

\[ G = \frac{G_0}{1 - \Sigma(G)G_0} \]
1.3 Random Phase Approximation

The (RPA) is one of the primary tools in studying susceptibilities. It was originally developed in the 1950s by Bohm and Pines\cite{14,15,16} and later work on the approximation by Lindhard was very important for understanding plasmons and electric field screening. There are many different approaches to the RPA, that can be found in textbooks like Vonsovsky and Katsnelson\cite{1}. Here a Green’s function formalism will be used to describe the RPA, since this is closest to the formalism used in the remainder of this thesis. We will summarize some results on the RPA and study the consequences of the RPA at large wavelength. More information on this formalism can be found in\cite{13,6,8,7}.

1.3.1 Formalism

The Random Phase Approximation is used to calculate susceptibilities in electron system. Every electron has a kinetic energy which, due to translational symmetry, depends only on their momentum \( k \). This kinetic energy is denoted by \( t_k \). Examples of \( t_k \) are the Hubbard dispersion (1.7) or the free electron gas \( t_k \propto k^2 \). When there is no additional interaction, the state of the full system can be obtained by filling the one-particle modes according to the Fermi-Dirac distribution. This changes when there is an interaction. Consider an interaction between electrons that depends on the distance between the electrons. Due to translational symmetry, this interaction also only depends on a single momentum and it will be denoted as \( V_k \). Now, the likelihood to fill a certain mode depends on which other modes are already filled, since the different modes interact via \( V \).

The Random Phase Approximation start from the non-interacting system. Remember that the non-interacting Matsubara Green’s function is given by (1.81):

\[
G(k, \nu) = \frac{1}{i\nu + \mu - t_k} \quad (1.108)
\]

The non-interacting charge susceptibility is obtained from Wick’s theorem as a bubble of the Green’s function, as shown in figure 1.4. This bubble diagram is a simple convolution of Green’s functions:

\[
\Pi(k, \omega) = \sum_{q,\nu,\sigma} G(q, \nu, \sigma)G(q - k, \nu - \omega, \sigma) \quad (1.109)
\]

\[
= 2 \sum_{q} \frac{f(\xi_q) - f(\xi_{q-k})}{\xi_q - \xi_{q-k} + i\omega} \quad (1.110)
\]

Here, \( f \) is the Fermi distribution function and \( \omega \) denotes a bosonic Matsubara frequency as is usual in this thesis. The notation \( \xi_q = t_q - \mu \) was used to simplify the expression. After analytical continuation from Matsubara frequency to real energy this results in:

\[
\Pi(k, E) = 2 \sum_{q} \frac{f(\xi_q) - f(\xi_{q-k})}{\xi_q - \xi_{q-k} - E + i\delta} \quad (1.111)
\]

Here \( \delta \) is some small broadening constant. This expression is called the dynamical Lindhard function.
In the interacting theory, free electron Green’s functions can couple to $V_k$ via a vertex with an incoming and outgoing fermion propagator and a single $V_k$ line. The Random Phase Approximation then assumes that for the two-particle correlation, it is sufficient to treat a series of bubble diagrams connected by the interaction $V_k$. An example of such a diagram is shown in figure 1.5. This results in a geometric series expression for the charge-charge correlator:

$$X(k, E) = \prod \frac{\Pi(k, E)}{1 - V_k \Pi(k, E)}$$  \hspace{1cm} (1.112)

This formula would be exact if the bubble $\Pi$ was replaced by the sum of all diagrams with the same endpoints that are one-particle irreducible with respect to $V_k$. However, this is not the case since a diagram like figure 1.6 is not included in the RPA. This is a large approximation which is valid in the limit of small $V_k$.

Another quantity that is often used to describe the collective excitations in the RPA is the dielectric function $\epsilon$. This dielectric function is defined as the ratio between an externally applied field and the resulting effective field after the field has been screened. In the RPA this dielectric function follows easily from the bubble diagram:

$$\epsilon(k, E) = 1 - V_k \Pi(k, E)$$ \hspace{1cm} (1.113)

$$\frac{1}{\epsilon(k, E)} = 1 + V_k X(k, E)$$ \hspace{1cm} (1.114)

In particular, we see that $\epsilon = 1$ if $V_k = 0$. No screening takes place in a non-interacting system. The relation (1.114) is true in general, not only in the RPA.
1.3.2 Long- and short-range interactions

The fundamental difference between long- and short-range interactions is visible in the RPA. The Fourier transform of a short-range interaction goes to a constant at small $k$, while the Fourier transform of a long-range interaction diverges for $k \to 0$. This means that the inverse dielectric function (1.114) does not have to go to zero even though $X(k, E)$ goes to zero for $k \to 0, E \neq 0$. This is illustrated by the prototypical example of a long range interaction, the Coulomb potential in 3D. The Coulomb potential $V_{\text{Coulomb}}(k) = U k^{-2}$ diverges for long wavelengths.

If we study the RPA for $k = 0$ and $E > 0$, from (1.111) we get $\Pi(k = 0, E) = 0$, and then it follows from (1.112) that $X(k = 0, E) = 0$. When $E = 0$, both the numerator and denominator in (1.111) vanish and the situation requires more analysis. So we find that any system will have a charge susceptibility dispersion that goes to 0 for $k \to 0, E \neq 0$.

In case of a long-range interaction, $\Pi(k, E)$ has the same behaviour since it does not depend on $V$, so $X(k, E)$ also vanishes for $k \to 0, E \neq 0$. But in the long wavelength limit $V_k X(k, E)$ will not vanish anymore, it can become independent of $k$ for small $k$. There can be a $E'$ where $V_k X(k, E)$ has a pole for $k \to 0, E \to E'$. This means that there is a finite energy mode at $k = 0$. This mode is typically called the plasmon mode and the energy $E'$ is called the plasma energy.

1.3.3 Non-interacting limit of the Hubbard model

The only dependence on the interaction is in the relation between $X$ or $\epsilon$ and $\Pi$. It is useful to study $\Pi$ since it determines the physics in the non-interacting case, which is easiest to consider. $\Pi$ is big when the denominator is almost zero. This is when the difference in the non-interacting $\xi$ terms is approximately $E$. Using the Hubbard dispersion in two dimensions (1.7), this difference can be rewritten as:

$$\xi_q - \xi_{q-k} = t_q - t_{q-k} = -4t \left( \sin\left(\frac{1}{2}k_x\right) \sin\left(\frac{1}{2}k_x - q_x\right) + \sin\left(\frac{1}{2}k_y\right) \sin\left(\frac{1}{2}k_y - q_y\right) \right)$$

This means that the condition $E \approx \xi_q - \xi_{q-k}$ results in:

$$|E| \leq 4t \left( \sin\left(\frac{1}{2}k_x\right) + \sin\left(\frac{1}{2}k_y\right) \right)$$

At $k = (\pi, 0)$, this gives $|E| \leq 4t$, while at $k = (\pi, \pi)$ it gives $|E| \leq 8t$.

For small $E, k$ and along the $k_x$ direction, the dispersion function is linear and the coefficient can be determined:

$$E(k_x) \approx 4t \sin\left(\frac{1}{2}k_x\right) \approx 2tk_x$$

In the interacting case, the calculation of $\Pi$ is still the most expensive part of the calculation, since it requires a sum over $q$ for every $k$. After $\Pi$ has been calculated, (1.112) and (1.113) directly give the dielectric function and the charge-charge correlator.
Figure 1.7: Π(k, E) and \( \epsilon^{-1}(k, E) \) in the 3D cubic Hubbard model on a 36 by 36 by 36 lattice at \( \beta = 50, \delta = 0.1, t = 0.25 \), with a Coulomb interaction with strength \( U = 1 \). Π shows the non-interacting Hubbard model with a mode with zero energy for long wavelengths. The inverse dielectric function has a finite energy plasmon mode due to the long-range Coulomb interaction.

So for \( k \) small, there is a clearly defined dispersion relation while for \( k \approx (\pi, \pi) \) there are available modes at all \( E \in [0, 8t] \). The highest energy modes there correspond to \( q \approx 0 \) while the lower energy modes correspond to \( q \approx (\frac{\pi}{2}, \frac{\pi}{2}) \).

1.3.4 Results

Numerical calculations can be done using (1.111), (1.112) and (1.114). A finite size lattice is used. The Coulomb interaction in a three-dimensional system \( V_{\text{Coulomb}} = U k^{-2} \) diverges at \( V(k = 0) \). This corresponds to the interaction of a homogeneous charge distribution. In materials, the homogeneous part of the negative charge of the itinerant electrons is compensated by the positive charge of the ions. This means that the correct way to describe the Coulomb interaction in an electron system is \( V_{\text{Coulomb}} = U k^{-2} \) for \( k \neq 0 \) and \( V_{\text{Coulomb}} = 0 \) for \( k = 0 \). The simulations in figure 1.7 are done using nearest neighbour hopping for electrons on a 3D cubic lattice: \( t_k = -2t (\cos(k_x) + \cos(k_y) + \cos(k_z)) \). The parameters for these simulations were \( t = 0.25, \beta = 50 \), the lattice size is 36 by 36 by 36. At small \( k \) the long-range interaction generates a finite plasmon energy in \( \epsilon^{-1} \), while short range interaction only have modes that go to zero.

It is also possible to study the 2D Hubbard Model on a square lattice using the RPA. In that case, take \( V_{\text{Hubbard}} = U \) and \( t_k = -2t (\cos(k_x) + \cos(k_y)) \). Π(k, E) can be calculated using (1.111), this gives the result shown in 1.8. This Π is the exact susceptibility at \( U = 0 \).

These calculations can also be done in the 3D cubic lattice Hubbard model. The nearest neighbour hopping then gives \( t_k = -2t (\cos(k_x) + \cos(k_y) + \cos(k_z)) \). These calculations were done on a 36 by 36 by 36 lattice, at \( \beta = 50, t = 0.25, \delta = 0.1 \). The results of this calculation for different \( U \) are shown in figure 1.9. Several things are clear from these figures. In the almost non-interacting case \( U = 0.01 \), everything is obviously very similar to the non-interacting case. At small \( k \), the dispersion is linear. At \( X = (\pi, 0, 0) \), the maximal energy is \( 4t \), at \( M = (\pi, \pi, 0) \) it is \( 8t \) and at \( R = (\pi, \pi, \pi) \) it is \( 12t \). Around the \( R \) and to a lesser extent the \( M \) point, there is a wider particle-hole continuum. As the interaction is increased to \( U = 1.00 \), the energies at the \( X, M \) and \( R \) points shift slightly up and the continuum modes are damped. This trend continues for \( U = 2.00 \) and for \( U = 5.00 \) the continuum modes are not visible anymore and the energies are clearly higher. For example, at the \( M \) point the energy is now \( 3 \) instead of \( 8t = 2 \).
Figure 1.8: The bubble $\Pi(k,E)$ in the 2D Hubbard model on a 64 by 64 lattice at $\beta = 50$, $\delta = 0.1$, $t = 0.25$.

Figure 1.9: $X(k,E)$ as a function of $U$ in the 3D cubic Hubbard model on a 32 by 32 by 32 lattice at $\beta = 50$, $\delta = 0.1$, $t = 0.25$. For small interactions, there is a broad continuum of modes, but as $U$ is increased this continuum vanishes, until there are only narrow bands left at $U = 5.00$. 
1.3.5 RPA starting from an interacting system

In the previous derivation of the RPA, it was assumed that only the non-interacting Green’s function was known exactly and this was used to calculate the susceptibility in the interacting system. Essentially, the interaction $V_k$ acted as a self-energy for the bare susceptibility $\Pi$. It is possible to have a system with an interaction $V + V'$ with $V$ simple enough to approximately calculate the susceptibility caused by $V$, but big enough that it is not appropriate to treat it in the RPA. On the other hand $V'$ describes a more complicated interaction, but it is smaller so it can be treated as a perturbation via the RPA. In this case, it is possible to use the RPA formalism, where $X_0$ has the role of the bare (with respect to $V'$) susceptibility $\Pi$. The full susceptibility is then given by:

$$X = \frac{X_0}{1 - V'X_0} \quad (1.120)$$

It is easy to check that this procedure produces a sensible result if $V$ was also treated in RPA:

$$X_0 = \frac{\Pi}{1 - V\Pi} \quad (1.121)$$

$$X = \frac{X_0}{1 - V'X_0} \quad (1.122)$$

$$= \frac{\Pi}{1 - V\Pi} \frac{1}{1 - V'\Pi} \quad (1.123)$$

$$= \frac{\Pi}{1 - V\Pi - V'\Pi} \quad (1.124)$$

$$= \frac{\Pi}{1 - (V + V')\Pi} \quad (1.125)$$

This is the same result as one would get from doing the RPA with $V + V'$ immediately.

Such an approach can be useful to relate results in the Hubbard model to results in a system with a long range Coulomb interaction. The Hubbard $U$ (and the extended Hubbard $V$) treats the largest part of the interaction, that can not be handled perturbatively but can be dealt with in dual boson like methods. The longer range parts of the interaction are smaller and can be treated in the RPA.

1.3.6 Charge ordering in the RPA

The extended Hubbard model can have a charge-ordered phase when the nearest neighbour interaction $V$ starts to dominate over the local interaction $U$. This is associated with a checkerboard ordering, so $k = (\pi, \pi)$ in two dimensions, $k = (\pi, \pi, \pi)$ in three dimensions, $k = (\pi, \pi, \ldots, \pi)$ in dimension $n$. This point will be denoted as $k_\pi$. The phase transition to this phase occurs when the susceptibility at $k_\pi$ diverges. According to (1.112) this happens when $1 - V_k\Pi(k, E) = 0$. $\Pi(k, E)$ does not depend on $V_k$ in the RPA scheme, so as a function of $U$ and $V$ the condition for a phase transition is:

$$V_{k_\pi} = \Pi(k_\pi, E = 0)^{-1} \quad (1.126)$$

$$U - 2nV = \Pi(k_\pi, E = 0)^{-1} \quad (1.127)$$

Observe that $2n = z$ is the number of nearest neighbours. In a $UV$-phasediagram based on the RPA, the charge-ordered phase transition will occur at $V_c(U) = V_c(U = 0) + \frac{z}{2}U$. 

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1.3.7 Conclusion

The RPA is a useful tool for studying charge susceptibilities. It shows the qualitative difference between long- and short-range interactions. Long-range interactions give rise to plasmons, excitations with a finite energy for \( k \to 0 \). Short-range interactions give rise to Goldstone modes with a vanishing energy for \( k \to 0 \). The RPA is exact in the limit of small interaction, so it can be used as a benchmark for other methods. It is also possible to apply the RPA to go from Hubbard susceptibilities to susceptibilities in systems with a longer range interaction.
Chapter 2

The dual boson method

In this chapter the dual boson method will be introduced. This method was originally proposed by Rubtsov et al.\cite{Rubtsov17} and is an extension of the dual fermion method\cite{Rubtsov18}. A derivation of the dual boson method analogous to the treatment of dual fermion by Hafermann\cite{Hafermann19} will be given. Dual boson will be compared to dual fermion, EDMFT+GW, EDMFT and DMFT. Some details of the derivation given in this chapter can be found in the appendices.

2.1 The dual transformation

In the action formalism, the generalized Hubbard model is given by the action:

\[ S_{\text{lat}} = -\sum_{\text{site} i} \sum_{\text{spin} \sigma} c_{i\sigma\nu}^\dagger (i \nu + \mu) c_{i\sigma\nu} + \sum_{\text{site} i} U n_{i,\uparrow,\omega} n_{i,\downarrow,\omega} + \sum_{\text{spin} \sigma} \sum_{\text{momentum} k} c_{k\sigma\nu}^\dagger c_{k\sigma\nu} + \frac{1}{2} \sum_{\omega} \rho_{K\omega} V_{K\omega} \rho_{K\omega} \]

(2.1)

Here, \( \mu \) is the chemical potential, \( \nu \) and \( \omega \) are respectively fermionic and bosonic Matsubara frequencies, \( k, K \) are momentum labels, \( U \) is the on-site interaction, \( V_K \) is the off-site interaction and \( t_k \) is the fermionic hopping. \( \rho \) is the density fluctuation \( n - \langle n \rangle \). The difference between using \( n \) and \( \rho \) can be compensated by an appropriate shift of \( \mu \). A factor \( \frac{1}{\beta} \) is implied in all sums over \( \nu, \omega \).

The theory presented here is a generalization of dual fermion theory. In dual fermion, \( V_K = 0 \). The derivation presented here is very similar to the derivation of dual fermion, the difference is that in the case of dual boson there are always fermionic and bosonic quantities, while dual fermion only has the former. The equations for the fermions and the bosons are very similar, as will be visible.

Parts of the action are local (\( k \)-independent), while other parts have an explicit \( k \)-dependence. The idea of the dual transformation is to collect all of the local contributions into one part of the action called the impurity part, and to use a Hubbard-Stratonovich transformation on the remainder. When writing \( S = S_{\text{imp}} + S_{\text{other}} \), there is of course a freedom to add/subtract an arbitrary \( k \)-independent term to/from the impurity and the other part. This freedom will be denoted by \( \Delta \) and \( \Lambda \) here.
The non-impurity part of the action is quadratic in $c$ and $\rho$. It can be decoupled using two Hubbard-Stratonovich transformations, introducing new (dual) variables $f, \phi$. More information on the Hubbard-Stratonovich transformation can be found in B. Technically the Hubbard-Stratonovich transformation requires positive definiteness. Ping Sun and Gabriel Kotliar have shown that this can be achieved by applying shifts which don’t affect any physical observables\cite{20} and Rubtsov, Katsnelson and Lichtenstein have shown that these problems can be avoided when using a complex Hubbard-Stratonovich transformation\cite{17}, so we will not spend much time on this issue here.

The partition function can then be written as an integral over both the old and the newly introduced variables. The impurity part of the action only depends on the original parameters.

$$Z = \int D[c^*, c] e^{-S_{\text{lat}}[c^*, c]}$$

$$= \int D[c^*, c] \left[ \int D[f^*, f; \phi] \sqrt{\det[\alpha_k(\Lambda_{\omega} - V_K)^{-1} \alpha_{\omega}]} \det[\alpha_f^{-1}(\Delta_{\nu} - t_k) \alpha_f^{-1}] \right.$$

$$\left. \times e^{-\sum_i S_{\text{site}}[c^*_i, c_i; f^*, f, \phi] - \sum_{k\nu\sigma} f^*_k \omega n_{\nu\sigma} \epsilon^*_k \nu \sigma (\Delta_{\nu} - t_k) \alpha_f^{-1} f^*_k \nu \sigma - \frac{1}{2} \sum_{\omega} \phi_{\omega} \chi_{\omega}^{-1} \phi_{\omega} - V[f^*, f; \phi]} \right]$$

where

$$e^{-\sum_i S_{\text{site}}[c^*_i, c_i; f^*, f, \phi]} = \prod_i e^{-S_{\text{imp}}[c^*_i, c_i]} e^{\sum_{i\nu\sigma} f^*_i \nu \sigma c_i \nu \sigma + c^*_i \nu \sigma f_i \nu \sigma + \phi_i \omega n_{i\omega}}$$

The dependence on $c^*, c$ is now restricted to $S_{\text{site}}$. The integral over $c^*, c$ can be performed. With a function $V[f^*, f; \phi]$ to be determined, it is possible to write:

$$\frac{1}{Z_{\text{imp}}} \int D[c^*, c] \exp(-S_{\text{site}}[c^*, c; f^*, f, \phi])$$

$$= \exp \left( -\sum_{i\nu\sigma} f^*_i \nu \sigma g_{\nu \sigma} f_{i \nu \sigma} - \frac{1}{2} \sum_{\omega} \phi_{\omega} \chi_{\omega}^{-1} \phi_{\omega} - V[f^*, f; \phi] \right)$$

The second exponential in (2.6) which appears in the first line of (2.7) can be expanded in terms of expectation values of the impurity problem to find the expression for $V$:

$$\langle A \rangle = \frac{1}{Z_{\text{imp}}} \int D[c^*, c] \exp(-S_{\text{imp}}[c^*, c]) A$$

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Choosing $\alpha_f = g^\nu_\nu^{-1}$ and $\alpha_b = \chi^{-1}$ with the $g, \chi$ that appeared in (2.7) given by:

$$g_{\sigma,\nu} = (c_{\sigma,\nu} c^*_{\sigma,\nu})$$  \hspace{1cm} (2.9)

$$\lambda = \rho_{\nu \rho_{\nu}}$$  \hspace{1cm} (2.10)

Collecting all the terms, and remembering that $\langle \rho \rangle = 0$ by definition of $\rho$ and that the average of an odd number of Grassmann variables is zero, one finally gets:

$$V[f^*, f; \phi] = \lambda_{\sigma,\nu,\omega} f^*_{\sigma,\nu,\omega} f_{\sigma,\nu,\omega} - \frac{1}{4} \gamma_{\sigma,\sigma',\nu,\nu'} f^*_{\sigma,\nu} f_{\sigma',\nu'} f_{\sigma',\nu'} f_{\sigma,\nu} + \ldots$$  \hspace{1cm} (2.11)

$$\lambda_{\sigma,\nu,\omega} = -\langle c_{\sigma}(\nu + \omega) c^*_\rho(\nu) n(\omega) \rangle - \beta g_{\nu}(\rho) \delta_{\omega,\nu}$$  \hspace{1cm} (2.12)

$$\gamma_{\sigma,\sigma',\nu,\nu'} = \langle c_{\sigma}(\nu + \omega) c^*_\rho(\nu) c^*_\sigma(\nu') c_{\sigma'}(\nu' + \omega) \rangle - \beta g_{\sigma,\nu} g_{\sigma',\nu'} \delta_{\omega,\nu} + \beta g_{\sigma,\nu} + \omega g_{\sigma,\nu} \delta_{\sigma,\sigma'} \delta_{\nu',\nu}$$  \hspace{1cm} (2.13)

The vertices $\lambda$ and $\gamma$ are amputated connected correlation functions of the impurity. Note that we use the convention $(cc^*cc^*)$ here. Rubtsov et al.\cite{rubtsov} use the convention $(cc^*c^*)$. These quantities can easily be related by commuting the Grassmann numbers and relabeling the associated frequencies. The convention chosen here coincides with the impurity solver that is used.

Inserting (2.7) into (2.5), the original fermions have been integrated out and the result is a partition function purely in terms of the dual fields.

$$Z = \int D[f^*, f; \phi] \sqrt{\det[\chi^{-1}_{\omega}(\Delta_{\nu} - V_{\mathbf{K}})^{-1} \chi^{-1}_{\omega}]} \det[g_{\nu}(\Delta_{\nu} - t_{\mathbf{k}}) g_{\nu}]
\times e^{-\sum_{k_{\nu,\sigma}} f_{k_{\nu,\sigma}} \left[ g_{\nu}^{-1}(\Delta_{\nu} - t_{\mathbf{k}})^{-1} g_{\nu}^{-1} + g_{\nu}^{-1} \right] f_{k_{\nu,\sigma}} - \frac{1}{2} \sum_{k_{\omega}} \phi_{k_{\omega}} \left[ \chi^{-1}_{\omega}(\Lambda_{\omega} - V_{\mathbf{K}})^{-1} \chi^{-1}_{\omega} + \chi^{-1}_{\omega} \right] \phi_{k_{\omega}} - V[f^*, f; \phi]
= \int D[f^*, f; \phi] e^{-S_0[f^*, f; \phi]}$$  \hspace{1cm} (2.14)

$$S_0[f^*, f; \phi] = -\sum_{k_{\nu,\sigma}} f_{k_{\nu,\sigma}} \left( \tilde{G}^{(0)}_{\nu,\mathbf{k}} \right)^{-1} f_{k_{\nu,\sigma}} - \frac{1}{2} \sum_{k_{\omega}} \phi_{k_{\omega}} \left( \tilde{X}^{(0)}_{\omega,\mathbf{K}} \right)^{-1} \phi_{k_{\omega}} + V[f^*, f; \phi]$$  \hspace{1cm} (2.15)

The fermionic and bosonic bare dual Green’s functions have been introduced here, they are given by:

$$\tilde{G}^{(0)}_{\nu,\mathbf{k}} = -\left[ g_{\nu}^{-1}(\Delta_{\nu} - t_{\mathbf{k}})^{-1} g_{\nu}^{-1} + g_{\nu}^{-1} \right]^{-1}$$  \hspace{1cm} (2.16)

$$\tilde{X}^{(0)}_{\omega,\mathbf{K}} = -\left[ \chi^{-1}_{\omega}(\Lambda_{\omega} - V_{\mathbf{K}})^{-1} \chi^{-1}_{\omega} + \chi^{-1}_{\omega} \right]^{-1}$$  \hspace{1cm} (2.17)

$$\tilde{X}^{(0)}_{\omega,\mathbf{K}} = -\left[ \chi^{-1}_{\omega}(\Lambda_{\omega} - V_{\mathbf{K}})^{-1} \chi^{-1}_{\omega} + \chi^{-1}_{\omega} \right]^{-1}$$  \hspace{1cm} (2.18)

$$\tilde{X}^{(0)}_{\omega,\mathbf{K}} = -\left[ \chi^{-1}_{\omega}(\Lambda_{\omega} - V_{\mathbf{K}})^{-1} \chi^{-1}_{\omega} + \chi^{-1}_{\omega} \right]^{-1}$$  \hspace{1cm} (2.19)

There exist exact relations between the lattice and dual Green’s functions. These can be derived by taking the derivative of the partition function with respect to $t_{\mathbf{k}}$ and $V_{\mathbf{K}}$ for fermions and bosons. The derivation for the fermionic Green’s function can be found in appendix A.6 of\cite{rubtsov}, in appendix E a similar derivation for the bosonic Green’s function is presented.

$$G_{\nu,\mathbf{k}} = \left( \left( g_{\nu} + g_{\nu} \tilde{G}_{\nu,\mathbf{k}} g_{\nu} \right)^{-1} + \Delta_{\nu} - t_{\mathbf{k}} \right)^{-1}$$  \hspace{1cm} (2.20)

$$X_{\omega,\mathbf{K}} = \left( \left( \chi_{\omega} + \chi_{\omega} \tilde{X}_{\omega,\mathbf{K}} \chi_{\omega} \right)^{-1} + \Delta_{\omega} - V_{\mathbf{K}} \right)^{-1}$$  \hspace{1cm} (2.21)
It is also possible to represent these relations in terms of the lattice and dual self-energies:

\[
\Sigma_{\nu,k} = \Sigma_{\text{Imp}}(\nu) + \frac{\tilde{\Sigma}_{\nu,k}}{1 + g_{\nu} \Sigma_{\nu,k}} \tag{2.22}
\]

\[
\Pi_{\omega,K} = \Pi_{\text{Imp}}(\omega) + \frac{\tilde{\Pi}_{\omega,K}}{1 + \chi_{\omega} \Pi_{\omega,K}} \tag{2.23}
\]

### 2.2 Impurity problems and solvers

In (2.2) an impurity problem was defined. This is a system with a finite and small number of sites, that should be much simpler to solve than the original lattice problem. For the dual theory, several expectation values of the impurity problem are required: \(g_{\nu}, \chi_{\omega}, \lambda_{\omega}, \gamma_{\nu,\nu}, \omega\). \(\gamma\) depends on 3 frequency labels, so it is the most expensive to store and calculate. Typically, \(\gamma\) is calculated for \(\nu_n = (2n + 1)\pi\beta^{-1}\), \(n = -N_{\nu}, -N_{\nu} + 1, \ldots, N_{\nu} - 1\) and \(\omega_n = 2n\pi\beta^{-1}\), \(n = 0, \ldots, N_{\omega} - 1\).

There exist some symmetry relations for the vertex which can help reduce the computational requirements, these can be found in appendix C.

There are different methods to solve these impurity problems. The solution of the impurity problem is usually the most computationally intensive part of DMFT or dual fermion/boson calculation schemes. Because of this, there has been a lot of work on efficient impurity solvers in recent years. For this thesis, a CT-HYB solver adopted by Hartmut Hafermann and based on the ALPS project\(^{21,22,23}\) was used. A full explanation of efficient impurity solvers goes beyond the scope of this thesis, for this we refer to the references\(^{24,25,26}\).

![Figure 2.1: A graphical illustration of the impurity model.](image)

The impurity problem describes an impurity coupled to a bath via a hybridization \(\Delta_{\nu}\). This is illustrated in figure 2.1. Electrons can come from the bath to the impurity and go back after a certain amount of (imaginary) time. This means that the charge on the impurity is not a conserved quantity. It should be compared to the total charge on a single lattice site, which is also not conserved.
2.3 Dual Perturbation Theory

One of the main results of the dual transformation is the dual action (2.15). This action describes a new, dual system where the parameters in the action depend on the solution of the impurity problem. If one can solve the dual system, (2.20) and (2.21) can be used to find the exact solution of the original lattice problem. Exactly solving the dual action is not possible, but it is expected that an approximate solution to the dual action using perturbation theory will give a good approximation to the lattice problem. There is an advantage of doing perturbation theory in dual quantities over doing perturbation theory in the original quantities. This is that in the dual theory $\Delta_\nu, \Lambda_\omega$ can be chosen in a way that the local correlation effects are taken into account in the impurity problem, which can be solved exactly. This means that the dual perturbation theory only needs to take into account the non-local correlation effects, which are smaller and typically have better convergence properties.

2.3.1 Feynman rules

The dual action is given by (2.15):

$$S_d[f^*, f; \phi] = -\sum_{k\nu\sigma} f_{k\nu\sigma}^* (\hat{\mathcal{G}}_{\nu k}^{(0)})^{-1} f_{k\nu\sigma} - \frac{1}{2} \sum_{K\omega} \phi_{K\omega} (\hat{\mathcal{X}}_{\omega K}^{(0)})^{-1} \phi_{K\omega} + V[f^*, f, \phi] \quad (2.24)$$

This action has a Gaussian part given by the bare propagators $\hat{\mathcal{G}}^{(0)}$ and $\hat{\mathcal{X}}^{(0)}$ and an interaction given by $\lambda$ and $\gamma$.

$$S_{d,0}[f^*, f; \phi] = -\sum_{k\nu\sigma} f_{k\nu\sigma}^* (\hat{\mathcal{G}}_{\nu k}^{(0)})^{-1} f_{k\nu\sigma} - \frac{1}{2} \sum_{K\omega} \phi_{K\omega} (\hat{\mathcal{X}}_{\omega K}^{(0)})^{-1} \phi_{K\omega} \quad (2.25)$$

$$V[f^*, f; \phi] = \lambda_{\sigma,\nu,\omega} f_{\sigma,\nu+\omega}^* f_{\sigma,\nu} \phi_{\omega} - \frac{1}{4} \gamma_{\sigma,\sigma',\nu,\nu',\omega} f_{\sigma,\nu+\omega}^* f_{\sigma,\nu} f_{\sigma',\nu'}^* f_{\sigma',\nu'} f_{\sigma',\nu'+\omega} + \ldots \quad (2.26)$$

The exponent of the dual action can be expanded in terms of the interaction $V$. In this way, the full propagators of the dual action can be found. The different contributions to this expression can be described by Feynman diagrams. In this case, the diagrams are built up from 4 components: a fermion line $\hat{\mathcal{G}}^{(0)}$, a boson line $\hat{\mathcal{X}}^{(0)}$, a vertex $\gamma$ with two incoming and two outgoing fermion lines and a vertex $\lambda$ with one incoming and one outgoing fermion line and one external boson line. These can be seen in figure 2.2. There are also higher order terms in $V$, like a vertex with six fermion lines and a vertex with four fermion lines and one boson line. The corresponding Feynman diagrams are expected to give small contributions, like they do in dual fermion\cite{19}, so these vertices will not be treated here.

Figure 2.2: Diagrammatic building blocks

The goal of the perturbation theory is to calculate the full dual Green’s functions. These are
defined by $\tilde{G}_{12} = -(f_1 f_2^*)_{S_d}$ and $\tilde{X}_{12} = -\langle \phi_1 \phi_2 \rangle_{S_d}$. The expansion of the exponent gives:

$$X_{12} = \int \mathcal{D}[f^*, f, \phi] \exp \left( -S_d[f^*, f; \phi] \right) \phi_1 \phi_2$$

(2.27)

$$= \int \mathcal{D}[f^*, f; \phi] \exp \left( -S_{d,0}[f^*, f; \phi] \right) \exp \left( -V[f^*, f, \phi] \right) \phi_1 \phi_2$$

(2.28)

$$= \langle \exp \left( -V[f^*, f; \phi] \right) \phi_1 \phi_2 \rangle_{S_{d,0}}$$

(2.29)

$$= \langle \phi_1 \phi_2 - V[f^*, f, \phi] \phi_1 \phi_2 + \frac{1}{2} V[f^*, f, \phi] V[f^*, f, \phi] \phi_1 \phi_2 + \ldots \rangle_{S_{d,0}}$$

(2.30)

$$= \langle \phi_1 \phi_2 \rangle_{S_{d,0}} - \langle V[f^*, f, \phi] \phi_1 \phi_2 \rangle_{S_{d,0}} + \langle \frac{1}{2} V[f^*, f, \phi] V[f^*, f, \phi] \phi_1 \phi_2 \rangle_{S_{d,0}} + \ldots$$

(2.31)

Now one fills in the expression for $V$ in terms of $f^*, f, \phi$. One can use Wick’s theorem to contract all the resulting terms, with the contraction of $f_1 f_2$ given by $-\tilde{G}_0^0$ and the contraction of $\phi_1 \phi_2$ given by $-\tilde{X}_0^0$.

The first few diagrams for the full fermionic propagator, in which only fermionic lines and $\gamma$ occur, also appear in dual fermion. These diagrams are worked out nicely, including prefactors in appendix A.4 of [19]. In appendix D of this thesis, the additional diagrams generated by the dual boson theory are treated in a similar way.

### 2.3.2 Limits

Physically there are two interesting limits to consider, very strong and very weak interaction $U$. In the case of small interaction, regular perturbation theory works pretty well. It can be shown [19] that dual fermion corresponds to regular perturbation theory in the limit of small $U$. The dual perturbation theory is well behaved for small $U$, since the vertex $\gamma$ is small in that case. This means that the higher order diagrams give relatively small contributions.

In the opposing limit of large $U$, the system is very localized. This means that the non-local part of the Green’s function is small. The dual Green’s function is equal to the non-local part of the Green’s function according to (2.17). This means that the dual fermionic Green’s function is small, so all higher order diagrams are small.

In the two opposing limits of strong and weak interaction, different elements of the perturbation theory vanish. No formal proof exists that the perturbation theory also converges in between, but at least these limits give some confidence about the perturbation theory.
2.4 Self-consistency

Until now, the hybridization quantities $\Delta_\nu$ and $\Lambda_\omega$ were free parameters. The choice of these parameters is important, since it determines the quantities that enter the dual perturbation theory. If these parameters can be chosen in such a way that the perturbation theory converges better, the final lattice results will also be better. In Dual Fermion this is typically done by demanding

$$\tilde{G}_{\text{loc}} = 0 \quad (2.32)$$

This means that all diagrams with local lines, especially the first-order diagram, yield zero. This condition is called the self-consistency condition, although this name is somewhat confusing. In the dual theory any choice of $\Delta_\nu$ and $\Lambda_\omega$ can in principle be used, however some are preferable since the associated perturbation theory is easier to handle. The choice $\tilde{G}_{\text{loc}} = 0$ means that the first order fermionic self-energy diagram shown in figure 2.3 is zero.

![Figure 2.3: First order diagram that is zero due to the self-consistency condition.](image)

Another self-consistency condition is $G_{\text{loc}} = g$, which says that the impurity describes the local part of the lattice Green’s function. In case $\Sigma = 0$, these conditions are equivalent:

$$\tilde{G}_{\text{loc}} = 0 \quad (2.33)$$

$$\frac{1}{N} \sum_k \left( \frac{1}{g_\nu + \Delta_\nu - t_k} \right)^{-1} - g_\nu = 0 \quad (2.34)$$

$$\frac{1}{N} \sum_k \left( \frac{1}{g_\nu + \Delta_\nu - t_k} \right)^{-1} = g_\nu \quad (2.35)$$

$$G_{\text{loc}} = g \quad (2.36)$$

However, if $\tilde{\Sigma} \neq 0$, the conditions are no longer equivalent.

Since the equations for the bosonic part are similar to the fermionic part, there are also two possible self-consistency conditions here, either $\tilde{X}_{\text{loc}} = 0$ or $X_{\text{loc}} = \chi$. Both conditions are equivalent in case no self-energy diagrams are calculated.

Typically, the scheme starts with some assumption for $\Delta_\nu$ and $\Lambda_\omega$. The impurity problem is solved and a set of self-energy diagrams can be calculated. This gives a $\tilde{G}, \tilde{X}$, which will not satisfy the self-consistency relation yet. Then, one needs to make a guess for a new $\Delta_\nu, \Lambda_\omega$ that will improve the self-consistency. This is called an update formula. These update formulas can be used to generate the two previously mentioned self-consistency conditions:

$$\Lambda_{\text{new}} - \Lambda_{\text{old}} = \xi \chi_\omega^{-1} (X_{\text{local},\omega} - \chi_\omega) X_{\text{local},\omega}^{-1} \quad (2.37)$$

The mixing parameter $\xi$ is introduced here. Every new iteration generates a guess for $\Lambda_\omega$. If $\xi < 1$, the previous guess for $\Lambda$ is still taken partially into account. Taking $\xi < 1$ can prevent some numerical instabilities in regimes where it is difficult to do calculations.
2.5 Dynamical mean field theories

The impurity formalism employed in the derivation of dual boson is reminiscent of Dynamical Mean Field Theory (DMFT). In this approach, a fermionic lattice problem is mapped to a self-consistent impurity problem. This mapping takes into account all local correlations and becomes exact in the limit of infinite dimensions, where non-local correlations vanish. A review of DMFT can be found in [27]. To treat non-local interactions, an extension of DMFT called Extended Dynamical Mean Field Theory (EDMFT) was developed [20]. Here the non-local interactions introduce a frequency dependence for the impurity interaction [28].

In the dual perturbation theory, dual self-energy diagrams are calculated. These diagrams give a correction to the impurity self-energy. The zeroth order in this perturbation theory, with no diagrams and \( \tilde{\Sigma} = 0 \), together with the usual self-consistency relation is exactly the same as Dynamical Mean Field Theory [29]. In the same way, the zeroth order in dual boson perturbation theory results in EDMFT.

In (E)DMFT it is assumed that non-local effects are small. This approximation works well in many cases. However, when considering dynamical susceptibility, non-local effects are very important. The impurity problem that forms the basis of (E)DMFT does not conserve charge, since it represents a single site. Charge conservation manifests itself as a K-dependence of the correlation function \( X_{\omega, K} \), since it requires this function to be zero for \( K = 0, \omega \neq 0 \), while it is non-zero for other K. K-dependence means non-locality, so the conservation of the total charge can only be achieved by taking into account non-local effects. This means that the results from (E)DMFT for \( X_{\omega, K} \) will not conserve charge. It is needed to go beyond dynamical mean field theories, for example using dual boson. In the next section this statement will be further explained within the dual boson formalism.

2.6 Charge conservation

In 1.1.4 it was shown that charge conservation requires:

\[
X_{\omega, K=0} = \langle pp \rangle_{\omega, K=0} = 0 \text{ for } \omega \neq 0
\]  

(2.38)

In dual theory, this quantity is calculated using (2.21):

\[
X_{\omega, K} = \left( \chi_{\omega} + \chi_{\omega} \tilde{\Pi}_{\omega, K} \chi_{\omega} \right)^{-1} + \Lambda_{\omega} - V_K
\]

(2.39)

This can only be 0 for all \( \omega \) if \( \chi_{\omega} + \chi_{\omega} \tilde{\Pi}_{\omega, K=0} \chi_{\omega} = 0 \), so if \( \tilde{\Pi}_{\omega, K=0} \chi_{\omega} = -1 \).

This means that the no-diagrams approximation (EDMFT) can never satisfy charge conservation, since it has \( \tilde{\Pi} = 0 \). At least some bosonic self-energy diagrams are needed to calculate the lattice susceptibility accurately. This shines some light on the relation between Dual Boson and EDMFT versus Dual Fermion and DMFT. DMFT is the lowest order approximation to Dual Fermion and in some parts of parameter space, where \( \gamma \) is small, it is effectively the same as Dual Fermion since the dual self-energy diagrams give just a small contribution. EDMFT is also the lowest order approximation to Dual Boson, but here, the diagrams always give a correction of order 1 to the bosonic Green’s function. This means that the EDMFT approximation is never justified for calculating a K-dependent susceptibility.
Note that the requirement $\Pi_{\omega,K=0}\chi_\omega = -1$ means that the bosonic lattice self-energy diverges according to (2.23)

$$\Pi_{\omega,K} = \Pi_{\text{Imp}}(\omega) + \frac{\Pi_{\omega,K}}{1 + \chi_\omega \Pi_{\omega,K}}$$  \hspace{1cm} (2.40)

This means that (2.21) is computationally more stable than (2.23)

2.6.1 Asymptotics

The fermionic impurity and lattice Green’s function scale as $g_\nu \propto \frac{1}{\nu}$ for large frequencies. The dual fermionic Green’s function is a correction to the lattice Green’s function and scales as $\tilde{G} \propto \frac{1}{\nu^2}$. The impurity bosonic Green’s function scales as $\chi_\omega \propto \frac{1}{\omega^2}$. According to $\Pi_{\omega,K=0}\chi_\omega = -1$, this means that $\Pi_{\omega,K=0} \propto \omega^2$. This is another indication of the difference between dual fermion and dual boson. The dual fermion correction to the impurity self-energy decays as $\frac{1}{\nu^2}$, which is faster than the decay of the impurity self-energy. The dual boson self-energy correction on the other hand increases in magnitude as a function of $\omega$.

2.7 GW-like approximation

In the previous sections it was shown that EDMFT is not a good scheme to calculate $X_{\omega,K}$, since it can not generate the right results at $K = 0$. It is necessary to calculate the polarization using a perturbation theory in $\gamma$ and $\lambda$. However these impurity quantities are expensive to calculate and store. It would be good to have an approximate scheme that does not require $\gamma$ and $\lambda$ and can still give reasonable results, at least in parts of the parameter space. Just like DMFT is a lot quicker and computationally cheaper than dual fermion and works well when $\gamma \approx 0$. The $\gamma \approx 0$ can also be used in dual boson. Given the relation between $\gamma$ and $\lambda$ (C.16) this results in $\lambda_{\nu,\omega} = \frac{-1}{\chi_\omega}$. Using this approximation for $\lambda$, the diagram in figure 2.4 can be calculated:

$$\Pi_{\omega,K} = \lambda_\omega (\tilde{G}\tilde{G})_{\omega,K}\lambda_\omega$$ \hspace{1cm} (2.41)

Then use Dynson’s equation for the dual propagator:

$$\tilde{X}_{\omega,K} = \frac{\tilde{X}_0^{\omega,K}}{1 - \tilde{X}_0^{\omega,K}\Pi_{\omega,K}}$$ \hspace{1cm} (2.42)

The fermionic self-energy can be calculated in real space using the diagram in figure 2.5:

$$\tilde{\Sigma}_{\nu,x} = \sum_\omega \lambda_\omega \tilde{G}_{\nu-\omega,x} \tilde{X}_{\omega,x}\lambda_\omega$$ \hspace{1cm} (2.43)
This is rather like the expression for the fermionic self-energy in a GW+EDMFT-scheme\textsuperscript{[28,13,20]}. There, the non-local part of $\Sigma = GW$ is used. In (2.43), the non-local part is selected by $\tilde{G}$, since starting from EDMFT gives $\tilde{G} = G_{\text{non-local}}$. So the approximation used here gives

$$W_{\omega, \mathbf{K}} = \frac{1}{\lambda_{\omega}} \tilde{X}_{\omega, \mathbf{K}} \lambda_{\omega}$$  \hspace{1cm} (2.44)

$$= \frac{1}{\lambda_{\omega}^2} \frac{X_{\omega, \mathbf{K}}^0}{1 - X_{\omega, \mathbf{K}}^0 \Pi_{\omega, \mathbf{K}}}$$  \hspace{1cm} (2.45)

$$= \frac{X_{\omega, \mathbf{K}}^0}{\lambda_{\omega}^2} \frac{1}{1 - \frac{X_{\omega, \mathbf{K}}^0}{\lambda_{\omega}^2} (\tilde{G} \tilde{G})_{\omega, \mathbf{K}}}$$  \hspace{1cm} (2.46)

This can be simplified using:

$$\frac{X_{\omega, \mathbf{K}}^0}{\chi_{\omega} \chi_{\omega}} = \frac{1}{\chi_{\omega}} \left( \frac{1}{\chi_{\omega}^2 + \Lambda_{\omega} - V_\mathbf{K}} - \chi_{\omega} \right) \frac{1}{\chi_{\omega}}$$  \hspace{1cm} (2.47)

$$= \frac{1}{\chi_{\omega}} \left( \frac{1}{1 - \chi_{\omega} (V_\mathbf{K} - \Lambda_{\omega})} - 1 \right)$$  \hspace{1cm} (2.48)

$$= \frac{V_\mathbf{K} - \Lambda_{\omega}}{1 - (V_\mathbf{K} - \Lambda_{\omega}) \chi_{\omega}}$$  \hspace{1cm} (2.49)

Resulting in:

$$W_{\omega, \mathbf{K}} = \frac{V_\mathbf{K} - \Lambda_{\omega}}{1 - (V_\mathbf{K} - \Lambda_{\omega}) (\chi_{\omega} + (\tilde{G} \tilde{G})_{\omega, \mathbf{K}})}$$  \hspace{1cm} (2.50)

Typically, GW uses $W = \frac{V}{1 - \frac{U - \Lambda}{\chi}}$. The approximation presented here differs from that scheme by the replacement $V \to V - \Lambda$ and by using $\chi_{\omega} + (\tilde{G} \tilde{G})_{\omega, \mathbf{K}}$ as the bare bosonic lattice Green’s function. The latter seems legitimate, since $\chi$ represents the impurity part of the susceptibility, while $\tilde{G} \tilde{G}$ is the non-local part of the fermion bubble, which generates a non-local susceptibility.

The former property solves one of the problems that is noted in\textsuperscript{[28]}. There is some ambiguity in the way $U$ is treated in the Hubbard-Stratonovich decoupling. It can be treated as part of the impurity action, but it can also be considered as the local part of $V_\mathbf{K}$\textsuperscript{1}. This is just a matter of choice and should not have any influence on the predictions of physical quantities. However, in EDMFT+GW it does. This is because the regular GW scheme uses $V_\mathbf{K}$ in the definition of $W$. The approximation derived from dual boson, and in fact anything calculated within dual boson, depends on $V_\mathbf{K} - \Lambda_{\omega}$ only. If $U$ is included in $V_\mathbf{K}$, this results in a shift of $\Lambda_{\omega}$ by $U$, and $V_\mathbf{K} - \Lambda_{\omega}$ stays the same.

\textsuperscript{1}e.g. $V_\mathbf{K} = U + v_1 (\cos(kx) + \cos(ky))$
2.7.1 Asymptotics of the polarization diagram

It is instructive to study the asymptotic behaviour of (2.41). The diagram should have a $\omega^2$ scaling behaviour to get charge conservation. The two triangle vertices contribute:

$$\lambda_\omega = \frac{1}{\lambda_\omega} \propto \omega^2$$  \hspace{1cm} (2.51)

The dual bubble has $\tilde{G}_\nu \tilde{G}_{\nu+\omega}$, which is peaked around $\nu \approx 0$ and $\nu \approx -\omega$. In that case, one Green’s function has a frequency close to zero, the other has a frequency close to $\pm \omega$. Since $\tilde{G}_\nu \propto \frac{1}{i\nu}$, this means that the bubble has two leading contributions that vanish as $\frac{1}{\omega^2}$, so after summing over the internal frequency $\nu$, it is expected that $(\tilde{G}\tilde{G})_\omega$ decays as $\frac{1}{\omega^2}$ as well.\(^2\)

Multiplying the three parts of the diagram results in $\Pi_\omega \propto \omega^2$, as expected.

---

\(^2\)This assumes the contributions at different $\nu$ do not cancel. Numerically, the $\frac{1}{\omega^2}$ behaviour can be verified.
2.8 Ladder approximation and the Bethe-Salpeter equation

In the previous section, an approximation to the perturbation theory with $\gamma = 0$ was considered. In general this will not be sufficient to accurately describe the dual perturbation theory. Diagrams that include the impurity vertices $\gamma$ and $\lambda$ are needed. It is possible to take into account a finite number of these diagrams and calculate them explicitly. Better results can be obtained by summing an infinite series of diagrams via the ladder equation. This approach has previously been used in dual fermion$^{[30]}$ and can be generalized to dual boson with little extra computational cost. A renormalized vertex $\Gamma$ is calculated, that contains vertices chained together by Green’s function bubbles.

The motivation for the ladder approach lies in the work of Baym and Kadanoff on conserving approximations$^{[31]}$. The ladder dual fermion approach is conserving in this sense since it is derivable from a Luttinger-Ward functional. More information on the ladder approximation in dual fermion can be found in chapter 11 of Hafermann$^{[19]}$, more information on the ladder approximation in general in Toschi, Katanin and Held$^{[32]}$.

Pictorially, the ladder approximation can be described by the Bethe-Salpeter equation:

$$\Gamma = \gamma + \gamma \Gamma$$

This equation can be used to generate $\Gamma$ iteratively, or it can be inverted to solve for $\Gamma$. This corresponds to solving a geometric sum, which in this case requires the eigenvalue of $[\gamma]$ to be smaller than 1. A more elaborate explanation of the Bethe-Salpeter can be found in chapter 5 of Altland and Simons$^{[8]}$.

2.8.1 Computational details

In the ladder approximation, the renormalized vertex $\Gamma$ is calculated. This $\Gamma$ replaces the impurity quantity $\gamma$ in the self-energy diagrams. The impurity $\gamma$ is local, since it is an impurity quantity, but the renormalization makes it non-local (or $\mathbf{K}$-dependent). So $\Gamma$ depends on 3 frequencies and 1 momentum, which would make it too large to store in memory. The parts of $\Gamma$ with different bosonic frequencies $\omega$ do not influence each other, which makes it possible to calculate the different $\omega$ one by one and even in parallel on different computational cores. At any moment, $\Gamma$ only has to be stored for the two fermionic frequencies and for one momentum, which greatly reduces the memory requirements.

2.8.2 Diagrams in the ladder approximation

The diagrams for the ladder approach can be obtained from the normal diagrams in appendix D by replacing the vertex $\gamma$ by the renormalized vertex $\Gamma$. The signs and numerical factors are identical.

The diagrams for the bosonic dual self-energy are:

---

$^{[3]}$The sign of the second diagram has to be determined based on the way the vertices are labeled, see$^{[19]}$
The fermionic dual self-energy has these mixed diagrams:

The purely fermionic ladder diagram also appears, in the same way as in dual fermion\textsuperscript{30}.

2.9 Spin interactions

The formalism introduced in this chapter can also be applied to spin susceptibilities and non-local spin-spin interactions. In the derivation of dual boson, one just needs to replace $\rho = n - \langle n \rangle$ by $\rho = S_z - \langle S_z \rangle$, or a similar expression for $S$ instead of $S_z$. A boson branch label $j$ can be introduced to treat these all at the same time. The most important feature of the charge susceptibility was that $\rho$ commutes with $H$, so $\rho$ is a conserved quantity which physically implies charge conservation. The commutator between the spin operator and the Hamiltonian is also zero, which means that the spin susceptibility has very similar conservation laws as the charge susceptibility. So it is possible to generate the entire formalism in a similar way as presented here for spin.

The extra label to describe the boson branch also occurs in the bosonic hybridization $\Lambda$, the bosonic impurity Green’s function $\chi$ and the vertex $\lambda$. To use the formalism with spin, it is necessary to have an impurity solver which can calculate these $\chi$ and $\lambda$ and take a spin hybridization as input. At the moment, this is in principle possible for $S_z$ interactions, but these will not be treated in this thesis. Recently there has been work on having the full $S$\textsuperscript{33} in the impurity problem.

One of the current problems in the dual fermion approach is that the eigenvalue of the ladder equation in the spin channel becomes larger than one at low temperatures. This means that the Bethe-Salpeter equation can not be inverted anymore. This is problematic, since it signals a divergence in the dual perturbation theory. This divergence corresponds to ferromagnetic checkerboard ordering. This is problematic since the starting point of the perturbation theory is a lattice of identical impurities. In an ordered state, the impurities are not identical. It is believed that when non-local (screening) effects are taken into account in dual boson, this ferromagnetic ordering will be suppressed. This means that dual boson theory should be able to handle lower temperatures than dual fermion.
2.10 Summary of the computation scheme

Various computational schemes have been introduced in this chapter. Here a short pictorial summary of these schemes will be given. First, the so-called outer loop will be described. Then, some of the sets of diagrams that can be calculated are given.

The outer loop or outer self-consistency describes the self-consistent determination of the hybridization. In EDMFT, this is the only self-consistency that happens. One starts with a certain initial guess for the hybridization, this is put into the impurity solver. The impurity solver calculates $g, \chi$ and uses these to calculate $\tilde{G}^0, \tilde{X}^0$ via equations 2.17 and 2.19. Then the self-consistency condition 2.37 (and similar for fermions) is used to determine the new guess for the hybridization functions. This process is repeated until convergence is reached. The entire scheme can be summarized as:

\[
\begin{array}{c}
\text{Impurity solver} \\
\Delta, \Lambda \\
\tilde{G}^0, \tilde{X}^0 \\
\text{Self-consistency}
\end{array}
\]

The simplest dual boson scheme has only a single shot of dual boson. It only uses the EDMFT hybridizations and does not use an update formula. Contrary to EDMFT, the impurity now also calculates the vertices $\gamma$ and $\lambda$ and uses these to calculate some dual self-energy diagrams. The diagrammatic corrections are then applied to the lattice Green’s functions.

\[
\begin{array}{c}
\Delta_{\text{EDMFT}}, \Lambda_{\text{EDMFT}} \\
\text{Impurity solver} \\
\tilde{G}^0, \tilde{X}^0, \gamma, \lambda \\
\text{Diagrams} \\
\tilde{\Sigma}, \tilde{\Pi} \\
\text{Exact transformation} \\
G, X
\end{array}
\]

An outer self-consistent dual boson scheme will renormalize the hybridization functions using one of the update formulas 2.37.
In the diagrams part of the dual boson, there is a choice of diagrams. It is possible to calculate only diagrams without the vertex \( \gamma \), this corresponds to GW+EDMFT. If the vertex is known, the simplest possibility is calculating the diagrams in D. The next possibility is using the Bethe-Salpeter equation to calculate the renormalized vertex \( \Gamma \) in the ladder approximation. This \( \Gamma \) can be used to calculate diagrams as explained in 2.8.

The calculation of the diagrams can be done self-consistently using skeleton diagrams, as explained in 1.2.10. This will be denoted as inner self-consistency in this thesis, to distinguish it from outer self-consistency.

### 2.11 Conclusion

The dual boson formalism uses exact Hubbard-Stratonovich transformations to map the strongly interacting lattice system to a lattice of weakly interacting impurities. The impurities can be solved using numerically exact QMC impurity solvers. The lattice of weakly interacting impurities is treated perturbatively. It leads to a field theory with bosonic and fermionic fields. Self-energies for both fields can be calculated using Feynman diagrams. The zero diagrams approximation corresponds to (E)DMFT. It was shown that this approximation violates charge conservation. It is possible to recover a GW-like approximation by ignoring all vertex corrections. In general, it is necessary to include the vertex corrections to achieve charge conservation, this can be done using the ladder approximation.
Chapter 3

Implementation details

A large part of the work done for this thesis involved the implementation of the dual boson theory into a computer program that allows for computations. In this chapter, some of the challenges encountered and techniques used will be explained. This chapter is partially meant as an introduction for future users of the code developed in this thesis. The casual reader may skip this chapter and proceed straight to the results in chapter 4.

3.1 Numerical and physical details

3.1.1 Fourier transforms and diagrams

The computational effort of the scheme can be significantly reduced by a clever use of Fourier theory. When calculating Feynman diagrams, it is often necessary to sum over one of the internal degrees of freedom, such as the momentum on one of the lines in a bubble. This has the mathematical structure of a convolution. Under a Fourier transform, convolutions and products are interchanged. Products are less computationally expensive, so it can be advantageous to first do a Fourier transform, then do the product and then do a Fourier transform back.

To give a simple example of this, imagine there is a bubble-like quantity $h$ which is obtained as a convolution in momentum space:

$$h(k) = \sum_{k'} g(k)g(k + k') \quad (3.1)$$

When $g$ is known, determining $h$ for a single $k$ requires a sum over $N_k$ values of $k'$. In position space, this equation takes on the simpler form:

$$h(x) = g(x)g(x) \quad (3.2)$$

Typically, bubbles of Green’s function can be calculated most easily in position space, while the Dyson equation should be calculated in momentum space. This means that several Fourier transforms take place in the program.
3.1.2 Finite number of frequencies

The impurity problem is solved numerically. It does not give analytical results for the expectation values like \( \chi_\omega \) and \( \lambda_{\nu'\omega'} \), but only gives values for a finite number of frequencies \( N_\nu, N_\omega \). Formally, it is necessary to sum over all Matsubara frequencies in the calculation of Feynman diagrams. So the numerical implementation misses the part of the self-energy contributions with internal frequencies that are too high. For the calculation of the Fermionic self-energy diagrams that occur within dual fermion, this is a problem that can easily be minimized by including a sufficiently large number of frequencies. The decay of the fermionic self-energy diagram is very quick \( \frac{1}{(i\nu)^2} \), so introducing a cut-off \( N_\nu \) here typically has a small impact. For the dual bosons, the case is a bit different. Even the high \( \omega \) diagrams are important for charge conservation. The associated bubble of dual Green’s function is a convolution of the Green’s function:

\[
\tilde{B}(\omega) = \sum_\nu \tilde{G}(\nu)\tilde{G}(\nu + \omega)
\]

(3.3)

This has large contributions at \( \nu \approx 0 \) and \( \nu + \omega \approx 0 \). This means that it is necessary to know \( \tilde{G} \) for large fermionic frequencies of the order of \( N_\omega \). As \( \omega \) increases, \( \tilde{G}(\nu)\tilde{G}(\nu + \omega) \) becomes less sharply peaked around specific fermionic frequencies \( \nu \), so even more frequencies should be necessary. To alleviate these problems, it is possible to use some symmetry relations that are proven in chapter C. These give equalities like \( \gamma_{\nu,\nu',\omega} = \gamma_{\nu',\nu,\omega} \) that reduce the number of frequencies the impurity problem has to calculate. Still, the cut-off problems are visible at large bosonic frequencies, for example in figure 4.6.

3.1.3 Implementing equations

In the Hubbard model with \( V = 0 \), some quantities like \( \tilde{X} \) are zero. To make sure that the program is able to do calculations in this (important) case, it is necessary to write all of the formulas in a way that avoids zero division problems. An example of this is the bosonic Dyson equation. This can be written as:

\[
\tilde{X} = \frac{1}{\tilde{X}_0^{-1} - \Pi}
\]

(3.4)

But this will lead to a division by zero. Multiplying the numerator and denominator by \( \tilde{X}_0 \) solves this problem:

\[
\tilde{X} = \frac{\tilde{X}_0}{1 - \Pi \tilde{X}_0}
\]

(3.5)

Similar care must be taken in other equations that involve \( \tilde{X} \).

3.2 Technical details

3.2.1 C++ and Python

The heavy work of the dual boson calculation is done using C++. The object-oriented features of C++ allow a separation between the physical equations and the implementation details like
storage and access. It also allows a similar treatment of data containers and functions. For example, it is possible to define a class \texttt{GREENFUNCTION} that can have both exact formulas, like the non-interacting Green’s function, and data containers, like the impurity Green’s function. These different Green’s functions can be accessed in a uniform way. At the same time, C++ is sufficiently fast to do the heavy calculations that are sometimes necessary.

The impurity problem is solved in a separate program. It can sometimes be useful to use a different impurity solver in specific situations. Some solvers work better at large, small or intermediate $U$. This makes it useful to be able to easily change the solver that is used. The solver and the necessary solver parameters can be controlled from the outer part of the program.

This outer part is written in Python. This part of the program makes sure that all of the data is stored and backed up in a nice directory structure, that the input and output of the solver is formatted in the proper way and that the correct parameters are sent to the different parts of the program. For these simple tasks, it is easier to use Python than C++ and Python also allows easier customization for specific cases.

All of the data analysis is also done in Python. Since Python does not have to be compiled, it can easily be modified to generate exactly the data that is required. Specific Python classes have been written that give similar functionality to what is available within the C++ code.

### 3.2.2 Code management

The dual boson project involves many similar versions of code that are developed in parallel. At the beginning of the dual boson project, there was already a working version of the dual fermion code. It is important to keep this working and even to allow bugs in this code to be fixed, while at the same time having another version of the code where the dual boson equations can be implemented. Later on, the dual boson code was in a testing phase and the first results were produced with the code, and at the same time the first work on implementing $S_z S_z$ interactions was starting. Again it was necessary to have different versions of the code, to be able to use and work on both at the same time and to easily copy improvements made in one version to the other versions. All of this had to happen in a collaborative environment, where different people were working on and with different versions and different parts of the code from different locations. To allow all of this to happen smoothly, the version control software Git is used.

### 3.2.3 Data storage

The data produced in the dual boson program often consists of large structured objects. As an example, one of the main quantities of interest $X_{K,\omega}$ holds data that depends on a momentum $K$, and a frequency $\omega$. This is a pretty large array. To do further calculations with the object, it is also necessary to know the lattice it is based on, the $\beta$ used in the calculation and similar data. This could all be stored in a simple text file, but there are several disadvantages with this. When reading and writing binary data to text-files some rounding is often unavoidable. This can be problematic when doing sensitive calculations like analytical continuation. It is also a lot of work to reliably read the data from a text file back into a program. For this project, binary storage using HDF5 is used. This allows streamlined access and modification of all the data.
Chapter 4

Results

In this chapter some results obtained with the dual boson method are given. To illustrate the possibilities of the method, several different systems are studied: In two and three dimensions, half-filled and away from half-filling. Highly accurate dual boson calculations are rather expensive. A proper publication-level analysis, especially the analytical continuation, requires more statistics than the results in this chapter have. This would require more sweeps in the Quantum Monte Carlo solution of the impurity problem. Higher quality data, especially on the Mott transition, is currently being produced in collaboration with Hartmut Hafermann (Institut de Physique Théorique, CEA, CNRS, France).

4.1 Mott Transition

The Mott transition was described in 1.1.7. It occurs in the half-filled Hubbard model as $U$ increases. Here the transition is studied in a 2 dimensional square lattice using a hopping parameter $t = 0.25$, at inverse temperature $\beta = 50$. Only an on-site interaction $U$ is used, so there is no need to use the EDMFT formalism and the retarded interaction $\Lambda_\omega$ is zero. The simulations are done in DMFT until convergence is reached. Then $\gamma$ is calculated, the Bethe-Salpeter equation is used to determine $\Gamma$ and the dual bosonic self-energy $\tilde{\Pi}$ is calculated. This is used to determine the lattice susceptibility $X$. A lattice of 64 by 64 sites is used.

DMFT describes the physics of the Mott transition. However it does not include non-local correlations. When these correlations are included, for example using Dual Fermion, the critical values of the parameters (in this case $U$) change, but the physics stays mostly the same. In the simulations presented here, no renormalization of the dual fermion lines was done, so the phase transition still occurs at the DMFT value. This means no inner self-consistency is done.

4.1.1 Density of states

The evolution of the local density of states can already be calculated within DMFT. This quantity is usually used as an indicator of the Mott transition. As $U$ increases, the spectral weight at the Fermi level ($E = 0$) vanishes. This can be shown by looking at $\frac{1}{2}G(\tau = \frac{\beta}{2})$ according to (1.91). $G(\tau)$ is plotted in figure 4.1 for various values of $U$. For higher $U$, the system becomes more
Figure 4.1: The imaginary time Green’s function in DMFT in a 2D Hubbard model for different values of $U$, with $t = 0.25$, $\beta = 50$. As $U$ increases, the system becomes more insulating and the Green’s function has a smaller absolute value. The value $\frac{\beta}{\pi} G(\tau = \frac{\beta}{2}) \approx A(0)$ is plotted in figure 4.2.

Figure 4.2: $\frac{\beta}{\pi} G(\tau = \frac{\beta}{2}) \approx A(0)$ as a function of $U$, calculated in DMFT in a 2D Hubbard model with $t = 0.25$, $\beta = 50$. This quantity drops to zero as the system goes across the Mott transition.

The density of states can be determined for different $U$ (figure 4.3). The different non-interacting density of states compared to the infinite dimensional result in figure 1.2 is apparent. Just like in figure 1.2, the Mott transition occurs as $U$ increases. Spectral weight shifts from the quasiparticle peak at $E = 0$ to the Hubbard bands at $E = \pm \frac{U}{2}$.
4.1.2 Susceptibility at $K = 0$

According to charge conservation, the susceptibility $X$ at $K = 0$ should be 0 for all $\omega \neq 0$. For $\omega = 0$, it is related to the variation of the total charge within the grand-canonical ensemble. If the density of states has a gap at the Fermi level, it is expensive to add extra particles. On the other hand, if there is spectral weight at the Fermi level then it is relatively easy to add another particle. So $X_{K=0,\omega=0}$ can be used as an indicator of a metallic or insulating state. It can be related to $\frac{\partial \langle n \rangle}{\partial \mu}$ as:

$$\frac{1}{2} X_{K=0,\omega=0} = \frac{\partial \ln Z}{\partial V_{K,\omega}}$$  \hspace{1cm} (4.1)

$$= \frac{1}{2} < \rho \rho >_{K=0,\omega=0}$$ \hspace{1cm} (4.2)

$$= \frac{1}{2} \text{Var}(n)$$ \hspace{1cm} (4.3)

$$\text{Var}(n) = \frac{1}{\beta^2} \frac{\partial^2 \ln Z}{\partial \mu^2}$$ \hspace{1cm} (4.4)

$$= \frac{1}{\beta} \frac{\partial \langle n \rangle}{\partial \mu}$$ \hspace{1cm} (4.5)

This quantity $X_{K=0,\omega=0}$ is shown as a function of $U$ in figure 4.4.
Figure 4.4: $-X(K=0,\omega=0)$ as a function of $U$, calculated in dual boson in a 2D Hubbard model with $t = 0.25$, $\beta = 50$. Values smaller than zero were set to zero. As the insulating phase is approached, $\text{Var}(n)$ vanishes.

In figure 4.5, the impurity susceptibility and the susceptibility at $K = 0$ are plotted as a function of Matsubara frequency.\textsuperscript{1} In the EDMFT approximation to dual boson these quantities are the same, but here it is possible to see the huge impact of the polarization diagrams.

The condition for charge conservation is $\chi_\omega \Pi_{K=0,\omega} = -1$ for $\omega \neq 0$. This condition is shown to hold in 4.6 and can be seen to be approximately true. This condition leads to $X_{K=0,\omega} = 0$ for $\omega \neq 0$. This is shown in 4.7 and 4.8. The fluctuations around zero have order of magnitude $10^{-4}$, while the non-zero parts of $X$ typically have an order of magnitude of $10^{-1}$, so the charge conservation is numerically very well fulfilled.

\textsuperscript{1}The lines in the figure, and in all other plots on Matsubara frequencies, are just guides to the eye. The function is only defined on the Matsubara frequencies. The susceptibility in dual boson is defined with a minus sign, here $-X$ is plotted which is positive.
Figure 4.5: $X_{\mathbf{K}=0,\omega}$ and $\chi_{\text{imp}}(\omega)$, calculated in dual boson in a 2D Hubbard model with $t = 0.25$, $\beta = 50$, $U = 1.51$. The polarization at $\mathbf{K} = 0$ ensures the charge conservation, bringing $X_{\mathbf{K}=0,\omega}$ down all the way to zero for all $\omega \neq 0$.

Figure 4.6: $\chi_{\omega,\Pi_{\mathbf{K}=0}}$ for different $U$, calculated in dual boson in a 2D Hubbard model with $t = 0.25$, $\beta = 50$. This quantity should be equal to $-1$ for charge conservation.
Figure 4.7: $X_{K=0,\omega}$ for different $U$. Zoomed in around $\omega \approx 0$, for the higher frequencies the line remains essentially flat. The higher frequencies are shown in figure 4.8.

Figure 4.8: $X_{K=0,\omega}$ for different $U$. Zoomed in around $X \approx 0$ to see the order of magnitude of fluctuations.
4.1.3 Local susceptibility

The local susceptibility $X_{\text{local}}$ can be obtained by a $K$-average over $X_{K,\omega}$. In (E)DMFT this quantity corresponds to the impurity susceptibility $\chi_\omega$, but in dual boson there is a correction due to diagrams. This quantity can be analytically continued to get $X_{\text{local}}(E)$. This quantity is shown for various $U$ in figure 4.9. The same color scheme as in figure 4.3 is used. The low energy behaviour was very stable under analytical continuation, but the exact height and location of the maximum depended more strongly on the number of frequencies used for analytical continuation.

The small $E$ behaviour of $X_{\text{local}}(E)$ is linear in $E$ for all $U$, but the coefficient depends on $U$. As $U$ increases, low energy excitations become more difficult. In figure 4.10 this coefficient is shown as a function of $U$. Near the Mott transition, the quantity vanishes.

It is also possible to look at $\langle 1 \rangle_X = \int_0^\infty dEX_{\text{local}}(E)$. This is called the zeroth moment of $X_{\text{local}}$. For fermions, this quantity has a fixed volume (see 1.2.7), but for bosons this is not the case. As can already be seen in figure 4.9, the surface under the graph decreases for increasing $U$.

Another quantity of interest is the first moment $\langle E \rangle_X = \int_0^\infty dEX_{\text{local}}(E)$. This gives an indication of the typical energy scale of $X$. In RPA, there were excitations with energies between 0 and 2, so $\langle E \rangle$ is expected to be around 1. These two quantities are shown in figures 4.11 and 4.12 as a function of $U$. The quantities had some variation with respect to the Padé parameters, but the general trends were stable.

In [28], the first moment of the impurity $\chi$ is shown as a function of $U$ in figure 16. This graph shows a jump around the Mott transition. A similar feature is visible in figure 4.12, the first moment increases almost linearly until the transition is approached. There it increases discontinuously. Above the transition, the first moment is approximately equal to $U$, which signals excitations from the lower to the upper Hubbard band.
Figure 4.10: For small $E$, $X_{\text{local}}(E)$ behaves as $X(E) \approx aE$. This coefficient $a$ is plotted as a function of $U$, calculated in dual boson in a 2D Hubbard model with $t = 0.25$, $\beta = 50$. Analytical continuation using a Padé scheme with $\delta = 0.1$, $N_\omega = 60$. As $U$ increases, the coefficient vanishes.

Figure 4.11: Zeroth moment $\int dE X_{\text{local}}(E)$ as a function of $U$, calculated in dual boson in a 2D Hubbard model with $t = 0.25$, $\beta = 50$. Analytical continuation using a Padé scheme with $\delta = 0.1$, $N_\omega = 60$. In the metallic phase, the zeroth moment decreases gradually as $U$ increases. It then becomes a constant in the insulating phase.
4.1.4 Static susceptibilities

Static susceptibilities are especially interesting since they can be measured in cold atom experiments. The evolution of the static susceptibility for various $U$ is shown in figure 4.13. Something interesting seems to happen at the $\Gamma = (0, 0)$ point, at high $U$ there is a maximum in $X$ at $\Gamma$, but at lower $U$ the situation is more complicated. In the direction of $X = (\pi, 0)$ the value of $X$ goes up, while in the direction of $M = (\pi, \pi)$ it goes down. These directions are not orthogonal, so $\Gamma$ is not a simple saddle point, but a more complicated point. Such a shape can be described by $f(x, y) = (x^2 - y^2)^2 - x^2 y^2$.

4.1.5 Lattice susceptibility along high symmetry path

Dual boson allows a look not only at local quantities, but also at $\mathbf{K}$-dependent ones. In figure 4.14 the lattice susceptibility $X(\mathbf{K}, E)$ is plotted along the high symmetry path $\Gamma = (0, 0) \rightarrow M = (\pi, 0) \rightarrow X = (\pi, \pi) \rightarrow \Gamma = (0, 0)$. Some artifacts of the analytical continuation are still visible, the analytical continuation of $\mathbf{K}$-dependent data is more difficult than the continuation of $\mathbf{K}$-averaged data. The analytical continuation was done using a Padé scheme with $\delta = 0.1$, $N_\omega = 15$. The non-interacting result is done using RPA (see 1.3), which is exact at $U = 0$.

In the non-interacting result, there is a large particle-hole continuum visible around $X = (\pi, \pi)$. For $U = 0.51$, this continuum is still visible, but for increasing $U$ it disappears. As $U$ increases, the overall amplitudes decrease, which was already visible in the $\mathbf{K}$-averaged result in figure 4.9. A careful analysis of the data also shows that the entire branch is moving slightly upward to higher $E$. Initially, the spectral weight is disappearing for all $\mathbf{K}$, but as the transition is approached the
Figure 4.13: $-X_{K,E=0}$ for various $U$. Note the different color scales in the various plots. For high $U$ the susceptibility at $K = 0$ vanishes, while it is non-zero for all $K$ below the Mott transition. Remarkably, the shape of the static susceptibility changes earlier, between $U = 1.51$ and $U = 2.21$. 

(a) $U = 0.51$

(b) $U = 1.01$

(c) $U = 1.51$

(d) $U = 2.21$

(e) $U = 2.251$

(f) $U = 2.51$

(g) $U = 2.61$
Figure 4.14: Spectral functions $X_{K,E}$ along high symmetry path for various $U$. Analytical continuation using a Padé scheme with $\delta = 0.1$, $N_\omega = 60$. The overall intensity decreases and in the insulating phase the spectral weight at small $K$ vanishes. The RPA result is from 1.3. Note the different color scales. Many artifacts of the analytical continuation remain.
Figure 4.15: The bubble of DMFT Green's functions at \( K = 0 \) as a function of \( \omega \) for different \( U \), calculated in DMFT in a 2D Hubbard model with \( t = 0.25, \beta = 50 \). For charge conservation this should be zero for all \( \omega > 0 \).

end points of the branch near \( K = 0 \) disappear completely. The RPA does describe the narrowing of the branch as the interaction is turned on, but it can not describe the Mott transition which is a non-perturbative effect. So using dual boson instead of the RPA is necessary for strong interactions.

### 4.1.6 Comparison to DMFT susceptibility

An alternative way to calculate the susceptibility is simply as a bubble of DMFT Green’s functions. This will not lead to charge conservation, since it uses a \( \Sigma(\nu) \), as explained in appendix F. To illustrate this, the \( K = 0 \) part of this bubble is shown in figure 4.15. The result should be zero for all \( \omega > 0 \), but this is clearly not the case. This violation of charge conservation grows as \( U \) increases, since it is caused by the self-energy \( \Sigma(\nu) \), which also increases in magnitude as \( U \) increases. For \( U = 0 \), DMFT is equal to the exact solution and the DMFT bubble is just the non-interacting bubble, which is the exact susceptibility in that case. Non-local effects of vertex corrections to the susceptibility are necessary to consider when vertex corrections are used in the impurity problem, as is done in the impurity solver.

It is also possible to study the analytically continued DMFT bubble. For small \( U \), this should still give reasonable results, but as \( U \) increases, the charge conservation will get worse. This is visible in figure 4.16. The large \( U \) results show an almost \( K \)-independent susceptibility, which is not physical since the susceptibility should vanish at \( K = 0 \), but should be non-zero for other \( K \). Since the bubble depends on a convolution of \( G \) with itself, even parts of \( G \) with relatively high frequency \( \nu \) can give important contributions, which means that the noise in these parts can have a big effect on the result of the bubble.
Figure 4.16: DMFT bubble \((GG)_{K,E}\) along high symmetry path for various \(U\). Analytical continuation using a Padé scheme with \(\delta = 0.1\), \(N_\omega = 60\). The higher values of \(U\) violate charge conservation, since they do not have the right behaviour at small \(K\). Vertex corrections are needed when \(U\) becomes bigger. Note the different color scales. Artifacts of analytical continuation remain at some values of \(U\).
4.1.7 Conclusion

The dual boson formalism can be used to study the charge susceptibility in the Hubbard model. To get charge conservation, it is necessary to include vertex corrections. The charge susceptibility is strongly $K$-dependent, so it is necessary to go beyond mean field theory to describe it. In the half-filled Hubbard model, the system undergoes a phase transition to an insulating state when $U$ is increased. This phase transition is usually studied by looking at single fermion properties like the density of states. Here it was shown that the transition is also visible in the charge susceptibility. As the system becomes insulating, low energy charge excitations disappear. These low energy modes were mainly present near the $\Gamma$ point, so this is where the Mott transition is most visible.
4.2 The Hubbard model away from half-filling

The Mott transition to an insulating phase only occurs in the half-filled model. There is one electron per site and the repulsion makes it very hard to doubly occupy a site. The local density of states consists of two Hubbard bands at \( E = \pm \frac{U}{2} \) separated by a gap. The lower band is fully filled and the upper band is empty, so the system is insulating. The susceptibility is very small. When the filling is decreased, the lower band is no longer fully filled. Excitations within the band become possible. This increases the susceptibility. Some lattice sites do not have an electron and it is possible for charge to move via these empty sites. The susceptibility will depend on the number of empty sites.

In this section simulation results for the Hubbard model away from half-filling are shown. Computationally, it is easier to fix the chemical potential \( \mu \) than the filling \( \langle n \rangle \). This means that the fillings in these simulations are not round numbers. These simulations were performed at \( \beta = 50, t = 0.25 \) on a 64 by 64 square lattice. All simulations are done at \( U = 4 \), which would be deep in the insulating phase in the half-filled case. This means that the quasi-particle peak is totally gone and only the Hubbard bands are left.

When the lower Hubbard band is almost entirely filled, \( \langle n \rangle \approx 1 \), only a small region of unfilled states in the lower Hubbard band remains. The susceptibility is mainly caused by excitations from the filled part of the lower Hubbard band to the unfilled part. At energies of roughly half the bandwidth, where the susceptibility is highest, these excitations come from the middle of the lower Hubbard band, with an energy \( E \) around half the width of the Hubbard band. When the filling changes, the number of empty states that can be the target of an excitation increases proportionally to \( 1 - \langle n \rangle \), but the number of origins of the excitation stays roughly the same, since when you go down \( E \) from the lowest empty state, you are still in within the band. This means the susceptibility is proportional to \( 1 - \langle n \rangle \). This can be verified in figure 4.17.

![Figure 4.17: The local susceptibility normalized by 1 - \( \langle n \rangle \) for different fillings. Analytical continuation using a Padé scheme with \( \delta = 0.1, N_\omega = 60 \). This shows the susceptibility is proportional to 1 - \( \langle n \rangle \).](image)

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Another point which is interesting is that there is a significant difference in the local susceptibility between the impurity susceptibility and susceptibility from the dual boson calculation. This is shown in figure 4.15. This behaviour is different from the half-filled case where both susceptibilities are very comparable. This shows that the non-local part of the susceptibility is important. This means that doing outer self-consistency might be more important away from half-filling.

It is useful to study the wavevector dependence of the susceptibility in the doped system. This is shown in figure 4.19. The susceptibility on Matsubara frequencies is shown for the $\mathbf{K}$-average (local part) and for two high symmetry points in the Brillouin zone: The $X$ point at $\mathbf{K} = (\pi, 0)$ and the $M$ point at $\mathbf{K} = (\pi, \pi)$. The susceptibility at the $X$ point is a lot higher than the other two quantities. This difference is much less pronounced in the half-filled case shown in the other part of the figure.
4.3 Three-dimensional Hubbard Model and non-local interactions

The three-dimensional cubic extended Hubbard model is another system of interest. Some aspects of the physics in three dimensions differ from the two dimensional case. Plasmons in three dimensions are especially of interest. Here we study the system at $\beta = 50$, $t = 0.25$ for various $U$ and $V$.

4.3.1 Screening and the impurity problem

In the extended Hubbard model the non-local interaction has the effect of a retarded interaction on the impurity problem. The effective impurity interaction $U$ becomes frequency dependent, which means there is interaction between different times $\tau, \tau'$. This $U(\omega) = U + \Lambda(\omega)$ shows screening at small frequencies, but at high frequencies screening is not possible and the effective interaction is equal to the bare interaction. This already happens in EDMFT. The retarded interaction in EDMFT is shown in figure 4.20.

![Figure 4.20: $U(\omega) = U + \Lambda(\omega)$ for various $V$, for $t = \frac{1}{4}$, $U = 1$, $\beta = 50$. This shows the impact of screening on the impurity problem. For larger $V$, there is more screening.](image)

At $V = 0$, the bare dual propagator $\tilde{X}^0 = 0$ for $\Lambda = 0$, so there is no retarded interaction induced by EDMFT. As $V$ increases, the retarded interaction increases. In figure 4.21 it is shown that the retarded interaction is proportional to $\frac{V^2}{\omega^2}$ for large frequencies. The coefficient of proportionality can still depend on $U$ and $\beta$. For smaller $\omega$, the screening is stronger than the asymptotic result. Large in this case is large with respect to the typical energy scales of the problem: $U$, $\beta$ and $t$. 
Figure 4.21: $\omega^2 \Lambda(\omega)/V^2$ for various $V$, for $t = \frac{1}{4}$, $U = 1$, $\beta = 50$. For large frequencies, $\Lambda(\omega) \approx -5.5 \frac{V^2}{\omega^2}$. The coefficient 5.5 can still depend on $\beta$ and $U$.

The retarded interaction also influences the behaviour of the fermions. In particular, it is possible to look at the fermionic impurity self-energy $\Sigma_{\text{imp}}(\nu)$. This is shown in figure 4.22. The fermionic self-energy decays as $\frac{1}{\nu}$, but the coefficient of the decay depends on $V$, it gets bigger as $V$ increases. This is in accordance with\cite{36} but it is different from the results obtained in figure 6 of Ayral\cite{28}. The same effect should have been present in those results, but it is probably obscured by the relatively low $\frac{V}{U}$ ratio and the significant noise in the high frequency region.

For large frequencies $\Sigma_{\nu} \propto \frac{\Sigma_1(U,V)}{\nu}$. The constant of proportionality $\Sigma_1(U,V)$ can be determined from the results presented here. It is well known that in the regular half-filled Hubbard model $\Sigma_1(U) = \frac{U^2}{4}$. The self-energies described shown here are well-described by $\Sigma_1(U = 1, V) = 0.25 + 2V^2$. In general, the prefactor of $V^2$ can depend on $U$ and $\beta$.

### 4.3.2 Local susceptibility

The non-local interaction influences the local part of the susceptibility. This is shown in figure 4.23. As $V$ increases, some of the spectral weight shifts to lower energy and the overall spectral weight increases. This is associated with the system becoming more metallic. The off-site interaction reduces the effective on-site repulsion due to screening.
Figure 4.22: $\Sigma_{\text{imp}}(\nu)$ for various $V$, for $t = \frac{1}{4}$, $U = 1$, $\beta = 50$. The tail behaviour of $\Sigma$ depends on $V$.

### 4.3.3 Towards charge-ordering

In 1.3.6 the charge-ordering transition was treated in the RPA framework. As $V$ increases, at some point the system will start displaying charge order. This is visible in a divergence of the susceptibility at the point $R = (\pi, \pi, \pi)$ at $E = 0$. In 4.24 $X_{K,E}$ it is clear that as $V$ increases, the susceptibility at $R$ increases strongly.

In the imaginary time data, the same divergence is visible at $R = (\pi, \pi, \pi)$, $\omega = 0$. This is shown in figure 4.25.

### 4.3.4 Conclusion

The extended three-dimensional Hubbard model was studied in this paragraph. The non-local interaction influences the impurity problem by reducing the effective impurity interaction due to screening. The extended Hubbard model has a charge ordering transition when the non-local interaction becomes more important than the local repulsion. The charge-ordering transition is visible in the momentum dependent susceptibility. This charge susceptibility diverges at the R point, associated with checkerboard order, when the charge ordered phase is approached.
Figure 4.23: \( X_{\text{loc}}(E) \) for various \( V \), for \( t = \frac{1}{2} \), \( U = 1 \), \( \beta = 50 \). Analytical continuation using a Padé scheme with \( N_w = 80 \), \( \delta = 0.1 \). The low energy behaviour is very stable under analytical continuation but the height and width of the maximum is less stable. Increasing \( V \) makes the system more metallic and increases the spectral weight at small \( E \).
Figure 4.24: $X_{K,E}$ for various $V$, for $t = \frac{1}{4}$, $U = 1$, $\beta = 50$, analytical continuation using a Padé scheme with $N_w = 80$, $\delta = 4\pi\beta^{-1}$. Note the different scales. Artifacts of analytical continuation remain at some values of $V$. As $V$ increases, the susceptibility near the $R$ point diverges, which shows the charge-ordering transition.
Figure 4.25: $-X(K = R, \omega)$ for various $V$, for $t = \frac{1}{4}$, $U = 1$, $\beta = 50$. There is a divergence as $V$ increases.
Chapter 5

Conclusion and outlook

Susceptibilities are an important property of physical systems. They can shine light on phase transitions and they are often experimentally accessible. So it is useful to have the theoretical tools to compute susceptibilities in (model) systems. Susceptibilities in electronic systems are often studied using the Random Phase Approximation. This is a weak interaction approximation, which means that it is not sufficient to study strongly correlated systems. Strongly correlated systems are usually treated in Dynamical Mean Field Theory, but this does not directly allow for a calculation of frequency and wavevector dependent susceptibilities, since it ignores non-local correlations which are very important for conservation laws. The dual boson theory was developed to solve this problem.

A treatment of the charge susceptibility in dual boson theory was given in this thesis. The dual boson formalism was derived with a focus on preparing for a numerical implementation of the scheme. It was shown that diagrammatic corrections to the mean field susceptibility are necessary to achieve charge conservation. An improvement to GW+DMFT was suggested but it was shown that even this is generally not sufficient to achieve charge conservation. The ladder approximation was introduced. This approximation includes vertex corrections in the particle hole channel to all orders and is important for achieving a charge conserving approximation.

During this thesis a numerical implementation of the dual boson formalism was created. Chapter 4 illustrated the possibilities of the method. Results in both two and three dimensions were obtained. In two dimensions the Mott transition in the Hubbard model was studied. It was shown that the Mott transition is very visible in the charge susceptibility. Previous studies of the Mott transition mostly focussed on the fermionic Green’s function. The extended Hubbard model was studied in three dimension. This model shows a charge order transition when the non-local interaction becomes stronger than the local interaction. This shows as a divergence in the wavevector dependent charge susceptibility at the wavevector associated with checkerboard ordering. Dual boson excels at calculating this kind of k-dependent susceptibility.

The calculations shown here only included single shot dual boson calculations. It is also possible to study fully self-consistent dual boson. The computational cost of such an approach is a lot higher, so the importance of the self-consistency should be studied. It is also important to find an appropriate self-consistency condition.

The focus in this thesis has been on the bosonic propagators and self-energies. The dual bosons also give a contribution to the fermionic self-energy. The behaviour of this self-energy can
be studied. This additional renormalization of the dual Green’s function could prove to be important for preventing a spurious ferromagnetic transition in low temperature studies of the two dimensional square lattice.

One of the current prospects in the dual boson theory is the implementation of $S_z S_z$ or even $\mathbf{S} \cdot \mathbf{S}$ coupling. This will allow the computation of magnetic susceptibilities. These should have conservation laws similar to the charge susceptibility studied in this thesis. Studying these susceptibilities around the various transitions in the Hubbard model can prove to be very interesting. The new interactions can also give rise to new phase transitions.

Concluding, dual boson is a valuable tool in the study of susceptibilities in correlated systems.
Appendix A

The non-interacting 2D Hubbard model

The dispersion of the half-filled non-interacting 2D Hubbard model is given by:

\[ t_k = -2t (\cos(k_x) + \cos(k_y)) \quad (A.1) \]

\[ = -4t \cos(\frac{1}{2}(k_x - k_y)) \cos(\frac{1}{2}(k_x + k_y)) \quad (A.2) \]

For some \( E \), we are looking for the number of states with energy smaller than \( E \) and the derivative of this function:

\[ N_<(E') = \frac{1}{(2\pi)^2} \int d\mathbf{k} \Theta(E - t_k) \quad (A.3) \]

\[ n(E') = \frac{\partial}{\partial E} N_<(E)|_{E=E'} \quad (A.4) \]

We are considering the half-filled case, so it is sufficient to determine \( n(E') \) for \( E' < 0 \), from (A.2) it is clear that when \([-\pi, \pi] \times [-\pi, \pi]\) is taken as the Brillouin zone, that the \( k \)-points with \( t_k < 0 \) lie within the square with corners \((0, \pi), (\pi, 0), (0, -\pi)\) and \((-\pi, 0)\). Transfer to coordinates \( \alpha = \frac{1}{2}(k_x + k_y), \beta = \frac{1}{2}(k_x - k_y) \). This linear transformation has a determinant \( \frac{1}{2} \).

With \( t = 0.25 \), this gives:

\[ t_k = -\cos(\alpha) \cos(\beta) \quad (A.5) \]

\( E' < 0 \) means \( \alpha, \beta \in [\frac{1}{4}, \frac{1}{4}] \). It is sufficient to consider \( \alpha > 0 \) and multiply the end result by two, this exactly cancels the determinant introduced previously. Since the proper normalization of the density of states is known, it is enough to determine the shape of the density of states. The equation \( E' < t_k \) is equivalent to \( E > -t_k = \cos(\alpha) \cos(\beta) \) and this saves a lot of minus signs in the calculation. Since \( \cos(\beta) \leq 1 \), it follows that \( \alpha \leq \arccos(E) \). For fixed \( \alpha \), this then means

\[ \cos(\beta) \leq \frac{E}{\cos(\alpha)} \quad (A.6) \]

\[ \beta \leq \arccos\left( \frac{E}{\cos(\alpha)} \right) \quad (A.7) \]

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\[ N_<(E) = \frac{1}{(2\pi)^2} \int_0^{\arccos(E)} d\alpha \int_{\text{arccos}(\frac{E}{\cos(\alpha)})}^{\pi} d\beta \quad (A.8) \]

\[ = \frac{2}{(2\pi)^2} \int_0^{\arccos(E)} d\alpha \arccos \left( \frac{E}{\cos(\alpha)} \right) \quad (A.9) \]

This leads to
\[ n(E) = \frac{\partial}{\partial E_i} N_<(E_i)|_{E_i=E'} \quad (A.10) \]

\[ n(E) \propto \arccos \left( \frac{E}{\cos(\alpha)} \right) \frac{1}{\sqrt{1 - \frac{E}{E_i}^2}} + \int_0^{\arccos(E)} d\alpha \frac{1}{\sqrt{\cos^2(\alpha) - E^2}} \quad (A.11) \]

\[ = 0 + \int_0^{\arccos(E)} d\alpha \frac{1}{\sqrt{\cos^2(\alpha) - E^2}} \quad (A.12) \]

\[ = \frac{1}{\sqrt{1 - E^2}} F(\arccos(E)|\frac{1}{1 - E^2}) \quad (A.13) \]

Here it was used that:
\[ \left( \frac{\partial}{\partial y} \int_0^{g(y)} dx f(x, y) \right) |_{y=y_0} = f(g(y_0)) \frac{dg(y)}{dy} |_{y=y_0} + \int_0^{g(y_0)} dx \frac{\partial f(x, y)}{\partial y} |_{y=y_0} \quad (A.15) \]

The function F is the elliptic integral of the first kind.

So for \( 1 > E > 0 \), the density of states is given by:
\[ n(E) \propto \frac{1}{\sqrt{1 - E^2}} F(\arccos(E)|\frac{1}{1 - E^2}) \quad (A.16) \]

The density of states for \( -1 < E < 0 \) follows by symmetry. This result is shown in figure A.1.

At zero temperature, the local susceptibility in the non-interacting system is given by:
\[ X_{\text{loc}}(E) = \int dE' n(E' + E) \Theta(-E') \Theta(E' + E) = \int_{-E}^0 dE' n(E') n(E' + E) \quad (A.17) \]

At finite temperature, the step function \( \Theta \) should be replaced by one minus the Fermi-Dirac distribution. In particular, for zero temperature \( \chi(E = 0) = 0 \) since the integral is over an interval of measure zero.

\[ X_{\text{loc}}(E) \] can be calculated numerically at zero temperature. This is shown in figure A.2.
Figure A.1: The non-interacting density of states $n(E)$ for the 2D Hubbard model in units of $t = 0.25$. 
Figure A.2: The non-interacting local susceptibility $X_{\text{loc}}(E)$ for the 2D Hubbard model in units of $t = 0.25$. 
Appendix B

Hubbard-Stratonovich transformation

Mathematically the Hubbard-Stratonovich transformation can be seen as a generalisation of the Gaussian integral. However, the way the transformation is used is different from how the Gaussian integral is used. Normally the integral over a function is replaced by a number using the Gaussian identity:

$$\int_{\mathbb{R}} dx \frac{1}{\sqrt{2\pi}} \exp(-\frac{x^2}{2}) = 1$$  \hspace{1cm} (B.1)

Or, by using $(x - y)^2 = x^2 - 2yx + y^2$:

$$\int_{\mathbb{R}} dx \frac{1}{\sqrt{2\pi}} \exp(-\frac{x^2}{2} + yx) = \exp(-\frac{y^2}{2})$$  \hspace{1cm} (B.2)

The left hand side has variables $x$ and $y$ and $x$ is eliminated using the Gaussian identity. In the Hubbard-Stratonovich transformation, the philosophy is the other way round. The exponent which contained $y^2$ is replaced by an exponent which only contains $y$ linearly, by introducing a new variable (degree of freedom) $x$ that is integrated over. So the Hubbard-Stratonovich transformation is essentially (B.2) read from right to left.

The same transformation can be done for a case with more variables. The Hubbard-Stratonovich transformation then reads:

$$\int \prod_i d\phi_i \frac{1}{\sqrt{(2\pi)^N}} e^{-\frac{1}{2} \phi_i A_{ij} \phi_j + \alpha \phi_i n_i} = \frac{1}{\sqrt{\det A}} e^{\frac{1}{2} n_i A_{ij}^{-1} n_j}$$  \hspace{1cm} (B.3)

Here $A$ is a symmetric and invertible matrix that is diagonalized by the rotation matrix $O$. All eigenvalues should be positive to guarantee convergence of the integral. To prove this, first complete the square in the exponential on the left-hand side by the linear shift transformation:

$$x_i = \alpha \phi_i - A_{ij}^{-1} n_j$$  \hspace{1cm} (B.4)

The quadratic term becomes:

$$-\frac{1}{2} x_i A_{ij} x_j = -\frac{1}{2} \alpha \phi_i A_{ij} \alpha \phi_j + \alpha \phi_i n_i - \frac{1}{2} n_i A_{ij}^{-1} n_j$$  \hspace{1cm} (B.5)
Filling this in gives:

\[ e^{-\frac{1}{2} n_i A_{ij} n_j} \int d\phi_i e^{-\frac{1}{2} \alpha \phi_i A_{ij} \alpha \phi_j + \alpha n_i \phi_i} = \frac{1}{\alpha^N} \int d\phi_i e^{-\frac{1}{2} x_i A_{ij} x_j} \]

\[ = \frac{1}{\alpha^N} \prod_i d\phi_i e^{-\frac{1}{2} \alpha \phi_i^2} \]

\[ = \frac{1}{\alpha^N} \prod_i \int d\phi_i e^{-\frac{1}{2} \alpha \phi_i^2} \]

\[ = \prod_i \sqrt{\frac{2\pi}{\alpha^2 a_i}} \]

\[ = \sqrt{\frac{(2\pi)^N}{\det \alpha^2 A}} \]  

(B.6)

The first transformation has \( dx_i = d\phi_i / \alpha \), the second transformation \( z_i = O^{-1}_{ij} x_j \) which diagonalizes \( A \) has Jacobian unity.

Redefining \( A = W^{-1} \) gives

\[ \sqrt{\det [\alpha W^{-1} \alpha]} \prod_i \frac{d\phi_i}{\sqrt{(2\pi)^N}} e^{-\frac{1}{2} \phi_i \alpha W_{ij}^{-1} \alpha \phi_j + \alpha n_i \phi_i} = e^{\frac{1}{2} n_i W_{ij} n_j} \]  

(B.7)

which is in the same form as the corresponding identity in Rubtsov et al.\(^{[17]}\).

The Hubbard-Stratonovich transformation presented here describes a real field \( \phi \). It is also possible to use a complex field (this is done in Rubtsov et al.\(^{[17]}\)). A Hubbard-Stratonovich transformation for fermions also exists. This equation is derived by Hafermann\(^{[19]}\), only the result is presented here:

\[ \frac{1}{\det a} \int \exp(-f^* a f + f^* b c + c^* b f) df^* df = \exp (c^* b a^{-1} c) \]  

(B.8)
Appendix C

Definition and symmetry of the vertex

C.1 The effect of conjugation on Grassmann numbers

For Grassmann numbers, conjugation is defined as:

\[ (c_1 c_2)^* = c_2^* c_1^* \]  \hspace{1cm} (C.1)

\[ (c^*)^* = c \] \hspace{1cm} (C.2)

The time evolution of operators is introduced as \( c(\tau) = \exp(\tau H)c\exp(-\tau H) \). This can be used to derive the effect of conjugation on a time-dependent Grassmann number:

\[ (c(\tau))^* = (\exp(\tau H)c\exp(-\tau H))^* \]
\[ = \exp(-\tau H)c^* \exp(\tau H) \]
\[ = c^*(-\tau) \] \hspace{1cm} (C.3)

The imaginary time argument changes sign. Contrast this with the normal real time evolution where \( (c(t))^* = c^*(t) \). To establish relations between objects with frequency indices, one should add the corresponding exponential and use the previous relations for \( c(\tau) \). Spin and space labels are not altered under conjugation.

For fermionic Green’s functions there is the simple relation \( g(\sigma,\nu,x)^* = g(\sigma,-\nu,-x) \). For a real field, like the charge, the relation \( n(\omega)^* = n(\omega) \) holds.

C.2 The vertex \( \gamma \)

The vertex is defined as:

\[ \gamma_{\nu\nu'}^{\sigma\sigma'} = \frac{\langle c_{\sigma'}(\nu + \omega)c_{\sigma'}^*(\nu)c_{\sigma'}(\nu')c_{\sigma'}^*(\nu' + \omega)\rangle - \beta g_{\sigma}(\nu)g_{\sigma'}(\nu')\delta_{\omega} + \beta g_{\sigma}(\nu + \omega)g_{\sigma'}(\nu)\delta_{\sigma\sigma'}\delta_{\nu\nu'}}{g_{\sigma}(\nu + \omega)g_{\sigma}(\nu)g_{\sigma'}(\nu')g_{\sigma'}(\nu' + \omega)} \] \hspace{1cm} (C.4)
The expectation value $\langle cc^* c^* c^* \rangle$ is abbreviated by $\chi$. The Fourier transform in this case is defined as:

$$
\chi(\nu_1, \nu_2, \nu_3, \nu_4) = \frac{1}{\beta} \int_0^\beta \int_0^\beta \int_0^\beta \int_0^\beta d\tau_1 d\tau_2 d\tau_3 d\tau_4 \chi(\tau_1, \tau_2, \tau_3, \tau_4) e^{i\nu_1 \tau_1} e^{-i\nu_2 \tau_2} e^{i\nu_3 \tau_3} e^{-i\nu_4 \tau_4}
$$

(C.5)

The two particles in the vertex can be interchanged, which changes the frequencies:

$$
\chi(\sigma, \sigma', \nu, \nu', \omega) = \int d\tau_1 c_\sigma(\tau_1) c_\sigma^*(\tau_2) c_\sigma(\tau_3) c_\sigma^*(\tau_4) \exp(i [(\nu + \omega)\tau_1 - \nu\tau_2 + \nu'\tau_3 - (\nu' + \omega)\tau_4])
\begin{equation}
= \int d\tau_1 c_\sigma^*(-\tau_4) c_\sigma(-\tau_3) c_\sigma(-\tau_2) c_\sigma^*(-\tau_1) \exp(i [-(\nu + \omega)\tau_1 + \nu\tau_2 - \nu'\tau_3 + (\nu' + \omega)\tau_4])
\end{equation}
\begin{equation}
= \int d\tau_1 c_\sigma^*(\tau_4) c_\sigma(\tau_2) c_\sigma(\tau_3) c_\sigma^*(\tau_1) \exp(i [(\nu + \omega)\tau_1 + \nu\tau_2 - \nu'\tau_3 - (\nu' + \omega)\tau_4])
\end{equation}
\begin{equation}
= \chi(\sigma', \sigma, \nu', \nu, \omega, -\omega)
\end{equation}

(C.6)

Now, for the complex conjugation of $\chi$, relabeling the dummy indices results in:

$$
\chi(\sigma, \sigma', \nu, \nu', \omega) = \left(\int d\tau_1 c_\sigma(\tau_1) c_\sigma^*(\tau_2) c_\sigma(\tau_3) c_\sigma^*(\tau_4) \exp(i [(\nu + \omega)\tau_1 - \nu\tau_2 + \nu'\tau_3 - (\nu' + \omega)\tau_4])\right)^*
\begin{equation}
= \int d\tau_1 c_\sigma^*(-\tau_4) c_\sigma(-\tau_3) c_\sigma(-\tau_2) c_\sigma^*(-\tau_1) \exp(i [-(\nu + \omega)\tau_1 + \nu\tau_2 - \nu'\tau_3 + (\nu' + \omega)\tau_4])
\end{equation}
\begin{equation}
= \int d\tau_1 c_\sigma^*(\tau_4) c_\sigma(\tau_2) c_\sigma(\tau_3) c_\sigma^*(\tau_1) \exp(i [(\nu + \omega)\tau_1 + \nu\tau_2 - \nu'\tau_3 - (\nu' + \omega)\tau_4])
\end{equation}
\begin{equation}
= \chi(\sigma, \sigma', -\nu, -\nu', -\omega)
\end{equation}

(C.7)

The vertex is the amputated connect part of the $\chi$ introduced earlier, and it satisfies the same symmetry relations:

$$
\gamma_{\nu, \nu', \omega}^{\sigma, \sigma'} = \gamma_{-\nu, -\nu', -\omega}^{\sigma, \sigma'}
$$

(C.8)

$$
\gamma_{\nu, \nu', \omega}^{\sigma', \sigma} = \gamma_{\nu' + \omega, \nu + \omega, -\omega}^{\sigma', \sigma}
$$

(C.9)

$$
\gamma_{-\nu', -\omega, -\nu, -\omega}^{\sigma', \sigma} = \left(\gamma_{\nu, \nu', \omega}^{\sigma, \sigma'}\right)^*
$$

(C.10)

### C.3 The mixed vertex $\lambda$

Recall the definition of the mixed vertex:

$$
\lambda_{\nu, \omega}^\sigma = \frac{-\langle c_\sigma(\nu + \omega)c_\sigma^*(\nu)n(\omega) \rangle - \beta g(\nu)|n\rangle_\delta_{\nu, \omega}}{g_\sigma(\nu + \omega)g_\sigma(\nu)\chi(\omega)}
$$

(C.11)

---

1It is easy to check that the subtractions and the denominator obey these symmetry relations
The mixed vertex is related to $\gamma$, since the $n$ that occurs in $\langle cc^*n \rangle$ is closely related to $c^*c$.

$$g_\sigma(\nu + \omega) g_\sigma(\nu) \chi(\omega) \chi^{\nu}_{\omega} = - \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu)n(\omega) \rangle - \beta g(\nu) \langle n \rangle \delta_\omega$$

$$= - \frac{1}{\beta} \sum_{\sigma', \nu'} \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu') c_{\sigma'}(\nu') c_{\sigma'}(\nu') \rangle - g(\nu) \sum_{\sigma', \nu'} \langle c^*_\sigma(\nu' + \omega) c_{\sigma'}(\nu') \rangle \delta_\omega$$

$$= + \frac{1}{\beta} \sum_{\sigma', \nu'} \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu') c_{\sigma'}(\nu') c_{\sigma'}(\nu' + \omega) \rangle + g(\nu) \sum_{\sigma', \nu'} \langle c_\sigma(\nu') c^*_\sigma(\nu') \rangle \delta_\omega$$

$$= + \frac{1}{\beta} \sum_{\sigma', \nu'} \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu') c_{\sigma'}(\nu') c_{\sigma'}(\nu' + \omega) \rangle - g(\nu) \sum_{\sigma', \nu'} g_{\sigma'}(\nu) \delta_\omega$$  \hspace{1cm} (C.12)

$\gamma$ satisfies:

$$g_\sigma(\nu + \omega) g_\sigma(\nu) \gamma^{\sigma \sigma'}_{\nu \nu'} g_{\sigma'}(\nu') g_{\sigma'}(\nu' + \omega) = \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu) c_{\sigma'}(\nu') c^*_\sigma(\nu' + \omega) \rangle$$

$$- \beta g_\sigma(\nu) g_{\sigma'}(\nu') \delta_\omega + \beta g_\sigma(\nu + \omega) g_\sigma(\nu) \delta_{\sigma \sigma'} \delta_{\nu \nu'}$$  \hspace{1cm} (C.13)

Further:

$$g_\sigma(\nu + \omega) g_\sigma(\nu) \frac{1}{\beta} \sum_{\sigma', \nu'} \gamma^{\sigma \sigma'}_{\nu \nu'} g_{\sigma'}(\nu') g_{\sigma'}(\nu' + \omega) = \frac{1}{\beta} \sum_{\sigma', \nu'} \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu) c_{\sigma'}(\nu') c^*_\sigma(\nu' + \omega) \rangle$$

$$- g_\sigma(\nu) \sum_{\sigma', \nu'} g_{\sigma'}(\nu') \delta_\omega + g_\sigma(\nu + \omega) g_\sigma(\nu)$$  \hspace{1cm} (C.14)

or

$$g_\sigma(\nu + \omega) g_\sigma(\nu) \left[ \frac{1}{\beta} \sum_{\sigma', \nu'} \gamma^{\sigma \sigma'}_{\nu \nu'} g_{\sigma'}(\nu') g_{\sigma'}(\nu' + \omega) - 1 \right] = \frac{1}{\beta} \sum_{\sigma', \nu'} \langle c_\sigma(\nu + \omega) c^*_\sigma(\nu) c_{\sigma'}(\nu') c^*_\sigma(\nu' + \omega) \rangle$$

$$- g_\sigma(\nu) \sum_{\sigma', \nu'} g_{\sigma'}(\nu') \delta_\omega$$  \hspace{1cm} (C.15)

which is the same has the right-hand side of (C.12). From this it follows that:

$$\lambda^\sigma_{\nu \omega} = \chi^{-1}(\omega) \left[ \frac{1}{\beta} \sum_{\sigma', \nu'} \gamma^{\sigma \sigma'}_{\nu \nu'} g_{\sigma'}(\nu') g_{\sigma'}(\nu' + \omega) - 1 \right]$$  \hspace{1cm} (C.16)
Appendix D

Explicit calculation of diagrams in Dual Perturbation theory

Recall the expression for the dual action and potential.

\[
\tilde{S}[f^*, f; \phi] = - \sum_{k \nu} f_{k \nu}^{-1} \tilde{G}_{\psi k} f_{k \nu} - \frac{1}{2} \sum_{K \omega} \phi_{K \omega} \tilde{X}_{K K}^{-1} \phi_{K \omega} + V[f^*, f, \phi] \quad (D.1)
\]

\[
V[f^*, f; \phi] = - \chi^{-1} \langle n \rangle \phi + \lambda f^* f \phi - \frac{1}{4} \gamma^{(4)} f^* f f^* f \quad (D.2)
\]

Introduce a bare dual action:

\[
\tilde{S}_0 = \sum_{1,2} - f_{1}^{*} \tilde{G}^{-1} f_{2} - \frac{1}{2} \phi_{1}^{*} \tilde{X}^{-1} \phi_{2} \quad (D.3)
\]

\[
\tilde{X}_{12} = - \langle \phi_{1} \phi_{2} \rangle \tilde{S} \quad (D.4)
\]

\[
= - \langle \phi_{1} \phi_{2} \exp(-V[f^*, f; \phi]) \rangle \tilde{S}_0 \quad (D.5)
\]

\[
\tilde{G}_{12} = - \langle f_{1} f_{2} \rangle \tilde{S} \quad (D.6)
\]

\[
= - \langle f_{1} f_{2} \exp(-V[f^*, f; \phi]) \rangle \tilde{S}_0 \quad (D.7)
\]

Now, expand \(-V\), so that only averages of products of \(\phi, f^*, f\) in terms of the non-interacting dual action \(\tilde{S}_0\) remain. These can be calculated using Wick’s theorem, since the bare dual action is Gaussian. This leads to certain Feynman diagrams. Here, the terms appearing in this expansion are determined. There is one minus sign due to the minus in the definition of the Green’s function, there is a \((-1)^n\) for the \(n\)-th order contribution due to the expansion of the exponential, and there are further factors from counting pairings and determining their sign. In the following, Latin indices indicate a space-time point and Greek indices indicate other variables such as spin and orbital. The Greek indices \(\gamma\) and \(\lambda\) are used and should not be confused with the vertices.

To get the self-energy corresponding to a diagram, the two external Green’s functions need to be amputated.

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D.1 Definitions

One needs to treat the labels and frequencies of the lines consistently. Here write \((\alpha, \nu)\) is written for a fermionic line with label \(\alpha\) and frequency \(\nu\) and \(\gamma_{\alpha\beta\gamma,\nu,\nu'}\) has incoming lines \((\alpha, \nu)\) and outgoing \((\beta, \nu')\) and \(\lambda_{\alpha,\beta,\gamma,\omega}\) has an incoming/going boson \((\alpha, \omega)\), an incoming fermion \((\beta, \nu)\) and an outgoing fermion \((\gamma, \nu + \omega)\).

D.2 Bosonic dual self-energy

At order 0 in \(V\), there is no self-energy contribution:

\[-\phi_1 \phi_2\] (D.8)

At order 2 in \(V\) (the prefactor of the term \(\lambda\lambda\) in \((\lambda + \gamma)^2\) is 1):

\[1 \sim 1\]

\[-\frac{1}{2} \sum_{ij, \alpha, \beta, \gamma, \delta, \epsilon, \zeta} \frac{(-1)^2}{2} \phi_1 \phi_2 \lambda_{i, \alpha \beta \gamma} \phi_{i, \alpha} f_{i, \beta} f_{i, \gamma} \lambda_{j, \delta \epsilon \zeta} \phi_{j, \delta} f_{j, \epsilon} f_{j, \zeta}\] (D.9)

\[\frac{1}{2} \sum_{ij, \alpha, \beta, \gamma, \delta, \epsilon, \zeta} \lambda_{i, \alpha \beta \gamma} \lambda_{j, \delta \epsilon \zeta} \phi_{i, \alpha} \phi_{j, \beta} f_{j, \delta} f_{j, \epsilon} f_{j, \zeta}\] (D.10)

\[\frac{1}{2} \sum_{ij, \alpha, \beta, \gamma, \delta, \epsilon, \zeta} \lambda_{i, \alpha \beta \gamma} \lambda_{j, \delta \epsilon \zeta} \tilde{X}_{1, i, \alpha} \tilde{X}_{k, \delta} \tilde{G}_{j, \epsilon, i, \beta} \tilde{G}_{i, \gamma, j, \delta}\] (D.11)

\[\tilde{\Pi}_{ij, \alpha \beta}(\omega) = \sum_{\gamma, \delta, \epsilon, \zeta} \lambda_{i, \alpha \beta \gamma}(\nu, \omega) \lambda_{j, \delta \epsilon \zeta}(\nu + \omega, -\omega) \tilde{G}_{j, \zeta, i, \beta}(\nu + \omega)\] (D.12)

At order 3 in \(V\) (the prefactor of the term \(\lambda\lambda\gamma\) in \((\lambda + \gamma)^3\) is 3):

\[3 \sum_{ijk, \alpha, \beta, \gamma, \delta, \epsilon, \zeta, \kappa, \lambda, \mu} \frac{(-1)^3}{3!} \phi_1 \phi_2 \phi_{i, \alpha} \phi_{j, \beta} f_{j, \gamma} f_{j, \delta} f_{j, \zeta} f_{j, \epsilon} f_{j, \kappa} f_{j, \lambda} f_{j, \mu} \lambda_{k, \kappa \lambda \mu} \phi_{k, \kappa} f_{k, \lambda} f_{k, \mu}\] (D.13)

\[-3 \sum_{ijk, \alpha, \beta, \gamma, \delta, \epsilon, \zeta, \kappa, \lambda, \mu} \frac{1}{4!} \lambda_{i, \alpha \beta \gamma} \gamma_{j, \delta \epsilon \zeta} \phi_{i, \alpha} \phi_{j, \beta} f_{j, \delta} f_{j, \epsilon} f_{j, \zeta} f_{j, \kappa} f_{j, \lambda} f_{j, \mu} f_{j, \kappa} f_{j, \lambda} f_{j, \mu}\] (D.14)

\[-3 \sum_{ijk, \alpha, \beta, \gamma, \delta, \epsilon, \zeta, \kappa, \lambda, \mu} \frac{1}{4!} \lambda_{i, \alpha \beta \gamma} \gamma_{j, \delta \epsilon \zeta} \phi_{i, \alpha} \phi_{j, \beta} \tilde{X}_{1, i, \alpha} \tilde{X}_{k, \delta} \tilde{G}_{j, \epsilon, i, \beta} \tilde{G}_{i, \gamma, j, \delta} \tilde{G}_{j, \theta, k, \lambda} \tilde{G}_{k, \mu, \zeta}\] (D.15)
There are 8 pairings that correspond to this diagram. The incoming boson 1 can be connected to \(\alpha\) or \(\kappa\). \(\beta\) can be connected to \(\theta\) or \(\epsilon\), and independently \(\gamma\) can be connected to \(\delta\) or \(\zeta\). Once these three choices have been made, all other lines are fixed. This leads to an overall contribution of:

\[
\tilde{\Pi}_{ik,\alpha\kappa}(\omega) = -\sum_{j,\beta,\gamma,\delta,\zeta,\theta,\lambda,\mu} \lambda_{i,\alpha\beta\gamma}(\nu,\omega)\gamma_{j,\delta,\zeta,\theta}(\nu,\nu',\omega)\lambda_{k,\kappa,\lambda}(\nu',-\omega) \\
\times \tilde{G}_{f_{j,\beta,\gamma}}(\nu)\tilde{G}_{f_{i,\delta,\zeta,\theta}}(\nu + \omega)\tilde{G}_{\beta,\zeta,\lambda}(\nu' + \omega)\tilde{G}_{\kappa,\lambda}(\nu')
\]  
(D.16)

Here, frequency labels have been added and the external bosonic Green’s functions have been amputated. In practice this diagram is calculated in k-space, so the space labels \(ik\) are replaced by a momentum \(K\).

### D.3 Mixed diagram

There is a diagram for the fermionic self-energy that includes dual bosonic lines. This originates from the same diagram in the Luttinger-Ward functional as the previously considered diagram. Here we consider it, and some of the ladder-like vertex corrections. For now, we ignore the space labels.

At order 2 \(((\lambda + \gamma)^2\text{ gives } 1 \lambda^2)\):

\[
\frac{(-1)^2}{2!} \sum_{\alpha,\beta,\gamma,\delta,\zeta} -f_1f_2^\ast \lambda_{\alpha,\beta,\gamma}(\nu,\omega)\lambda_{\delta,\zeta}(\nu,\nu',\omega)\tilde{X}_{\alpha,\beta}(\omega)\tilde{G}_{1,\beta}(\nu)\tilde{G}_{\gamma,\theta}(\nu + \omega)\tilde{G}_{\zeta,\lambda}(\nu')
\]  
(D.17)

There are two possible pairings (interchange of the two vertices), so the resulting self-energy contribution is:

\[
\tilde{\Sigma}_{\beta\zeta}(\nu) = \sum_{\alpha,\gamma,\delta,\lambda} \lambda_{\alpha,\beta,\gamma}(\nu,\omega)\lambda_{\delta,\zeta}(\nu,\nu',\omega)\tilde{X}_{\alpha,\beta}(\omega)\tilde{G}_{\gamma,\theta}(\nu + \omega)\tilde{G}_{\zeta,\lambda}(\nu')
\]  
(D.18)

At order 3 \(((\lambda + \gamma)^3\text{ gives } 3 \lambda^2\gamma)\):

\[
3\frac{(-1)^3}{3!} \sum_{\alpha,\beta,\gamma,\delta,\zeta,\theta,\lambda,\mu} -f_1f_2^\ast(-\frac{1}{4})\gamma_{\alpha,\beta,\gamma,\delta,\zeta,\theta,\lambda,\mu}(\nu,\nu',\omega)\tilde{X}_{\alpha,\beta}(\omega)\tilde{G}_{\gamma,\theta}(\nu)\tilde{G}_{\delta,\zeta,\lambda}(\nu + \omega)
\]  
(D.19)
There are 8 possible pairings (interchange the two triangle vertices, interchange the two incoming points of the box, interchange the two outgoing points of the box), which results in a self-energy contribution of:

$$\tilde{\Sigma}(\nu) = \sum_{\alpha,\beta,\delta,\eta,\theta,\kappa} \gamma_{\alpha,\beta,\delta}(\nu', \nu, \omega) \lambda_{\alpha,\beta,\delta}(\nu' + \omega, -\omega) \tilde{X}_{\theta,\kappa}(\omega) \tilde{G}_{\beta,\delta}(\nu' + \omega) \tilde{G}_{\delta,\kappa}(\nu + \omega)$$

(D.20)

There is a second diagram at order 3, where the box is paired with the outgoing fermion 2 instead of the incoming fermion 1, this gives a similar contribution of.

$$\tilde{\Sigma}(\nu) = \sum_{\alpha,\gamma,\delta,\eta,\theta,\kappa} \gamma_{\alpha,\gamma,\delta}(\nu', \nu, \omega) \lambda_{\alpha,\gamma,\delta}(\nu' + \omega, -\omega) \tilde{X}_{\alpha,\delta}(\omega) \tilde{G}_{\gamma,\eta}(\nu + \omega) \tilde{G}_{\eta,\theta}(\nu' + \omega) \tilde{G}_{\theta,\kappa}(\nu' + \omega)$$

(D.21)

At order 4 ($\lambda + \gamma$) gives $6\lambda^2\gamma^2$:

$$6\frac{(-1)^4}{4!} \times -f_{1,2} \sum_{\alpha, \ldots, \xi} \frac{1}{4} \gamma_{\alpha,\beta,\gamma,\delta}(\nu', \nu, \omega) \lambda_{\alpha,\beta,\gamma,\delta}(\nu'' + \omega, -\omega) \tilde{X}_{\xi,\eta}(\omega) \tilde{G}_{\beta,\gamma}(\nu'' + \omega) \tilde{G}_{\gamma,\delta}(\nu' + \omega) \tilde{G}_{\delta,\xi}(\nu + \omega)$$

(D.22)

There are 64 pairings (interchanging the endpoints of the boxes gives 16 pairings, interchanging the two triangles gives 2, interchanging the two boxes gives 2), which gives a self-energy of:

$$\tilde{\Sigma}(\nu) = \sum_{\alpha,\beta,\delta,\eta,\theta,\kappa} \gamma_{\alpha,\beta,\delta}(\nu', \nu, \omega) \lambda_{\alpha,\beta,\delta}(\nu' + \omega, -\omega) \gamma_{\mu,\gamma,\delta}(\nu'' + \omega, -\omega) \lambda_{\gamma,\delta,\mu}(\nu'' + \omega, -\omega) \gamma_{\mu,\xi,\eta}(\nu, \nu'', \omega) \gamma_{\gamma,\xi,\eta}(\nu, \nu'', \omega) \gamma_{\xi,\eta,\mu}(\nu, \nu'', \omega) \gamma_{\eta,\mu,\xi}(\nu, \nu'', \omega) \gamma_{\mu,\eta,\xi}(\nu, \nu'', \omega) \gamma_{\xi,\eta,\mu}(\nu, \nu'', \omega)$$

(D.23)

### D.4 Remarks on factors

Like in the Dual Fermion case, the diagrams without any indistinguishable lines have a prefactor of 1. The factors caused by the expansion of the exponential exactly cancel with the number of permutations of the vertices. In principle, the sign of a diagram can also be determined by counting fermion loops, similar to section A.4.4 of Hafermann\cite{109}, where triangle vertices and bosonic propagators also have to be replaced by wiggly lines.
Appendix E

The exact relation between $X$ and $\tilde{X}$

A derivation of the relation between $X$ and $\tilde{X}$ is presented here analogous to the relation between $G$ and $\tilde{G}$ derived in appendix A.6 of Hafermann\textsuperscript{[19]}. The basic idea is that the lattice bosonic Green’s function can formally be found as a derivative of the partition function with respect to the interaction $V$.\textsuperscript{1} The factors of $\beta$ are not written explicitly in this derivation. The equations all have the correct dimensionality on both sides, so it is sufficient to consider them in units where $\beta = 1$.

\[
\frac{1}{Z} \frac{\delta Z}{\delta V_{\mathbf{K},\omega}} = -\frac{1}{2} \langle \rho \rho \rangle_{\mathbf{K},\omega} = \frac{1}{2} X_{\mathbf{K},\omega} \tag{E.1}
\]

The same derivative can be applied after the dual degrees of freedom have been introduced. Start with the expression:

\[
\int \exp(-S[c^*, c]) \mathcal{D}[c^*, c] = Z_f Z_b \int \int \int \exp(-S[c^*, c; f^*, f, \phi]) \mathcal{D}[c^*, c; f^*, f, \phi] \tag{E.2}
\]

where $Z_f Z_b$ is defined by:

\[
\frac{Z}{Z_f Z_b} = \int \int \int \exp(-S[c^*, c; f^*, f, \phi]) \mathcal{D}[c^*, c; f^*, f, \phi] \tag{E.3}
\]

Then use the chain rule,

\[
+ \frac{1}{Z} \frac{Z}{\delta V_{\mathbf{K},\omega}} = \frac{1}{Z} \frac{Z_f}{Z_f Z_b} \left( \frac{\delta Z_b}{\delta V_{\mathbf{K},\omega}} \right) \frac{Z}{Z_f Z_b} + Z_b \frac{\delta}{\delta V_{\mathbf{K},\omega}} \left( \frac{Z}{Z_f Z_b} \right) \tag{E.4}
\]

\textsuperscript{1}Which we we generalize to also have a frequency label.

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The second term can be evaluated using

\[
\frac{Z_f Z_b}{Z} \frac{\delta}{\delta V_{K,\omega}} \frac{Z_f(Z_f Z_b)}{Z} = \langle -\frac{1}{2} \phi_{K,\omega} \chi_{\omega}^{-1} \delta(A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} \phi_{K,\omega} \rangle \tag{E.5}
\]

\[
= \langle -\frac{1}{2} \phi_{K,\omega} \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \delta(A_{\omega} - V_{K,\omega}) (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} \phi_{K,\omega} \rangle \tag{E.6}
\]

\[
= \langle -\frac{1}{2} \phi_{K,\omega} \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} \phi_{K,\omega} \rangle \tag{E.7}
\]

\[
= \frac{1}{2} \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \bar{X}_{K,\omega} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} \tag{E.8}
\]

where the full dual boson Green’s function is defined as:

\[
\bar{X}_{K,\omega} = -\langle \phi \phi \rangle_{K,\omega} \tag{E.9}
\]

The quantities \( V \) and \( \Lambda \) are parameters and \( \chi \) is the parameter introduced in the Hubbard-Stratonovich transformation, so these can all be taken out of the average.

Here it was used that:

\[
\frac{\delta 1}{\delta V} = 0 \tag{E.10}
\]

\[
\frac{\delta A A^{-1}}{\delta V} = 0 \tag{E.11}
\]

\[
A \frac{\delta A^{-1}}{\delta V} + \frac{\delta A}{\delta V} A^{-1} = 0 \tag{E.12}
\]

\[
\frac{\delta A^{-1}}{\delta V} = -A^{-1} \frac{\delta A}{\delta V} A^{-1} \tag{E.13}
\]

And also, using \( \text{Tr} \ln A = \ln \det A \):

\[
\frac{\delta \text{Tr} \ln A}{\delta V} = \text{Tr} \left[ \frac{\delta \ln A}{\delta V} \right] \tag{E.14}
\]

\[
\frac{\delta \ln \det A}{\delta V} = \text{Tr} \left[ \frac{\delta \ln A}{\delta V} \right] \tag{E.15}
\]

\[
\frac{1}{\det A} \frac{\delta \det A}{\delta V} = \text{Tr} \left[ A^{-1} \frac{\delta A}{\delta V} \right] \tag{E.16}
\]

\[
\frac{\delta \det A}{\delta V} = \det A \text{Tr} \left[ A^{-1} \frac{\delta A}{\delta V} \right] \tag{E.17}
\]

The following derivative was also used:

\[
\frac{\delta (A_{\omega} - V_{K,\omega})^{-1}}{\delta V_{K,\omega}} = -(A_{\omega} - V_{K,\omega})^{-1} \frac{\delta (A_{\omega} - V_{K,\omega})}{\delta V_{K,\omega}} (A_{\omega} - V_{K,\omega})^{-1} \tag{E.18}
\]

\[
= +(A_{\omega} - V_{K,\omega})^{-1} (A_{\omega} - V_{K,\omega})^{-1} \tag{E.19}
\]

Furthermore, the derivative of \( Z_b \) can be calculated. First, using (E.17) establish the general
matrix relation:

\[
\frac{\delta}{\delta V} \sqrt{\det A} = \frac{1}{2} \frac{1}{\sqrt{\det A}} \frac{\delta}{\delta V} \det A \\
= \frac{1}{2} \frac{1}{\sqrt{\det A}} \det A \text{Tr}[A^{-1} \frac{\delta A}{\delta V}] \\
= \frac{1}{2} \sqrt{\det A} \text{Tr}[A^{-1} \frac{\delta A}{\delta V}] 
\] (E.20)

Apply (E.22) to \( Z_b \):

\[
\frac{\delta Z_b}{\delta V_{K,\omega}} = \frac{\delta}{\delta V_{K,\omega}} \sqrt{\det[\chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1}]} \\
= \frac{1}{2} \sqrt{\det[\chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1}]} \text{Tr}[\chi_{\omega} (A_{\omega} - V_{K,\omega}) \chi_{\omega} \chi_{\omega}^{-1} \delta (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} \chi_{\omega}^{-1} \delta V_{K,\omega}] 
\] (E.23)

Using (E.19) yields:

\[
\frac{\delta Z_b}{\delta V_{K,\omega}} = \frac{1}{2} \sqrt{\det[\chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1}]} \text{Tr}[\chi_{\omega} (A_{\omega} - V_{K,\omega}) \chi_{\omega} \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1}] \\
= \frac{1}{2} \sqrt{\det[\chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1}]} (A_{\omega} - V_{K,\omega})^{-1} \\
= \frac{1}{2} Z_b (A_{\omega} - V_{K,\omega})^{-1} 
\] (E.24)

Putting these results into (E.4) finally yields

\[
\frac{1}{2} X_{K,\omega} = \frac{1}{Z} \frac{\delta Z}{\delta V} \\
= \frac{1}{2} (A_{\omega} - V_{K,\omega})^{-1} + \frac{1}{2} \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \tilde{X} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} 
\] (E.25)

so that finally

\[
X_{K,\omega} = (A_{\omega} - V_{K,\omega})^{-1} + \chi_{\omega}^{-1} (A_{\omega} - V_{K,\omega})^{-1} \tilde{X}_{K,\omega} (A_{\omega} - V_{K,\omega})^{-1} \chi_{\omega}^{-1} 
\] (E.26)
It is possible to express this relation purely in terms of the dual self-energy $\tilde{\Pi}$.

$$\tilde{X}_{K,\omega} = \frac{1}{(\tilde{X}^0_{K,\omega})^{-1} - \tilde{\Pi}_{K,\omega}}$$  \hspace{1cm} (E.31)

$$\tilde{X}^0 = \frac{1}{\chi^{-1}_\omega + \Lambda - V_{K,\omega}} - \chi$$  \hspace{1cm} (E.32)

$$\frac{\chi^2}{\tilde{X}^0_{K,\omega}} = \frac{1 - (V_{K,\omega} - \Lambda)\chi}{V_{K,\omega} - \Lambda}$$  \hspace{1cm} (E.33)

$$X_{K,\omega} = (\Lambda - V_{K,\omega})^{-1} + \chi^{-1}_\omega (\Lambda - V_{K,\omega})^{-1} \tilde{X}_{K,\omega} (\Lambda - V_{K,\omega})^{-1} \chi^{-1}_\omega$$  \hspace{1cm} (E.34)

$$= (\Lambda - V_{K,\omega})^{-1} + \chi^{-1}_\omega (\Lambda - V_{K,\omega})^{-1} \frac{1}{(\tilde{X}^0_{K,\omega})^{-1} - \tilde{\Pi}_{K,\omega}} (\Lambda - V_{K,\omega})^{-1}$$  \hspace{1cm} (E.35)

$$= (\Lambda - V_{K,\omega})^{-1} + (\Lambda - V_{K,\omega})^{-1} \frac{1}{\chi_\omega (\tilde{X}^0_{K,\omega})^{-1} \chi_\omega - \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega} (\Lambda - V_{K,\omega})^{-1}$$  \hspace{1cm} (E.36)

$$= (\Lambda - V_{K,\omega})^{-1} (1 - \frac{1}{(\Lambda - V_{K,\omega})\chi_\omega + 1 + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega (\Lambda - V_{K,\omega})})$$  \hspace{1cm} (E.37)

$$= (\Lambda - V_{K,\omega})^{-1} \frac{(\Lambda - V_{K,\omega})\chi_\omega + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega (\Lambda - V_{K,\omega})}{(\Lambda - V_{K,\omega})\chi_\omega + 1 + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega (\Lambda - V_{K,\omega})}$$  \hspace{1cm} (E.38)

$$= \frac{\chi_\omega + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega}{(\Lambda - V_{K,\omega})\chi_\omega + 1 + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega (\Lambda - V_{K,\omega})}$$  \hspace{1cm} (E.39)

$$= \frac{\chi_\omega + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega}{1 + (\chi_\omega + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega (\Lambda - V_{K,\omega})}$$  \hspace{1cm} (E.40)

$$= \frac{1}{\chi_\omega + \chi_\omega \tilde{\Pi}_{K,\omega} \chi_\omega} + (\Lambda - V_{K,\omega})$$  \hspace{1cm} (E.41)
Appendix F

Asymptotics of bubbles

In the calculation of susceptibilities, bubbles of Green’s functions are often calculated. To study
the asymptotic behaviour of such quantities, it is necessary to know how these bubbles behave.
Some examples are given here. We consider expressions of the form

\[ X(\omega) = \sum_{\nu} G(\nu)G(\nu + \omega) \] (F.1)

and study how they depend on \( \omega \).

F.1 Non-interacting Green’s functions

A non-interacting Green’s function is simply given by

\[ G_0(\nu) = \frac{1}{i\nu + a} \] (F.2)

where \( a \) does not depend on \( \nu \). In this case, the bubble can easily be calculated. There are two
distinct cases, \( \omega = 0 \) and \( \omega \neq 0 \).

\[ X(0) = \sum_{\nu} G_0(\nu)G_0(\nu) \] (F.3)
\[ = \sum_{\nu} \frac{1}{i\nu + a} \frac{1}{i\nu + a} \] (F.4)
\[ = \sum_{\nu} \frac{1}{(i\nu + a)^2} \] (F.5)
is some non-zero constant. The sum is convergent as long as \(i\nu + a \neq 0\) for all Matsubara frequencies \(\nu\). This is typically the case, since \(a\) has a real part. For \(\omega \neq 0\), the result is different:

\[
X(\omega) = \sum_\nu G_0(\nu)G_0(\nu + \omega)
\]

(F.6)

\[
= \sum_\nu \frac{1}{i\nu + a} \frac{1}{i\nu + i\omega + a}
\]

(F.7)

\[
= \sum_\nu \frac{1}{i\omega} \left( \frac{1}{i\nu + a} - \frac{1}{i\nu + i\omega + a} \right)
\]

(F.8)

\[
= 0
\]

(F.9)

since the two terms in brackets give the same sum, just shifted by a bosonic Matsubara frequency \(\omega\).

If \(a\) is not a constant, but a function of \(k\), then the formula for the bubble is of the form

\[
X(\omega, K) = \sum_\nu G(\nu, k)G(\nu + \omega, k + K)
\]

(F.10)

The previous argument that \(X = 0\) no longer applies generally, but it still works for \(\omega \neq 0, K = 0\).

### F.2 Dynamical Mean Field

The Green’s function in a dynamical mean field theory is given by

\[
G_{\text{DMFT}}(\nu) = \frac{1}{i\nu + a + \Sigma(\omega)}
\]

(F.11)

In this case, the previous argument no longer applies due to the frequency dependence of \(G\). This means \(X(\omega \neq 0, K = 0)\) is no longer zero, should charge conservation can be violated.

### F.3 Dual Green’s function

If \(G(\nu)\) decays as \(G(\nu) \propto \frac{1}{(\nu)}\) for \(\nu \to \infty\), then for \(\omega\) large, the main contributions to the bubble are at \(\nu \approx 0\) and \(\nu + \omega \approx 0\).

\[
X(\omega) = \sum_\nu G(\nu)G(\nu + \omega)
\]

(F.12)

\[
\approx G(\nu \approx 0)G(\nu \approx \omega) + G(\nu \approx -\omega)G(\nu \approx 0)
\]

(F.13)

\[
\approx G(\nu \approx 0) \left( G(\nu \approx \omega) + G(\nu \approx -\omega) \right)
\]

(F.14)

\[
\propto G(\nu \approx \omega)
\]

(F.15)

\[
\propto \frac{1}{\omega^2}
\]

(F.16)

So a bubble of dual Green’s functions decays as \(\frac{1}{\omega^2}\) as a function of \(\omega\). In the same way, if the Green’s function decays as \(\frac{1}{(\nu)}\), the bubble is expected to decay as \(\frac{1}{\omega}\), unless some special cancellations occur (like in the non-interacting case).

This behaviour was used in section 2.7.1.
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