Ultracold Fermions in Two-Dimensional Planes with Dipolar Interaction

Diplomarbeit
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Abstract

Many-Body quantum systems are difficult to describe, due to their strong correlations in general. In the field of fermionic ultracold quantum gases, a usual assumption beyond others is that one deals with dilute weak interacting gases. In order to see if these beyond other approximations are still valid in the case of the strong dipole-dipole interaction within two-dimensional systems, we are going to recapitulate the Hartree-Fock equation starting from first principles. Then we will derive in the leading order for large particle numbers the self-energy $\Sigma(\mathbf{k}, \mathbf{R})$ within Hartree-Fock approximation often used as a basic input for the calculation of many-body physical quantities. Furthermore we will calculate this self-energy within the semiclassical approximation commonly used in the field of ultracold quantum gases. Finally we compare both approximations.

Selbstständigkeitserklärung

Hiermit versichere ich, die vorliegende Arbeit ohne unzulässige Hilfe Dritter und ohne Benutzung anderer als der angegebenen Hilfsmittel angefertigt zu haben. Die aus fremden Quellen direkt oder indirekt übernommenen Gedanken sind als solche kenntlich gemacht. Die Arbeit wurde bisher weder im In- nochAusland in gleicher oder ähnlicher Form einer anderen Prüfungsbehörde vorgelegt.

(Ort, Datum)

(Marek Xavier Schiffer)

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Chapter 1

Introduction

1.1 Introduction Ultracold Atomic Quantum Gases

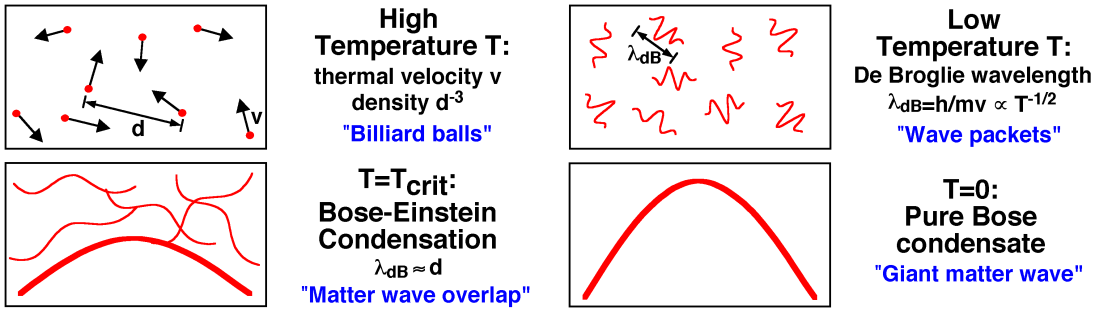


Figure 1.1: A schematic overview on the transition from a classical gas at high temperatures to a Bose-Einstein condensate below a critical temperature. Made and popularized by Wolfgang Ketterle. [1]

The field of ultracold quantum gases investigates the behavior of atomic gases below a certain temperature, called the critical temperature, where the quantum mechanical nature of the considered particles takes effect. Before we engage ourselves deeper with the interesting physical phenomena at low temperatures, we will give a short outline of the history of ultracold quantum gases, which starts with two groundbreaking discoveries. The experimental discovery of superfluidity in liquid Helium ^{4}He in 1938 by Pyotar Kapitza [2], John Allen and Don Misener [3] portrait a stunning demonstration, that in order to describe this directly visual observable phenomenon classical physics was not sufficient. In the same year Fritz London [4] suggested that the transition between liquid He I and liquid He II might be the result of the same process which causes Bose-Einstein condensation, which again was proposed by Albert Einstein in 1925 in his two succeeding papers [5,6] and takes the part of the first groundbreaking discovery.

Based on Satyendra Nath Bose's new derivation of Max Planck's black body radiation formula [7] using only the assumption to split the phase space in quanta of $\hbar\nu$, Einstein expanded the model in his paper [6] to particles with non vanishing rest mass and elaborated on the idea in the following year, where he made the stunning proposal that by compressing the gas and therefore increasing the density to a given temperature, a large number of particles would condense in the ground state.

Although this statement doesn't seem too remarkable from a modern point of view, since alone due to the Heisenberg uncertainty principle $\delta x\, \delta p \geq \frac{\hbar}{2}$ and the thermodynamic estimate $\delta p \propto \sqrt{mk_BT}$ one has the relation $\delta x \geq \frac{\hbar}{2\sqrt{mk_BT}}$ and the de'Broglie wavelength λ_{dB} would increase with lowering the temperature, it was very groundbreaking for that time. See also Figure 1.1.

Maybe just as remarkable as the idea of Bose-Einstein condensation was the idea of applying the concept to liquid Helium, since Einstein's derivation was made for an ideal gas which has no interaction, while liquid Helium, on the contrary, possess strong interaction. Not surprisingly London's idea was at first dismissed and replaced by Lev Davidovich Landau's two fluid model [8, 9]. For his contributions to condensate matter physics and especially the explanation of liquid Helium, Landau later received the Nobel Prize in physics in 1962. Contrary to London's idea of connecting superfluidity with Bose-Einstein condensation, Landau's model had no such connection.

During 1953 and 1958 Richard P. Feynman provided several papers on liquid Helium and superfluidity [10–12] supporting Landau's theory from first principles and supporting London's idea that, the superfluidity could indeed be based on the same process as Bose-Einstein condensation. A theoretical proof that Bose-Einstein condensation does indeed occur in liquid Helium was then given by Onsager and Penorose [13].

1.2 Experimental Breakthrough

While liquid Helium provided a natural substance to investigate superfluidity due to the fairly easily accessible transition to quantum degeneracy at 2.172K. The experimental progress was pushed forward by the illusive goal of reaching Bose-Einstein condensation. The first big step towards this goal was the invention of laser cooling, which was proposed by Theodor Hänch in 1975 and finally realized by Steven Chu [14] in 1985. The main principle is to shine lasers from several directions on a cloud of atoms, where the lasers have to be chosen in such a way, that the frequency is slightly below the excitation frequency of the atoms. If an atom now moves towards the laser it sees the laser light red shifted due to the Doppler shift, while it sees the laser coming from behind blue shifted. As a consequence the atom will only absorb a photon if it moves towards it. After the absorption of the photon, the atom will be exited and shortly afterwards emits again a photon. But since the direction of this emission is randomly given, the atoms will eventually cool down. This cooling process however has a natural limit, since the photons have a finite momenta, there exists a certain temperature, where the atoms will be accelerated by the momenta of the photons and end up jiggling around. The natural limit of laser cooling lies around $1\mu K$ and in order to achieve Bose-Einstein condensation a second cooling process was needed.

Once the limit of laser cooling is reached the second mechanism called evaporative cooling comes into play. By applying a magnetic or optical trap the atoms will be held into place. Driven by the collisions between the atoms the most energetic atoms will leave the trapping potential and the remaining atoms can then rethermalize, consequently lowering the temperature of the system. Once the critical temperature $T_c \sim$ nK, is reached the phenomena of Bose-Einstein condensation was observed.

By combining this two cooling mechanisms the groups of Eric Cornell and Carl Wiemann as well as Wolfgang Ketterle archived almost simultaneously the first experimental realized Bose-Einstein condensate back in 1995 [15, 16]. All three gained the Nobel Prize in physics 2001. After the discovery in 1995 the field of ultracold atoms raised dramatically.

1.3 Reaching Degeneracy for Fermi Gases

Once the goal of realizing Bose-Einstein condensation was archived it was the obvious step to work towards degeneracy of ultracold Fermi gases. However the cooling mechanism for bosons were not appropriate for cooling down fermions, hence as just described collisions between the atoms are a fundamental part of evaporative cooling. It took 4 years, to overcome some of the difficulties and in 1999 the group of Deborah Jin finally succeeded using ^{40}K [17]. The novelty here was to trap two different spin states of ^{40}K, so that collision was again possible. This mechanism is now called sympathetic cooling. Sympathetic cooling describes the process of cooling down two species of fermions with distinguishable atoms or in different spin

states, since then s-wave collisions are again possible and evaporative cooling can be applied. The experiment had then to be performed in such a way, that the two spin state populations are in balance.

The next step considering fermions was now to not only cool down atoms but molecules composed of two fermionic atoms. This goal was reached within a short time frame in the year 2004 by the groups of JILA again using ^{40}K [18] and among others by the group of Wolfgang Ketterle at MIT using ^{6}Li [19].

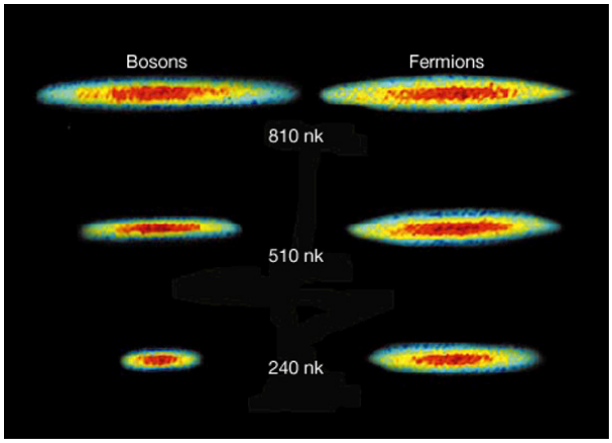


Figure 1.2: Difference of the momentum distribution of a bosonic ^{7}Li (left) and a fermionic ^{6}Li (right) at different temperatures due to the Fermi pressure in a dilute gas measured by Ref. [20]

Although the desired goal of superfluidity was not reached yet it was obvious that the degeneracy was archived. Especially interesting was the comparison of ^{7}Li and ^{6}Li, were the difference of the bosonic to the fermionic cloud could be observed by sheer comparison of the size difference caused by the Fermi pressure see Figure 1.2. We should stress the fact that all descriptions up to this point are exclusively done for dilute Fermi gases. The degeneracy is therefore only caused by the quantum nature of the system and not due to the interaction. In dilute quantum gases the distance between the atoms are normally large enough to neglect interactions other than contact interaction.

1.4 Dense Fermi Gases with Dipole-Dipole Interaction

The consideration of dense gases, which include long-range interaction such as the dipole-dipole interaction opens up new possibilities, especially due to the anisotropic nature of the interaction. Particularly interesting is the fact, that one can change the interaction from attractive to repulsive simply by adjusting an electric field relative to the trapping potential. Alone due to that reason one can hope to find new physics.

While Bose gases with dipolar interaction have been studied experimentally [21], the realization of a degenerated Fermi gas was much more difficult due to the forbidden s-wave scattering embedded by the Pauli-exclusion principle, which makes the magnetic dipole-dipole interaction difficult to observe [22].

The first experimental realization of a spin-polarized degenerated dipolar Fermi gas was accomplished by M. Lu [23]. With the help of sympathetic cooling, a mixture consisting of ^{161}Dy and the bosonic isotop ^{162}Dy were cooled down to $T/T_F \sim 0.2$.

The magnetic moment of atoms is still very small to fully appreciate the influences of the dipole-dipole interaction and for that matter the recent goal has more changed to cooling down diatomic molecules. The electric dipole-dipole interaction is of a magnitude 10^4 higher than the magnetic dipole-dipole moment. The cooling of such diatomic molecules again provide great difficulties for the experimentalists and two main strategies have been developed in order to overcome the same. The first problem consists of the enormous number of quantum states a diatomic molecule possesses, which makes it difficult to get the atom really

in the rovibrational ground state. The strategy which lead to success was to first cool down atoms and then coherently convert them to ground state molecules at low temperatures without heating the sample. Mainly this is done by the use of Feshbach resonance to switch the interaction after the cooling process from repulsive to attractive. In order to further lower the so created molecules, which at first are in a highly excited vibrational state into the rovibrational ground state one uses lasers to stimulate emission of the electronic states with appropriate lasers.

The second problem comes with the fact that most considered diatomic molecules such as the considered KRb+KRb $\rightarrow$ K_2 + Rb_2 are highly chemical reactive [24, 25]. As has been shown by Miranda et all [26] these chemical reactions can be significantly suppressed, if one confines the system of molecules in a quasi two-dimensional plane in such a way, that the dipole moments are perpendicular to the confining potential making the two-dimensional consideration of such systems not only interesting in regards of finding new physics moreover necessary to investigate such molecules. Nevertheless the new possibilities due to this confinement shouldn't be underestimated, since both the quantum and interaction effects are stronger in the case of two dimensions compared to three dimensions [27]. Experimentally the first two-dimensional Fermi gas within a harmonic trap was realized in 2010 by Martiyanov et al. [28]

One way to compare the theoretical results with experiments is by measuring the collective oscillations of the trapped sample in response to perturbations of the trapping potential. These oscillations then form the collective oscillations of the system [29]. As mentioned by Mehrtash Babadi and Eugene Demler the measurement of the frequency and the damping of these animations can be utilized to understand the properties of the ground state and to gain informations about self-energy corrections. [29]

1.5 Theoretical Description

While early phenomenological investigations of ultracold atoms such as the previously mentioned of Einstein and Landau, were very fruitful, a modern description has to be founded in the theoretical framework of quantum mechanics. In contrast to ultracold bosons being in the Bose condensate phase, which are described by a macroscopical wave function of one coordinate in position space, ultracold fermions have to be described by a quantum mechanical wave function depending on each coordinate of the particles. In order to obtain this wave function one can often use as the simplest approximation the Hartree-Fock method. Solving Hartree-Fock equations self-consistently, like done within the description of molecules, is at the present time not possible for a sample of ultracold atoms due to the sheer number of atoms. Within ultracold samples, one can distinguish between a collisionless regime, where the mean free path of the atoms is larger than the size of the sample and the hydrodynamic regime, where the mean free path of the atoms is smaller than the size of the sample. From a theoretical point of view interactions are considered negligibly weak or suppressed within the collisionless limit; while in the hydrodynamic limit the Fermi gas is supposed to be in the superfluid phase or at least a strongly interacting Fermi liquid. In three dimensions and for dipolar interaction these two regimes have been investigated by Sogo et al. [30] for the collisionless regime and by Lima et al. [31, 32] in the hydrodynamic regime.

Therefore Sogo et al. started from the Hartree Fock approximation and used a semiclassical approach by using a variational ansatz for the Wigner distribution, based on the Thomas-Fermi or local density approximation. Both approximations are used synonymously and assume that the local Fermi surface has the same form at each spatial point as in the homogeneous case [30]. While starting from a Hartree-Fock approximation and switching to the Wigner representation, one can derive the collisionless Boltzmann-Vlasov equation. Roughly speaking the difference to the collisional Boltzmann-Vlasov equation consists of an inhomogeneous term, called the collision integral in the differential equation. Before discussing the Boltzmann-Vlasov equation a little deeper, we mention the path taken by Lima et al. to describe the hydrodynamic regime. They used a variational approach to extremize the Hartree-Fock action with respect to a velocity potential as well as the time-even Wigner function. In order to implement this variational approach they restrict their

search to a velocity potential of a harmonic form and a time-even Wigner function within the local density approximation with a deformed Fermi surface. By doing so they arrive at equations which describe the static as well as the dynamic properties of a polarized dipolar Fermi gas. In a more recent work Babadi et al. [29] started to investigated the intermediate region within a two-dimensional system, between the collisionless and hydrodynamic limit by using the collisional Boltzmann-Vlasov equation, which considers the collisional regime and makes therefore no prior assumptions of being in the collisionless or hydrodynamic regime. As mentioned before and pointed out in [29], the Boltzmann-Vlasov equation can be viewed as a generalization of the classical Boltzmann transport equation by including Pauli exclusion effects in the collision integral and self-energy corrections to the quasiparticle dispersion. While their main goal is to study oscillation frequencies and damping of the generated collective excitations, they also consider self-energy corrections and find that the inclusion yields to significant corrections in the quantum degenerate regime. They consider the self-energy within the local density approximation, after correctly stating, that non-local Hartree contributions are neglectable. They then use the self-energy functional within a numerical calculation to obtain a equilibrium solution for the Boltzmann-Vlasov equation. Finally we note here that just recently a similar calculation has been carried out in three-dimensions be Wächtler et al. [33].

1.5.1 Motivation & Brief Overview

The importance of the self-energy corrections pointed out by [29] give reason to analyse the approximations needed to determine the self-energy. This is especially true for the dipole-dipole interaction which is rather strong at low distances, compared to the known Coulomb interaction. The confinement to two dimensions additionally increases this ultraviolet divergence behaviour. For this it is not a priori clear that standard assumptions within the field of ultracold quantum gases such as the local density approximation are still valid and what kind of approximations are needed in order to obtain a valid approximation for the electronic self-energy. In the following we restrict our investigation for the self-energy to the two-dimensional dipolar Fermi gas in a harmonic trap. We will thereby compare the standard semiclassical approach to the self-energy with a systematically calculated self-energy for large particle numbers. Both approaches are calculated within the Hartree-Fock approximation. Due to the anisotropy of the dipole-dipole interaction, there exist stable and unstable configurations. As we will see the semiclassical approximation describes the self-energy behaviour well for stable configurations, with increasing deviations for particles away of the center of the trap. The two approximations differs enormously for unstable dipole-dipole configurations.

The Thesis is structured as follows:
In **chapter two** we use a field theoretical description of the system by using the path integral formulation. To maintain the Pauli exclusion principle the use of Grassmann numbers is necessary. Therefore we start in **section one** with a detailed introduction to Grassmann algebras, where we develop some new notations in order to deal not only with Grassmann functions but also with Grassmann functionals. Then we follow the descriptions of [34] to introduce fermionic coherent states. Having worked out all the necessary tools, we further proceed in **section two** by introducing the fermionic coherent state path integral and derive formulas for the partition function as well as the free Green function. In order to deal with the dipole-dipole interaction we will use a perturbation theory approach. Therefore we review in **section three** briefly the Feynman rules for the partition function, with which we then derive the Feynman rules for the interacting Green function. Finally in **section four** we derive Dyson's equation from which we then obtain our Hartree-Fock equations. **Chapter three** starts with a detailed discussion of the dipole-dipole interaction. We derive the interaction behaviour and discuss the dipole-dipole interaction for three and two dimensions. **Section two** is devoted to deriving the Fourier transformations in preparation to describe the homogeneous system. In **section three** we then investigate the homogeneous three- and two-dimensional Fermi gas with dipolar interaction. This investigations have previously carried out in [35]. To see further differences between two and three dimensions, we compare our results with the corresponding Jellium systems. In **chapter four** we then calculate based on the previously derived Hartree-Fock equations systematically in large particle numbers the self-energy within a harmonic trap. In addition we calculate the same quantity in the semiclassical approximation and finally compare the results.

Chapter 2

Mathematical Background

"Since then I never pay any attention to anything by "experts." I calculate everything myself."

Richard P. Feynman [36]

2.1 Grassmann Algebra

We are going to discuss a fermionic system within the framework of the fermionic coherent state path integral. In order to do so one needs Grassmann algebra to maintain the Pauli exclusion principle, when dealing with fields instead of operators. In this chapter we will give an introduction to Grassmann algebra and elaborate all necessary calculation rules in order to derive the path integral and later the Dyson equation for fermionic functionals, which are consequently functionals of Grassmann functions. We will first start with the discrete Grassmann algebra, and then proceed to a Grassmann algebra of infinite dimensions.

2.1.1 Finite Dimensional Grassmann Algebra

One introduces a finite dimensional Grassmann algebra U over a body $\mathbb{K}$. $\mathbb{K}$ being either $\mathbb{R}$ or $\mathbb{C}$, with the two operations $\cdot : A \times A \longrightarrow A$; $(\eta_i, \eta_j) \longrightarrow \eta_i \cdot \eta_j$ which is associative and anticommutative and $+ : A \times A \longrightarrow A$; $(\eta_i, \eta_j) \longrightarrow \eta_i + \eta_j$ which is associative and commutative. Further, the following distribution law holds

$$\begin{aligned} &(\eta_1 + \eta_2)\eta_3 = \eta_1\eta_3 + \eta_2\eta_3 \ , \\ &\eta_1(\eta_2 + \eta_3) = \eta_1\eta_2 + \eta_1\eta_3 \ , \\ &\lambda(\eta_1\eta_2) = (\lambda\eta_1)\eta_2 = \eta_1(\lambda\eta_2) \ . \end{aligned} \tag{2.1.1}$$

The anticommutative property is mostly written as

$$\eta_i\eta_j = -\eta_i\eta_j \Longleftrightarrow \eta_i\eta_j + \eta_j\eta_i = 0 \Longleftrightarrow \{\eta_i, \eta_j\} = 0 \ . \tag{2.1.2}$$

Here $\{\bullet, \bullet\}$ is the anticommutator. One particular important property due to this relation is

$$\eta_k^2 = 0 \quad \forall_k \ . \tag{2.1.3}$$

A finite dimensional Grassmann algebra can be build from n such elements called generators $\{\eta_k\}\, k = 1, \ldots, n$. Due to the property (2.1.3), all elements of the algebra can then be expressed with a linear combination of these generators

$$\{1, \eta_{\lambda_1}, \eta_{\lambda_1}\eta_{\lambda_2}, \ldots, \eta_{\lambda_1}\eta_{\lambda_2} \cdot \ldots \cdot \eta_{\lambda_n}\} \ . \tag{2.1.4}$$

Where we have $0 < \eta_k \leq n$ and that the elements are by convention ordered as $\lambda_1 < \lambda_2 < \ldots < \lambda_n$. Since $\eta_k^2 = 0$ no element of the higher products contains more than one η_k. Any element of the n-dimensional Grassmann algebra can now be expressed as

$$f = f_0 + \sum_{p_1} f_{p_1}\eta_1 + \sum_{p_1<p_2} f_{p_1p_2}\eta_1\eta_2 + \ldots + \sum_{p_1<p_2<\ldots<p_n} f_{p_1p_2\ldots p_n}\eta_{p_1}\eta_{p_2}\ldots\eta_{p_n} \; . \tag{2.1.5}$$

The coefficients are complex numbers $f_k \in \mathbb{C}$ or complex functions, in which case f is a function of the generators and a complex variable. We will therefore refer to objects of the form (2.1.5) as Grassmann functions. In order to operate with Grassmann functions it is necessary to define analog operations to differentiation and integration for Grassmann functions.

Definition: Differentiation with respect to Grassmann Variables

Differentiation with respect to a Grassmann variable (generator) is defined as

$$\begin{aligned}\frac{d}{d\eta_j}\eta_{\lambda_1}\eta_{\lambda_2}\ldots\eta_{\lambda_n} &= \delta_{j\lambda_1}\eta_{\lambda_2}\cdot\ldots\cdot\eta_{\lambda_n} - \delta_{j\lambda_2}\eta_{\lambda_1}\eta_{\lambda_3}\cdot\ldots\cdot\eta_{\lambda_n} \\ &\quad + \ldots + (-1)^{n-1}\delta_{j\lambda_n}\eta_{\lambda_1}\eta_{\lambda_2}\ldots\eta_{\lambda_{n-1}} \; .\end{aligned} \tag{2.1.6}$$

Specifically the derivative is a left sided derivative. In essence one has to anticommute the variable to the left and apply the rules

$$\frac{d}{d\eta_i}1 = 0 \qquad \frac{d}{d\eta_i}\eta_j = \delta_{ij} \; . \tag{2.1.7}$$

Before we proceed to evaluate the derivation rules for Grassmann functions, we need to derive some peculiar properties of Grassmann generators.

1 Every even number of Grassmann numbers commute with another even number of Grassmann numbers.

$$[\eta_1\eta_2\ldots\eta_{2n}, \xi_1\xi_2\ldots\xi_{2k}] = 0 \; . \tag{2.1.8}$$

2 Any even number of Grassmann numbers commute with any odd number of Grassmann numbers.

$$[\eta_1\eta_2\ldots\eta_{2n}, \xi_1\xi_2\ldots\xi_{2k+1}] = 0 \; . \tag{2.1.9}$$

3 Any odd number of Grassmann numbers anticommutes with any odd number of Grassmann numbers.

$$\{\eta_1\eta_2\ldots\eta_{2n+1}, \xi_1\xi_2\ldots\xi_{2k+1}\} = 0 \; . \tag{2.1.10}$$

Proof of $[\xi_1\xi_2\ldots\xi_{2n}, \eta] = 0$

First we note that any even number of Grassmann numbers commute with another Grassmann number. This can easily be seen via induction. First we show

$$\begin{aligned}[\eta_1\eta_2, \xi] &= \eta_1\eta_2\xi - \xi\eta_1\eta_2 \\ &= -\eta_1\xi\eta_2 - \xi\eta_1\eta_2 \\ &= \xi\eta_1\eta_2 - \xi\eta_1\eta_2 \\ &= 0 \; .\end{aligned} \tag{2.1.11}$$

Now we assume

$$[\eta_1\eta_2\dots\eta_{2n},\xi]=0, \tag{2.1.12}$$

then the induction step reads

$$\begin{aligned}
[\eta_1\eta_2\dots\eta_{2n+2},\xi] &= \eta_1\eta_2\dots\eta_{2n}\eta_{2n+1}\eta_{2n+2}\xi-\xi\eta_1\eta_2\dots\eta_{2n}\eta_{2n+1}\eta_{2n+2}\\
&= -\eta_1\eta_2\dots\eta_{2n}\eta_{2n+1}\xi\eta_{2n+2}-\xi\eta_1\eta_2\dots\eta_{2n}\eta_{2n+1}\eta_{2n+2}\\
&= \eta_1\eta_2\dots\eta_{2n}\xi\eta_{2n+1}\eta_{2n+2}-\xi\eta_1\eta_2\dots\eta_{2n}\eta_{2n+1}\eta_{2n+2}\\
&= \left(\eta_1\eta_2\dots\eta_{2n}\xi-\xi\eta_1\eta_2\dots\eta_{2n}\right)\eta_{2n+1}\eta_{2n+2}\\
&= \underbrace{[\eta_1\eta_2\dots\eta_{2n},\xi]}_{=0\,\text{I.H}}\eta_{2n+1}\eta_{2n+2}\\
&= 0\,.
\end{aligned} \tag{2.1.13}$$

Proof of $[\eta_1\eta_2\dots\eta_{2n},\xi_1\xi_2\dots\xi_k]=0$

Next we verify that an arbitrary number of even Grassmann numbers commute with any other number of Grassmann numbers. Here and in the following proofs, we leave out the initial step as it is trivial. We are going to do the induction over k. I.e. the induction hypothesis holds true for

$$[\eta_1\eta_2\dots\eta_{2n},\xi_1\xi_2\dots\xi_k]=0 \tag{2.1.14}$$

and conclude

$$\begin{aligned}
[\eta_1\eta_2\dots\eta_{2n},\xi_1\xi_2\dots\xi_{k+1}] &= \eta_1\eta_2\dots\eta_{2n}\xi_1\xi_2\dots\xi_{k+1}-\xi_1\xi_2\dots\xi_{k+1}\eta_1\eta_2\dots\eta_{2n}\\
&= \eta_1\eta_2\dots\eta_{2n}\xi_1\xi_2\dots\xi_{k+1}-\xi_1\xi_2\dots\xi_k\xi_{k+1}\eta_1\eta_2\dots\eta_{2n}\\
&= \eta_1\eta_2\dots\eta_{2n}\xi_1\xi_2\dots\xi_{k+1}-\xi_1\xi_2\dots\xi_k\eta_1\eta_2\dots\eta_{2n}\xi_{k+1}\\
&= \left(\eta_1\eta_2\dots\eta_{2n}\xi_1\xi_2\dots\xi_k-\xi_1\xi_2\dots\xi_k\eta_1\eta_2\dots\eta_{2n}\right)\xi_{k+1}\\
&= \underbrace{[\eta_1\eta_2\dots\eta_{2n},\xi_1\xi_2\dots\xi_k]}_{=0\,\text{I.H}}\xi_{k+1}=0\,.
\end{aligned} \tag{2.1.15}$$

Proof of $\{\eta_1\eta_2\dots\eta_{2n+1},\xi_1\xi_2\dots\xi_{2k+1}\}=0$

Next we will verify that two arbitrary odd numbers of Grassmann numbers anticommute. So first we have to verify that one Grassmann number anticommute with an odd number of Grassmann variables, so we assume

$$\{\eta_1\eta_2\dots\eta_{2n+1},\xi\}=0\,, \tag{2.1.16}$$

then we get immediately

$$\begin{aligned}
\{\eta_1\eta_2\dots\eta_{2k+3},\xi\} &= \eta_1\eta_2\dots\eta_{2k+3}\xi+\xi\eta_1\eta_2\dots\eta_{2k+3}\\
&= \eta_1\eta_2\dots\eta_{2k+1}\eta_{2k+2}\eta_{2k+3}\xi+\xi\eta_1\eta_2\dots\eta_{2k+3}\\
&= \eta_1\eta_2\dots\eta_{2k+1}\xi\eta_{2k+2}\eta_{2k+3}+\xi\eta_1\eta_2\dots\eta_{2k+3}\\
&= \left(\eta_1\eta_2\dots\eta_{2k+1}\xi+\xi\eta_1\eta_2\dots\eta_{2k+1}\right)\eta_{2k+2}\eta_{2k+3}\\
&= \underbrace{\{\eta_1\eta_2\dots\eta_{2k+1},\xi\}}_{=0\,\text{I.H.}}\eta_{2k+2}\eta_{2k+3}=0\,.
\end{aligned} \tag{2.1.17}$$

Now we are ready to do the next induction for an arbitrary $n>0$ and do the induction over k. We assume

$$\{\eta_1\eta_2\dots\eta_{2n+1},\xi_1\xi_2\dots\xi_{2k+1}\}=0\,, \tag{2.1.18}$$

and do the induction

$$\begin{aligned}\{\eta_1\eta_2\dots\eta_{2n+1},\xi_1\xi_2\dots\xi_{2k+3}\} &= \eta_1\eta_2\dots\eta_{2n+1}\xi_1\xi_2\dots\xi_{2k+3}+\xi_1\xi_2\dots\xi_{2k+3}\eta_1\eta_2\dots\eta_{2n+1}\\ &= \eta_1\eta_2\dots\eta_{2n+1}\xi_1\xi_2\dots\xi_{2k+3}+\xi_1\xi_2\dots\xi_{2k+1}\xi_{2k+2}\xi_{2k+3}\eta_1\eta_2\dots\eta_{2n+1}\\ &= \eta_1\eta_2\dots\eta_{2n+1}\xi_1\xi_2\dots\xi_{2k+3}+\xi_1\xi_2\dots\xi_{2k+1}\eta_1\eta_2\dots\eta_{2n+1}\xi_{2k+2}\xi_{2k+3}\\ &= \left(\eta_1\eta_2\dots\eta_{2n+1}\xi_1\xi_2\dots\xi_{2k+1}+\xi_1\xi_2\dots\xi_{2k+1}\eta_1\eta_2\dots\eta_{2n+1}\right)\xi_{2k+2}\xi_{2k+3}\\ &= \underbrace{\left\{\eta_1\eta_2\dots\eta_{2n+1},\xi_1\xi_2\dots\xi_{2k+1}\right\}}_{=0\,\text{I.H.}}\xi_{2k+2}\xi_{2k+3}\,. \end{aligned} \tag{2.1.19}$$

We can now summarize the results as

$$[\text{even},\text{even}]=0 \qquad [\text{even},\text{odd}]=0 \qquad \{\text{odd},\text{odd}\}=0\,. \tag{2.1.20}$$

With this properties, it is clear from (2.1.5) that two arbitrary Grassmann functions do not commute. So in general we have

$$[f(\eta),g(\eta)]\neq 0\,. \tag{2.1.21}$$

This leads immediately to the definition of even and odd Grassmann functions. Naturally they are given by

$$\begin{aligned} f^+(\eta) &:= f_0+\sum_{p_1<p_2} f_{p_1p_2}\eta_{p_1}\eta_{p_2}+\sum_{p_1<p_2<p_3<p_4} f_{p_1p_2p_3p_4}\eta_{p_1}\eta_{p_2}\eta_{p_3}\eta_{p_4}+\dots+\sum_{p_1<p_2<\dots<p_{2n}} f_{p_1p_2\dots p_{2n}}\eta_{p_1}\eta_{p_2}\dots\eta_{p_{2n}}\,,\\ f^-(\eta) &:= f_0+\sum_{p_1} f_{p_1}+\sum_{p_1<p_2<p_3} f_{p_1p_2p_3}\eta_{p_1}\eta_{p_2}\eta_{p_3}+\dots+\sum_{p_1<p_2<\dots p_{2n+1}} f_{p_1p_2\dots p_{2n+1}}\eta_{p_1}\eta_{p_2}\dots\eta_{p_{2n+1}}\,, \end{aligned} \tag{2.1.22}$$

respectively. Another form to characterize the element of a Grassmann algebra is by introducing an automorphism P, which acts as a parity operator

$$P(\eta_{\lambda_1}\dots\eta_{\lambda_n})=(-1)^n\eta_{\lambda_1}\dots\eta_{\lambda_n}\,. \tag{2.1.23}$$

So, for an even function one has $P(f^+)=f^+$ and for an odd function one has $P(f^-)=-f^-$. Now all the elements of the algebra U can be expressed by an even and an odd part of the algebra. The even parts of the algebra will be called U^+ the odd parts of the algebra will be denoted by U^-. We will now write even functions as f^+ and odd functions as f^-. From the properties (2.1.8),(2.1.9),(2.1.10) it immediately follows:

$$\left[f^+,g^+\right]=0\,,\quad \left[f^+,g^-\right]=0\,,\quad \left[f^-,g^-\right]\neq 0\,,\quad \left[f,g^+\right]=0\,,\quad \left[f,g^-\right]\neq 0\,. \tag{2.1.24}$$

At this point we are ready to introduce some differentiation rules for Grassmann functions. First we note from formula (2.1.5), that with respect to any variable η_k we can write a Grassmann function as

$$f(\eta_k)=f_1^+ + f_1^- + \eta_k(f_2^+ + f_2^-)\,. \tag{2.1.25}$$

We translate the above given commutator relations to

$$\begin{aligned} [\text{even, even}]=0 \quad &\Leftrightarrow \quad [f_i^+,f_j^+]=0\,,\\ [\text{even, odd }]=0 \quad &\Leftrightarrow \quad [f_i^+,f_j^-]=0\,,\\ \{\text{odd, odd}\}=0 \quad &\Leftrightarrow \quad \left\{f_i^-,f_j^-\right\}=0\,. \end{aligned} \tag{2.1.26}$$

Now we take two arbitrary functions and write them with respect to η_k as

$$\begin{aligned} f &= f_1^+ + f_1^- + \eta\left(f_2^+ + f_2^-\right)\\ g &= g_1^+ + g_1^- + \eta\left(g_2^+ + g_2^-\right)\,, \end{aligned} \tag{2.1.27}$$

where we have now simply written η instead of η_k. Now we can simply form the product

$$\begin{aligned} fg &= f_1^+ g_1^+ + f_1^+ g_1^- + f_1^+ \eta(g_2^+ + g_2^-) + f_1^- g_1^+ + f_1^- g_1^- + f_1^- \eta(g_2^+ + g_2^-) \\ &\quad + \eta(f_2^+ + f_2^-) g_1^+ + \eta(f_2^+ + f_2^-) g_1^- + \eta(f_2^+ + f_2^-)\eta(g_2^+ + g_2^-) \\ &= f_1^+ g_1^+ + f_1^+ g_1^- + \eta f_1^+(g_2^+ + g_2^-) + f_1^- g_1^+ + f_1^- g_1^- - \eta f_1^-(g_2^+ + g_2^-) \\ &\quad + \eta(f_2^+ + f_2^-) g_1^+ + \eta(f_2^+ + f_2^-) g_1^- + \eta^2(f_2^+ - f_1^-)(g_2^+ + g_2^-)\,, \end{aligned} \tag{2.1.28}$$

and differentiate (2.1.28) as follows

$$\begin{aligned} \frac{\partial(fg)}{\partial\eta} &= f_1^+(g_2^+ + g_2^-) - f_1^-(g_2^+ + g_2^-) + (f_2^+ + f_2^-) g_1^+ + (f_2^+ + f_2^-) g_1^- \\ &= (f_1^+ - f_1^-)(g_2^+ + g_2^-) + (f_2^+ + f_2^-)(g_1^+ + g_1^-) \\ &= \left[f_1^+ - f_1^- - \eta(f_2^+ - f_2^-) + \eta(f_2^+ - f_2^-)\right](g_2^+ + g_2^-) + (f_2^+ + f_2^-)(g_1^+ + g_1^-) \\ &= \left[f_1^+ - f_1^- - \eta(f_2^+ - f_2^-)\right](g_2^+ + g_2^-) + \eta(f_2^+ - f_2^-)(g_2^+ + g_2^-) + (f_2^+ + f_2^-)(g_1^+ + g_1^-) \\ &= \left[f_1^+ - f_1^- - \eta(f_2^+ - f_2^-)\right](g_2^+ + g_2^-) + (f_2^+ + f_2^-)\eta(g_2^+ + g_2^-) + (f_2^+ + f_2^-)(g_1^+ + g_1^-) \\ &= \left[f_1^+ - f_1^- - \eta(f_2^+ - f_2^-)\right](g_2^+ + g_2^-) + (f_2^+ + f_2^-)[g_1^+ + g_1^- + \eta\left(g_2^+ + g_2^-\right)] \\ &= P(f)\frac{\partial g}{\partial\eta} + \frac{\partial f}{\partial\eta} g\,. \end{aligned} \tag{2.1.29}$$

In the last step we use the parity operator (2.1.23) on (2.1.25)

$$P(f) = f_1^+ - f_1^- - \eta(f_2^+ - f_2^-)\,. \tag{2.1.30}$$

Next we are going to need the chain rule. The chain rule for Grassmann functions seems to be omitted in the literature. It is one mentioned in [37], however this chain rule seems to be limited to one dimension[1]. In the standard introduction to Grassmann algebra from F.A. Berezin [38], there are also given just two examples of the chain rule for Grassmann functions. Here we present two chain rules for Grassmann functions, one combining Grassmann functions with analytic functions and one for actually chaining Grassmann functions. We start with the definition and the proof of the discrete Grassmann chain rule with an analytic function.

Chain Rule for an Analytic Function and a Grassmann Function

If we have an analytic function $f : \mathbb{C} \to \mathbb{C}$ and a Grassmann function $g : U^- \to U^+, \eta \to g(\eta)$, the following chain rule holds true

$$\frac{\partial}{\partial\eta} f(g(\eta)) = \frac{\partial g}{\partial\xi}\frac{\partial f}{\partial g}\bigg|_{\xi=0}\,. \tag{2.1.31}$$

Proof

First we note that any analytic function can be expressed with the Laurent series

$$f(z) = \sum_{n=0}^{\infty} c_n (z - z_0)^n\,, \quad U_R(z_0) \leq \infty\,. \tag{2.1.32}$$

[1]The chain rule is given as $\frac{\partial A}{\partial\eta} = \frac{\partial f}{\partial\eta}\frac{\partial A}{\partial f} + \frac{\partial g}{\partial\eta}\frac{\partial A}{\partial g}$ where g is an even and f an odd function of η. Here $A \equiv A(f, g)$. This chain rule can be proven by assuming A has the following form $A = a_1^+ + a_1^- + g\left(a_2^+ + a_2^-\right) + f\left(a_3^+ + a_3^-\right)$. However not all Grassmann functions follow this form.

The definition of chaining the analytic function and the Grassmann function is given via the Laurent expansion. With the above introduced notation we can write $g : U^- \to U^+$ in the form: $g = g_1^+ + \eta\, g_2^-$. Obviously then we have

$$P(g) = g_1^+ + (-\eta)(-g_2^-) = g_1^+ + \eta g_2^- = g \quad \Longrightarrow \quad g \in U^+ \,. \tag{2.1.33}$$

First we observe

$$\begin{aligned}
\left(g_1^+ + \eta g_2^-\right)^2 &= \left(g_1^+ + \eta g_2^-\right)\left(g_1^+ + \eta g_2^-\right) = \left(g_1^+\right)^2 + g_1^+ \eta g_2^- + \eta g_2^- g_1^+ \\
&= \left(g_1^+\right)^2 + \eta g_2^- g_1^+ + \eta g_2^- g_1^+ \\
&= \left(g_1^+\right)^2 + 2\eta g_2^- g_1^+ \\
\left(g_1^+ + \eta g_2^-\right)^3 &= \left(g_1^+ + \eta g_2^-\right)\left[\left(g_1^+\right)^2 + 2\eta g_2^- g_1^+\right] \\
&= \left(g_1^+\right)^3 + 2g_1^+ \eta g_2^- g_1^+ + \eta g_2^- (g_1^+)^2 \\
&= \left(g_1^+\right)^3 + 2\eta g_2^- (g_1^+)^2 + \eta g_2^- (g_1^+)^2 \\
&= \left(g_1^+\right)^3 + 3\eta g_2^- (g_1^+)^2 \\
&\vdots \\
\left(g_1^+ + \eta g_2^-\right)^n &= (g_1^+)^n + n\,\eta g_2^- (g_1^+)^{n-1} \,,
\end{aligned} \tag{2.1.34}$$

and look at

$$\begin{aligned}
f(g) &= \sum_{n=0}^{\infty} c_n g^n = \sum_{n=0}^{\infty} c_n \left(g_1^+ + \eta g_2^-\right)^n \\
&= \sum_{n=0}^{\infty} c_n \left[(g_1^+)^n + n\eta g_2^- (g_1^+)^{n-1}\right] \\
&= \sum_{n=0}^{\infty} c_n (g_1^+)^n + \sum_{n=0}^{\infty} c_n n \eta g_2^- (g_1^+)^{n-1} \,,
\end{aligned} \tag{2.1.35}$$

then we have

$$\begin{aligned}
\frac{\partial f(g)}{\partial \eta} &= \sum_{n=0}^{\infty} c_n n g_2^- (g_1^+)^{n-1} \\
&= g_2^- \sum_{n=0}^{\infty} c_n n (g_1^+)^{n-1} = \frac{\partial g}{\partial \eta} \sum_{n=0}^{\infty} c_n \frac{\partial}{\partial g} g^n \bigg|_{\eta=0} \\
&= \frac{\partial g}{\partial \eta}\frac{\partial}{\partial g} \sum_{n=0}^{\infty} c_n g^n = \frac{\partial g}{\partial \eta}\frac{\partial f}{\partial g}\bigg|_{\eta=0} \,.
\end{aligned}$$

Here we have used

$$\frac{\partial}{\partial g} g^n \bigg|_{\eta=0} n g^{n-1} \bigg|_{\eta=0} = n \left(g_1^+ + \eta g_2^-\right)^{n-1} \bigg|_{\eta=0} = n (g_1^+)^{n-1}$$

and

$$\frac{\partial g}{\partial \eta} = \frac{\partial}{\partial \eta}\left(g_1^+ + \eta g_2^-\right) = g_2^- \,. \tag{2.1.36}$$

The same chain rule doesn't hold true for odd Grassmann functions of the form $g : U^- \to U^-$. Which can easily be seen by a counter example. However a very similar chain rule can be shown for this type of functions.

The last chain rule is (2.1.31) in contrast to the following chain rule, which only holds true for functions of the form $g : U^- \to U^-$.

Chain Rule for Two Grassmann Functions

Be F an arbitrary Grassmann function. That is we don't make any restrictions for F to be even or odd. Further be $\eta_1, \ldots, \eta_n$ odd Grassmann functions: $\eta_k \in U^-$ then we have

$$\frac{\partial}{\partial \xi} F\left(\eta_1(\xi)\eta_2(\xi), \ldots \eta_n(\xi)\right) = \sum_k \frac{\partial \eta_k}{\partial \xi} \frac{\partial F}{\partial \eta_k}\bigg|_{\xi=0} . \tag{2.1.37}$$

Proof

Each η_k depends on $\xi_1, \ldots, \xi_n$. For each ξ_ℓ we can write $\eta_k(\xi_\ell) = u^-_{1k} + \xi_\ell u^+_{2k}$. We are now going to write ξ for our specific selected ξ_ℓ. Then we can write for any product

$$\begin{aligned}\prod_{\ell=1}^{n} \eta_{p_\ell} &= \prod_{\ell=1}^{n} u^-_{1p_\ell} + (-1)^{n-1}\xi \sum_{k=n}^{1} (-1)^{n+2-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n} u^-_{1p_\ell} u^+_{2p_k} \\ &= \prod_{\ell=1}^{n} u^-_{1p_\ell} + \xi \sum_{k=n}^{1} (-1)^{2n+1-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n} u^-_{1p_\ell} u^+_{2p_k} \ . \end{aligned} \tag{2.1.38}$$

Now let us look at an arbitrary function f for an odd transformation.

$$\begin{aligned} f &= f_0 + \sum_{p_1} f_{p_1}\eta_{p_1} + \sum_{p_1<p_2} f_{p_1p_2}\eta_{p_1}\eta_{p_2} + \sum_{p_1<p_2<p_3} f_{p_1p_2p_3}\eta_{p_1}\eta_{p_2}\eta_{p_3} \\ &\quad + \ldots + \sum_{p_1<p_2<\ldots<p_n} f_{p_1p_2\ldots p_n}\eta_{p_1}\eta_{p_2}\ldots\eta_{p_n} \\ &= f_0 + \sum_{p_1} f_{p_1}(u^-_{1p_1} + \xi u^+_{2p_1}) + \sum_{p_1<p_2} f_{p_1p_2}\left(\prod_{\ell=1}^{2} u^-_{1p_\ell} + \xi\sum_{k=2}^{1}(-1)^{5-k}\prod_{\substack{\ell=1\\\ell\neq k}}^{2} u^-_{1p_\ell}u^+_{2p_k}\right) \\ &\quad + \sum_{p_1<p_2<p_3}\left(\prod_{\ell=1}^{3} u^-_{1p_\ell} + \xi\sum_{k=3}^{1}(-1)^{7-k}\prod_{\substack{\ell=1\\\ell\neq k}}^{3} u^-_{1p_\ell}u^+_{2p_k}\right) \\ &\quad + \ldots + \sum_{p_1<p_2<\ldots<p_n}\left(\prod_{\ell=1}^{n} u^-_{1p_\ell} + \xi\sum_{k=n}^{1}(-1)^{2n+1-k}\prod_{\substack{\ell=1\\\ell\neq k}}^{n} u^-_{1p_\ell}u^+_{2p_k}\right) \\ &= \xi\left[\sum_{p_1} f_{p_1}u^+_{2p_1} + \sum_{p_1<p_2} f_{p_1p_2}\sum_{k=2}^{1}(-1)^{5-k}\prod_{\substack{\ell=1\\\ell\neq k}}^{2} u^-_{1p_\ell}u^+_{2p_k}\right. \\ &\quad \left. + \ldots + \sum_{p_1<p_2<\ldots<p_n}\left(\sum_{k=n}^{1}(-1)^{2n+1-k}\prod_{\substack{\ell=1\\\ell\neq k}}^{n} u^-_{1p_\ell}u^+_{2p_k}\right)\right] + \text{Terms without } \xi \ , \end{aligned} \tag{2.1.39}$$

now follows

$$\frac{\partial f}{\partial \xi} = \sum_{p_1} f_{p_1} u^+_{2p_1} + \sum_{p_1<p_2} f_{p_1p_2} \sum_{k=2}^{1} (-1)^{5-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{2} u^-_{1p_\ell} u^+_{2p_k}$$
$$+ \ldots + \sum_{p_1<p_2<\ldots<p_n} \left(\sum_{k=n}^{1} (-1)^{2n+1-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n} u^-_{1p_\ell} u^+_{2p_k} \right) . \tag{2.1.40}$$

A few words about the notation. Obviously the sums run over a given set of coefficients to a given function f. If in f a certain coefficient is not present it is zero. Equally if a coefficient in a given odd transformation is not present.

Now we look at a function f (2.1.5) again, the derivation with respect to a certain η_k leads

$$\begin{aligned}
\frac{\partial f}{\partial \eta_k} &= f_k + (-1)^{P^{(2)}_{p_k}} \sum_{p_1/p_k} \hat{f}_{k\,p_1} \eta_{p_1} + (-1)^{P^{(3)}_{p_k}} \sum_{(p_1<p_2)/p_k} \hat{f}_{k\,p_1p_2} \eta_{p_1} \eta_{p_2} \\
&\quad + \ldots + (-1)^{P^{(n)}_{p_k}} \sum_{(p_1<p_2<\ldots<p_{n-1})/p_k} \hat{f}_{k\,p_1\ldots p_{n-1}} \eta_{p_1} \ldots \eta_{p_{n-1}} \\
&= f_k + (-1)^{P^{(2)}_{p_k}} \sum_{p_1/p_k} \hat{f}_{kp_1} \left(\prod_{\ell=1}^{1} u^-_{1p_\ell} + \xi \sum_{k=1}^{1} (-1)^{5-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{1} u^-_{1p_\ell} u^+_{2p_k} \right) \\
&\quad + (-1)^{P^{(3)}_{p_k}} \sum_{(p_1<p_2)/p_k} \hat{f}_{k\,p_1p_2} \left(\prod_{\ell=1}^{2} u^-_{1p_\ell} + \xi \sum_{k=2}^{1} (-1)^{7-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{2} u^-_{1p_\ell} u^+_{2p_k} \right) \\
&\quad + \ldots + \\
&\quad + (-1)^{P^{(n)}_{p_k}} \sum_{(p_1<p_2<\ldots<p_{n-1})/p_k} \hat{f}_{kp_1\ldots p_{n-1}} \left(\prod_{\ell=1}^{n-1} u^-_{1p_1} + \xi \sum_{k=n-1}^{1} + (-1)^{2n+1-k} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n-1} u^-_{1p_\ell} u^+_{2p_k} \right) .
\end{aligned} \tag{2.1.41}$$

Here the notation has to be understood as follows, $P^{(2)}_{p_k}$ gives either an even or odd number, depending in which position η_k in a given function stands. For example, for the first place $p_k = 1$ $P^{(n)}_{p_1} = 0$, for the second place $P^{(n)}_{p_2} = 1$ and so on. The sums again run over a set of given functions. Here the notation $(p_1 < p_2)/p_k$ means, that no summand includes η_k. Finally we put a hat above f, hence by convention the generators are ordered and the coefficients are also ordered by convention. Here we wrote k at the first place and therefore introduced the hat.

$$\left.\frac{\partial f}{\partial \eta_k}\right|_{\xi=0} = f_k + (-1)^{P^{(2)}_{p_k}} \sum_{p_1/p_k} \hat{f}_{kp_1} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{1} u^-_{p_\ell} + (-1)^{P^{(3)}_{p_k}} \sum_{(p_1<p_2)/p_k} \hat{f}_{kp_1p_2} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{2} u^-_{1p_\ell}$$
$$+ \ldots + (-1)^{P^{(n)}_{p_k}} \sum_{(p_1<p_2<\ldots<p_{n-1})/p_k} \hat{f}_{kp_1\ldots p_{n-1}} \prod_{\substack{\ell=1 \\ \ell\neq k}}^{n-1} u^-_{1p_\ell} . \tag{2.1.42}$$

Now for each $\eta_k = u^-_{1k} + \xi u^+_{2k}$ we have $\frac{\partial \eta_k}{\partial \xi} = u^+_{2k}$. So it follows

$$\sum_k \frac{\partial \eta_k}{\partial \xi}\frac{\partial f}{\partial \eta_k}\bigg|_{\xi=0} = \sum_k f_k u^+_{2k} + \sum_k (-1)^{P^{(2)}_{p_k}} \sum_{p_1/p_k} \hat{f}_{kp_1} \prod_{\substack{\ell=1\\ \ell\neq k}}^{1} u^-_{1p_\ell} u^+_{2k} + \sum_k (-1)^{P^{(3)}_{p_k}} \sum_{(p_1<p_2)/p_k} \hat{f}_{kp_1p_2} \prod_{\substack{\ell=1\\ \ell\neq k}}^{2} u^-_{1p_\ell} u^+_{2k}$$
$$+ \ldots + \sum_k (-1)^{P^{(n)}_{p_k}} \sum_{(p_1<p_2<\ldots<p_{n-1})/p_k} \hat{f}_{kp_1\ldots p_{n-1}} \prod_{\substack{\ell=1\\ \ell\neq k}}^{n-1} u^-_{1p_\ell} u^+_{2k} \,. \tag{2.1.43}$$

That the two expressions (2.1.40), (2.1.43) are equal is evident except for the minus sign. So first we notice that in the second expression (2.1.43) each k-sum term has always alternating signs and starts with a plus. The sum over k here goes over each η_k present in a given monomial to a given function, so each k-sum runs over $1, 2, \ldots, n$ summands. In the first expression (2.1.40) the sum starts either with a plus or minus sign, but the sum runs through the expressions from k to 1 in opposite to the second expression, (2.1.43) which runs from 1 to k. Hence we can have even and odd monomials and since the terms within the first expression (2.1.40) alternates, starting with a minus sign due to $2n + 1 - k$ starting from $k = n$, the last summand within this k-sum corresponds with the first summand in the second expression (2.1.43). We note that the sign change in (2.1.43) is due to the outer product of the chain rule, which is always present if one defines the chain rule in the common way. The alternation of the minus sign in the first expression (2.1.40) is only present in the case of odd functions. That is why the chain rule dose not work for even functions. Before we conclude the section on the discrete Grassmann algebra, we have to look at the following properties.

Exponential Function of Grassmann Numbers

Next we use the Baker-Campbell-Hausdorff formula [39] which reads as follows

$$e^x e^y = e^z \quad \text{with} \quad Z = X + \int_0^1 \mathrm{d}t\, g\left(e^{\mathrm{ad}_x} e^{t\,\mathrm{ad}_y}\right)[y] \quad \text{and} \quad g(z) = \frac{z\log(z)}{z-1}\,. \tag{2.1.44}$$

Where for $\mathscr{G}$ being a Lie algebra. $\mathrm{ad}_x : \mathscr{G} \to \mathscr{G}$ is a linear map defined by

$$\mathrm{ad}_x[y] := [x, y]\,. \tag{2.1.45}$$

Now expanding Z till the third order one gets

$$Z \approx x + y + \frac{1}{2}[x,y] + \frac{1}{12}\left([x,[x,y]] - [y,[x,y]]\right) - \frac{1}{24}[x,[y,[x,y]]] + \ldots \,. \tag{2.1.46}$$

From the expansion of the integral as done in Appendix D, it is evident that all higher cascading commutators depend on $[x, y]$ as the innermost commutator. Hence if $[x, y]$ vanishes, all higher commutators vanish as well. So we get immediately

$$e^{\sum_{\lambda_k} \eta_{\lambda_k}\eta_{\lambda_{k+1}}\cdots\eta_{\lambda_{2k}}} = \prod_{\lambda_k} e^{\eta_{\lambda_k}\eta_{\lambda_{k+1}}\cdots\eta_{\lambda_{2k}}} \quad \Leftrightarrow \quad e^{\sum_{\lambda_k}^{2n}\prod_k \eta_{\lambda_k}} = \prod_{\lambda_k}^{2n} e^{\prod_k \eta_{\lambda_k}}\,. \tag{2.1.47}$$

Now the following relation is obvious

$$\left[e^{\sum_\lambda \xi_{\lambda_1}\xi_{\lambda_2}\cdots\xi_{\lambda_{2k}}}, \eta_1\ldots\eta_n\right] = \prod_{\lambda_k}\left[e^{\xi_{\lambda_1}\xi_{\lambda_2}\cdots\xi_{\lambda_{2k}}}, \eta_1\ldots\eta_n\right] = \prod_{\lambda_k}[1 - \xi_{\lambda_1}\xi_{\lambda_2}\ldots\xi_{\lambda_{2k}}, \eta_1\ldots\eta_n]$$
$$= \prod_{\lambda_k}(\underbrace{[1,\eta_1\ldots\eta_n]}_{=0} - \underbrace{[\xi_{\lambda_1}\xi_{\lambda_2}\ldots\xi_{\lambda_{2k}}, \eta_1\ldots\eta_n]}_{=0}) = 0\,. \tag{2.1.48}$$

In the same manner we can show

$$\left[e^{\sum_{\lambda_n}\eta_{\lambda_1}\dots\eta_{\lambda_{2n}}}, e^{\sum_{\lambda_k}\xi_{\lambda_1}\dots\xi_{\lambda_{2k}}}\right] = \prod_{\lambda_n}^{2n}\prod_{\lambda_k}^{2k}[1-\eta_{\lambda_n}, 1-\eta_{\lambda_k}] = \prod_{\lambda_k}^{2n}\prod_{\lambda_k}^{2k}[\eta_{\lambda_n}, \eta_{\lambda_k}] = 0\,. \tag{2.1.49}$$

Furthermore, we immediately get the relation

$$\left[e^{f^+(\eta)}, g(\eta)\right] = 0\,, \tag{2.1.50}$$

for any even Grassmann function $f^+(\eta)$ and any Grassmann function $g(\eta)$. The last result will be used extensively.

Involution of Grassmann Numbers

On every even Grassmann algebra of $n = 2p$, one can introduce an involution operation by associating with each generator η_k one generator $\overline{\eta}_k$ and demand the following properties

$$\begin{aligned}\overline{(\eta_k)} &= \overline{\eta}_k\,,\\ \overline{(\overline{\eta}_k)} &= \eta_k\,,\\ \overline{(\lambda\eta_k)} &= \overline{\lambda}\overline{\eta}_k\lambda \in \mathbb{C}\,,\end{aligned} \tag{2.1.51}$$

as well as

$$\overline{(\eta_{\lambda_1}, \eta_{\lambda_2}\dots\eta_{\lambda_n})} = \overline{\eta}_{\lambda_n}\overline{\eta}_{\lambda_{n-1}}\dots\overline{\eta}_{\lambda_1}\,. \tag{2.1.52}$$

The two generators η_k and $\overline{\eta}_k$ are completely independent and so all derived rules above are applicable. Sometimes involuted Grassmann numbers are also called complex Grassmann numbers. However one should keep in mind that there are also objects of the form $\eta_1 + \eta_2$, which are then called complex Grassmann numbers.

It is worth pointing out that this relation (2.1.48) includes the often used relations

$$\left[e^{\sum_\lambda \overline{\xi}_\lambda\xi_\lambda}, \eta\right] = 0 \quad \text{and} \quad \left[e^{\sum_\lambda \overline{\xi}_\lambda\xi_\lambda}, \eta_1, \dots \eta_n\right] = 0\,, \tag{2.1.53}$$

We note that the general Hamiltonian in normal order is an operator of the form

$$\hat{H} = \frac{1}{n!}\sum_{\lambda_1,\dots\lambda_n}\sum_{\mu_1\dots\mu_n}\langle\lambda_1\dots\lambda_n|\,H\,|\mu_1\dots\mu_n\rangle\, a^\dagger_{\lambda_1}\dots a^\dagger_{\lambda_n}a_{\mu_n}\dots a_{\mu_1} \tag{2.1.54}$$

so for any operator there is always an even combination of creation and annihilation operators, so we conclude that we have

$$\left[e^{-i\frac{\varepsilon}{\hbar}H[\overline{\varphi},\varphi]}, \xi_k\right] = 0\,. \tag{2.1.55}$$

Berezin Integration

The definition of Grassmann integration was introduced by F.A. Berezin [38] and we will call it explicitly Berezin integration. Since every second derivative of a Grassmann variable vanishes, it is not possible to define Grassmann integration as the inverse of differentiation. The idea now is rather to define Berezin integrals by

$$\begin{aligned}\int \mathrm{d}\eta\, 1 &= 0\,,\\ \int \mathrm{d}\eta_k\, \eta_\ell &= \delta_{k\,\ell}\,.\end{aligned} \tag{2.1.56}$$

Surprisingly this definition is sufficient to deal with Grassmann integrals. If we have involuted Grassmann numbers, we shall write these to the left of the normal Grassmann integrals. So we will write

$$\int \mathrm{d}\overline{\eta} \int \mathrm{d}\eta \quad \text{and not} \quad \int \mathrm{d}\eta \int \mathrm{d}\overline{\eta}\,, \tag{2.1.57}$$

since obviously these two operations are not the same. We will need Berezin integrals in order to introduce the overcompleteness relation within the fermionic coherent states and occasionally to solve a Grassmann Gauss integral. The only non trivial thing when dealing with Berezin integration is the transformation law for interchanging the integration variable. We outline here an elegant proof from [34]. The transformation law to be shown is

$$\int d\overline{\eta}_1 d\eta_1 \dots \overline{\eta}_n d\eta_n P(\overline{\eta},\eta) = \left|\frac{\partial(\overline{\xi},\xi)}{\partial(\overline{\eta},\eta)}\right| \int d\overline{\xi}_1 d\xi_1 \dots d\overline{\xi}_n d\xi_n P(\overline{\eta}(\overline{\xi},\xi),\eta(\overline{\xi},\xi))\,. \tag{2.1.58}$$

Now the idea is to write the variables as

$$\begin{aligned} \left(\overline{\eta}_1\overline{\eta_2}\dots\overline{\eta}_n\eta_n\eta_{n-1}\dots\eta_1\right) &\equiv \left(\tilde{\eta}_1\tilde{\eta}_2\dots\tilde{\eta}_{2n}\right)\,, \\ \left(\overline{\xi}_1\overline{\xi_2}\dots\overline{\xi}_n\xi_n\xi_{n-1}\dots\xi_1\right) &\equiv \left(\tilde{\xi}_1\tilde{\xi}_2\dots\tilde{\xi}_{2n}\right)\,, \end{aligned} \tag{2.1.59}$$

and rewrite them as

$$\tilde{\eta}_k = M_{k\ell}\,\tilde{\xi}_\ell\,. \tag{2.1.60}$$

So it is clear that in relation (2.1.58) only terms survive, which contain each $\tilde{\eta}_\ell$ in one factor only once. This can be written as $p\prod_{\ell=1}^{2n}\tilde{\eta}$. Thus the only thing remaining, is to determine J in the equation

$$\int d\overline{\eta}_1 d\eta_1 \dots \overline{\eta}_n d\eta_n p \prod_{\ell=1}^{2n}\tilde{\eta}_\ell = J\int d\overline{\xi}_1 d\xi_1 \dots d\overline{\xi}_n d\xi_n p \prod_{\ell=1}^{2n}\left(\sum_k M_{k\ell}\tilde{\xi}_k\right)\,. \tag{2.1.61}$$

The left side can directly be evaluated to $p(-1)^n$. Since each summand on the right side can include each Grassmann variable only once, and there are $2n$ variables, the only non vanishing contribution on the right arises, if the $(2n)!$ permutations are present. Now one can calculate

$$\begin{aligned} p(-1)^n &= Jp\int d\overline{\xi}_1\, d\xi_1 \dots d\overline{\xi}_n d\xi_n \sum_P \prod_\ell M_{\ell P_\ell}\tilde{\xi}_{P_\ell} \\ &= Jp\sum_P \prod_\ell M_{\ell P_\ell}(-1)^{P_\ell}\int d\overline{\xi}_1 d\xi_1 \dots \overline{\xi}_n d\xi_n \tilde{\xi}_1\tilde{\xi}_2\dots\tilde{\xi}_{2n} \\ &= Jp(-1)^n \det(M)\,, \end{aligned} \tag{2.1.62}$$

and therefore $J = (\det(M))^{-1}$. The Gauss integral is summarized with the other integrals in the Appenix C .

2.1.2 Infinite Dimensional Grassmann Algebra

If we are dealing with Grassmann algebra in the limit $n \to \infty$ and we have functionals instead of functions. The basic property for Grassmann generators in infinite dimensions goes over in

$$\{\eta(x),\eta(y)\} = 0\,. \tag{2.1.63}$$

The functional reads

$$F[\eta] = f_0 + \int dx\, f_1(x)\eta(x) + \int dx_1 dx_2 f_2(x_1, x_2)\eta(x_1)\eta(x_2) + \dots \tag{2.1.64}$$

The functions $f \in \mathbb{C}$ are chosen to be antisymmetric with respect to any two arguments. This property is going to be important for the next properties. The derivative of a generator is simply given by the Dirac delta distribution [40]

$$\frac{\delta\eta(x)}{\delta\eta(z)} = \delta(x - z)\,. \tag{2.1.65}$$

The derivative is defined in analogy to the discrete form as

$$\begin{aligned}\frac{\delta}{\delta\eta(z)}&\left[\eta(x_1)\,\eta(x_2)\,\dots\,\eta(x_n)\right]\\ &= \delta(z - x_1)\eta(x_2)\dots\eta(x_n) - \delta(z - x_2)\eta(x_1)\eta(x_3)\dots\eta(x_n)\\ &\quad + \dots + (-1)^{n-1}\delta(z - x_n)\eta(x_1)\eta(x_2)\dots\eta(x_{n-1})\,.\end{aligned} \tag{2.1.66}$$

In particular, we interested in functionals of two independent fields. As in the discrete form the complex Grassmann fields $\eta(x)$ and $\overline{\eta}(x)$ are independent. We define

$$\begin{aligned}F[\overline{\eta}, \eta] := f_0 &+ \int dx_1 \left\{f_0(x_1)\eta(x) + f_1(x_1)\overline{\eta}(x_1)\right\}\\ &+ \int dx_1 dx_2 \left\{f_0(x_1, x_2)\eta(x_1)\eta(x_2) + f_1(x_1, x_2)\overline{\eta}(x_1)\eta(x_2) + f_2(x_1, x_2)\overline{\eta}(x_1)\overline{\eta}(x_2)\right\}\\ &+ \int dx_1 dx_2 dx_3 \left\{f_0(x_1, x_2, x_3)\eta(x_1)\eta(x_2)\eta(x_3) + f_1(x_1, x_2, x_3)\overline{\eta}(x_1)\eta(x_2)\eta(x_3)\right.\\ &\qquad \left. + f_2(x_1, x_2, x_3)\overline{\eta}(x_1)\overline{\eta}(x_2)\eta(x_3) + f_3(x_1, x_2, x_3)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\right\}\\ &+ \dots \quad .\end{aligned} \tag{2.1.67}$$

In general we can write such a functional of two independent fields as

$$F[\overline{\eta}, \eta] = \sum_{n=0}^{\infty}\sum_{k=0}^{n}\prod_{\ell=1}^{n}\left[\int dx_\ell\right] f_k(x_1, ..., x_n)\prod_{i=1}^{k}\overline{\eta}(x_i)\prod_{j=k+1}^{n}\eta(x_j)\,, \tag{2.1.68}$$

with $f_0(x_1) \equiv f_0$. We are now going to derive the derivation rules for such functionals. First we consider the derivation with respect to $\eta(z)$ and then with respect to $\overline{\eta}(z)$, for the first case we have

$$\begin{aligned}\frac{\delta F[\overline{\eta}, \eta]}{\delta\eta(z)} &= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\prod_{\ell=1}^{n}\left[\int dx_\ell\right]\sum_{m=0}^{n-k-1}(-1)^{k+m} f_k(x_1, \dots, x_n)\delta(x_{k+m+1} - z)\prod_{i=1}^{k}\overline{\eta}(x_i)\prod_{\substack{j=k+1\\ j\neq k+1+m}}^{n}\eta(x_j)\\ &= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\sum_{m=0}^{n-k-1}\prod_{\ell=1}^{n}\left[\int dx_\ell\right](-1)^{k+m} f_k(x_1, \dots, x_n)\delta(x_{k+m+1} - z)\prod_{i=1}^{k}\overline{\eta}(x_i)\prod_{\substack{j=k+1\\ j\neq k+1+m}}^{n}\eta(x_j)\\ &= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\sum_{m=0}^{n-k-1}\prod_{\substack{\ell=1\\ \ell\neq k+m+1}}^{n}\left[\int dx_\ell\right](-1)^{k+m} f_k(x_1, \dots \underbrace{z}_{k+m+1}, \dots x_n)\prod_{i=1}^{k}\overline{\eta}(x_i)\prod_{\substack{j=k+1\\ j\neq k+m+1}}^{n}\eta(x_j)\\ &= \sum_{n=0}^{\infty}\sum_{k=0}^{n}(-1)^k(n-k)\prod_{\ell=1}^{n-1}\left[\int dx_\ell\right] f_k(x_1, \dots, \underbrace{z}_{k+1}, \dots x_{n-1})\prod_{i=1}^{k}\overline{\eta}(x_i)\prod_{j=k+1}^{n-1}\eta(x_j)\,.\end{aligned} \tag{2.1.69}$$

The last formula gives a practical way to obtain the derivative. In essence the sign is determined by the number k of $\overline{\eta}$ generators before the first η by $(-1)^k$. The value of the derived functional is then inserted at the position $k+1$ of the function f, and the pre-factor $(n-k)$ is defined by the number of generators η. Let us now consider

$$\begin{aligned}
\frac{\delta F[\overline{\eta},\eta]}{\delta\overline{\eta}(z)} &= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\prod_{\ell=1}^{n}\left[\int dx_\ell\right]\sum_{m=1}^{k}(-1)^{m+1}f_k(x_1,\ldots,x_n)\delta(x_m-z)\prod_{\substack{i=1\\ i\neq m}}^{k}\overline{\eta}(x_i)\prod_{j=k+1}^{n}\eta(x_j)\\
&= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\sum_{m=1}^{k}\prod_{\ell=1}^{n}\left[\int dx_\ell\right](-1)^{m+1}f_k(x_1,\ldots,x_n)\delta(x_m-z)\prod_{\substack{i=1\\ i\neq m}}^{k}\overline{\eta}(x_i)\prod_{j=k+1}^{n}\eta(x_j)\\
&= \sum_{n=0}^{\infty}\sum_{k=0}^{n}\sum_{m=1}^{k}\prod_{\substack{\ell=1\\ \ell\neq m}}^{k}\left[\int dx_\ell\right](-1)^{m+1}f_k(x_1,\ldots,\underbrace{z}_{m},x_n)\prod_{\substack{i=1\\ i\neq m}}^{k}\overline{\eta}(x_i)\prod_{j=k+1}^{n}\eta(x_j)\\
&= \sum_{n=0}^{\infty}\sum_{k=0}^{n}k\prod_{\ell=1}^{n-1}\left[\int dx_\ell\right]f_k(z,\ldots,x_{n-1})\prod_{i=1}^{k-1}\overline{\eta}(x_i)\prod_{j=k}^{n-1}\eta(x_j)\,. \qquad (2.1.70)
\end{aligned}$$

By derivatating the value of the functional with respect to $\overline{\eta}$, one has simply to take the number of the generators $\overline{\eta}$ and insert the variable of the derivated function $\overline{\eta}(z)$ in the function f_k at the first position

Next we want to have a short look what happens, if we have a general product of two functionals. For that matter we simply look at one summand of the product given by $F[\overline{\eta},\eta]G[\overline{\eta},\eta]$. One such summand for fixed n_1,n_2 and corresponding k_1,k_2 is, according to (2.1.67), given by

$$\begin{aligned}
M = \prod_{\ell=1}^{n_1+n_2}\left[\int dx_\ell\right] & f_{k_1}(x_1,\ldots,x_{n_1})g_{k_2}(x_{n_1+1},\ldots,x_{n_1+n_2})\\
&\times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\times\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1+1}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2+1}^{n_1+n_2}\overline{\eta}(x_{j_2})\,. \qquad (2.1.71)
\end{aligned}$$

Now the derivative with respect to η yields

$$\begin{aligned}
\frac{\delta M}{\delta\eta(z)} &= \prod_{\ell=1}^{n_1+n_2}\left[\int dx_\ell\right]\sum_{m=0}^{n_1-k_1-1}(-1)^{k_+1+m} f_{k_1}(x_1,\ldots,x_{n_1})g_{k_2}(x_{n_1+1},\ldots,x_{n_1+n_2})\delta(x_{k_1+1+m}-z)\\
&\quad\times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{\substack{j_1=k_1+1\\ j_1\neq k_1+1+m}}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1+1}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2+1}^{n_1+n_2}\eta(x_{j_2})\\
&\quad+\prod_{\ell=1}^{n_1+n_2}\left[\int dx_\ell\right]\sum_{m=0}^{n_2-k_2-1}(-1)^{n_1+k_2+m} f_{k_1}(x_1,\ldots,x_{n_1})g_{k_2}(x_{n_1+1},\ldots,x_{n_1+n_2})\delta(x_{n_1+k_2+1+m}-z)\\
&\quad\times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1+1}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{\substack{j_2=n_1+k_2+1+m\\ j_2\neq n_1+k_2+1+m}}^{n_1+n_2}\eta(x_{j_2})\\
&=(-1)^{k_1}\prod_{\ell=1}^{n_1+n_2-1}\left[\int dx_\ell\right] f_{k_1}(x_1,\ldots,\underbrace{z}_{k_1+1}\ldots x_{n_1-1})g_{k_2}(x_{n_1},\ldots,x_{n_1+n_2-1})\\
&\quad\times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1-1}\eta(x_{j_1})\prod_{i_2=n_1}^{n_1+k_2-1}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2}^{n_1+n_2-1}\eta(x_{j_2})\\
&\quad+(-1)^{n_1+k_2}\prod_{\ell=1}^{n_1+n_2-1}\left[\int dx_\ell\right] f_{k_1}(x_1,\ldots x_{n_1})g_{k_2}(x_{n_1+1},\ldots,\underbrace{z}_{n_1+k_2+1}\ldots x_{n_1+n_2-1})\\
&\quad\times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1+1}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2+1}^{n_1+n_2-1}\eta(x_{j_2})\,. \qquad (2.1.72)
\end{aligned}$$

and corresponding for $\overline{\eta}$

$$\begin{aligned}
\frac{\delta M}{\delta\overline{\eta}(z)} = & \prod_{\ell=1}^{n_1+n_2}\left[\int dx_\ell\right]\sum_{m=0}^{k_1-1}(-1)^m f_{k_1}(x_1,\dots x_{n_1})g_{k_2}(x_{n_1+1},\dots x_{n_1+n_2})\delta(x_{1+m}-z) \\
& \times\prod_{\substack{i_1=1\\ i_1\neq m+1}}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1+1}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2+1}^{n_1+n_2}\eta(x_{j_2}) \\
& + \prod_{\ell=1}^{n_1+n_2}\left[\int dx_\ell\right]\sum_{m=0}^{k_2-1}(-1)^{n_1+m}f_{k_1}(x_1\dots x_{n_1})g_{k_2}(x_{n_1+1},\dots,x_{n_1+n_2})\delta(x_{n_1+1+m}-z) \\
& \times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{\substack{i_2=n_1+1\\ i_2\neq n_1+1+m}}^{n_1+k_2}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2+1}^{n_1+n_2}\eta(x_{j_2}) \\
= & \prod_{\ell=1}^{n_1+n_2-1}\left[\int dx_\ell\right]f_{k_1}(z,x_1,\dots,x_{n_1-1})g_{k_2}(x_{n_1},\dots,x_{n_1+n_2-1}) \\
& \times\prod_{i_1=1}^{k_1-1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1}^{n_1-1}\eta(x_{j_1})\prod_{i_2=n_1}^{n_1+k_2-1}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2}^{n_1+n_2-1}\eta(x_{j_2}) \\
& + \prod_{\ell=1}^{n_1+n_2-1}\left[\int dx_\ell\right](-1)^{n_1}f_{k_1}(x_1,\dots x_{n_1})g_{k_2}(x_{n_1+1},\dots,\underbrace{z}_{n_1+1},\dots x_{n_1+n_2-1}) \\
& \times\prod_{i_1=1}^{k_1}\overline{\eta}(x_{i_1})\prod_{j_1=k_1+1}^{n_1}\eta(x_{j_1})\prod_{i_2=n_1}^{n_1+k_2-1}\overline{\eta}(x_{i_2})\prod_{j_2=n_1+k_2}^{n_1+n_2-1}\eta(x_{j_2})\,. \qquad (2.1.73)
\end{aligned}$$

Now that we know how this monomials act under the functional derivative, we can introduce the following notation

$$\begin{aligned}
&\overline{u}_f u_f := \\
&\int dx_1dx_2 f(x_1,x_2)\overline{\eta}(x_1)\eta(x_2)+\int dx_1dx_2dx_3dx_4 f_1(x_1,x_2,x_3,x_4)\overline{\eta}(x_1)\eta(x_2)\eta(x_3)\eta(x_4) \\
&\quad +\dots+ \\
&\quad \int dx_1dx_2dx_3dx_4 f_2(x_1,x_2,x_3,x_4)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\eta(x_4) \\
&\quad +\dots \qquad (2.1.74)
\end{aligned}$$

So we gather up all monomials which are both uneven in η and in $\overline{\eta}$. Likewise we define

$$\begin{aligned}
\overline{g}_f g_f :&= \int dx_1dx_2dx_3dx_4 f(x_1,x_2,x_3,x_4)\overline{\eta}(x_1)\overline{\eta}(x_2)\eta(x_3)\eta(x_4) \\
&\quad +\int dx_1dx_2dx_3dx_4dx_5dx_6 f(x_1,x_2,x_3,x_4,x_5,x_6)\overline{\eta}(x_1)\overline{\eta}(x_2)\eta(x_3)\eta(x_4)\eta(x_5)\eta(x_6) \\
&\quad +\dots+ \\
&\quad +\int dx_1dx_2dx_3dx_4dx_5dx_6 f(x_1,x_2,x_3,x_4,x_5,x_6)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\overline{\eta}(x_4)\eta(x_5)\eta(x_6) \\
&\quad +\dots \qquad (2.1.75)
\end{aligned}$$

Where we gathered all terms which consists of integrals, which are both even in $\overline{\eta}$ and η

$$\begin{aligned}\overline{u}_f g_f := &\int dx_1 dx_2 dx_3 f(x_1,x_2,x_3)\overline{\eta}(x_1)\eta(x_2)\eta(x_3)\\ &+\ldots+\\ &+\int dx_1 dx_2 dx_3 dx_4 dx_5 f(x_1,x_2,x_3,x_4,x_5)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\eta(x_4)\eta(x_5)\\ &+\int dx_1 dx_2 dx_3 dx_4 dx_5 dx_6 dx_7 f(x_1,x_2,x_3,x_4,x_5,x_6,x_7)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\eta(x_4)\eta(x_5)\eta(x_6)\eta(x_7)\\ &+\ldots\end{aligned} \tag{2.1.76}$$

Also we have gathered all the terms which are uneven in $\overline{\eta}$ and are even in η.

$$\begin{aligned}\overline{g}_f u_f := &\int dx_1 dx_2 dx_3 f(x_1,x_2,x_3)\overline{\eta}(x_1)\overline{\eta}(x_2)\eta(x_3)\\ &+\int dx_1 dx_2 dx_3 dx_4 dx_5 f(x_1,x_2,x_3,x_4,x_5)\overline{\eta}(x_1)\overline{\eta}(x_2)\eta(x_3)\eta(x_4)\eta(x_5)\\ &+\ldots+\\ &+\int dx_1 dx_2 dx_3 dx_4 dx_5 f(x_1,x_2,x_3,x_4,x_5)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\overline{\eta}(x_4)\eta(x_5)\\ &+\int dx_1 dx_2 dx_3 dx_4 dx_5 dx_6 dx_7 f(x_1,x_2,x_3,x_4,x_5,x_6,x_7)\overline{\eta}(x_1)\overline{\eta}(x_2)\overline{\eta}(x_3)\overline{\eta}(x_4)\eta(x_5)\eta(x_6)\eta(x_7)\\ &+\ldots\end{aligned} \tag{2.1.77}$$

Finally here we have gathered all the integrals which are even in $\overline{\eta}$ and uneven in η. Now with our new notation we can write any functional as

$$F[\overline{\eta},\eta] := \overline{u}_{f_1} u_{f_1} + \overline{g}_{f_1} g_{f_1} + \overline{u}_{f_2} g_{f_2} + \overline{g}_{f_2} u_{f_2}\ . \tag{2.1.78}$$

The notation has to be seen as a minimalistic wrtiting form. The indices f_1 and f_2, have only be introduced to destinquish between $\overline{u}$ of the term $\overline{u}_{f_1} u_{f_1}$ and $\overline{u}$ out of $\overline{u}_{f_2} g_{f_2}$

Product Rule for Grassmann Functionals

We are now going to prove the product rule for functionals, where F and G are arbitrary Grassmann functionals

$$\begin{aligned}F &= \overline{g}_{f_1} g_{f_1} + \overline{u}_{f_1} u_{f_1} + \overline{g}_{f_2} u_{f_2} + \overline{u}_{f_2} g_{f_2}\\ G &= \overline{g}_{g_1} g_{g_1} + \overline{u}_{g_1} u_{g_1} + \overline{g}_{g_2} g_{g_2} + \overline{u}_{g_2} g_{g_2}\ .\end{aligned} \tag{2.1.79}$$

The derivatives can then be written as follows

$$\begin{aligned}\frac{\delta F}{\delta\eta(z)} &= \overline{g}_{f_1} \overset{-1}{\underset{\downarrow}{g}}_{f_1} - \overline{u}_{f_1} \overset{-1}{\underset{\downarrow}{u}}_{f_1} + \overline{g}_{f_2} \overset{-1}{\underset{\downarrow}{u}}_{f_2} - \overline{u}_{f_2} \overset{-1}{\underset{\downarrow}{g}}_{f_2}\\ \frac{\delta G}{\delta\eta(z)} &= \overline{g}_{g_1} \overset{-1}{\underset{\downarrow}{g}}_{g_1} - \overline{u}_{g_1} \overset{-1}{\underset{\downarrow}{u}}_{g_1} + \overline{g}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2} - \overline{u}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2}\end{aligned} \tag{2.1.80}$$

Here we have introduced the notation $\overset{-1}{\underset{\downarrow}{g/u}}$ for the derivative regarding to the formulas (2.1.69),(2.1.70). Obviously the derivative of an even integral term gives an odd integral term and vice versa. We are now

going to look at the product of two functionals.

$$
\begin{aligned}
F\cdot G = &\left(\overline{g}_{f_1}g_{f_1}+\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_2}u_{f_2}+\overline{u}_{f_2}g_{f_2}\right)\cdot\left(\overline{g}_{g_1}g_{g_1}+\overline{u}_{g_1}u_{g_1}+\overline{g}_{g_2}g_{g_2}+\overline{u}_{g_2}g_{g_2}\right)\\
&\overline{g}_{f_1}g_{f_1}\overline{g}_{g_1}g_{g_1}+\overline{g}_{f_1}g_{f_1}\overline{u}_{g_1}u_{g_1}+\overline{g}_{f_1}g_{f_1}\overline{g}_{g_2}g_{g_2}+\overline{g}_{f_1}g_{f_1}\overline{u}_{g_2}g_{g_2}\\
&+\overline{u}_{f_1}u_{f_1}\overline{g}_{g_1}g_{g_1}+\overline{u}_{f_1}u_{f_1}\overline{u}_{g_1}u_{g_1}+\overline{u}_{f_1}u_{f_1}\overline{g}_{g_2}g_{g_2}+\overline{u}_{f_1}u_{f_1}\overline{u}_{g_2}g_{g_2}\\
&+\overline{g}_{f_2}u_{f_2}\overline{g}_{g_1}g_{g_1}+\overline{g}_{f_2}u_{f_2}\overline{u}_{g_1}u_{g_1}+\overline{g}_{f_2}u_{f_2}\overline{g}_{g_2}g_{g_2}+\overline{g}_{f_2}u_{f_2}\overline{u}_{g_2}g_{g_2}\\
&+\overline{u}_{f_2}g_{f_2}\overline{g}_{g_1}g_{g_1}+\overline{u}_{f_2}g_{f_2}\overline{u}_{g_1}u_{g_1}+\overline{u}_{f_2}g_{f_2}\overline{g}_{g_2}g_{g_2}+\overline{u}_{f_2}g_{f_2}\overline{u}_{g_2}g_{g_2}\\
=\;&\overline{g}_{f_1}\overline{g}_{g_1}g_{f_1}g_{g_1}+\overline{g}_{f_1}\overline{u}_{g_1}g_{f_1}u_{g_1}+\overline{g}_{f_1}\overline{g}_{g_2}g_{f_1}g_{g_2}+\overline{g}_{f_1}\overline{u}_{g_2}g_{f_1}g_{g_2}\\
&+\overline{u}_{f_1}\overline{g}_{g_1}u_{f_1}g_{g_1}-\overline{u}_{f_1}\overline{u}_{g_1}u_{f_1}u_{g_1}+\overline{u}_{f_1}\overline{g}_{g_2}u_{f_1}g_{g_2}-\overline{u}_{f_1}\overline{u}_{g_2}u_{f_1}g_{g_2}\\
&+\overline{g}_{f_2}\overline{g}_{g_1}u_{f_2}g_{g_1}-\overline{g}_{f_2}\overline{u}_{g_1}u_{f_2}u_{g_1}+\overline{g}_{f_2}\overline{g}_{g_2}u_{f_2}g_{g_2}-\overline{g}_{f_2}\overline{u}_{g_2}u_{f_2}g_{g_2}\\
&+\overline{u}_{f_2}\overline{g}_{g_1}g_{f_2}g_{g_1}+\overline{u}_{f_2}\overline{u}_{g_1}g_{f_2}u_{g_1}+\overline{u}_{f_2}\overline{g}_{g_2}g_{f_2}g_{g_2}+\overline{u}_{f_2}\overline{u}_{g_2}g_{f_2}g_{g_2}\,.
\end{aligned}
\tag{2.1.81}
$$

Now the products are of course again a sum which now corresponds to integrals, which have a certain combination of $\overline{\eta}$ and η in them. In the second line we have brought each term in the sum to what one might call normal form. That is all the $\overline{\eta}$ are on the left. Of course the sign changes accordingly to the normal Grassmann commutator rules. We can now again apply the derivation rule (2.1.72),(2.1.73),(2.1.81) and get

$$
\begin{aligned}
&\frac{\delta(FG)}{\delta\eta(z)}\\
=\;&\overline{g}_{f_1}\overline{g}_{g_1}\overset{-1}{\downarrow}g_{f_1}g_{g_1}+\overline{g}_{f_1}\overline{g}_{g_1}g_{f_1}\overset{-1}{\downarrow}g_{g_1}-\overline{g}_{f_1}\overline{u}_{g_1}\overset{-1}{\downarrow}g_{f_1}u_{g_1}-\overline{g}_{f_1}\overline{u}_{g_1}g_{f_1}\overset{-1}{\downarrow}u_{g_1}+\overline{g}_{f_1}\overline{g}_{g_2}\overset{-1}{\downarrow}g_{f_1}g_{g_2}+\overline{g}_{f_1}\overline{g}_{g_2}g_{f_1}\overset{-1}{\downarrow}g_{g_2}\\
&-\overline{g}_{f_1}\overline{u}_{g_2}\overset{-1}{\downarrow}g_{f_1}g_{g_2}-\overline{g}_{f_1}\overline{u}_{g_2}g_{f_1}\overset{-1}{\downarrow}g_{g_2}-\overline{u}_{f_1}\overline{g}_{g_1}\overset{-1}{\downarrow}u_{f_1}g_{g_1}+\overline{u}_{f_1}\overline{g}_{g_1}u_{f_1}\overset{-1}{\downarrow}g_{g_1}-\overline{u}_{f_1}\overline{u}_{g_1}\overset{-1}{\downarrow}u_{f_1}u_{g_1}+\overline{u}_{f_1}\overline{u}_{g_1}u_{f_1}\overset{-1}{\downarrow}u_{g_1}\\
&-\overline{u}_{f_1}\overline{g}_{g_2}\overset{-1}{\downarrow}u_{f_1}g_{g_2}+\overline{u}_{f_1}\overline{g}_{g_2}u_{f_1}\overset{-1}{\downarrow}g_{g_2}-\overline{u}_{f_1}\overline{u}_{g_2}\overset{-1}{\downarrow}u_{f_1}g_{g_2}+\overline{u}_{f_1}\overline{u}_{g_2}u_{f_1}\overset{-1}{\downarrow}g_{g_2}+\overline{g}_{f_2}\overline{g}_{g_1}\overset{-1}{\downarrow}u_{f_2}g_{g_1}-\overline{g}_{f_2}\overline{g}_{g_1}u_{f_2}\overset{-1}{\downarrow}g_{g_1}\\
&+\overline{g}_{f_2}\overline{u}_{g_1}\overset{-1}{\downarrow}u_{f_2}u_{g_1}-\overline{g}_{f_2}\overline{u}_{g_1}u_{f_2}\overset{-1}{\downarrow}u_{g_1}+\overline{g}_{f_2}\overline{g}_{g_2}\overset{-1}{\downarrow}u_{f_2}g_{g_2}-\overline{g}_{f_2}\overline{g}_{g_2}u_{f_2}\overset{-1}{\downarrow}g_{g_2}+\overline{g}_{f_2}\overline{u}_{g_2}\overset{-1}{\downarrow}u_{f_2}g_{g_2}-\overline{g}_{f_2}\overline{u}_{g_2}u_{f_2}\overset{-1}{\downarrow}g_{g_2}\\
&-\overline{u}_{f_2}\overline{g}_{g_1}\overset{-1}{\downarrow}g_{f_2}g_{g_1}-\overline{u}_{f_2}\overline{g}_{g_1}g_{f_2}\overset{-1}{\downarrow}g_{g_1}+\overline{u}_{f_2}\overline{u}_{g_1}\overset{-1}{\downarrow}g_{f_2}u_{g_1}+\overline{u}_{f_2}\overline{u}_{g_1}g_{f_2}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{f_2}\overline{g}_{g_2}\overset{-1}{\downarrow}g_{f_2}g_{g_2}-\overline{u}_{f_2}\overline{g}_{g_2}g_{f_2}\overset{-1}{\downarrow}g_{g_2}\\
&+\overline{u}_{f_2}\overline{u}_{g_2}\overset{-1}{\downarrow}g_{f_2}g_{g_2}+\overline{u}_{f_2}\overline{u}_{g_2}g_{f_2}\overset{-1}{\downarrow}g_{g_2}\,.
\end{aligned}
\tag{2.1.82}
$$

Next we evaluate the desired terms for the product rule. Here we will carry out the derivation rule and leave them as they are.

$$P(F)\frac{\delta G}{\delta \eta} = \left(\overline{g}_{f_1} g_{f_1} + \overline{u}_{f_1} u_{f_1} - \overline{g}_{f_2} u_{f_2} - \overline{u}_{f_2} g_{f_2}\right)\left(\overline{g}_{g_1} \overset{-1}{\downarrow} g_{g_1} - \overline{u}_{g_1} \overset{-1}{\downarrow} u_{g_1} + \overline{g}_{g_2} \overset{-1}{\downarrow} g_{g_2} - \overline{u}_{g_2} \overset{-1}{\downarrow} g_{g_2}\right) = \tag{2.1.83}$$

$$\begin{aligned}
&= \overline{g}_{f_1} g_{f_1} \overline{g}_{g_1} \overset{-1}{\downarrow} g_{g_1} - \overline{g}_{f_1} g_{f_1} \overline{u}_{g_1} \overset{-1}{\downarrow} u_{g_1} + \overline{g}_{f_1} g_{f_1} \overline{g}_{g_2} \overset{-1}{\downarrow} g_{g_2} - \overline{g}_{f_1} g_{f_1} \overline{u}_{g_2} \overset{-1}{\downarrow} g_{g_2} \\
&+ \overline{u}_{f_1} u_{f_1} \overline{g}_{g_1} \overset{-1}{\downarrow} g_{g_1} - \overline{u}_{f_1} u_{f_1} \overline{u}_{g_1} \overset{-1}{\downarrow} u_{g_1} + \overline{u}_{f_1} u_{f_1} \overline{g}_{g_2} \overset{-1}{\downarrow} g_{g_2} - \overline{u}_{f_1} u_{f_1} \overline{u}_{g_2} \overset{-1}{\downarrow} g_{g_2} \\
&- \overline{g}_{f_2} u_{f_2} \overline{g}_{g_1} \overset{-1}{\downarrow} g_{g_1} + \overline{g}_{f_2} u_{f_2} \overline{u}_{g_1} \overset{-1}{\downarrow} u_{g_1} - \overline{g}_{f_2} u_{f_2} \overline{g}_{g_2} \overset{-1}{\downarrow} g_{g_2} + \overline{g}_{f_2} u_{f_2} \overline{u}_{g_2} \overset{-1}{\downarrow} g_{g_2} \\
&- \overline{u}_{f_2} g_{f_2} \overline{g}_{g_1} \overset{-1}{\downarrow} g_{g_1} + \overline{u}_{f_2} g_{f_2} \overline{u}_{g_1} \overset{-1}{\downarrow} u_{g_1} - \overline{u}_{f_2} g_{f_2} \overline{g}_{g_2} \overset{-1}{\downarrow} g_{g_2} + \overline{u}_{f_2} g_{f_2} \overline{u}_{g_2} \overset{-1}{\downarrow} g_{g_2} .
\end{aligned} \tag{2.1.84}$$

Finally we have to evaluate the second part of the product rule, which reads

$$\frac{\delta F}{\delta \eta(z)} G = \left(\overline{g}_{f_1} \overset{-1}{\downarrow} g_{f_1} - \overline{u}_{f_1} \overset{-1}{\downarrow} u_{f_1} + \overline{g}_{f_2} \overset{-1}{\downarrow} u_{f_2} - \overline{u}_{f_2} \overset{-1}{\downarrow} g_{f_2}\right)\left(\overline{g}_{g_1} g_{g_1} + \overline{u}_{g_1} u_{g_1} + \overline{g}_{g_2} g_{g_2} + \overline{u}_{g_2} g_{g_2}\right)$$

$$\begin{aligned}
&= \overline{g}_{f_1} \overset{-1}{\downarrow} g_{f_1} \overline{g}_{g_1} g_{g_1} + \overline{g}_{f_1} \overset{-1}{\downarrow} g_{f_1} \overline{u}_{g_1} u_{g_1} + \overline{g}_{f_1} \overset{-1}{\downarrow} g_{f_1} \overline{g}_{g_2} g_{g_2} + \overline{g}_{f_1} \overset{-1}{\downarrow} g_{f_1} \overline{u}_{g_2} g_{g_2} \\
&- \overline{u}_{f_1} \overset{-1}{\downarrow} u_{f_1} \overline{g}_{g_1} g_{g_1} - \overline{u}_{f_1} \overset{-1}{\downarrow} u_{f_1} \overline{u}_{g_1} u_{g_1} - \overline{u}_{f_1} \overset{-1}{\downarrow} u_{f_1} \overline{g}_{g_2} g_{g_2} - \overline{u}_{f_1} \overset{-1}{\downarrow} u_{f_1} \overline{u}_{g_2} g_{g_2} \\
&+ \overline{g}_{f_2} \overset{-1}{\downarrow} u_{f_2} \overline{g}_{g_1} g_{g_1} + \overline{g}_{f_2} \overset{-1}{\downarrow} u_{f_2} \overline{u}_{g_1} u_{g_1} + \overline{g}_{f_2} \overset{-1}{\downarrow} u_{f_2} \overline{g}_{g_2} g_{g_2} + \overline{g}_{f_2} \overset{-1}{\downarrow} u_{f_2} \overline{u}_{g_2} g_{g_2} \\
&- \overline{u}_{f_2} \overset{-1}{\downarrow} g_{f_2} \overline{g}_{g_1} g_{g_1} - \overline{u}_{f_2} \overset{-1}{\downarrow} g_{f_2} \overline{u}_{g_1} u_{g_1} - \overline{u}_{f_2} \overset{-1}{\downarrow} g_{f_2} \overline{g}_{g_2} g_{g_2} - \overline{u}_{f_2} \overset{-1}{\downarrow} g_{f_2} \overline{u}_{g_2} g_{g_2} .
\end{aligned} \tag{2.1.85}$$

Comparing the results (2.1.84), (2.1.85) with (2.1.82) we finally have

$$\frac{\delta F[\overline{\eta}, \eta] G[\overline{\eta}, \eta]}{\delta \eta(z)} = P\left(F[\overline{\eta}, \eta]\right) \frac{\delta G[\overline{\eta}, \eta]}{\delta \eta(z)} + \frac{\delta F[\overline{\eta}, \eta]}{\delta \eta(z)} G[\overline{\eta}, \eta] . \tag{2.1.86}$$

In the special case that F is even we have

$$P\left(F[\overline{\eta}, \eta]\right) = \overline{g}_{f_1} g_{f_1} + (-\overline{u}_{f_1})(-u_{f_1}) = \overline{g}_{f_1} g_{f_2} + \overline{u}_{f_1} u_{f_1} = F[\overline{\eta}, \eta] \tag{2.1.87}$$

and therefore

$$\frac{\delta F[\overline{\eta}, \eta] G[\overline{\eta}, \eta]}{\delta \eta(z)} = F[\overline{\eta}, \eta] \frac{\delta G[\overline{\eta}, \eta]}{\delta \eta(z)} + \frac{\delta F[\overline{\eta}, \eta]}{\delta \eta(z)} G[\overline{\eta}, \eta] . \tag{2.1.88}$$

And in the same manner for F odd we have

$$P\left(F[\overline{\eta}, \eta]\right) = \overline{g}_{f_2}(-u_{f_2}) + (-\overline{u}_{f_2}) = g_{f_2} = \left[\overline{g}_{f_2} u_{f_2} + \overline{u}_{f_2} g_{f_2}\right] = -F[\overline{\eta}, \eta] \tag{2.1.89}$$

and consequently

$$\frac{\delta F[\overline{\eta}, \eta] G[\overline{\eta}, \eta]}{\delta \eta(z)} = -F[\overline{\eta}, \eta] \frac{\delta G[\overline{\eta}, \eta]}{\delta \eta(z)} + \frac{\delta F[\overline{\eta}, \eta]}{\delta \eta(z)} G[\overline{\eta}, \eta] . \tag{2.1.90}$$

Finally we note that the same product rule (2.1.86) holds for derivations with respect to $\overline{\eta}(z)$.

Chain Rule for an Analytic Function with a Grassmann Functional

We are now going to prove the Grassmann chain rule for an analytic function f and a functional,

$$\frac{\delta}{\delta\eta(z)}f(F) = \left[\frac{\delta F}{\delta\eta(z)}\right] f'(F) \; . \tag{2.1.91}$$

Where we again restrict the functional to be an even functional. According to our above introduced notation we can write it as

$$F = \overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1} \; . \tag{2.1.92}$$

The analytic function is again given by the Laurent series (2.1.32). We are now going derivate the series term by term. The square of the functional is given by

$$\begin{aligned} F^2 = \left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right)^2 &= \left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right)\left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right) \\ &= \overline{u}_{f_1}u_{f_1}\overline{u}_{f_1}u_{f_1} + \overline{u}_{f_1}u_{f_1}\overline{g}_{f_1}g_{f_1} + \overline{g}_{f_1}g_{f_1}\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\overline{g}_{f_1}g_{f_1} \\ &= -\overline{u}_{f_1}\overline{u}_{f_1}u_{f_1}u_{f_1} + \overline{u}_{f_1}\overline{g}_{f_1}u_{f_1}g_{f_1} + \overline{g}_{f_1}\overline{u}_{f_1}g_{f_1}u_{f_1} + \overline{g}_{f_1}\overline{g}_{f_1}g_{f_1}g_{f_1} \; . \end{aligned} \tag{2.1.93}$$

Now if we derivate this term, we have to keep track, which two terms belong to the same function $f$in the integral expression. In order to do so we will underline them, thus giving

$$\begin{aligned} \frac{\delta F^2}{\delta\eta(z)} = \; & -\underline{\overline{u}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}u_{f_1} + \overline{u}_{f_1}\underline{\overline{u}_{f_1}}u_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1} - \underline{\overline{u}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}g_{f_1} + \overline{u}_{f_1}\underline{\overline{g}_{f_1}}u_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1} \\ & - \overline{g}_{f_1}\underline{\overline{u}_{f_1}}g_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1} + \underline{\overline{g}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}g_{f_1} + \overline{g}_{f_1}\underline{\overline{g}_{f_1}}g_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1} \\ = \; & -\underline{\overline{u}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}u_{f_1} - \underline{\overline{u}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}u_{f_1} - \underline{\overline{u}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}g_{f_1} - \underline{\overline{g}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}g_{f_1} \\ & - \underline{\overline{g}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}u_{f_1} - \underline{\overline{u}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{g_1}g_{f_1} + \underline{\overline{g}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}g_{f_1} + \underline{\overline{g}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}g_{f_1} \\ = \; & -2\underline{\overline{u}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}u_{f_1} - 2\underline{\overline{u}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}g_{f_1} - 2\underline{\overline{g}_{f_1}}\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}u_{f_1} + 2\underline{\overline{g}_{f_1}}\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}g_{f_1} \; . \end{aligned} \tag{2.1.94}$$

Now we look at the expected expression

$$\begin{aligned} & 2\left(-\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1} + \overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\right)\left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right) \\ & = -2\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}\underline{\overline{u}_{f_1}u_{f_1}} - 2\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1}\underline{\overline{g}_{f_1}g_{f_1}} + 2\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\underline{\overline{u}_{f_1}u_{f_1}} + 2\overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\underline{\overline{g}_{f_1}g_{f_1}} \\ & = -2\overline{u}_{f_1}\underline{\overline{u}_{f_1}}\overset{-1}{\underset{\downarrow}{u}}_{f_1}\underline{u_{f_1}} - 2\overline{u}_{f_1}\underline{\overline{g}_{f_1}}\overset{-1}{\underset{\downarrow}{u}}_{f_1}\underline{g_{f_1}} - 2\overline{g}_{f_1}\underline{\overline{u}_{f_1}}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\underline{u_{f_1}} + 2\overline{g}_{f_1}\underline{\overline{g}_{f_1}}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\underline{g_{f_1}} \end{aligned} \tag{2.1.95}$$

and we see, that the two expressions (2.1.94)(2.1.95) are in fact equal. Now we can show the other terms via induction by using the previous derived product rule (2.1.85). We therefore assume

$$\frac{\delta}{\delta\eta(z)}\left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right)^n = n\left(-\overline{u}_{f_1}\overset{-1}{\underset{\downarrow}{u}}_{f_1} + \overline{g}_{f_1}\overset{-1}{\underset{\downarrow}{g}}_{f_1}\right)\left(\overline{u}_{f_1}u_{f_1} + \overline{g}_{f_1}g_{f_1}\right)^{n-1} \; , \tag{2.1.96}$$

then

$$\begin{aligned}
&\frac{\delta}{\delta\eta(z)}\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)^{n+1}=\left[\frac{\delta}{\delta\eta(z)}\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)^{n}\right]\\
&=P\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)\frac{\delta}{\delta\eta(z)}\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)^{n}+\left[\frac{\delta}{\delta\eta(z)}\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)\right]\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)^{n}\\
&=P\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)n(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n-1}+(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n}\\
&=\left(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1}\right)n(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n-1}+(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n}\\
&=n(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n-1}+(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n}\\
&=(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(n+1)(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n}\\
&=(n+1)(-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1})(\overline{u}_{f_1}u_{f_1}+\overline{g}_{f_1}g_{f_1})^{n}\,. \qquad (2.1.97)
\end{aligned}$$

Now all that remains is to take out the derivatives to the left and resume the Laurent series to get the chain rule (2.1.91).

Chain Rule for Grassmann Functionals

Finally we want to prove the following chain rule. Be $\eta[\overline{\xi},\xi]$ and $\overline{\eta}[\overline{\xi},\xi]$ odd functionals of the form $\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}$ and F an arbitrary Grassmann functional $F[\overline{\eta},\eta]:=\overline{u}_{f_1}\overline{u}_{f_1}+\overline{g}_{f_1}g_{f_1}+\overline{g}_{f_2}u_{f_2}+\overline{u}_{f_2}g_{f_2}$, then we have

$$\frac{\delta F[\overline{\eta},\eta]}{\delta\xi(z)}=\int ds\left\{\frac{\delta\eta(s)}{\delta\xi(z)}\frac{\delta F[\overline{\eta},\eta]}{\delta\eta(s)}+\frac{\delta\overline{\eta}(s)}{\delta\xi(z)}\frac{\delta F[\overline{\eta},\eta]}{\delta\overline{\eta}(s)}\right\} \qquad (2.1.98)$$

Proof

Now we remember that $\overline{u}_{f_1}u_{f_1}$ stands for a sum of integrals, where each term has an uneven number of $\overline{\eta}$ and η. According to (2.1.72),(2.1.73) we loose one η or $\overline{\eta}$ by derivating and one integral, due to the delta function and the function of the summand will be evaluate at that particular point, given by the number of proceeding $\overline{\eta}$. Let us first derivate F with respect to η, thus leading

$$\begin{aligned}
\frac{\delta F}{\delta\eta(s)}&=-\overline{u}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_1}\overset{-1}{\downarrow}_{f_1}+\overline{g}_{f_2}\overset{-1}{\downarrow}_{f_2}-\overline{u}_{f_2}\overset{-1}{\downarrow}_{f_2}\,,\\
\frac{\delta F}{\delta\overline{\eta}(s)}&=\overset{-1}{\downarrow}_{f_1}u_{f_1}+\overset{-1}{\downarrow}_{f_1}g_{f_1}+\overset{-1}{\downarrow}_{f_2}u_{f_2}+\overset{-1}{\downarrow}_{f_2}g_{f_2}\,, \qquad (2.1.99)
\end{aligned}$$

Each $\overline{\eta}$ is given by

$$\overline{\eta}=\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2} \qquad (2.1.100)$$

and each η as

$$\eta=\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\,, \qquad (2.1.101)$$

where u/g are dependent on ξ and $\overline{u}/\overline{g}$ are dependent on $\overline{\xi}$. We start with the derivative regarding ξ, by

$$\begin{aligned}\frac{\delta\overline{\eta}}{\delta\xi(z)} &= \left(\overline{g}_{h_1}\overset{-1}{\underset{\downarrow}{u}}_{h_1} - \overline{u}_{h_2}\overset{-1}{\underset{\downarrow}{g}}_{h_2}\right) ,\\ \frac{\delta\eta}{\delta\xi(z)} &= \left(\overline{g}_{g_1}\overset{-1}{\underset{\downarrow}{u}}_{g_1} - \overline{u}_{g_2}\overset{-1}{\underset{\downarrow}{g}}_{g_2}\right) .\end{aligned} \tag{2.1.102}$$

Each monomial of F consists of a combination of even/odd generating functionals. For each such functional one $\eta/\overline{\eta}$ (2.1.100) (2.1.2) has to be inserted. We will now denote these products by the exponents k_ℓ and n_ℓ. The combination of even and odd monomials is given by the functional F. We can now write the derivative of F (2.1.99) with respect to η as

$$\begin{aligned}\frac{\delta F}{\delta\overline{\eta}(s)} = (2k_1+1)\quad & f_1\Big|_{s=1}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1+1}\\ +2k_2\quad & f_1\Big|_{s=1}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2}\\ +2k_3\quad & f_2\Big|_{s=1}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_3-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3+1}\\ +(2k_4+1)\quad & f_2\Big|_{s=1}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4} .\end{aligned} \tag{2.1.103}$$

The same procedure for the derivative of F with respect to $\overline{\eta}$ yields

$$\begin{aligned}\frac{\delta F}{\delta\eta(s)} = -(2n_1+1)\quad & f_1\Big|_{s=2n_1+2}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1+1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1}\\ +2n_2\quad & f_1\Big|_{s=2n_2+1}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2-1}\\ +(2n_3+1)\quad & f_2\Big|_{s=2n_s+2}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_3}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3}\\ -2n_4\quad & f_2\Big|_{s=2n_4+2}\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4+1}\left(\overline{g}_{g_1}g_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4-1}\end{aligned} \tag{2.1.104}$$

Using the above expressions the desired chain rule yields to the following result.

$$
\begin{aligned}
&\int ds \left\{ \frac{\delta\overline{\eta}}{\delta\xi(z)} \frac{\delta F}{\delta\overline{\eta}(s)} + \frac{\delta\eta(s)}{\delta\xi(z)} \frac{\delta F}{\delta\eta} \right\} \\
&= (2k_1+1)\, f_1\Big|_{s=1} \left(g_{h_1} \overset{-1}{\underset{\downarrow}{u}}_{h_1} - \overline{u}_{h_2} \overset{-1}{\underset{\downarrow}{g}}_{h_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_1+1} \\
&\quad + (2k_2)\, f_1\Big|_{s=1} \left(g_{h_1} \overset{-1}{\underset{\downarrow}{u}}_{h_1} - \overline{u}_{h_2} \overset{-1}{\underset{\downarrow}{g}}_{h_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_2-1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_2} \\
&\quad + (2k_3) \quad f_2\Big|_{s=1} \left(g_{h_1} \overset{-1}{\underset{\downarrow}{u}}_{h_1} - \overline{u}_{h_2} \overset{-1}{\underset{\downarrow}{g}}_{h_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_3-1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_3+1} \\
&\quad + (2k_4+1)\, f_2\Big|_{s=1} \left(g_{h_1} \overset{-1}{\underset{\downarrow}{u}}_{h_1} - \overline{u}_{h_2} \overset{-1}{\underset{\downarrow}{g}}_{h_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_4} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_4} \\
&\quad - (2n_1+1)\, f_1\Big|_{s=2n_1+2} \left(g_{g_1} \overset{-1}{\underset{\downarrow}{u}}_{g_1} - \overline{u}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_1+1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_1} \\
&\quad + (2n_2) \quad f_1\Big|_{s=2n_2+1} \left(g_{g_1} \overset{-1}{\underset{\downarrow}{u}}_{g_1} - \overline{u}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_2} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_2-1} \\
&\quad + (2n_3+1)\, f_2\Big|_{s=2n_3+2} \left(g_{g_1} \overset{-1}{\underset{\downarrow}{u}}_{g_1} - \overline{u}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_3} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_3} \\
&\quad - (2n_4) \quad f_2\Big|_{s=2n_4+2} \left(g_{g_1} \overset{-1}{\underset{\downarrow}{u}}_{g_1} - \overline{u}_{g_2} \overset{-1}{\underset{\downarrow}{g}}_{g_2} \right) \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_4+1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_4-1} \quad . \qquad (2.1.105)
\end{aligned}
$$

We will now insert the transformations (2.1.100) directly in F and then use the product rule in order to derivate the functional with respect to ξ.

$$
\begin{aligned}
F = &\left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_1+1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_1+1} + \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_2} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_2} \\
&+ \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_3} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_3+1} + \left(\overline{g}_{h_1} u_{h_1} + \overline{u}_{h_2} g_{h_2} \right)^{2k_4+1} \left(\overline{g}_{g_1} u_{g_1} + \overline{u}_{g_2} g_{g_2} \right)^{2n_4} \quad . \qquad (2.1.106)
\end{aligned}
$$

Now derivating leads

$$
\begin{aligned}
\frac{\delta F}{\delta\xi(z)} = {} & P\left[\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1+1}\right](2n_1+1)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1} \\
& +(2k_1+1)\left(g_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1+1} \\
& +P\left[\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2}\right](2n_2)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2-1} \\
& +(2k_2)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2} \\
& +P\left[\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_3}\right](2n_3+1)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3} \\
& +(2k_3)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_3-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3+1} \\
& +P\left[\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4+1}\right](2n_4)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4-1} \\
& +(2k_4+1)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4} \\
= {} & -(2n_1+1)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1+1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1} \\
& +(2k_1+1)\left(g_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}u_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_1+1} \\
& +(2n_2)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2-1} \\
& +(2k_2)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_2-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_2} \\
& +(2n_3+1)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{g_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2n_3}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3} \\
& +(2k_3)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_3-1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_3+1} \\
& -(2n_4)\left(\overline{g}_{g_1}\overset{-1}{\downarrow}u_{g_1}-\overline{u}_{g_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4+1}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4-1} \\
& +(2k_4+1)\left(\overline{g}_{h_1}\overset{-1}{\downarrow}u_{h_1}-\overline{u}_{h_2}\overset{-1}{\downarrow}g_{h_2}\right)\left(\overline{g}_{h_1}u_{h_1}+\overline{u}_{h_2}g_{h_2}\right)^{2k_4}\left(\overline{g}_{g_1}u_{g_1}+\overline{u}_{g_2}g_{g_2}\right)^{2n_4} \quad . \qquad (2.1.107)
\end{aligned}
$$

If we now compare the result of (2.1.107) and (2.1.105), the crucial point here is that any odd product of odd functionals contains an odd number of u and $\overline{u}$. Likewise an even product of odd functionals contains and

even number of u and $\overline{u}$, so that the P operator gives a minus/plus sign respectively. For even functionals this is not the case and the chain rule does not hold true.

2.1.3 Fermionic Coherent States

In this section we are going to briefly introduce fermionic coherent states. Coherent states are defined to be eigenstates of the annihilation operator a_λ. So we require

$$a_\lambda |\varphi\rangle = \varphi_\lambda |\varphi\rangle \ . \tag{2.1.108}$$

Then it becomes evident, that we need Grassman numbers in order to proceed. To see this, we assume for a moment that φ_{λ_1} and φ_{λ_2} are ordinary numbers. Then we can write

$$\begin{aligned} a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} |\varphi\rangle = a^\dagger_{\lambda_1} \varphi_{\lambda_2} |\varphi\rangle = \varphi_{\lambda_1}\varphi_{\lambda_2} |\varphi\rangle = \varphi_{\lambda_2}\varphi_{\lambda_1} |\varphi\rangle \\ a^\dagger_{\lambda_2} a^\dagger_{\lambda_1} |\varphi\rangle = a_{\lambda_2}\varphi_{\lambda_1} |\varphi\rangle = \varphi_{\lambda_2}\varphi_{\lambda_1} |\varphi\rangle \end{aligned} \tag{2.1.109}$$

out of this two equations we get the relation $a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} |\varphi\rangle = a^\dagger_{\lambda_2} a^\dagger_{\lambda_1} |\varphi\rangle$ which contradicts the anticommutator relation $\left\{a^\dagger_{\lambda_1}, a^\dagger_{\lambda_2}\right\} = 0$, so that we need Grassmann numbers in order to define fermionic coherent states. Hence the regular Fock space is build up of the direct sum of all n-dimensional Hilbert spaces, it has to be extended in order to contain Grassmann numbers. One now associates for each annihilation operator a_λ one Grassmann generator η_λ and for each $a^\dagger_\lambda$ one Grassmann generator $\overline{\eta}_\lambda$. The extended Fock space is then formed by building the linear combination of the regular Fock space states and the Grassmann coefficients. That is

$$|\varphi\rangle = \sum_\lambda \chi_\lambda |\psi_\lambda\rangle \ . \tag{2.1.110}$$

Where χ_λ are Grassmann numbers, and $|\psi_\lambda\rangle$ is a state of the regular Fock space. In order to build coherent states analog to the bosonic ones, one has to demand the following relations

$$\begin{aligned} \{\eta, a\} = 0, \qquad & \qquad \{\eta, a^\dagger\} = 0, \\ \{\overline{\eta}, a\} = 0 \qquad \text{and} \qquad & \qquad \{\overline{\eta}, a^\dagger\} = 0. \end{aligned} \tag{2.1.111}$$

as well as the following operations for involution

$$\begin{aligned} (\eta a)^\dagger = a^\dagger \overline{\eta}, \qquad & \qquad (\eta a^\dagger)^\dagger = a\overline{\eta}, \\ (\overline{\eta} a)^\dagger = a^\dagger \eta \qquad \text{and} \qquad & \qquad (\overline{\eta} a^\dagger)^\dagger = a\eta \ . \end{aligned} \tag{2.1.112}$$

The coherent states are now defined as

$$|\varphi\rangle = e^{-\sum_\lambda \eta_\lambda a^\dagger_\lambda} |0\rangle \ . \tag{2.1.113}$$

Due to the Baker-Campbell-Hausdorff formula (2.1.44) and the fact that

$$\left[\eta_{\lambda_k} a^\dagger_{\lambda_k} \eta_{\lambda_\ell} a^\dagger_{\lambda_\ell}\right] = 0 \ , \tag{2.1.114}$$

it follows

$$|\varphi\rangle = \prod_\lambda (1 - \eta_\lambda a^\dagger_\lambda) |0\rangle \ . \tag{2.1.115}$$

With this definition it follows directly that $|\varphi\rangle$ is indeed an eigenstate of a_λ. To see this, first observe

$$\begin{aligned} a_\lambda (1 - \eta_\lambda a^\dagger_\lambda) |0\rangle &= a_\lambda |0\rangle - a_\lambda \eta_\lambda |\lambda\rangle = \eta_\lambda a_\lambda |\lambda\rangle = \eta_\lambda |0\rangle \\ &= (\eta_\lambda - 0) |0\rangle = (\eta_\lambda - \eta^2_\lambda a^\dagger_\lambda) |0\rangle \\ &= \eta_\lambda (1 - \eta_\lambda a^\dagger_\lambda) |0\rangle \ , \end{aligned} \tag{2.1.116}$$

and thus

$$\begin{aligned}
a_\lambda |\eta\rangle &= a_\lambda e^{-\sum_\mu a_\mu^\dagger} |0\rangle \\
&= a_\lambda \prod_\mu (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= a_\lambda \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger)(1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&= \prod_{\substack{\mu \\ \mu\neq\lambda}} (a_\lambda + \eta_\mu a_\lambda a_\mu^\dagger)(1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&= \prod_{\substack{\mu \\ \mu\neq\lambda}} (a_\lambda - \eta_\mu a_\mu^\dagger a_\lambda)(1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&= \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) a_\lambda (1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&\overset{2.1.116}{=} \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) \eta_\lambda (1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&= \eta_\lambda \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger)(1-\eta_\lambda a_\lambda^\dagger) |0\rangle \\
&= \eta_\lambda \prod_\mu (1-\eta_\mu a_\mu^\dagger) |0\rangle = \eta_\lambda |\eta\rangle \ . \qquad (2.1.117)
\end{aligned}$$

Next we notice

$$\begin{aligned}
a_\lambda^\dagger |\lambda\rangle = a_\lambda^\dagger e^{-\sum_\mu \eta_\mu a_\mu^\dagger} |0\rangle &= a_\lambda^\dagger \prod_\mu (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= a_\lambda^\dagger (1-\eta_\lambda a_\lambda^\dagger) \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= (a_\lambda^\dagger + \eta_\lambda \underbrace{(a_\lambda^\dagger)^2}_{=0}) \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= a_\lambda^\dagger \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= -\frac{\partial}{\partial \eta_\lambda} (1-\eta_\lambda a_\lambda^\dagger) \prod_{\substack{\mu \\ \mu\neq\lambda}} (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= -\frac{\partial}{\partial \eta_\lambda} \prod_\mu (1-\eta_\mu a_\mu^\dagger) |0\rangle \\
&= -\frac{\partial}{\partial \eta_\lambda} |\varphi\rangle \ . \qquad (2.1.118)
\end{aligned}$$

The overlap of two coherent states is easily determined by

$$\begin{aligned}
\langle \eta | \eta' \rangle &= \langle 0 | \, e^{\sum_\lambda \overline{\eta}_\lambda a_\lambda} e^{-\sum_\lambda \eta'_\lambda a^\dagger_\lambda} \, | 0 \rangle \\
&= \langle 0 | \prod_\lambda (1 + \overline{\eta}_\lambda a_\lambda) \prod_\lambda (1 - \eta'_\lambda a^\dagger_\lambda) \, | 0 \rangle \\
&= \prod_\lambda \langle 0 | \, (1 + \overline{\eta}_\lambda a_\lambda)(1 - \eta'_\lambda a^\dagger_\lambda) \, | 0 \rangle \\
&= \prod_\lambda \langle 0 | \, 1 - \eta'_\lambda a^\dagger_\lambda + \overline{\eta}_\lambda a_\lambda - \overline{\eta}_\lambda a_\lambda \eta'_\lambda a^\dagger_\lambda \, | 0 \rangle \\
&= \prod_\lambda \left(\langle 0 | 0 \rangle - \eta'_\lambda \langle 0 | \lambda \rangle + \langle 0 | \, \overline{\eta}_\lambda \underbrace{a_\lambda \, | 0 \rangle}_{=0} + \overline{\eta}_\lambda \eta'_\lambda \underbrace{\langle 0 | \, \alpha_\lambda a^\dagger_\lambda \, | 0 \rangle}_{=1} \right) \\
&= \prod_\lambda (1 + \overline{\eta}_\lambda \eta'_\lambda) \\
&= e^{\sum_\lambda \overline{\eta}_\lambda \eta'_\lambda} \, .
\end{aligned} \tag{2.1.119}$$

Finally we prove the overcompleteness relation

$$\int \prod_\lambda d\overline{\eta}_\lambda d\eta_\lambda e^{-\sum_\lambda \overline{\eta}_\lambda \eta_\lambda} \, | \varphi \rangle \, \langle \varphi | = \mathbb{1} \, . \tag{2.1.120}$$

Proof

In order to prove this relation, we show that

$$\begin{aligned}
&\langle \eta' | \left[\int \prod_n d\overline{\varphi}_n d\varphi_n e^{-\sum_n \overline{\varphi}_n \varphi_n} \, | \varphi \rangle \, \langle \varphi | \right] | \eta \rangle \\
&= \int \prod_n d\overline{\varphi}_n d\varphi_n \, \langle \eta' | \varphi \rangle \, e^{-\sum_n \overline{\varphi}_n \varphi_n} \, \langle \varphi | \eta \rangle \\
&= \int \prod_n d\overline{\varphi}_n d\varphi_n e^{\sum_n \overline{\eta}'_n \varphi_n} e^{-\sum_n \overline{\varphi}_n \varphi_n} e^{\sum_n \overline{\varphi}_n \eta_n} \\
&\overset{2.1.53}{=} \int \prod_{\substack{n \\ n \neq N}} d\overline{\varphi}_n d\varphi_n \left(\int d\overline{\varphi}_N d\varphi_N e^{\sum_{n_{n \neq N}} \overline{\eta}'_n \varphi_n} e^{\overline{\eta}'_N \varphi_N} e^{-\overline{\varphi}_N \varphi_N} e^{\overline{\varphi}_N \eta_N} e^{-\sum_{n_{n \neq N}} \overline{\varphi}_n \varphi_n} e^{\sum_{n_{n \neq N}} \overline{\varphi}_n \eta_n} \right) \\
&= \int \prod_{\substack{n \\ n \neq N}} d\overline{\varphi}_n d\varphi_n \\
&\quad \times \int d\overline{\varphi}_N d\varphi_N e^{\sum_{n_{n \neq N}} \overline{\eta}'_n \varphi_n} \left(1 - \overline{\varphi}_N \varphi_N + \eta'_N \varphi_N + \varphi_N \overline{\varphi}_N \overline{\eta}'_N \eta_N \right) e^{-\sum_{n_{n \neq N}} \overline{\varphi}_n \varphi_n} e^{\sum_{n_{n \neq N}} \overline{\varphi}_n \eta_n} \\
&= \int \prod_{\substack{n \\ n \neq N}} d\overline{\varphi}_n d\varphi_n \left(e^{\sum_{n_{n \neq N}} \overline{\eta}'_n \varphi_n} \left(1 + \overline{\eta}'_N \eta_N \right) e^{-\sum_{n_{n \neq N}} \overline{\varphi}_n \varphi_n} e^{\sum_{n_{n \neq N}} \overline{\varphi}_n \eta_n} \right) \\
&= \int \prod_{\substack{n \\ n \neq N}} d\overline{\varphi}_n d\varphi_n \left(e^{\sum_{n_{n \neq N}} \overline{\eta}'_n \varphi_n} e^{\overline{\eta}'_N \eta_N} e^{-\sum_{n_{n \neq N}} \overline{\varphi}_n \varphi_n} e^{\sum_{n_{n \neq N}} \overline{\varphi}_n \eta_n} \right) \\
&\quad \vdots \\
&= e^{\sum_\lambda^N \overline{\eta}'_N \eta_N} \, .
\end{aligned} \tag{2.1.121}$$

The overcompleteness relation can now be used to represent a state of the extended Fock space in terms of coherent states.

$$\begin{aligned} |\psi\rangle &= \int \prod_\lambda d\overline{\varphi}_\lambda d\varphi_\lambda e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} |\varphi\rangle \langle\varphi|\psi\rangle \\ &= \int \prod_\lambda d\overline{\varphi}_\lambda d\varphi_\lambda e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} \psi(\overline{\varphi}) |\varphi\rangle \ , \end{aligned} \tag{2.1.122}$$

where $\langle\varphi|\psi\rangle = \psi(\overline{\varphi})$. With this definition, we immediately get

$$\begin{aligned} \langle\varphi| a_\lambda |\psi\rangle &= \frac{\partial}{\partial\overline{\eta}_\lambda} \langle\varphi|\psi\rangle \\ &= \frac{\partial}{\partial\overline{\eta}_\lambda} \psi(\overline{\varphi}) \end{aligned} \tag{2.1.123}$$

and

$$\begin{aligned} \langle\varphi| a_\lambda^\dagger |\psi\rangle &= \overline{\eta}_\lambda \langle\varphi|\psi\rangle \\ &= \overline{\eta}_\lambda \psi(\overline{\varphi}) \ . \end{aligned} \tag{2.1.124}$$

Finally we have to evaluate the expectation value

$$\begin{aligned} \langle\varphi| A[a^\dagger, a] |\varphi'\rangle &= \langle\varphi| \sum_{k=1}^\infty c_n (a^\dagger a)^n |\varphi'\rangle \\ &= \langle\varphi| \sum_{k=1}^\infty c_n (\overline{\varphi}\,\varphi)^n |\varphi'\rangle \\ &= e^{\sum_\lambda \overline{\varphi}_\lambda \varphi'_\lambda} A[\overline{\varphi}\,\varphi'] \ . \end{aligned} \tag{2.1.125}$$

So we may also write

$$A[\overline{\varphi}, \varphi'] = \frac{\langle\varphi| A[a^\dagger, a] |\varphi'\rangle}{\langle\varphi|\varphi'\rangle} \ . \tag{2.1.126}$$

Finally we note that the inner product yields

$$\begin{aligned} \langle n|\varphi\rangle \langle\varphi|m\rangle &= \left(\varphi_{\lambda_p} \dots \varphi_{\lambda_1}\right) \left(\overline{\varphi}_{\lambda_1}, \dots \overline{\varphi}_{\lambda_p}\right) \\ &= \zeta^{p^2} \left(\overline{\varphi}_{\lambda_1} \dots \overline{\varphi}_{\lambda_p}\right) \left(\varphi_{\lambda_p} \dots \varphi_{\lambda_1}\right) \\ &= \zeta^p \left(\overline{\varphi}_{\lambda_1} \dots \overline{\varphi}_{\lambda_p}\right) \left(\varphi_{\lambda_p} \dots \varphi_{\lambda_1}\right) \\ &= \langle\zeta\varphi|m\rangle \langle n|\varphi\rangle \ . \end{aligned} \tag{2.1.127}$$

So if we have a complete set of states in the Fock space, the trace of an operator can be written as

$$\begin{aligned} \mathrm{Tr}(A) &= \sum_n \langle n| A |n\rangle \\ &= \int \prod_\lambda d\overline{\varphi}_\lambda d\varphi_\lambda e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} \sum_n \langle n|\varphi\rangle \langle\varphi| A |n\rangle \\ &= \int \prod_\lambda d\overline{\varphi}_\lambda d\varphi_\lambda e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} \sum_n \langle\zeta\varphi| A |n\rangle \langle n|\varphi\rangle \\ &= \int \prod_\lambda d\overline{\varphi}_\lambda d\varphi_\lambda e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} \langle\zeta\varphi| A |\varphi\rangle \ . \end{aligned} \tag{2.1.128}$$

Now it is important to point out contrasts to bosonic coherent states, which are quantum mechanical states, where a quantum mechanical system is near the classical limit. That is the classical field $\varphi(x)$ describes the same state as the coherent state $|\varphi\rangle = e^{\int dx \varphi(n)\varphi^\dagger(a)} |0\rangle$. The fermionic coherent states are not in the Fock space but rather in the extended Fock space. There is no classical fermionic field which is observable.

2.2 Fermionic Coherent State Path Integral

In this thesis we are applying the functional integral formalism. The purpose of this chapter is to give a short overview over the functional integral and setting the mathematical framework we are using throughout this thesis. We introduce the mathematical terminology used and establish certain conventions for the rest of the text.

Short Introduction of Functional Integrals

Although Norbert Wiener has introduced a functional integral back in 1921, [41] the real breakthrough for the functional integral came after Richard Feynman published his approach to quantum mechanics, which he called the space-time approach, in 1948 [42]. In his article Richard Feynman derived, starting from what he called a new composition law for probabilities, his path-integral formula. Later he repeated basically the same approach in his famous textbook "Quantum Mechanics and Path Integrals " [43], where he illustrated the probability laws on an imaginary double slit experiment.
While Richard Feynman always derived his path integral formula from the probability laws of quantum mechanics, the usual textbook approach today is to start from the time evolution operator and use its composition law N-times, while afterwards inserting the completeness relation $N-1$-times. Then the appearing integrals on the time-slice are approximated [39], [34], [44]. It should be mentioned that the so called path integral is also a functional integral, although the term seems to be used more in the context of quantum field theory. The original Feynman path integral, in configuration or momentum space, gives the probability amplitude of a particle starting at a given point (x_a, t_a) to arrive at a final point (x_b, t_b). The functional integral approach can also be used to calculate the partition function of a single particle[2] $Z = \mathrm{Tr} e^{-\beta \hat{H}}$. This so called imaginary-time or euclidean path integral is closely related to the original Feynman path integral over the so called Wick rotation, which is in essence an analytical continuation with a variable transformation $t = -i\tau$. It should be mentioned that although the two path integral formulations are closely related in this way, they are quite different. The standard path integral has an imaginary factor in the action and with that comes an imaginary measure. The convergence of the integral thus relies on interference, while the euclidean action in the imaginary-time path integral is given by the Wiener measure and so the integral can be given a precise mathematical definition [34], [45]. While the path integral seems to be quite cumbersome in quantum mechanics it provides a powerful tool in quantum field theory. Here we investigate a quantum gas in the grand-canonical ensemble and we want to write down a path integral formulation for this purpose. Hence the total number of particles is not conserved in the grand-canonical ensemble, we need a field theory approach which is given by reformulating non relativistic quantum mechanics in a field theory over the single particle wave functions, also known as second quantization. With the help of coherent states, which form an over complete set in the Fock space it is possible to derive a path integral formulation for the partition function.

Detailed Derivation of the Fermionic Coherent State Path Integral

The coherent state path integral can be derived directly from the partition function, but to see some properties regarding the time ordering, we are going to derive the path integral in three steps. The derivation is valid for both bosons and fermions, but naturally we will focus on the fermionic case and pay special attention

[2] The generalisation to N-particles is then trivial.

to derive the path integral with the fermionic rules given in the previous chapter. At some crucial points the Grassmann rules will be written explicitly above the $\equiv$ sign. First we will rewrite the overcompletness relation (2.1.122)

$$|\psi\rangle = \int \prod_{\lambda} \frac{d\overline{\varphi}_\lambda d\varphi_\lambda}{\mathrm{N}} e^{-\sum_\lambda \overline{\varphi}_\lambda \varphi_\lambda} \psi(\overline{\varphi}) \, |\varphi\rangle \qquad \text{with N} := \begin{cases} 2\pi i & \text{Bosons} \\ 1 & \text{Fermions} \end{cases} , \tag{2.2.1}$$

in order to include the bosonic case. Now we extend the closure relation (2.1.120)

$$\int \prod_{\lambda} \frac{d\overline{\varphi}_\lambda d\varphi_\lambda}{\mathrm{N}} e^{-\sum_n \overline{\varphi}_n \varphi_n} \, |\varphi\rangle \, \langle\varphi| = \mathbb{1} \tag{2.2.2}$$

for each time step k

$$\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{\mathrm{N}} e^{-\sum_\lambda \overline{\varphi}_{\lambda,k} \varphi_{\lambda,k}} \, |\varphi\rangle \, \langle\varphi| = \mathbb{1} \, . \tag{2.2.3}$$

While slicing the time in N steps. The procedure is then the same for each component as for the standard (non-field) coherent state path integral

$$\begin{aligned} \langle \psi_F t_F | \psi_I t_I \rangle &= \langle \psi_F | \, U(t_N, t_{N-1}) U(t_{N-1}, t_{N-2}) \dots U(t_2, t_1) U(t_1, t_0) \, |\psi_I\rangle \\ &= \prod_{k=1}^{N-1} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{\mathrm{N}} e^{-\sum_\lambda \overline{\varphi}_{\lambda,k} \varphi_{\lambda,k}} \right] \langle \psi_F | \, U(t_N, t_{N-1}) \, |\varphi_{N-1}\rangle \\ &\qquad \times \left(\prod_{k=2}^{N-1} \langle \varphi_k | \, U(t_k, t_{k-1}) \, |\varphi_{k-1}\rangle \right) \langle \varphi_1 | \, U(t_1, t_0) \, |\psi_I\rangle \, . \end{aligned} \tag{2.2.4}$$

Now in order to evaluate the necessary elements, we need to approximate the time evolution operator in the following manner. If we have a Hamiltonian in normal order all the creation operators are on the left, then we can write the time evolution operator in the following way

$$\begin{aligned} e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} &=: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : + e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} - : e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : \\ &=: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : + \sum_{n=0}^{\infty} \frac{\left(-i\frac{\varepsilon}{\hbar}\right)^n}{n!} \left(\hat{H}^n \left[a^\dagger, a\right] - : \hat{H}^n \left[a^\dagger, a\right] : \right) \\ &=: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : + 0 + 0 + \sum_{n=2}^{\infty} \frac{\left(-i\frac{\varepsilon}{\hbar}\right)^n}{n!} \left(\hat{H}^n \left[a^\dagger, a\right] - : \hat{H}^n \left[a^\dagger, a\right] : \right) \\ &=: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : + \sum_{n=0}^{\infty} \frac{\left(-i\frac{\varepsilon}{\hbar}\right)^{n+2}}{(n+2)!} \left(\hat{H}^{n+2} \left[a^\dagger, a\right] - : \hat{H}^{n+2} \left[a^\dagger, a\right] : \right) \\ &=: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : - \left(\frac{\varepsilon}{\hbar}\right)^2 \sum_{n=0}^{\infty} \frac{\left(-i\frac{\varepsilon}{\hbar}\right)^n}{(n+2)!} \left(\hat{H}^{n+2} \left[a^\dagger, a\right] - : \hat{H}^{n+2} \left[a^\dagger, a\right] : \right) . \end{aligned} \tag{2.2.5}$$

The first zero comes from the difference of two ones and the second from the fact that we assumed the Hamiltonian is in normal order. The operator $: \bullet :$ stands for the normal order operator, which is defined as putting all the creation operators to the left. In the fermionic case this has to be done under consideration of the necessary sign changes. The normal order is always defined with respect to the vacuum, which we will address shortly. So if we have the Hamiltonian in normal order, we can replace the time-evolution operator with

$$e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} \approx: e^{-i\frac{\varepsilon}{\hbar}\hat{H}[a^\dagger,a]} : + \mathscr{O}(\varepsilon^2) \, . \tag{2.2.6}$$

For the following calculation we will now assume, that the time evolution operator is in normal order and that we have ignored the error of $\mathscr{O}(\varepsilon^2)$. Now we will calculate the following elements

$$\begin{aligned}
\langle\varphi_1|\,U(t_0,t_1)\,|\Psi_I\rangle &= \langle\varphi_1|\,e^{-\frac{i}{\hbar}\varepsilon\hat{H}[a^\dagger,a]}\int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi(\overline{\varphi})\,|\varphi_0\rangle\\
&= \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi(\overline{\varphi})\,\langle\varphi_1|\,e^{-\frac{i}{\hbar}\varepsilon\hat{H}[a^\dagger,a]}\,|\varphi_0\rangle\\
&\approx \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi(\overline{\varphi})\,\langle\varphi_1|:e^{-\frac{i}{\hbar}\varepsilon\hat{H}[a^\dagger,a]}:+\mathscr{O}(\varepsilon^2)\,|\varphi_0\rangle\\
&= \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi(\overline{\varphi})\,\langle\varphi_1|\varphi_0\rangle\,e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,1},\varphi_{\lambda,0}]}\\
&= \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi(\overline{\varphi})e^{\sum_\lambda\overline{\varphi}_{\lambda,1}\varphi_{\lambda,0}}e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,1},\varphi_{\lambda,0}]}\,,
\end{aligned}\tag{2.2.7}$$

where the following Grassmann rules have been used (2.1.48), (2.1.49) and (2.1.53). When calculating the matrix element of the time evolution operator, the normal order has to be seen as ordering the summands of the power series in normal order and then after applying the coherent states on each term resuming the series. This is due to the definition of the normal order operator, which is given with respect to the vacuum [46]. The index λ on the Hamiltonian $H\left[\overline{\varphi}_{\lambda,1},\varphi_{\lambda,0}\right]$ is not to be confused with a sum index. The same applies later for the Hamiltonian $H[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}]$. The matrix element was evaluated by (2.1.126). So it should be noted, that if we later insert the Hamiltonian in normal order, it is given by

$$H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]\equiv\frac{\langle\varphi_k|\,\hat{H}[a_k^\dagger,a_k]\,|\varphi_{k-1}\rangle}{\langle\varphi_k|\varphi_{k-1}\rangle}\,,\tag{2.2.8}$$

hence the scalar product of (2.1.119) will be inserted in the formula for the path integral. This means, that later one can simply replace a Hamilton operator given in second quantization by one with the coherent states. We can now derive the other two elements in the same manner. With $c\,|a\rangle\leftrightarrow\langle a|\,\overline{c}$ we get

$$\langle\psi|=\int\prod_\lambda\frac{d\overline{\varphi}_\lambda d\varphi_\lambda}{N}e^{-\sum_n\overline{\varphi}_n\varphi_n}\overline{\psi}(\varphi)\,\langle\varphi|\ .\tag{2.2.9}$$

The element is then given by

$$\begin{aligned}
\langle\psi_F|\,U(t_N,t_{N-1})\,|\varphi_{N-1}\rangle &= \langle\psi_N|\,U(t_N,t_{N-1})\,|\varphi_{N-1}\rangle\\
&= \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,N}d\varphi_{\lambda,N}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}\overline{\psi}(\varphi)\,\langle\varphi_N|\,U(t_N,t_{N-1})\,|\varphi_{N-1}\rangle\\
&\approx \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,N}d\varphi_{\lambda,N}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}\overline{\psi}(\varphi)\,\langle\varphi_N|\varphi_{N-1}\rangle\,e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,N},\varphi_{\lambda,N-1}]}\\
&= \int\prod_\lambda\frac{d\overline{\varphi}_{\lambda,N}d\varphi_{\lambda,N}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}\overline{\psi}(\varphi)e^{\sum_\lambda\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N-1}}e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,N},\varphi_{\lambda,N-1}]}\,.
\end{aligned}\tag{2.2.10}$$

And finally we can calculate the element

$$\begin{aligned}
\langle\varphi_k|\,U(t_k,t_{k-1})\,|\varphi_k\rangle &= \langle\varphi_k|\,e^{-\frac{i}{\hbar}\varepsilon\hat{H}[a^\dagger,a]}\,|\varphi_{k-1}\rangle\\
&\approx \langle\varphi_k|\varphi_{k-1}\rangle\,e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}]}\\
&= e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}}e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}]}\,,
\end{aligned}\tag{2.2.11}$$

where again the Grassmann rules (2.1.48), (2.1.49) and (2.1.53) have been used. Now we are ready to calculate the overlap for the coherent state path integral

$$
\begin{aligned}
&\langle\psi_F t_F|\psi_I t_I\rangle \\
&\quad= \langle\psi_F|\, U(t_N,t_{N-1})U(t_{N-1},t_{N-2})\dots U(t_2,t_1)U(t_1,t_0)\,|\psi_I\rangle \\
&\quad= \prod_{k=1}^{N-1}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\langle\psi_F|\, U(t_N,t_{N-1})\,|\varphi_{N-1}\rangle \\
&\qquad\times\left(\prod_{k=2}^{N-1}\langle\varphi_k|\, U(t_k,t_{k-1})\,|\varphi_{k-1}\rangle\right)\langle\varphi_1|\, U(t_1,t_0)\,|\psi_I\rangle \\
&= \prod_{k=1}^{N-1}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\left(\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,0}d\varphi_{\lambda,0}}{N}e^{-\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}\overline{\psi}_F(\varphi_\lambda)e^{\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N-1}}e^{-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N-1}\right]}\right) \\
&\qquad\times\left(\prod_{k=2}^{N-1}e^{\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}}e^{-\frac{i}{\hbar}\varepsilon H[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}]}\right)\left(\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,N}d\varphi_{\lambda,N}}{N}e^{-\sum_\lambda \overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}\psi_I(\overline{\varphi}_\lambda)e^{\sum_\lambda \overline{\varphi}_{\lambda,1}\varphi_{\lambda,0}}e^{-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,1},\varphi_{\lambda,0}\right]}\right) \\
&\overset{\substack{2.1.48\\2.1.49\\2.1.53}}{=} \prod_{k=0}^{N}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\overline{\psi}_F(\varphi_\lambda)\left(\prod_{k=1}^{N}e^{\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}}e^{-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)\psi_I(\overline{\varphi}_\lambda) \\
&\overset{2.1.47}{=} \prod_{k=0}^{N}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\overline{\psi}_F(\varphi_\lambda)e^{\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\psi_I(\overline{\varphi}_\lambda) \\
&\overset{2.1.53}{=} \prod_{k=0}^{N}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\overline{\psi}_F(\varphi_\lambda)\psi_I(\overline{\varphi}_\lambda)\,. \qquad (2.2.12)
\end{aligned}
$$

At this point one can differentiate two cases:
Case 1

$$
\begin{aligned}
&e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\quad\overset{2.1.53}{=} e^{-\sum_\lambda \overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}e^{-\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\quad= e^{-\sum_\lambda \overline{\varphi}_{\lambda,0}\varphi_{\lambda,0}}e^{\frac{i}{\hbar}\varepsilon\sum_{k=1}^{N}\sum_\lambda\, i\hbar\overline{\varphi}_{\lambda,k}\left(\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}\right)-H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\,. \qquad (2.2.13)
\end{aligned}
$$

Case 2

$$
\begin{aligned}
&e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\quad= e^{-\sum_{k=0}^{N}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=0}^{N-1}\sum_\lambda \overline{\varphi}_{\lambda,k+1}\varphi_{\lambda,k}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k+1},\varphi_{\lambda,k}\right]} \\
&\quad\overset{2.1.53}{=} e^{-\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}e^{-\sum_{k=0}^{N-1}\sum_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=0}^{N-1}\sum_\lambda \overline{\varphi}_{\lambda,k+1}\varphi_{\lambda,k}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k+1},\varphi_{\lambda,k}\right]} \\
&\quad= e^{-\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}e^{\sum_{k=0}^{N-1}\sum_\lambda\left(\overline{\varphi}_{\lambda,k+1}-\overline{\varphi}_{\lambda,k}\right)\varphi_{\lambda,k}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k+1},\varphi_{\lambda,k}\right]} \\
&\quad= e^{-\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}e^{\sum_{k=1}^{N}\sum_\lambda\left(\overline{\varphi}_{\lambda,k}-\overline{\varphi}_{\lambda,k-1}\right)\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\quad= e^{-\sum_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}}e^{\frac{i}{\hbar}\varepsilon\sum_{k=1}^{N}\sum_\lambda(-i\hbar)\left(\frac{\overline{\varphi}_{\lambda,k}-\overline{\varphi}_{\lambda,k-1}}{\varepsilon}\right)\varphi_{\lambda,k-1}-H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\,. \qquad (2.2.14)
\end{aligned}
$$

We can now define a symmetric path integral in the following way

$$\langle\psi_F t_F|\psi_I t_I\rangle = \prod_{k=0}^{N}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{-\frac{1}{2}\sum_\lambda\left(\overline{\varphi}_{\lambda,I}\varphi_{\lambda,I}+\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}\right)} \times e^{\frac{i}{\hbar}\varepsilon\sum_{k=1}^{N}\sum_\lambda\frac{i\hbar}{2}\left[\overline{\varphi}_{\lambda,k}\left(\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}\right)-\left(\frac{\overline{\varphi}_{\lambda,k}-\overline{\varphi}_{\lambda,k-1}}{\varepsilon}\right)\varphi_{\lambda,k-1}\right]-H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\overline{\psi}_F(\varphi_\lambda)\psi_I(\overline{\varphi}_\lambda)\ , \tag{2.2.15}$$

if the final and initial states are also coherent states, we get instead

$$\langle\varphi_F t_F|\varphi_I t_I\rangle = \prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{\frac{1}{2}\sum_\lambda\left(\overline{\varphi}_{\lambda,I}\varphi_{\lambda,I}+\overline{\varphi}_{\lambda,N}\varphi_{\lambda,N}\right)} \times e^{\frac{i}{\hbar}\varepsilon\sum_{k=1}^{N}\sum_\lambda\frac{i\hbar}{2}\left[\overline{\varphi}_{\lambda,k}\left(\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}\right)-\left(\frac{\overline{\varphi}_{\lambda,k}-\overline{\varphi}_{\lambda,k-1}}{\varepsilon}\right)\varphi_{\lambda,k-1}\right]-H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\ . \tag{2.2.16}$$

We note here that the symmetrization is not necessary if we are interested in the partition function, since due to the trace another factor $e^{-\sum_\lambda\overline{\varphi}_\lambda\varphi_\lambda}$ comes in and the sum on the left side of the coherent state form of (2.2.12), which only differs in the change of k, N from 0 and N to 1 and $N-1$, as in (2.2.16). In the case that the initial and final states are coherent states the overlap (2.2.12) reads

$$\langle\varphi_F t_F|\varphi_I t_I\rangle = \prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\ . \tag{2.2.17}$$

We are now performing the Wick rotation in the discrete form, that is due to the transformation $t=-i\tau$ we get

$$\varepsilon_t = t_n - t_{n-1} = -i\tau_n + i\tau_{n-1} = -i(\tau_n-\tau_{n-1}) = -i\varepsilon_\tau\ . \tag{2.2.18}$$

If we now introduce the Hamiltonian $\hat{H}-\mu\hat{N}$, where μ is the chemical potential and $\hat{N}$ is the particle operator, we arrive with

$$\begin{aligned}
&\langle\varphi_I,0|\,e^{-\beta(\hat{H}-\mu\hat{N})}\,|\varphi_F,\hbar\beta\rangle \\
&\quad=\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{1}{\hbar}\varepsilon\left(H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]-N\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]\right)} \\
&\quad=\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{1}{\hbar}\varepsilon\left(H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]-\mu\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right)}\ .
\end{aligned} \tag{2.2.19}$$

The partition function can now be expressed in the form

$$
\begin{aligned}
Z &= \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} \\
&= \int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda} d\varphi_{\lambda}}{N} e^{-\sum_{\lambda}\overline{\varphi}_{\lambda}\varphi_{\lambda}} \left\langle \zeta\varphi \right| e^{-\beta(\hat{H}-\mu\hat{N})} \left|\varphi\right\rangle \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\sum_{k=1}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}} e^{\sum_{k=1}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1} - \frac{1}{\hbar}\varepsilon\left(H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]-\mu\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right)} \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{\sum_{k=1}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\left(\varphi_{\lambda,k-1}-\varphi_{\lambda,k}\right) - \frac{1}{\hbar}\varepsilon\left(H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]-\mu\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right)} \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\frac{\varepsilon}{\hbar}\sum_{k=1}^{N}\sum_{\lambda}\hbar\overline{\varphi}_{\lambda,k}\left(\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}\right)+H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]-\mu\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}} \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\frac{\varepsilon}{\hbar}\sum_{k=1}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right)+H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} .
\end{aligned}
\tag{2.2.20}
$$

Now due to the cycling property of the trace

$$
\mathrm{Tr}\left\langle\varphi_F\right| U(t_N,t_{N-1})U(t_{N-1},t_{N-2})\ldots U(t_1,t_0)\left|\varphi_I\right\rangle = \mathrm{Tr}\left\langle\varphi_F\right| U(t_1,t_0)U(t_N,t_{N-1})\ldots U(t_2,t_1)\left|\varphi_I\right\rangle \tag{2.2.21}
$$

we obtain the periodic, antiperiodic boundary condition

$$
\zeta\varphi_{\lambda,N} = \varphi_{\lambda,0} \,. \tag{2.2.22}
$$

This can be expressed explicitly by writing

$$
\begin{aligned}
Z &= \mathrm{Tr} e^{-\beta(\hat{H}-\mu\hat{N})} \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\frac{\varepsilon}{\hbar}\sum_{k=2}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right)+H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\qquad + \frac{\varepsilon}{\hbar}\left[\sum_{\lambda}\overline{\varphi}_{\lambda,1}\left(\hbar\frac{\varphi_{\lambda,1}-\varphi_{\lambda,0}}{\varepsilon}-\mu\varphi_{\lambda,0}\right) + H\left[\overline{\varphi}_{\lambda,1},\varphi_{\lambda,0}\right]\right] \\
&= \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\frac{\varepsilon}{\hbar}\sum_{k=2}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right)+H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]} \\
&\qquad + \frac{\varepsilon}{\hbar}\left[\sum_{\lambda}\overline{\varphi}_{\lambda,1}\left(\hbar\frac{\varphi_{\lambda,1}-\zeta\varphi_{\lambda,N}}{\varepsilon}-\mu\zeta\varphi_{\lambda,N}\right) + H\left[\overline{\varphi}_{\lambda,1},\zeta\varphi_{\lambda,N}\right]\right] .
\end{aligned}
\tag{2.2.23}
$$

Now it is common to define the discrete action

$$
\begin{aligned}
S^N[\overline{\varphi},\varphi] &= \frac{\varepsilon}{\hbar}\sum_{k=2}^{N}\sum_{\lambda}\overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right) + H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right] \\
&\quad + \frac{\varepsilon}{\hbar}\left[\sum_{\lambda}\overline{\varphi}_{\lambda,1}\left(\hbar\frac{\varphi_{\lambda,1}-\zeta\varphi_{\lambda,N}}{\varepsilon}-\mu\zeta\varphi_{\lambda,N}\right) + H\left[\overline{\varphi}_{\lambda,1},\zeta\varphi_{\lambda,N}\right]\right] ,
\end{aligned}
\tag{2.2.24}
$$

so we have the path integral

$$
Z = \lim_{N\to\infty}\prod_{k=1}^{N}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right] e^{-S^N[\overline{\varphi},\varphi]} \,, \tag{2.2.25}
$$

introducing the trajectory notation

$$\begin{aligned}\overline{\varphi}_\lambda(\tau)\hbar\frac{\partial\varphi_\lambda(\tau)}{\partial\tau} &:= \overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}\right)\\ \varphi_\lambda(\tau) &:= \varphi_{\lambda,k-1}\\ H[\overline{\varphi}_\lambda(\tau),\varphi_\lambda(\tau)] &:= H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]\ ,\end{aligned} \tag{2.2.26}$$

we obtain the trajectory path integral form

$$Z=\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\sum_\lambda\overline{\varphi}_\lambda\left(\hbar\frac{\partial\varphi_\lambda(\tau)}{\partial\tau}-\mu\varphi_\lambda(\tau)\right)+H[\overline{\varphi}_\lambda(\tau),\varphi_\lambda(\tau)]}\ . \tag{2.2.27}$$

It should be pointed out, that the trajectory form of the path integral is merely a symbolic form of the discrete definition (2.2.25). This is also most evident from the fact that the derivative $\partial_\tau := \frac{1}{\varepsilon}\left(\varphi_{\lambda,k}-\varphi_{\lambda,k-1}\right)$ is indeed a derivative for bosons but does not make sense for Grassmann numbers in which case just the limit is defined. Furthermore the above form has been derived in an $\mathscr{O}(\varepsilon^2)$ approximation. There are cases in which this approximation is not sufficient and higher orders have to be considered as has for example been pointed out in [47] in the context of the Chern-Simons theory. Although the trajectory notation is a nice way to write down the path integral, the calculations should be checked within the discrete form [34]. Finally it should not be left unnoticed that sometimes it can be useful to rewrite the path integral with the help of fields in space coordinates as done uniformly in [48]. We will quickly outline the procedure to do so. First recall the transformation rule

$$a_\lambda^\dagger=\sum_{\tilde{\lambda}}\langle\tilde{\lambda}|\lambda\rangle a_{\tilde{\lambda}}^\dagger \qquad\leftrightarrow\qquad a_{\tilde{\lambda}}=\sum_{\tilde{\lambda}}\langle\lambda|\tilde{\lambda}\rangle a_\lambda^\dagger\ . \tag{2.2.28}$$

which in the case for the continuous space coordinates yields

$$\hat{\psi}^\dagger(\mathbf{x}):=a_{\mathbf{x}}^\dagger=\sum_{\tilde{\lambda}}\langle\tilde{\lambda}|\mathbf{x}\rangle a_{\tilde{\lambda}}^\dagger \qquad\leftrightarrow\qquad a_{\tilde{\lambda}}^\dagger=\int\mathrm{d}^3\mathrm{x}\,\langle\mathbf{x}|\tilde{\lambda}\rangle\hat{\psi}^\dagger(\mathbf{x})=\int\mathrm{d}^3\mathbf{x}\,\varphi_{\tilde{\lambda}}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\ . \tag{2.2.29}$$

Now every coherent state can be rewritten as

$$|\varphi\rangle=e^{\zeta\sum_\lambda\varphi_\lambda a_\lambda^\dagger}|0\rangle=e^{\zeta\sum_\lambda\varphi_\lambda\left(\int\mathrm{d}\mathbf{x}\varphi_\lambda(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})\right)}|0\rangle=e^{\zeta\int\mathrm{d}\mathbf{x}\left(\sum_\lambda\varphi_\lambda\varphi_\lambda(\mathbf{x})\right)\hat{\psi}^\dagger(\mathbf{x})}|0\rangle=:e^{\zeta\int\mathrm{d}\mathbf{x}\chi(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})}|0\rangle\ , \tag{2.2.30}$$

so the transition can simply be made by replacing the sum with the integral, through the functions in fact do change. The path integral in this form reads

$$Z=\int\mathscr{D}\overline{\psi}\mathscr{D}\psi e^{\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\int\mathrm{d}^3\mathbf{x}\left\{\overline{\psi}(\mathbf{x},\tau)(\hbar\partial\tau-\mu)\psi(\mathbf{x},\tau)+H[\overline{\psi}(\mathbf{x},\tau),\psi(\mathbf{x},\tau)]\right\}}\ . \tag{2.2.31}$$

Time Ordered Property of the Functional Integral

We are now going to take one step back to see the time ordered property of the functional integral. The standard way of showing the time ordered property for the path integral is to add two operators evaluated at two different times t_1 and t_2 to the path integral formula and then use the composition law as well as the definition for the probability amplitude via the time evolution operator, to show that in the cases, where $t_1 > t_2$ and $t_1 < t_2$, the path integral automatically orders the two operators in the right way, that is as demanded from the time order operator. In the case of the coherent state path integral we have to go back to the discrete form of the path integral and bring the operators to the right position of the time-slice. It is very instructive to do this in the same way as for the normal path integral, i.e., consider two operators evaluated at two different times, and bring them to the right time-slice point for the both cases $t_1 > t_2$ and $t_1 < t_2$. The main difference here is that one evaluated operator has to be brought to the right of the time evolution operator and the other to the left. This is due to the fact, that the creation operator has to act on the bra of the inserted closure relation and the annihilation operator has to act on the corresponding ket. In both cases the time-slice is the same and one has to identify the discrete time close to the time where the operator is evaluated. Here we are going to show the principle directly via the time ordered operator $\hat{\mathrm{T}}$, which is defined as

$$\hat{\mathrm{T}}\left[O_{\lambda_1}(t_1)O_{\lambda_2}(t_2)\dots O_{\lambda_3}(t_3)\right] := \zeta^P \hat{O}_{\lambda_{P_1}}(t_{\lambda_{P_1}})\hat{O}_{\lambda_{P_2}}(t_{\lambda_{P_2}})\dots\hat{O}_{\lambda_{P_n}}(t_{\lambda_{P_n}})\,, \tag{2.2.32}$$

where the operators are now ordered such that

$$t_{P_1} > t_{P_2} > \ldots > t_{P_n}\,. \tag{2.2.33}$$

The time order operator is tailor-made for fermions and bosons, so that in the fermionic case the anticommutation takes place due to the time ordering. Furthermore, the time ordering process shall be in such a way, that the operators at the same time are in normal order, if we have to order creation and annihilation operators at the same time. We will now indicate the operator with $\tilde{a}$ for being either a creation or annihilation operator. So we will start with

$$\begin{aligned}
&\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]\varphi_{\lambda_1}(t_1)\dots\varphi_{\lambda_n}(t_n)\overline{\varphi}_{\lambda_{n+1}}(t_{n+1})\dots\overline{\varphi}_{\lambda_{2n}}(t_{2n})e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\\
&\qquad\qquad\times e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\\
&=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]\tilde{\varphi}_{\lambda_{P_1}}(t_{P_1})\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(t_{P_{2n}})e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\,.
\end{aligned} \tag{2.2.34}$$

Now we find depending on whether we have a creation or annihilation operator the corresponding time-slice element

$$\begin{aligned}
\exists_{t_{m-1}}\,t_{P_1}\sim t_{m-1}\quad&\vee\quad\exists_{t_m}\,t_{P_1}\sim t_m\\
\exists_{t_{n-1}}\,t_{P_2}\sim t_{n-1}\quad&\vee\quad\exists_{t_n}\,t_{P_2}\sim t_n\\
&\vdots\\
\exists_{t_{\ell-1}}\,t_{P_{2n}}\sim t_{\ell-1}\quad&\vee\quad\exists_{t_\ell}\,t_{P_{2n}}\sim t_\ell\,.
\end{aligned} \tag{2.2.35}$$

We can now proceed with

$$\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]\tilde{\varphi}_{\lambda_{P_1}}(t_{P_1})\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(t_{P_{2n}})e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}$$
$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]\tilde{\varphi}_{\lambda_{P_1}}(\tilde{t}_m)\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(\tilde{t}_\ell)e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}$$
$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\tilde{\varphi}_{\lambda_{P_1}}(\tilde{t}_m)\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(\tilde{t}_\ell)e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}$$
$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\tilde{\varphi}_{\lambda_{P_1}}(\tilde{t}_m)\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(\tilde{t}_\ell)e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}$$

We now split the time slice, according to where the fields are evaluated, and bring them to the left or right of the time-evolution

$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\tilde{\varphi}_{\lambda_{P_1}}(\tilde{t}_m)\dots\tilde{\varphi}_{\lambda_{P_{2n}}}(\tilde{t}_\ell)\left(\prod_{k=m+1}^{N}e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)$$
$$\times e^{\sum_\lambda\overline{\varphi}_{\lambda,m}\varphi_{\lambda,m-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,m},\varphi_{\lambda,m-1}\right]}$$
$$\times\left(\prod_{k=\ell+1}^{m-1}e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)e^{\sum_\lambda\overline{\varphi}_{\lambda,\ell}\varphi_{\lambda,\ell-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,n},\varphi_{\lambda,n-1}\right]}\left(\prod_{k=1}^{\ell-1}e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)$$
$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\left(\prod_{k=m+1}^{N}e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)$$
$$\times e^{\sum_\lambda\overline{\varphi}_{\lambda,m}\varphi_{\lambda,m-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,m},\varphi_{\lambda,m-1}\right]}\tilde{\varphi}_{\lambda_{P_1}}(\tilde{t}_m)$$
$$\times\dots\times\tilde{\varphi}_{\lambda_{P_{2n}}}(\tilde{t}_\ell)e^{\sum_\lambda\overline{\varphi}_{\lambda,\ell}\varphi_{\lambda,\ell-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,n},\varphi_{\lambda,n-1}\right]}\left(\prod_{k=1}^{\ell-1}e^{\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\right)$$

Next we will use de definition of the time evolution operator and then define temporarily an operator $\tilde{U}$,$\tilde{U}^\dagger$ depending on the position of a or $a^\dagger$.

$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\left(\prod_{k=m+1}^{N}\langle\varphi_k|\,\hat{U}(t_k,t_{k-1})\,|\varphi_{k-1}\rangle\right)\langle\varphi_m|\,\hat{U}(t_m,t_{m-1})\hat{a}_{\lambda_{P_1},m-1}\,|\varphi_{m-1}\rangle$$
$$\times\dots\times\langle\varphi_\ell|\,\hat{a}^\dagger_{\lambda_{P_{2n}}}\hat{U}(t_\ell,t_{\ell-1})\,|\varphi_{\ell-1}\rangle\left(\prod_{k=1}^{\ell-1}\langle\varphi_k|\,\hat{U}(t_k,t_{k-1})\,|\varphi_{k-1}\rangle\right)$$
$$=\zeta^{P_{2n}}\prod_{k=1}^{N-1}\left[\int\prod_{\lambda}\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}}\right]\left(\prod_{k=m+1}^{N}\langle\varphi_k|\,\hat{U}(t_k,t_{k-1})\,|\varphi_{k-1}\rangle\right)\langle\varphi_m|\,\tilde{U}(t_m,t_{m-1})\,|\varphi_{m-1}\rangle$$
$$\times\dots\times\langle\varphi_\ell|\,\tilde{U}^\dagger(t_\ell,t_{\ell-1})\,|\varphi_{\ell-1}\rangle\left(\prod_{k=1}^{\ell-1}\langle\varphi_k|\,\hat{U}(t_k,t_{k-1})\,|\varphi_{k-1}\rangle\right)$$
$$=\zeta^{P_{2n}}\langle\psi_F|\,U(t_N,t_{N-1})U(t_N,t_{N-2})\dots U(t_{m+1},t_m)\tilde{U}(t_m,t_{m-1})\dots\tilde{U}^\dagger(t_\ell,t_{\ell-1})U(t_\ell,t_{\ell-1})\dots U(t_2,t_1)U(t_1,t_0)\,|\varphi_I\rangle$$
$$=\zeta^{P_{2n}}\langle\psi_F|\,U(t_N,t_{N-1})U(t_N,t_{N-2})\dots U(t_{m+1},t_m)\underbrace{U(t_m,t_{m-1})\hat{a}_{\lambda_{P_1},m-1}}_{\tilde{U}(t_m,t_{m-1})}\dots\underbrace{\hat{a}^\dagger_{\lambda_{P_{2n}},\ell}U(t_\ell,t_{\ell-1})}_{\tilde{U}^\dagger(t_\ell,t_{\ell-1})}\dots U(t_2,t_1)U(t_1,t_0)\,|\varphi_I\rangle$$
$$=\langle\psi_F t_F|\,\hat{\mathrm{T}}\,a_{\lambda_1}(t_1)\dots a_{\lambda_n}(t_n)a^\dagger_{\lambda_{n+1}}(t_{n+1})\dots a^\dagger_{\lambda_{2n}}(t_{2n})\,|\psi_I t_I\rangle \tag{2.2.36}$$

The only question remaining is, what happens if two operators are acting at the same time t_k. Then we must in order to be consistent with the definition of the time-order operator bring the operators at equal times in normal order. By doing so, two coherent states can be brought to one time evolution operator. That is one will have an element like

$$\langle\varphi_m|\,\hat{a}^\dagger_{\lambda_{P_2},m-1}\hat{U}(t_m,t_{m-1})\hat{a}_{\lambda_{P_1},m-1}\,|\varphi_{m-1}\rangle \tag{2.2.37}$$

and the pre-factor $\zeta^{P_{2n}}$ will be in accordance with the definition of the time order operator. That means if we have a creation and annihilation operator acting at the same time, the creation operator will be evaluated one time step later than the corresponding annihilation operator. So finally we obtain the identity

$$\begin{aligned}
&\langle\psi_F t_F|\,\hat{\mathrm{T}}\,a_{\lambda_1}(t_1)\dots a_{\lambda_n}(t_n)a^\dagger_{\lambda_{n+1}}(t_{n+1})\dots a^\dagger_{\lambda_{2n}}(t_{2n})\,|\psi_I t_I\rangle \\
&= \prod_{k=1}^{N-1}\left[\int\prod_\lambda \frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]\varphi_{\lambda_1}(t_1)\dots\varphi_{\lambda_n}(t_n)\overline{\varphi}_{\lambda_{n+1}}(t_{n+1})\dots\overline{\varphi}_{\lambda_{2n}}(t_{2n})e^{-\sum_{k=1}^{N-1}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}} \\
&\qquad\qquad\times e^{\sum_{k=1}^{N}\sum_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{i}{\hbar}\varepsilon H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]}\,.
\end{aligned} \tag{2.2.38}$$

2.2.1 Derivation of the Free Partition Function with the Path Integral

We want to express the Green function with the path integral, and then thread the interaction via perturbation theory. Derive the partition function for the free Hamiltonian. In this chapter we follow the way taken by John W. Negele and Henri Orland from [34] and evaluate the partition function and the Green function in the discrete form of the path integral. For that matter we are now considering the Hamiltonian of a free particle

$$H_0 = \sum_\lambda \varepsilon_\lambda a_\lambda^\dagger a_\lambda \ . \tag{2.2.39}$$

The discrete action (2.2.24) can then be rewritten as follows

$$\begin{aligned}
S^N[\overline{\varphi},\varphi] &= \frac{\varepsilon}{\hbar}\sum_{k=2}^{N}\left[\sum_\lambda \overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right)+H\left[\overline{\varphi}_{\lambda,k},\varphi_{\lambda,k-1}\right]\right] \\
&\quad+\frac{\varepsilon}{\hbar}\left[\sum_\lambda \overline{\varphi}_{\lambda,1}\left(\hbar\frac{\varphi_{\lambda,1}-\zeta\varphi_{\lambda,N}}{\varepsilon}-\mu\zeta\varphi_{\lambda,N}\right)+H\left[\overline{\varphi}_{\lambda,1},\zeta\varphi_{\lambda,N}\right]\right] \\
&= \frac{\varepsilon}{\hbar}\sum_{k=2}^{N}\sum_\lambda\left[\overline{\varphi}_{\lambda,k}\left(\hbar\frac{\varphi_{\lambda,k}-\varphi_{\lambda,k-1}}{\varepsilon}-\mu\varphi_{\lambda,k-1}\right)+\varepsilon_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right] \\
&\quad+\frac{\varepsilon}{\hbar}\sum_\lambda\overline{\varphi}_{\lambda,1}\left[\left(\hbar\frac{\varphi_{\lambda,1}-\zeta\varphi_{\lambda,N}}{\varepsilon}-\mu\zeta\varphi_{\lambda,N}\right)+\zeta\varepsilon_\lambda\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right] \\
&= \sum_{k=2}^{N}\sum_\lambda\left[\overline{\varphi}_{\lambda,k}\left(\varphi_{\lambda,k}-\varphi_{\lambda,k-1}-\frac{\varepsilon}{\hbar}\mu\varphi_{\lambda,k-1}\right)+\frac{\varepsilon}{\hbar}\varepsilon_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right] \\
&\quad+\sum_\lambda\left[\overline{\varphi}_{\lambda,1}\left(\varphi_{\lambda,1}-\zeta\varphi_{\lambda,N}-\frac{\varepsilon}{\hbar}\mu\zeta\varphi_{\lambda,N}\right)+\frac{\varepsilon}{\hbar}\zeta\varepsilon_\lambda\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right] \\
&= \sum_{k=2}^{N}\sum_\lambda\left[\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}-\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}-\frac{\varepsilon}{\hbar}\mu\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}+\frac{\varepsilon}{\hbar}\varepsilon_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right] \\
&\quad+\sum_\lambda\left[\overline{\varphi}_{\lambda,1}\varphi_{\lambda,1}-\zeta\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}-\frac{\varepsilon}{\hbar}\mu\zeta\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}+\frac{\varepsilon}{\hbar}\zeta\varepsilon_\lambda\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right] \\
&= \sum_{k=2}^{N}\sum_\lambda\left[\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}-\left[1-\frac{\varepsilon}{\hbar}\left(\varepsilon_\lambda-\mu\right)\right]\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right] \\
&\quad+\sum_\lambda\left[\overline{\varphi}_{\lambda,1}\varphi_{\lambda,1}-\zeta\left[1-\frac{\varepsilon}{\hbar}\left(\varepsilon_\lambda-\mu\right)\right]\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right] \\
&= \sum_{k=2}^{N}\sum_\lambda\left(\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k}-a_\lambda\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1}\right)+\sum_\lambda\left(\overline{\varphi}_{\lambda,1}\varphi_{\lambda,1}-\zeta a_\lambda\overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right) \ .
\end{aligned} \tag{2.2.40}$$

Where we have defined

$$a := 1-\frac{\varepsilon}{\hbar}\left(\varepsilon_\lambda-\mu\right) \ . \tag{2.2.41}$$

The advantage of writing the action in this form is that we can now express it in matrix form. The fact that no interaction is present makes the matrix almost diagonal and we will be able to solve the partition function.

We now define the matrix M as:

$$M^{(\lambda)} = \begin{pmatrix} 1 & 0 & & \dots & 0 & -\zeta a_\lambda \\ -a_\lambda & 1 & 0 & & & 0 \\ 0 & -a_\lambda & 1 & \ddots & & \vdots \\ & 0 & -a_\lambda & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a_\lambda & 1 \end{pmatrix} , \tag{2.2.42}$$

where the last entry in first line takes care of the boundary term. If we first derive

$$M^{(\lambda)} \cdot \varphi = \begin{pmatrix} 1 & 0 & & \dots & 0 & -\zeta a_\lambda \\ -a_\lambda & 1 & 0 & & & 0 \\ 0 & -a_\lambda & 1 & \ddots & & \vdots \\ & 0 & -a_\lambda & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a_\lambda & 1 \end{pmatrix} \cdot \begin{pmatrix} \varphi_{\lambda,1} \\ \varphi_{\lambda,2} \\ \vdots \\ \\ \varphi_{\lambda,N-1} \\ \varphi_{\lambda,N} \end{pmatrix} = \begin{pmatrix} \varphi_{\lambda,1} - \zeta a_\lambda \varphi_{\lambda,N} \\ -a_\lambda \varphi_{\lambda,1} + \varphi_{\lambda,2} \\ -a_\lambda \varphi_{\lambda,2} + \varphi_{\lambda,3} \\ \vdots \\ -a_\lambda \varphi_{\lambda,N-2} + \varphi_{\lambda,N-1} \\ -a_\lambda \varphi_{\lambda,N-1} + \varphi_{\lambda,N} \end{pmatrix} , \tag{2.2.43}$$

we can next evaluate the element

$$\begin{aligned} \overline{\varphi}_\lambda \cdot M^{(\lambda)} \cdot \varphi_\lambda &= \left(\overline{\varphi}_{\lambda,1}, \overline{\varphi}_{\lambda,2}, \dots, \overline{\varphi}_{\lambda,N}\right) \cdot \begin{pmatrix} \varphi_{\lambda,1} - \zeta a_\lambda \varphi_{\lambda,N} \\ -a_\lambda \varphi_{\lambda,1} + \varphi_{\lambda,2} \\ -a_\lambda \varphi_{\lambda,2} + \varphi_{\lambda,3} \\ \vdots \\ -a_\lambda \varphi_{\lambda,N-2} + \varphi_{\lambda,N-1} \\ -a_\lambda \varphi_{\lambda,N-1} + \varphi_{\lambda,N} \end{pmatrix} \\ &= \overline{\varphi}_{\lambda,1}\varphi_{\lambda,1} - \zeta a_\lambda \overline{\varphi}_{\lambda,1}\varphi_{\lambda,N} - a_\lambda \overline{\varphi}_{\lambda,2}\varphi_{\lambda,1} + \overline{\varphi}_{\lambda,2}\varphi_{\lambda,2} + \overline{\varphi}_{\lambda,3}\varphi_{\lambda,3} \\ &\qquad - \dots - a_\lambda \overline{\varphi}_{\lambda,N-1}\varphi_{\lambda,N-2} + \overline{\varphi}_{\lambda,N-1}\varphi_{N-1} - a_\lambda \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N-1} + \overline{\varphi}_{\lambda,N}\varphi_{\lambda,N} \\ &= \sum_{k=2}^{N} \left(\overline{\varphi}_{\lambda,k}\varphi_{\lambda,k} - a_\lambda \overline{\varphi}_{\lambda,k}\varphi_{\lambda,k-1} + \overline{\varphi}_{\lambda,1}\varphi_{\lambda,1} - \zeta a_\lambda \overline{\varphi}_{\lambda,1}\varphi_{\lambda,N}\right) . \end{aligned} \tag{2.2.44}$$

Comparing this with (2.2.40) we can finally rewrite the action as

$$S^N = \sum_\lambda \sum_{\substack{i=1 \\ j=1}}^{N} \overline{\varphi}_{\lambda,i} M^{(\lambda)}_{ij} \varphi_{\lambda,j} . \tag{2.2.45}$$

So we have rewritten the action in a Gaussian form, where the field components decouple but the time does not. In other words for each λ we get a sum of a λ^2 term times a sum over the time components. The

partition function now reads

$$\begin{aligned} Z_0 &= \lim_{N\to\infty} \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] e^{-\sum_\lambda \sum_{i,j=1}^{N} \overline{\varphi}_{\lambda,i} M_{ij}^{(\lambda)} \varphi_{\lambda,j}} \\ &= \lim_{N\to\infty} \prod_{k=1}^{N} \left[\int \prod_{\lambda} \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} \right] \prod_{\lambda} e^{-\sum_{i,j=1}^{N} \overline{\varphi}_{\lambda,i} M_{ij}^{(\lambda)} \varphi_{\lambda,j}} \\ &= \lim_{N\to\infty} \prod_{k=1}^{N} \prod_{\lambda} \left[\int \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} e^{-\sum_{i,j=1}^{N} \overline{\varphi}_{\lambda,i} M_{ij}^{(\lambda)} \varphi_{\lambda,j}} \right] \\ &= \lim_{N\to\infty} \prod_{\lambda} \left[\prod_{k=1}^{N} \int \frac{d\overline{\varphi}_{\lambda,k} d\varphi_{\lambda,k}}{N} e^{-\sum_{i,j=1}^{N} \overline{\varphi}_{\lambda,i} M_{ij}^{(\lambda)} \varphi_{\lambda,j}} \right] \\ &= \lim_{N\to\infty} \prod_{\lambda} \left[\det M^{(\lambda)} \right]^{-\zeta} . \end{aligned} \tag{2.2.46}$$

Since the determinant of $M^{(\lambda)}$ (2.2.42) is given by

$$\begin{aligned} \det \mathrm{M}^{(\lambda)} &= \lim_{N\to\infty} \left[1 - \zeta \left(1 - \frac{\beta(\varepsilon_\lambda - \mu)}{N} \right)^N \right] \\ &= 1 - \zeta e^{-\beta(\varepsilon_\lambda - \mu)} , \end{aligned} \tag{2.2.47}$$

one gets the standard expression for the free partition function

$$Z_0 = \prod_{\lambda} \left(1 - \zeta e^{\beta(\varepsilon_\lambda - \mu)} \right)^{-\zeta} . \tag{2.2.48}$$

Derivation of the Inverse Matrix

Next we need to determine the inverse of the matrix $\mathrm{M}^{(\lambda)}$, because it is related to the free Green function as we will see in a moment, thus

$$\begin{aligned} &\begin{pmatrix} 1 & 0 & & \dots & 0 & -\zeta a_\lambda \\ -a_\lambda & 1 & 0 & & & 0 \\ 0 & -a_\lambda & 1 & \ddots & & \vdots \\ & 0 & -a_\lambda & \ddots & 0 & \\ \vdots & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a_\lambda & 1 \end{pmatrix} \cdot \begin{pmatrix} \eta_{11} & \eta_{21} & \dots & \dots & \eta_{N1} \\ \eta_{12} & \eta_{22} & \dots & \dots & \eta_{N2} \\ \vdots & \vdots & & & \vdots \\ & & & & \\ & & & & \\ \eta_{1N} & \eta_{2N} & \dots & \dots & \eta_{NN} \end{pmatrix} \\ &= \begin{pmatrix} \eta_{11} - \zeta a_\lambda \eta_{1N} & \eta_{21} - \zeta a_\lambda \eta_{2N} & \dots & \dots & \eta_{N1} - \zeta a_\lambda \eta_{NN} \\ -a_\lambda \eta_{11} + \eta_{12} & -a_\lambda \eta_{21} + \eta_{22} & \dots & \dots & -a_\lambda \eta_{N1} + \eta_{N2} \\ -a_\lambda \eta_{12} + \eta_{13} & -a_\lambda \eta_{22} + \eta_{23} & \dots & \dots & -a_\lambda \eta_{N2} + \eta_{N3} \\ -a_\lambda \eta_{13} + \eta_{14} & -a_\lambda \eta_{23} + \eta_{24} & \dots & \dots & -a_\lambda \eta_{N3} + \eta_{N4} \\ \vdots & \vdots & & & \vdots \\ -a_\lambda \eta_{1N-2} + \eta_{1N-1} & -a_\lambda \eta_{2N-2} + \eta_{2N-1} & \dots & \dots & -a_\lambda \eta_{NN-2} + \eta_{NN-1} \\ -a_\lambda \eta_{1N-1} + \eta_{1N} & -a_\lambda \eta_{2N-1} + \eta_{2N} & \dots & \dots & -a_\lambda \eta_{NN-1} + \eta_{NN} \end{pmatrix} \stackrel{!}{=} \mathbb{1} . \end{aligned} \tag{2.2.49}$$

The rows can now be solved via recursion. I.e :

$$\begin{aligned}
\eta_{11} &= 1 + \zeta a_\lambda \eta_{1N} \\
\eta_{12} &= a_\lambda \, \eta_{11} = a_\lambda(1 + \zeta a_\lambda \eta_{1N}) = a_\lambda + \zeta a_\lambda^2 \eta_{1N} \\
\eta_{13} &= a_\lambda \, \eta_{12} = a_\lambda(a_\lambda + \zeta a_\lambda^2 \eta_{1N}) = a_\lambda^2 + \zeta a_\lambda^3 \eta_{1N} \\
&\vdots \\
\eta_{1k} &= a_\lambda^{k-1} + \zeta a_\lambda^k \eta_{1N} \, .
\end{aligned} \tag{2.2.50}$$

Now we can evaluate the last entry by

$$\eta_{1N} = a_\lambda^{N-1} + \zeta a_\lambda^N \eta_{1N} \quad \Leftrightarrow \quad \eta_{1N}(1 - \zeta \, a_\lambda^N) = a_\lambda^{N-1} \quad \Leftrightarrow \quad \eta_{1N} = \frac{a_\lambda^{N-1}}{1 - \zeta a_\lambda^N} \, , \tag{2.2.51}$$

$$\Longrightarrow \qquad \eta_{1k} = a_\lambda^{k-1} + \zeta a_\lambda^k \frac{a_\lambda^{N-1}}{1 - \zeta a_\lambda^N} = \frac{a_\lambda^{k-1}(1 - \zeta a_\lambda^N)}{1 - \zeta a_\lambda^N} + \frac{\zeta a_\lambda^{N+k-1}}{(1 - \zeta a_\lambda^N)} = \frac{a_\lambda^{k-1} - \zeta a_\lambda^{N+k-1} + \zeta a_\lambda^{N+k-1}}{1 - \zeta \, a_\lambda^N} = \frac{a_\lambda^{k-1}}{1 - \zeta a_\lambda^N}$$

Now we do the same thing for the second row

$$\begin{aligned}
\eta_{21} &= \zeta a_\lambda \eta_{2N} \\
\eta_{22} &= 1 + a_\lambda \eta_{21} = 1 + a_\lambda^2 \zeta \eta_{2N} \\
\eta_{23} &= a_\lambda \eta_{22} = a_\lambda(1 + a_\lambda^2 \zeta \eta_{2N}) = a_\lambda + a_\lambda^3 \zeta \eta_{2N} \\
&\vdots \\
\eta_{2k} &= a_\lambda^{k-2} + a_\lambda^k \zeta \eta_{2N} \, .
\end{aligned} \tag{2.2.52}$$

So now we can again calculate the last entry

$$\eta_{2N} = a_\lambda^{N-2} + a_\lambda^N \zeta \eta_{2N} \quad \Leftrightarrow \quad \eta_{2N}(1 - \zeta a_\lambda^N) = a_\lambda^{N-2} \quad \Leftrightarrow \quad \eta_{2N} = \frac{a_\lambda^{N-2}}{1 - \zeta a_\lambda^N} \tag{2.2.53}$$

$$\eta_{2k} = a_\lambda^{k-2} + a_\lambda^k \zeta \frac{a_\lambda^{N-2}}{1 - \zeta a_\lambda^N} = \frac{(1 - \zeta a_\lambda^N) a_\lambda^{k-2}}{(1 - \zeta a_\lambda^N)} + a_\lambda^k \zeta \frac{a_\lambda^{N-2}}{1 - \zeta a_\lambda^N} = \frac{a_\lambda^{k-2} - \zeta a_\lambda^{N+k-2} + \zeta a_\lambda^{N+k-2}}{1 - \zeta a_\lambda^N} = \frac{a_\lambda^{k-2}}{1 - \zeta a_\lambda^N}$$

and for the next entry follows

$$\begin{aligned}
\eta_{31} &= \zeta \alpha_\lambda \eta_{3N} \\
\eta_{32} &= a_\lambda \eta_{31} = a_\lambda^2 \zeta \eta_{3N} \\
\eta_{33} &= 1 + a_\lambda \eta_{32} = 1 + a_\lambda^3 \zeta \eta_{3N} \\
\eta_{34} &= a_\lambda \eta_{33} = a_\lambda(1 + a_\lambda^3 \zeta \eta_{3N}) = a_\lambda + a_\lambda^4 \zeta \eta_{3N} \\
\eta_{35} &= a_\lambda \eta_{34} = a_\lambda(a_\lambda + a_\lambda^4 \zeta \eta_{3N}) = a_\lambda^2 + a_\lambda^5 \zeta \eta_{3N} \\
&\vdots \\
\eta_{3k} &= a_\lambda^{k-3} + a_\lambda^k \zeta \eta_{3N} \, .
\end{aligned} \tag{2.2.54}$$

So for the last entry we get

$$\eta_{3N} = a_\lambda^{N-3} + a_\lambda^N \zeta \eta_{3N} \quad \Leftrightarrow \quad \eta_{3N}(1 - \zeta a_\lambda^N) = a_\lambda^{N-3} \quad \Leftrightarrow \quad \eta_{3N} = \frac{a_\lambda^{N-3}}{1 - \zeta a_\lambda^N} \tag{2.2.55}$$

$$\eta_{3k} = a_\lambda^{k-3} + a_\lambda^k \zeta \frac{a_\lambda^{N-3}}{1 - \zeta a_\lambda^N} = \frac{a_\lambda^{k-3}(1 - \zeta a_\lambda^N)}{(1 - \zeta a_\lambda^N)} + \zeta \frac{a_\lambda^{N+k-3}}{(1 - \zeta a_\lambda^N)} = \frac{a_\lambda^{k-3} - \zeta a_\lambda^{N+k-3} + \zeta a_\lambda^{N+k-3}}{1 - \zeta a_\lambda^N} = \frac{a_\lambda^{k-3}}{1 - \zeta a_\lambda^N} \, .$$

So now the pattern should be clear and in general we get

$$\eta_{\ell k} = a_\lambda^{k-\ell} + a_\lambda^k \zeta \frac{a_\lambda^{N-\ell}}{1-\zeta a_\lambda^N} = \frac{a_\lambda^{k-\ell}(1-\zeta a_\lambda^N)}{1-\zeta a_\lambda^N} + \frac{\zeta a_\lambda^{N+k-\ell}}{1-\zeta a_\lambda^N} = \frac{a_\lambda^{k-\ell} - \zeta a_\lambda^{N+k-\ell} + \zeta a_\lambda^{N+k-\ell}}{1-\zeta a_\lambda^N} = \frac{a_\lambda^{k-\ell}}{1-\zeta a_\lambda^N} \,. \tag{2.2.56}$$

With all of these terms we can now write down the inverse matrix as

$$M^{(\lambda)-1} = \frac{1}{1-\zeta a_\lambda^N} \begin{pmatrix} 1 & \zeta a_\lambda^{N-1} & \zeta a_\lambda^{N-2} & \dots & \zeta a_\lambda \\ a_\lambda & 1 & \zeta a_\lambda^{N-1} & & \zeta a_\lambda^2 \\ a_\lambda^2 & a_\lambda & 1 & & \\ \vdots & a_\lambda^2 & a_\lambda & & \vdots \\ & & a_\lambda^2 & & \\ a_\lambda^{N-3} & & & & \\ a_\lambda^{N-2} & a_\lambda^{N-3} & & \zeta a_\lambda^{N-1} & \\ a_\lambda^{N-1} & a_\lambda^{N-2} & a_\lambda^{N-3} & \dots & 1 \end{pmatrix} . \tag{2.2.57}$$

2.2.2 Derivation of the Free Green Function with the Path Integral

Definition of the Green Function

We will now define the imaginary Green function and then express it with the help of the path integral. We start with the definition

$$G^{(n)}(\lambda_1\tau_1\dots\lambda_n\tau_n|\lambda_1'\tau_1'\dots\lambda_n'\tau_n') := \langle \hat{\mathrm{T}} a_{\lambda_1}(\tau_1)\dots a_{\lambda_n}(\tau_n) a^\dagger_{\lambda_n'}(\tau_n')\dots a^\dagger_{\lambda_1'}(\tau_1')\rangle \tag{2.2.58}$$

where the creation and annihilation operators are given in the Heisenberg representation

$$\begin{aligned} a_\lambda(\tau) &= e^{\frac{(\hat{H}-\mu\hat{N})\tau}{\hbar}} a_\lambda e^{\frac{-(\hat{H}-\mu\hat{N})\tau}{\hbar}} , \\ a^\dagger_\lambda(\tau) &= e^{\frac{(\hat{H}-\mu\hat{N})\tau}{\hbar}} a^\dagger_\lambda e^{\frac{-(\hat{H}-\mu\hat{N})\tau}{\hbar}} . \end{aligned} \tag{2.2.59}$$

The thermal average is defined as

$$\begin{aligned} \langle \hat{A}\rangle &= \frac{\sum_\lambda \langle\psi_\lambda| e^{-\beta(\hat{H}-\mu\hat{N})}\hat{A}\,|\psi_\lambda\rangle}{\sum_\lambda \langle\psi_\lambda| e^{\beta(\hat{H}-\mu\hat{N})}\,|\psi_\lambda\rangle} \\ &= \frac{1}{Z_0}\mathrm{Tr}\left(e^{-\beta(\hat{H}-\mu\hat{N})}\hat{A}\right) . \end{aligned} \tag{2.2.60}$$

with

$$Z_0 = \mathrm{Tr} e^{-\beta(\hat{H}-\mu\hat{N})} . \tag{2.2.61}$$

Now we will rewrite the Green function with the path integral formalism. The last step makes use of the time ordered property of the path integral which was shown (2.2.36) in the previous section, we again write $\tilde{a}$ for either a or $a^\dagger$

$$\begin{aligned} G^{(n)}&\left(\lambda_1\tau_1\dots\lambda_n\tau_n|\lambda_{2n}'\tau_{2n}'\dots\lambda_{n+1}'\tau_{n+1}'\right) = \langle \hat{\mathrm{T}} a_{\lambda_1}(\tau_1)\dots a_{\lambda_n}(\tau_n) a^\dagger_{\lambda_n'}(\tau_{n+1}')\dots a^\dagger_{\lambda_1'}(\tau_{2n}')\rangle \\ &= \frac{1}{Z_0}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\hat{\mathrm{T}} a_{\lambda_1}(\tau_1)\dots a_{\lambda_n}(\tau_n) a^\dagger_{\lambda_{n+1}'}(\tau_{n+1}')\dots a^\dagger_{\lambda_{2n}'}(\tau_{2n}')\right] \\ &= \frac{1}{Z_0}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\zeta^{\mathrm{P}}\tilde{a}_{\lambda_{\mathrm{P}_1}}(\tau_{\mathrm{P}_1})\tilde{a}_{\lambda_{\mathrm{P}_2}}(\tau_{\mathrm{P}_2})\dots\tilde{a}^\dagger_{\lambda_{\mathrm{P}_{2n}}}(\tau_{\mathrm{P}_{2n}})\right] \\ &= \frac{1}{Z_0}\zeta^{\mathrm{P}}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{\mathrm{P}_1}}(\tau_{\mathrm{P}_1})\tilde{a}_{\lambda_{\mathrm{P}_2}}(\tau_{\mathrm{P}_2})\dots\tilde{a}^\dagger_{\lambda_{\mathrm{P}_{2n}}}(\tau_{\mathrm{P}_{2n}})\right] \\ &= \frac{1}{Z_0}\zeta^{\mathrm{P}}\mathrm{Tr}\left[e^{-\beta(\hat{H}-\mu\hat{N})}e^{(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}}\tilde{a}_{\lambda_{\mathrm{P}_1}}(\tau_{\mathrm{P}_1})e^{-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}}e^{(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_2}}\tilde{a}_{\lambda_{\mathrm{P}_2}}(\tau_{\mathrm{P}_2})e^{-\tau_{\mathrm{P}_2}(\hat{H}-\mu\hat{N})}\right] \\ &\qquad\qquad \dots e^{(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_{2n}}}\tilde{a}_{\lambda_{\mathrm{P}_{2n}}}(\tau_{\mathrm{P}_{2n}})e^{-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_{2n}}}\Big] . \end{aligned} \tag{2.2.62}$$

Now we need (2.1.44)

$$\begin{aligned} e^{-\int_{\tau_{\mathrm{P}_1}}^{\beta}(\hat{H}-\mu\hat{N})} &= e^{-\left[\beta(\hat{H}-\mu\hat{N})-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}\right]} \\ &= e^{-\beta(\hat{H}-\mu\hat{N})}e^{(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}} , \end{aligned} \tag{2.2.63}$$

and

$$\begin{aligned} e^{-\int_{\tau_{\mathrm{P}_2}}^{\tau_{\mathrm{P}_1}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})} &= e^{-\left[(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_2}\right]} \\ &= e^{-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}+(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_2}} \\ &= e^{-(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_1}}e^{(\hat{H}-\mu\hat{N})\tau_{\mathrm{P}_2}} , \end{aligned} \tag{2.2.64}$$

and likewise

$$\begin{aligned} e^{-\int_{\tau_{k+1}}^{\tau_k} \mathrm{d}\tau'(\hat{H}-\mu\hat{N})} &= e^{-\left[(\hat{H}-\mu\hat{N})\tau_k-(\hat{H}-\mu\hat{N})\tau_{k+1}\right]} \\ &= e^{-(\hat{H}-\mu\hat{N})-\tau_k+(\hat{H}-\mu\hat{N})\tau_{k+1}} \\ &= e^{-(\hat{H}-\mu\hat{N})\tau_k} e^{(\hat{H}-\mu\hat{N})\tau_{k+1}} \,. \end{aligned} \tag{2.2.65}$$

With these expressions we can proceed

$$\begin{aligned} &G^{(n)}\left(\lambda_1\tau_1\dots\lambda_n\tau_n|\lambda'_{2n}\tau'_{2n}\dots\lambda'_{n+1}\tau'_{n+1}\right) \qquad (2.2.66)\\ &= \frac{1}{Z_0}\zeta^P \mathrm{Tr}\left[e^{-\int_{\tau_{P_1}}^{\beta}(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P_1}}(\tau_{P_1})e^{-\int_{\tau_{P_2}}^{\tau_{P_1}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P2}}(\tau_{P2})e^{-\int_{\tau_{P3}}^{\tau_{P2}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\right.\\ &\qquad\qquad \left.\dots e^{-\int_{\tau_{P_{2n}}}^{\tau_{P_{2n-1}}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P_{2n}}}(\tau_{P_{2n}})e^{-\int_{\tau_{P_{2n+1}}}^{\tau_{P_{2n}}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\right]\\ &= \frac{1}{Z_0}\zeta^P \mathrm{Tr}\left[e^{-\int_{\tau_{P_1}}^{\beta}(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P_1}}(\tau_{P_1})e^{-\int_{\tau_{P_2}}^{\tau_{P_1}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P_2}}(\tau_{P_2})e^{-\int_{\tau_{P_3}}^{\tau_{P_2}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\right.\\ &\qquad\qquad \left.\dots e^{-\int_{\tau_{P_{2n}}}^{\tau_{P_{2n-1}}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\tilde{a}_{\lambda_{P_{2n}}}(\tau_{P_{2n}})e^{-\int_{\tau_0}^{\tau_{P_{2n}}}\mathrm{d}\tau'(\hat{H}-\mu\hat{N})}\right]\\ &= \frac{1}{Z_0}\mathrm{Tr}\left[\hat{\mathrm{T}}e^{-\int_0^{\beta}(\hat{H}-\mu\hat{N})}a_{\lambda_1}(\tau_1)a_{\lambda_2}(\tau_2)\dots a_{\lambda_N}(\tau_N)a^{\dagger}_{\lambda_{N+1}}(\tau_{N+1})a^{\dagger}_{\lambda_{N+2}}(\tau_{N+2})\dots a^{\dagger}_{\lambda_{2N}}(\tau_{2N})\right]\\ &= \frac{1}{Z_0}\int D\overline{\varphi}_\lambda D\varphi_\lambda\, \varphi_{\lambda_1}(\tau_1)\varphi_{\lambda_2}(\tau_2)\dots\varphi_{\lambda_n}(\tau_n)\overline{\varphi}_{\lambda_{n+1}}(\tau_{n+1})\dots\overline{\varphi}_{\lambda_{2n}}(\tau_{2n})e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\sum_\lambda\overline{\varphi}_\lambda(\hbar\partial_\tau-\mu)\varphi_\lambda(\tau)+\mathrm{H}[\overline{\varphi}_\lambda,\varphi_\lambda]}\,. \end{aligned}$$

The last formula states, that we integrate over all field configurations of the system with different phases given by the Hamiltonian and multiplied by the fixed fields, $\varphi_{\lambda_k}(\tau_k)$ and $\overline{\varphi}_{\lambda'_k}(\tau'_k)$. Since these fields are only acting on a certain time and the rest of the integration is the same the Green function gives us the change of the system, when one particle $\varphi(\tau)$ at a given time is present or $\overline{\varphi}(\tau')$ absent. Next we will see, that the so defined Green function is indeed a Green function in the mathematical sense of being a solution to a differential equation, with a Delta distribution or an inhomogeneous local source term. Now we are going to calculate the free two point Green function with the discrete path integral. In order to do so, we associate

$$\tau_1 \sim q\frac{\beta}{N} \qquad \text{and} \qquad \tau_2 \sim r\frac{\beta}{N}\,, \tag{2.2.67}$$

then follows from (2.2.66) and (2.2.45) directly,

$$\begin{aligned} G_0(\alpha\tau_1|\beta\tau_2) &= \frac{1}{Z_0}\int D\overline{\varphi}_\lambda D\varphi_\lambda\, e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\sum_\lambda[\overline{\varphi}_\lambda(\hbar\partial_\tau-\mu)\varphi_\lambda(\tau)+\mathrm{H}_0[\overline{\varphi}_\lambda,\varphi_\lambda]]}\,\varphi_\alpha(\tau_1)\overline{\varphi}_\beta(\tau_2)\\ &= \lim_{N\to\infty}\frac{1}{Z_0^N}\prod_{k=1}^{N}\left[\prod_\lambda\int\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}\right]e^{-\sum_\lambda\sum_{i,j=1}^{N}\overline{\varphi}_{\lambda,i}M^{(\lambda)}_{ij}\varphi_{\lambda,j}}\,\varphi_{\alpha,q}\overline{\varphi}_{\beta,r}\\ &= \lim_{N\to\infty}\frac{1}{Z_0^N}\prod_{k=1}^{N}\prod_\lambda\left[\int\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_{i,j=1}^{N}\overline{\varphi}_{\lambda,i}M^{(\lambda)}_{ij}\varphi_{\lambda,j}}\,\varphi_{\alpha,q}\overline{\varphi}_{\beta,r}\right]\,. \end{aligned} \tag{2.2.68}$$

where Z_0^N stands for the discrete form of the partition function. Since the action does not couple to different field components, integrating an odd function over a symmetric interval, results to zero, thus we can write

$$\begin{aligned}
G_0(\alpha\tau_1|\beta\tau_2) &= \delta_{\alpha,\beta}\lim_{N\to\infty}\frac{1}{Z_0^N}\prod_{k=1}^{N}\prod_{\lambda}\left[\int\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_{i,j=1}^{N}\overline{\varphi}_{\lambda,i}M_{ij}^{(\alpha)}\varphi_{\lambda,j}}\,\varphi_{\alpha,q}\overline{\varphi}_{\beta,r}\right]\\
&= \delta_{\alpha,\beta}\lim_{N\to\infty}\frac{\zeta}{Z_0^N}\frac{\partial}{\partial\overline{J}_q\partial J_r}\prod_{k=1}^{N}\prod_{\lambda}\int\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_{i,j=1}^{N}\overline{\varphi}_{\lambda,i}M_{ij}^{(\alpha)}\varphi_{\lambda,j}+\sum_i\overline{J}_i\varphi_{\alpha,i}+\overline{\varphi}_{\beta,i}J_i}\Big|_{J=\overline{J}=0}\\
&= \delta_{\alpha,\beta}\lim_{N\to\infty}\frac{\zeta}{Z_0^N}\frac{\partial}{\partial\overline{J}_q\partial J_r}\prod_{\lambda}\prod_{k=1}^{N}\int\frac{d\overline{\varphi}_{\lambda,k}d\varphi_{\lambda,k}}{N}e^{-\sum_{i,j=1}^{N}\overline{\varphi}_{\lambda,i}M_{ij}^{(\alpha)}\varphi_{\lambda,j}+\sum_i\overline{J}_i\varphi_{\alpha,i}+\overline{\varphi}_{\beta,i}J_i}\Big|_{J=\overline{J}=0}\\
&= \delta_{\alpha,\beta}\lim_{N\to\infty}\frac{\zeta}{Z_0^N}\frac{\partial}{\partial\overline{J}_q\partial J_r}\prod_{\lambda}[\det(M)]^{-\zeta}\,e^{\sum_{i,j=1}^{N}\overline{J}_iM_{ij}^{(\alpha)^{-1}}J_j}\Big|_{\overline{J}=J=0}\\
&= \delta_{\alpha,\beta}\lim_{N\to\infty}\frac{\zeta}{Z_0^N}\frac{\partial}{\partial\overline{J}_q\partial J_r}\underbrace{\prod_{\lambda}[\det(M)]^{-\zeta}}_{=Z_0^N}\prod_{\lambda}e^{\sum_{i,j=1}^{N}\overline{J}_iM_{ij}^{(\alpha)^{-1}}J_j}\Big|_{\overline{J}=J=0}\\
&= \delta_{\alpha,\beta}\lim_{N\to\infty}\zeta\frac{\partial}{\partial\overline{J}_q\partial J_r}\prod_{\lambda}e^{\sum_{i,j=1}^{N}\overline{J}_iM_{ij}^{(\alpha)^{-1}}J_j}\Big|_{\overline{J}=J=0}\\
&= \lim_{N\to\infty}\delta_{\alpha,\beta}M_{qr}^{(\alpha)^{-1}}\,.
\end{aligned}\tag{2.2.69}$$

Here we see, that the matrix $M_{qr}^{(\alpha)^{-1}}$ gives the discrete version of the Green function. So we see, that $G_0(\alpha\tau_1|\alpha\tau_2)$ is indeed a Green function, as it is the (discrete) solution to the differential equation

$$(\hbar\partial_\tau+\varepsilon_\alpha-\mu)\,G_0(\alpha\tau_1|\alpha\tau_2)=\delta(\tau_1-\tau_2)\,.\tag{2.2.70}$$

Indeed, without the subtlety of what happens at equal times one can also solve the differential equation by considering the boundary conditions. See Appendix D. Elaborating on the above, we can now more precisely say, that the Green function gives the expectation value of a system, where a particle is inserted or created in a state φ_λ at a time τ_1, travels through the medium to a time τ_2 and is removed, destroyed there. We should say, that we have introduced the $\overline{J}$ and J terms, which again in the fermionic case are Grassmann numbers. These terms are called source terms and are eventually set to zero, so they do not have a physical significance. With the inverse matrix (2.2.57) we can now evaluate the two-point Green function. The diagonal represents the case when $\tau_q=\tau_r$. In the upper triangle we have $\tau_q\leq\tau_r$ and in the lower triangle $\tau_q\geq\tau_r$. According to our observation after (2.2.38) we have to use the upper triangle in case of equal times. Now we can calculate

for $q < r$

$$\begin{aligned}
\lim_{N\to\infty} M_{qr}^{(\alpha)^{-1}} &= \lim_{N\to\infty} \frac{a^{q-r}}{1-\zeta a^N} \\
&= \lim_{N\to\infty} a^{q-r}\left(\frac{1}{1-\zeta a^N}\right) \\
&= \lim_{N\to\infty} a^{q-r}\left(\frac{1-\zeta\, a^N}{1-\zeta a^N} + \frac{\zeta a^N}{1-\zeta a^N}\right) \\
&= \lim_{N\to\infty} a^{q-r}\left(1 + \frac{\zeta a^N}{1-\zeta a^N}\right) \\
&= \lim_{N\to\infty} a^{q-r}\left(1 - \frac{1}{a^{-N}-\zeta}\right) \\
&= \lim_{N\to\infty} (1 - \frac{\varepsilon}{\hbar}(\varepsilon_\alpha - \mu))^{q-r}\left(1 - \frac{1}{(1-\frac{\varepsilon}{\hbar}(\varepsilon_\alpha-\mu))^{-N}-\zeta}\right) \\
&= \lim_{N\to\infty} (1 - \frac{\beta}{N}(\varepsilon_\alpha - \mu))^{\frac{N}{\beta}(\tau_q-\tau_r)}\left(1 - \frac{1}{(1-\frac{\varepsilon}{\hbar}(\varepsilon_\alpha-\mu))^{-N}-\zeta}\right) \\
&= e^{-(\varepsilon_\alpha-\mu)(\tau_q-\tau_r)}\left(1 - \frac{\zeta}{e^{\beta(\varepsilon_\alpha-\mu)}-\zeta}\right)\,,
\end{aligned} \tag{2.2.71}$$

where we made use of (2.2.41). For $q \leq r$, we now get in the same manner

$$\begin{aligned}
\lim_{N\to\infty} M_{qr}^{(\alpha)^{-1}} &= \lim_{N\to\infty} \frac{\zeta a^{N+q-r}}{1-\zeta a^N} \\
&= \lim_{N\to\infty} a^{q-r}\frac{\zeta a^N}{1-\zeta a^N} \\
&= \lim_{N\to\infty} a^{q-r}\frac{\zeta}{a^{-N}-\zeta} \\
&= \lim_{N\to\infty} \left[1 - \frac{\varepsilon}{\hbar}(\varepsilon_\alpha-\mu)\right]^{q-r}\frac{\zeta}{(1-\frac{\varepsilon}{\hbar}\varepsilon_\alpha-\mu)^{-N}-\zeta} \\
&= \lim_{N\to\infty} \left[1 - \frac{\beta}{N}(\varepsilon_\alpha-\mu)\right]^{\frac{N}{\beta}(\tau_q-\tau_r)}\frac{\zeta}{(1-\frac{\varepsilon}{\hbar}\varepsilon_\alpha-\mu)^{-N}-\zeta} \\
&= e^{-(\varepsilon_\alpha-\mu)(\tau_q-\tau_r)}\frac{1}{e^{\beta(\varepsilon_\alpha-\mu)}-\zeta}\,.
\end{aligned} \tag{2.2.72}$$

If we further introduce the usual bosonic and fermionic occupation number

$$n_\alpha := \frac{1}{e^{\beta(\varepsilon_\alpha-\mu)}-\zeta}\,, \tag{2.2.73}$$

we can write the two point Green function as

$$\begin{aligned}
G_0(\alpha\tau_1|\beta\tau_2) &= \delta_{\alpha,\beta}e^{-(\varepsilon_\alpha-\mu)(\tau_1-\tau_2)}\Big[\theta(\tau_1-\tau_2-\eta)(1+\zeta n_\alpha) + \zeta\theta(\tau_2-\tau_1+\eta)n_\alpha\Big] \\
&= \delta_{\alpha,\alpha'}g_\alpha(\tau_1-\tau_2-\eta)\,,
\end{aligned} \tag{2.2.74}$$

where the η prescription acts as a reminder, that the second term is to be used if $\tau_1 = \tau_2$. The whole derivation in this manner was done in order to justify the evaluation of the path integral at equal times. Otherwise the continuous expression (2.2.70) could be used immediately as done in most textbooks. See also Appendix D.

2.3 Perturbation Theory

Since it is not possible to calculate the interacting Green function for our system because of the dipolar interaction, we have to use perturbation theory to take the interaction into account. Our goal is to express the interacting Green function via perturbation theory and then calculate the self-energy, which is given by the Dyson equation. Before we derive the perturbation theory for the Green function, we need the Wick theorem, which we will now derive first.

Wick Theorem

We can now easily show the Wick theorem by looking at the following identity. Again we concentrate on the fermionic case. We start with the following identity for Grassmann integrals. See Appendix C

$$G(\overline{J},J)=\frac{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi\, e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}=e^{\sum_{ij=1}\overline{J}_iM^{-1}_{ij}J_j}\ . \tag{2.3.1}$$

Now with the help of the chain rule for Grassmann functions (2.1.31) we get

$$\begin{aligned}\frac{\partial}{\partial J_1}G(\overline{J},J)&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi\,(\zeta\overline{\varphi}_1)\,e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\\&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\,(\zeta\overline{\varphi}_1)\ .\end{aligned} \tag{2.3.2}$$

Where in the second line we have used again the fact, that the exponent just consists of an even number of Grassmann variables. Now we can proceed as follows

$$\begin{aligned}\frac{\partial^2}{\partial J_2\partial J_1}G(\overline{J},J)&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi\,(\zeta\overline{\varphi}_2)\,e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i\overline{\varphi}_iJ_i}\,(\zeta\overline{\varphi}_1)\\&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i\overline{\varphi}_iJ_i}\left(\zeta^2\overline{\varphi}_2\overline{\varphi}_1\right)\ .\end{aligned} \tag{2.3.3}$$

Continuing in this way, we arrive at

$$\frac{\partial^n}{\partial J_n...\partial J_1}G(\overline{J},J)=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_i+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\,(\zeta^n\overline{\varphi}_n...\overline{\varphi}_1)\ . \tag{2.3.4}$$

Next up we proceed with the derivative with respect to $\overline{J}$ and get

$$\begin{aligned}\frac{\partial^{n+1}}{\partial\overline{J}_n\partial J_n...\partial J_1}G(\overline{J},J)&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{j}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi\,(\varphi_n)\,e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\,(\zeta^n\overline{\varphi}_n...\overline{\varphi}_1)\\&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{j}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_iM_{ij}\varphi_j+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\,(\zeta^n\varphi_n\overline{\varphi}_n...\overline{\varphi}_1)\\&\vdots\\\frac{\partial^{2n-1}}{\partial\overline{J}_{2n-1}...\partial\overline{J}_n\partial J_n...\partial J_1}G(\overline{J},J)&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_j}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_jM_{ij}\varphi_i+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\,(\zeta^n\varphi_{2n-1}...\varphi_n\overline{\varphi}_n...\overline{\varphi}_1)\\\frac{\partial^{2n}}{\partial\overline{J}_1...\partial\overline{J}_n\partial J_n...\partial J_1}G(\overline{J},J)&=\frac{1}{\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{\sum_{ij}\overline{\varphi}_iM^{-1}_{ij}\varphi_1}}\int\mathscr{D}\overline{\varphi}\mathscr{D}\varphi e^{-\sum_{ij}\overline{\varphi}_jM_{ij}\varphi_i+\sum_i\overline{J}_i\varphi_i+\overline{\varphi}_iJ_i}\zeta^n\,(\varphi_1...\varphi_n\overline{\varphi}_n...\overline{\varphi}_1)\ .\end{aligned} \tag{2.3.5}$$

In the next step we derivate the right side of the identity (2.3.1)

$$\begin{aligned}
\frac{\partial}{\partial J_1} G(\overline{J}, J) &= \left(\zeta \sum_i \overline{J}_i M^{-1}_{i1} \right) e^{\sum_{ij} \overline{J}_i M^{-1}_{ij} J_j} \\
\frac{\partial^2}{\partial J_2 \partial J_1} G(\overline{J}, J) &= \zeta^2 \left(\sum_i \overline{J}_i M^{-1}_{i2} \right) \left(\sum_i \overline{J}_i M^{-1}_{i1} \right) e^{\sum_{ij} \overline{J}_i M^{-1}_{ij} J_j} \\
&\vdots \\
\frac{\partial^n}{\partial J_n ... \partial J_1} G(\overline{J}, J) &= \zeta^n \left(\sum_{i=1} \overline{J}_i M^{-1}_{in} \right) \dots \left(\sum_{i=1} \overline{J}_i M^{-1}_{i2} \right) \left(\sum_i \overline{J}_i M^{-1}_{i1} \right) e^{\sum_{ij} \overline{J}_i M^{-1}_{ij} J_j} \, . \qquad (2.3.6)
\end{aligned}$$

Now obviously for Grassmann numbers only terms survive, which contain each J_k only once. Hence we derivated n-times, we have n^n-terms. The second index of M corresponds with $\overline{J}$, thus we can write the last line as

$$\frac{\partial^n}{\partial J_n ... \partial J_1} G(\overline{J}, J) = \zeta^n \sum_{\ell}^{n} \prod_{\substack{P_\ell \\ P_\ell \neq \ell}} \overline{J}_{P_\ell} M^{-1}_{P_\ell, \ell} e^{\sum_{ij} \overline{J}_i M^{-1}_{ij} J_j} \, . \qquad (2.3.7)$$

This sum is best pictured as a block of $n \times n$ summands. For Grassmann numbers all terms vanish, which contain any $\overline{J}_k$ more than once. Then of all the n^n-terms only $n!$ terms remain. Since in all of this terms all permutations of $\overline{J}_k$ are present, the derivation with respect to all $\overline{J}_k$ leave only terms, which are independent of $J, \overline{J}$ outside of the exponent plus terms which still contain $\overline{J}$ due to the product rule. However if we set $J = \overline{J} = 0$ only the $n!$ permutations independent of $J, \overline{J}$ outside of the exponential remain. In the bosonic case the terms of (2.3.7) are all present but if we derivate with respect to all $\overline{J}$ again only terms which had each $\overline{J}$ present survive. In this way we have arrived at the identity

$$\frac{\partial^{2n}}{\partial \overline{J}_1 \dots \partial \overline{J}_n \partial J_n \dots \partial J_1} \left(e^{\sum_{i,j=1} \overline{J}_i M^{-1}_{ij} J_j} \right) \Big|_{\overline{J}=J=0} = \sum_P \zeta^P M^{-1}_{P_n, n} \dots M^{-1}_{P_1, 1} \qquad (2.3.8)$$

Now by setting $\overline{J} = J = 0$ in (2.3.5) we arrive at the form

$$\frac{\int \mathscr{D}\overline{\varphi} \mathscr{D}\varphi \varphi_1 \dots \varphi_n \overline{\varphi}_n \dots \overline{\varphi}_1 e^{-\sum_{ij} \overline{\varphi}_i M_{ij} \varphi_j}}{\int \mathscr{D}\overline{\varphi} \mathscr{D}\varphi \, e^{\sum_{ij} \overline{\varphi}_i M^{-1}_{ij} \varphi_j}} = \sum_P \zeta^P M^{-1}_{P_n, n} \dots M^{-1}_{P_1, 1} \, . \qquad (2.3.9)$$

To write Wick's theorem in the standard form, one defines so called contractions:

$$\begin{aligned}
\overbrace{\varphi_\alpha(\tau_1) \overline{\varphi}_\beta(\tau_2)} &:= \langle \varphi_\alpha(\tau_1) \overline{\varphi}_\beta(\tau_2) \rangle_0 \\
\overbrace{\overline{\varphi}_\beta(\tau_2) \varphi_\alpha(\tau_1)} &:= \langle \overline{\varphi}_\beta(\tau_2) \varphi_\alpha(\tau_1) \rangle_0 \, . \qquad (2.3.10)
\end{aligned}$$

Hence the expectation value vanishes, if the two fields are both Grassmann fields, or both convoluted Grassmann fields (2.3.10) implies

$$\overbrace{\varphi_\alpha(\tau_1) \varphi_\beta(\tau_2)} = \overbrace{\overline{\varphi}_\beta(\tau_2) \overline{\varphi}_\alpha(\tau_1)} = 0 \, . \qquad (2.3.11)$$

We calculated the two point Green function as (2.2.74) so we can see the contractions as Green functions (propagators)

$$\begin{aligned}
\overbrace{\varphi_\alpha(\tau_1) \overline{\varphi}_\beta(\tau_2)} &:= \delta_{\alpha,\beta} g_\alpha(\tau_1 - \tau_2) \\
\overbrace{\overline{\varphi}_\beta(\tau_2) \varphi_\alpha(\tau_1)} &:= \zeta \delta_{\alpha,\beta} g_\alpha(\tau_1 - \tau_2) \, . \qquad (2.3.12)
\end{aligned}$$

With this definitions and the representation for the discrete Green function given by (2.2.69), we can write the Wick Theorem in the standard form

$$\langle\tilde{\psi}_{\lambda_1}(\tau_1)\dots\tilde{\psi}_{\lambda_n}(\tau_n)\rangle_0 = \sum \text{ all complete contractions} \tag{2.3.13}$$

2.3.1 Feynman Rules for the Partition Function

Since the dipole-dipole interaction will be seen as a two point interaction, we now have to consider a Hamiltonian of the form

$$H = \sum_\lambda \varepsilon_\lambda \overline{\psi}_\lambda(\tau)\psi_\lambda(\tau) - \frac{1}{2}\sum_{\alpha\,\beta\,\gamma\,\delta}\langle\alpha\,\beta|\,V\,|\gamma\,\delta\rangle\,\overline{\psi}_\alpha(\tau)\overline{\psi}_\beta(\tau)\psi_\gamma(\tau)\psi_\delta(\tau)\,, \tag{2.3.14}$$

where we have now written ψ, to emphasize that we are dealing with an interacting Hamiltonian. With the thermal average expressed for any functional F, with the path integral as

$$\begin{aligned}&\left\langle F\left[\overline{\psi}_\alpha(\tau_i),\overline{\psi}_\beta(\tau_j),\dots,\psi_\gamma(\tau_k),\psi_\delta(\tau_\ell),\dots\right]\right\rangle_0 \\ &\quad:= \frac{1}{Z_0}\int_{\psi(\hbar\beta)=\zeta\psi(0)}\mathscr{D}\overline{\psi}\mathscr{D}\psi e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\sum_\lambda\overline{\psi}_\lambda(\hbar\partial_\tau+\varepsilon_\lambda-\mu)\psi_\lambda}F\left[\overline{\psi}_\alpha(\tau_i),\overline{\psi}_\beta(\tau_j),\dots,\psi_\gamma(\tau_k),\psi_\delta(\tau_\ell),\dots\right]\end{aligned} \tag{2.3.15}$$

we can rewrite the partition function as

$$\begin{aligned}Z &= \int_{\psi(\hbar\beta)=\zeta\psi(0)}\mathscr{D}\overline{\psi}\mathscr{D}\psi e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\sum_\lambda\overline{\psi}_\lambda(\hbar\partial_\tau+\varepsilon_\lambda-\mu)\psi_\lambda+V[\overline{\psi}_\alpha(\tau_1)\overline{\psi}_\beta(\tau_j)\dots\psi_\gamma(\tau_k)\psi_\delta(\tau_\ell)\dots]} \\ &= \int_{\psi(\hbar\beta)=\zeta\psi(0)}\mathscr{D}\overline{\psi}\mathscr{D}\psi e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\sum_\lambda\overline{\psi}_\lambda(\hbar\partial_\tau+\varepsilon_\lambda-\mu)\psi_\lambda}e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,V[\overline{\psi}_\alpha(\tau_1)\overline{\psi}_\beta(\tau_j)\dots\psi_\gamma(\tau_k)\psi_\delta(\tau_\ell)\dots]} \\ &= Z_0\left\langle e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,V[\overline{\psi}_\alpha(\tau_1)\overline{\psi}_\beta(\tau_j)\dots\psi_\gamma(\tau_k)\psi_\delta(\tau_\ell)\dots]}\right\rangle_0\,.\end{aligned} \tag{2.3.16}$$

In order to apply perturbation theory, we use the series of the exponential function and rewrite the partition function as

$$\begin{aligned}\frac{Z}{Z_0} &= \left\langle\sum_{n=0}^\infty\frac{(-1)^n}{n!\,\hbar^n}\left[\int_0^{\hbar\beta}\mathrm{d}\tau\,V(\overline{\psi}_\alpha(\tau)\overline{\psi}_\beta(\tau),\dots,\psi_\gamma(\tau)\psi_\delta(\tau),\dots)\right]^n\right\rangle_0 \\ &= \left\langle\sum_{n=0}^\infty\frac{(-1)^n}{n!\,\hbar^n}\int_0^{\hbar\beta}\mathrm{d}\tau_1\dots\mathrm{d}\tau_n\,V(\overline{\psi}_\alpha(\tau_1)\overline{\psi}_\beta(\tau_1),\dots,\psi_\gamma(\tau_1)\psi_\delta(\tau_1),\dots)\right. \\ &\qquad\left.\times\dots\times V(\overline{\psi}_\alpha(\tau_n)\overline{\psi}_\beta(\tau_n),\dots,\psi_\gamma(\tau_n)\psi_\delta(\tau_n),\dots)\right\rangle_0 \\ &= \left\langle\sum_{n=0}^\infty\frac{(-1)^n}{n!\,\hbar^n}\prod_{k=1}^n\left[\int_0^{\hbar\beta}\mathrm{d}\tau_k V(\overline{\psi}_\alpha(\tau_k)\overline{\psi}_\beta(\tau_k),\dots,\psi_\gamma(\tau_k)\psi_\delta(\tau_k),\dots)\right]\right\rangle_0 \\ &= \sum_{n=0}^\infty\frac{(-1)^n}{n!\,\hbar^n}\prod_{k=1}^n\int_0^{\hbar\beta}\mathrm{d}\tau_k\left\langle V(\overline{\psi}_\alpha(\tau_k)\overline{\psi}_\beta(\tau_k),\dots,\psi_\gamma(\tau_k)\psi_\delta(\tau_k),\dots)\right\rangle_0\,.\end{aligned} \tag{2.3.17}$$

Considering a two-body interaction like the dipole-dipole interaction it follows from the Hamiltonian (2.3.14)

$$\begin{aligned}\frac{Z}{Z_0} &= \left\langle e^{-\frac{1}{2\hbar}\int_0^{\hbar\beta}\sum_{\alpha,\beta,\gamma,\delta}\langle\alpha\,\beta|V|\gamma\,\delta\rangle\overline{\psi}_\alpha(\tau)\overline{\psi}_\beta(\tau)\psi_\gamma(\tau)\psi_\delta(\tau)}\right\rangle_0 \\ &= \left\langle \sum_{n=0}^{\infty}\frac{(-1)^n}{(2\hbar)^n n!}\sum_{\alpha_1,\beta_1,\gamma_1,\delta_1}\cdots\sum_{\alpha_n,\beta_n,\gamma_n,\delta_n}\langle\alpha_1\,\beta_1|\,V\,|\gamma_1\,\delta_1\rangle\ldots\langle\alpha_n\,\beta_n|\,V\,|\gamma_n\,\delta_n\rangle\int_0^{\hbar\beta}d\tau_1\ldots d\tau_n\right. \\ &\qquad\left.\times\,\overline{\psi}_\alpha(\tau_1)\overline{\psi}_\beta(\tau_1)\psi_\gamma(\tau_1)\psi_\delta(\tau_1)\ldots\overline{\psi}_\alpha(\tau_n)\overline{\psi}_\beta(\tau_n)\psi_\gamma(\tau_n)\psi_\delta(\tau_n)\right\rangle_0 \\ &= \sum_{n=0}^{\infty}\frac{(-1)^n}{(2\hbar)^n n!}\prod_{k=1}^{n}\sum_{\alpha_k,\beta_k,\gamma_k,\delta_k}\langle\alpha_k\,\beta_k|\,V\,|\gamma_k\,\delta_k\rangle\prod_{k=1}^{n}\left[\int_0^{\hbar\beta}d\tau_k\right]\left\langle\prod_{k=1}^{n}\overline{\psi}_\alpha(\tau_k)\overline{\psi}_\beta(\tau_k)\psi_\gamma(\tau_k)\psi_\delta(\tau_k)\right\rangle_0 . \quad (2.3.18)\end{aligned}$$

With the help of Wick's theorem it is now possible to justify Feynman rules for the series expansion. Since we can expand the expectation value with the help of Wick's theorem in all the contractions, one represents the contractions, which are according to (2.3.12) Green functions, with a directed line from $\overline{\psi}_{\lambda_i}(\tau_i)$ to $\psi_{\lambda_j}(\tau_j)$. The corresponding interaction vertices $\langle\alpha_k\,\beta_k|\,V\,|\gamma_k\,\delta_k\rangle$ will be represented by vertices with the incoming lines $\gamma_k\,\delta_k$ and two outgoing lines $\alpha_k\,\beta_k$. Acting on a time τ_k. So we introduce:

(a) (b)

Figure 2.1: Diagrammatic representation of propagators and vertices

Going back to formula (2.3.18), we see that each summand of order n has n vertices and (for the two body interaction) $2n$ fields in the expectation value, leading to $(2n)!$ contractions. Since the diagrams are seen just as a representation of the contributing terms, they are not uniquely defined. Merely two diagrams are equal, if they can be transformed into each other smoothly. That is by conserving the arrows and labels of the diagram. Finally we must consider the pre-factor $\frac{(-1)^n}{2^n n!}$ for each diagram. But for fermions as can be seen from formula (2.3.12), each contraction brings a ζ factor and so one has to find the right sign. Each vertex has two incoming and two outgoing lines (propagators). Since we are only dealing with complete contractions, all vertices connections form a closed loop. Each of such a loop consists of less than n vertices. Each vertex has an even number of fields in it. A specific closed loop uses two of the given fields. Hence even Grassmann fields commute with even Grassmann fields, the enclosed fields can be brought to the left of a given closed cycle, so that the closed cycle has the form:

$$\overline{\psi}_1\psi_1\ldots\overline{\psi}_2\psi_2\ldots\ldots\overline{\psi}_n\psi_n\ldots\,, \quad (2.3.19)$$

so the inner contractions $\overline{\psi}\psi$ each lead to a $(+1)$ factor, while the outer contraction $\overline{\psi}\psi$ gives a ζ. Since the remaining loops are made of the remaining even Grassmann fields, they can be brought in the same form and have the same sign. So we conclude, that each closed loop leads to the factor ζ^{n_c}, where n_c is the number of closed loops. Thus we have the following rules for Feynmann diagrams for the partition function.

1 In order to construct all diagrams of order n, one has to draw all distinct diagrams with n vertices of the Figure 2.1b, and connect these with the propagators (2.1a). The diagrams are distinct, if they cannot be transformed into each other by conserving labels and propagator direction.

2 Each propagator gets an index and is assigned the quantity $g_\alpha(\tau_k - \tau_\ell)$ (2.2.74).

3 Each vertex stands for the matrix element $\langle \alpha\, \beta |\, V\, | \gamma\, \delta \rangle$.

4 Include the sum over each index and the integral over all times, where the integrals run from $[0, \hbar\beta]$.

5 Include the pre-factor consisting of $\frac{(-1)^n}{2^n\, n!}\zeta^{n_c}$.

It should be mentioned, that one can reduce the number of diagrams dramatically, by analysing which diagrams lead to the same contribution. In order to do so one has to define the symmetry factor, which in essence boils down to investigate in which cases the time integration and the spatial integration within the interaction overlap matrix can be interchanged. However, since we are interested in the Feynman rules for the Green function, we will skip this discussion here.

2.3.2 Feynman Rules for the Interacting Green Function

We are now going to derive the Feynman rules for the interacting Green function

$$G^{(n)}\left(\alpha_1\beta_1\ldots\alpha_n\beta_n|\alpha_1'\beta_1'\ldots\alpha_n'\beta_n'\right) = \frac{\left\langle e^{-\frac{1}{\hbar}\int d\beta V\left[\overline{\psi},\psi\right]}\psi_{\alpha_1}(\beta_1)\ldots\psi_{\alpha_n}(\beta_n)\overline{\psi}_{\alpha_n}(\beta_n')\ldots\overline{\psi}\alpha_1'(\beta_1')\right\rangle_0}{\left\langle e^{-\frac{1}{\hbar}\int d\beta V\left[\overline{\psi},\psi\right]}\right\rangle_0}\,. \quad (2.3.20)$$

The external time are now denoted β to distinguish these from the internal time. We now want to apply the so called replica trick, for that matter we introduce the n fields $\left\{\overline{\psi}_\lambda^\sigma, \psi_\lambda^\sigma\right\}$, with $1 \le \sigma \le n$ and define:

$$G_m := \frac{1}{Z_0^m}\int\prod_{\sigma=1}^m \mathscr{D}\overline{\psi}^\sigma\mathscr{D}\psi^\sigma\psi_\alpha(\beta_1)\ldots\psi_{\alpha_n}(\beta_n)\overline{\psi}_{\alpha_n'}(\beta_n')\ldots\overline{\psi}_{\alpha_1'}(\beta_1')e^{-\frac{1}{\hbar}\sum_{\sigma=1^n}\int d\tau\sum_\lambda\overline{\psi}_\lambda^\sigma(\hbar\partial_\tau+\epsilon_\lambda-\mu)\overline{\psi}_\lambda^\sigma+V\left[\overline{\psi}^\sigma\psi^\sigma\right]}\,. \quad (2.3.21)$$

Before we proceed in developing the Feynman rules for the interacting Green function it is useful to have a closer look at formula (2.3.20). According to formula (2.3.6), we can develop the nominator and denominator with the help of the above given perturbation theory. Then we see immediately that in the denominator only contractions between the interaction arise, which are not connected to the external fields, $\overline{\psi}_\ell(\beta)$, while the nominator does couple the interaction with the external fields. One now expects that the disconnected parts, that is disconnected to the external field, cancel with the disconnected fields in the denominator. We will now see, with the help of the replica method, that this is indeed the case. We already know that the Green function describes the expectation value of the system if a particle is (inserted) or removed in the system at a time τ_1 and (removed) inserted at a time τ_2. If the above expression is evaluated with the help of perturbation theory, the interacting Green function will be given, as the free Green function added by some correction terms.

Noting that the two fields corresponding to one time τ are an even number apart, it follows

$$\begin{aligned}
G_m &= \frac{1}{Z_0}\int\prod_{\sigma=1}^m\mathscr{D}\overline{\psi}^\sigma\mathscr{D}\psi^\sigma\psi_{\alpha_1}(\beta_1)\overline{\psi}_{\alpha_1'}(\beta_1')e^{-\frac{1}{\hbar}\sum_{\sigma=1}^n\int\mathrm{d}\tau\sum_\lambda\overline{\psi}_\lambda^\sigma(\hbar\partial_\tau+\varepsilon_\lambda-\mu)\psi_\lambda^\sigma+V[\overline{\psi}^\sigma,\psi^\sigma]}\\
&\quad\times\frac{1}{Z_0^{m-1}}\int\prod_{\sigma=2}^m\mathscr{D}\overline{\psi}^\sigma\mathscr{D}\psi^\sigma\psi_{\alpha_2}(\beta_2)\ldots\psi_{\alpha_n}(\beta_n)\overline{\psi}_{\alpha_n'}(\beta_n')\ldots\overline{\psi}_{\alpha_2'}(\beta_2')e^{-\frac{1}{\hbar}\sum_\sigma\int d\tau\sum_\lambda\overline{\psi}_\lambda(\hbar\partial_\tau+\epsilon_\lambda-\mu)\psi_\lambda V\left[\overline{\psi}^\sigma,\psi^\sigma\right]}\\
&= \left\langle e^{-\frac{1}{\hbar}\sum_\lambda\int d\tau V\left[\overline{\psi}^\sigma\psi^\sigma\right]}\psi_{\alpha_1}(\beta_1)\overline{\psi}_{\alpha_1'}(\beta_1')\right\rangle_0\left\langle e^{-\frac{1}{\hbar}\sum_{\sigma=1}^n\int d\tau V\left[\overline{\psi}^\sigma\psi^\sigma\right]}\psi_{\alpha_2}(\beta_2)\ldots\psi_{\alpha_n}(\beta_n)\overline{\psi}_{\alpha_n'}(\beta_n')\ldots\overline{\psi}_{\alpha_2'}(\beta_2')\right\rangle_0^{m-1}\,.
\end{aligned} \quad (2.3.22)$$

Now G_m produces $G^{(n)}$ (2.3.21) for $m = 0$. Now we can expand G_m as follows

$$G_m = \frac{1}{Z_0^m} \int \prod_{\sigma=1}^{m} \mathscr{D}\overline{\psi}^\sigma \mathscr{D}\psi^\sigma \psi^\sigma_{\alpha_1}(\beta_1) \dots \psi_{\alpha_n}(\beta_n) \overline{\psi}_{\alpha'_n}(\beta'_n) \dots \overline{\psi}_{\alpha'_1}(\beta'_1) e^{-\frac{1}{\hbar}\sum_\sigma \int d\tau \sum_\lambda \overline{\psi}_\alpha (\hbar\partial_\tau + \varepsilon_\lambda - \mu)\psi_\lambda} e^{-\frac{1}{\hbar}\sum_{\sigma=1}^n \int d\tau V\left[\overline{\psi}^\sigma \psi^\sigma\right]} . \tag{2.3.23}$$

Expanding the series

$$\begin{aligned} e^{-\frac{1}{\hbar}\sum_{\sigma=1}^m \int d\tau V\left[\overline{\psi}^\sigma \psi^\sigma\right]} &= \sum_{p=0}^{\infty} \frac{(-1)^p}{\hbar^p p!} \prod_{k=1}^{p} \sum_{\sigma_k} \int d\tau_k V\left[\overline{\psi}^{\sigma_k} \psi^{\sigma_k}\right] \\ &= 1 + \frac{(-1)}{\hbar} \sum_{\sigma_1} \int d\tau V\left[\overline{\psi}^{\sigma_1} \psi^{\sigma_1}\right] + \frac{(-1)^2}{\hbar^2 2!} \sum_{\sigma_1\sigma_2} \int d\tau_1 d\tau_2 V\left[\overline{\psi}^{\sigma_1} \psi^{\sigma_1}\right] V\left[\overline{\psi}^{\sigma_2} \psi^{\sigma_2}\right] \\ &\quad + \sum_{p=3} \frac{(-1)^p}{\hbar^p p!} \prod_{k=1}^{p} \sum_{\sigma_k} \int d\tau_k V\left[\overline{\psi}^{\sigma k} \psi^{\sigma_k}\right] , \end{aligned} \tag{2.3.24}$$

then yields

$$\begin{aligned} G_m &= \frac{1}{z_0^m} \int \prod_{\sigma=1}^{m} \mathscr{D}\overline{\psi}^\sigma \mathscr{D}\psi_\sigma e^{-\frac{1}{\hbar}\sum_\sigma \int d\tau \sum_\lambda \overline{\psi}^\sigma_\lambda (\hbar\partial_\tau + \epsilon_\lambda - \mu)\psi^\sigma_\lambda} \\ &\quad + \frac{(-1}{\hbar} \sum_{\sigma_1} \int d\tau_1 \left[\frac{1}{z_0^m} \int \prod_{\sigma=1}^{m} \mathscr{D}\overline{\psi}^\sigma \mathscr{D}\psi^\sigma e^{-\frac{1}{\hbar}\sum_\sigma \int d\tau \sum_\lambda \overline{\psi}^\sigma_\lambda (\hbar\partial_\tau + \epsilon_\lambda - \mu)\psi^\sigma_\lambda} \psi_{\alpha_1}(\beta_1) \overline{\psi}_{\alpha'_1}(\beta'_1) V\left[\overline{\psi}^{\sigma_1} \psi^{\sigma_1}\right] \right] \\ &\quad + \frac{1}{\hbar^2 2} \sum_{\sigma_1\sigma_2} \int d\tau_1 d\tau_2 \left[\frac{1}{z_0^m} \int \prod_{\sigma=1}^{m} \mathscr{D}\overline{\psi}^\sigma \mathscr{D}\psi^\sigma e^{-\frac{1}{\hbar}\sum_\sigma \int d\tau \sum_\lambda \overline{\psi}^\sigma_\lambda (\hbar\partial_\tau + \epsilon_\lambda - \mu)\psi^\sigma_\lambda} \psi_{\alpha_2}(\beta_2) \overline{\psi}_{\alpha'_2}(\beta'_2) V\left[\overline{\psi}^{\sigma_1} \psi^{\sigma_1}\right] V\left[\overline{\psi}^{\sigma_2} \psi^{\sigma_2}\right] \right] \\ &\quad + \frac{(-1)^p}{\hbar^p p!} \sum_{p=3}^{\infty} \prod_{k=1}^{p} \sum_{\sigma_k} \int d\tau_k \left[\frac{1}{z_0^m} \int \prod_{\sigma=1}^{m} \mathscr{D}\overline{\psi}^\sigma \mathscr{D}\psi^\sigma e^{-\frac{1}{\hbar}\sum_\sigma \int d\tau \sum_\lambda \overline{\psi}^\sigma_\lambda (\hbar\partial_\tau + \epsilon_\lambda - \mu)\psi^\sigma_\lambda} \right. \\ &\qquad \left. \times \psi_{\alpha_3}(\beta_3) \dots \psi_{\alpha_n}(\beta_n) \overline{\psi}_{\alpha'_n}(\beta'_n) \dots \overline{\psi}_{\alpha'_1}(\beta'_1) \dots V\left[\overline{\psi}^{\sigma_k} \psi^{\sigma_k}\right] \right] \\ &= 1 + \frac{(-1)}{\hbar} \sum_{\sigma} \int d\tau_1 \left\langle \psi_{\alpha_1}(\beta_1) \overline{\psi}_{\alpha'_1}(\beta'_1) V\left[\overline{\psi}^{\sigma_1}, \psi^{\sigma_1}\right] \right\rangle_0 \\ &\quad + \frac{(-1)^2}{\hbar^2 2} \sum_{\sigma_1\sigma_2} \int d\tau_1 d\tau_2 \left\langle \psi_{\alpha_2}(\beta_2) \overline{\psi}_{\alpha'_2}(\beta'_2) V\left[\overline{\psi}^{\sigma_1}, \psi^{\sigma_1}\right] V\left[\overline{\psi}^{\sigma_2} \psi^{\sigma_2}\right] \right\rangle_0 \\ &\quad + \sum_{p=3}^{\infty} \frac{(-1)^p}{\hbar^p p!} \prod_{k=1}^{p} \sum_{\sigma_k} \int d\tau_k \left\langle \psi_{\alpha_3}(\beta_3) \dots \psi_{\alpha_m}(\beta_m) \dots \overline{\psi}_{\alpha'_1}(\beta'_1) V\left[\overline{\psi}^{\sigma_1}, \psi^{\sigma_1}\right] \right\rangle_0 \\ &=: \sum_{p=0}^{\infty} \frac{(-1)^p}{\hbar^p p!} \prod_{k=1}^{p} \sum_{\sigma_k} \int d\tau_k \left\langle \prod_{k=1}^{p} \psi_{\alpha_k}(\beta_k) \dots \overline{\psi}_{\alpha'_k}(\beta'_k) V\left[\overline{\psi}^{\sigma_k} \psi^{\sigma_k}\right] \right\rangle_0 . \end{aligned} \tag{2.3.25}$$

As we can see the external vertices $\psi_i(\beta_i)$ and $\overline{\psi}_i(\beta_i)$ are associated with the index σ_1. The diagrams now have an index $\sigma \in [1, m]$. The propagators attached to the external fields $\psi_i(\beta_i)$ and $\overline{\psi}_i(\beta_i)$ all carry the index $\sigma = 1$. Furthermore all propagators connected to the same vertex conserve the replica index, since the propagators are given by $\delta_{\alpha,\alpha'} g_\alpha(\tau_1 - \tau_2)$. So the p parts that are not connected to the external legs are proportional to the replica index n^p. By setting $m = 0$, we get the Green function and thus only diagrams which are connected to the external legs.

Since we are only dealing with connected diagrams, the diagrams only consist of directed lines and closed loops connected by the vertex, but not connected over a propagator. Since the propagators within a loop are directed the time-label is fixed and cannot be permuted within a loop and we are dealing only with connected diagrams. One time label in a given loop fixes the time label in a connected loop. So by recursion, all time labels are fixed and cannot be permuted. Since therefore both interchanges of integration are suppressed, the symmetry factor for the Green function is always $S = 1$. Now the final task consist in determining the pre-factor sign of the Wick contractions. By definition of the Green function all $\overline{\psi}_{\alpha'_k}(\beta'_k)$ are an even number of fields separated from $\psi_{\alpha_k}(\beta_k)$, so that the contraction always gives +1. If one now fixes one arbitrary $\overline{\psi}_{\alpha'_k}(\beta'_k)$ and considers the contractions with a permutation of it's counterpart, the sign changes to ζ^P where P is the necessary permutation. Then one can add the other contractions to form a closed loop. By bringing them again in the form (2.3.19) one gets the additional factor ζ^{n_c}. being the closed propagator loops.
We are now ready to give the Feynman rules for the interacting Green function:

1 First one has to draw all distinct unlabeled diagrams, starting with the n external points and with the r interaction vertices. The diagrams are distinct if they cannot be transformed into each other by fixing the external points and keeping the direction of the propagators fixed.

2 The external legs are given by the to be calculated Green function, which have to be assigned first to the interaction vertices. Then the free legs have to be connected with propagators and each propagator is given an index. Then each propagator is assigned with the propagator (2.1a) .

3 Then include for each vertex the matrix element $\langle \alpha\, \beta |\, V\, | \gamma\, \delta \rangle$.

4 Finally for each internal index one includes a sum and for each internal time label one integral, where the integration runs from $[0, \hbar\beta]$.

5 Finally the pre-factor $(-1)^r \zeta^P \zeta^{n_c}$ is included.

Finally we note, that we can produce the n-particle Green function over a generating function defined by

$$\begin{aligned} G(\overline{J}_\lambda, J_\lambda) &= \left\langle e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_\lambda [\overline{J}_\lambda \psi_\lambda + \overline{\psi} J_\lambda]} \right\rangle \\ &= \frac{1}{Z} \int D\overline{\psi}_\lambda D\psi_\lambda e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_\lambda \overline{\psi}_\lambda (\partial_\tau - \mu)\psi_\lambda \psi_\lambda + \mathrm{H}[\overline{\psi_\lambda}, \psi_\lambda] + \overline{J}_\lambda \psi_\lambda + \overline{\psi}_\lambda J_\lambda} \,. \end{aligned} \tag{2.3.26}$$

Where the average is now to be taken with respect to the source field. Note that we have suppressed the τ of the functions, but kept it on the integral for better readabillity. Now the thermal n-point Green function can be expressed as

$$G^{(n)}(\alpha_1\tau_1 \ldots \alpha_n\tau_n | \alpha'_1\tau'_1 \ldots \alpha'_n\tau'_n) = \frac{\hbar^{2n}}{\zeta^n} \frac{\delta^{2n} G(\overline{J}_\lambda, J_\lambda)}{\delta\overline{J}_{\alpha_1}(\tau_1) \ldots \delta\overline{J}_{\alpha_n}(\tau_n) \delta J_{\alpha'_n}(\tau'_n) \ldots \delta J_{\alpha'_1}(\tau'_1)} \bigg|_{\overline{J}=J=0} . \tag{2.3.27}$$

Connected Green Function

Now that we have derived the Feynman rules for the Green function we see, that the diagrams are connected to all the external fields. However the diagrams are not all connected, which means they are build out of lower order Green functions. It is therefore useful to cut these parts off once again. Naturally this can be done with the replica technique once again. The connected parts will then again be proportional to p. So this time we simply write

$$\begin{aligned} W[\overline{J}_\lambda, J_\lambda] &= \lim_{p\to 0} \frac{\partial}{\partial p} G(\overline{J}_\lambda, J_\lambda)^p \\ &= \log\left(G(\overline{J}_\lambda, J_\lambda)\right) \end{aligned} \tag{2.3.28}$$

and the connected n-point Green function is then given by

$$G_{\mathrm{c}}^{(n)}(\alpha_1\tau_1\dots\alpha_n\tau_n|\alpha_1'\tau_1'\dots\alpha_n'\tau_n') = \zeta^n \frac{\delta^{2n}W(\overline{J}_\lambda, J_\lambda)}{\delta\overline{J}_{\alpha_1}(\tau_1)\dots\delta\overline{J}_{\alpha_n}(\tau_n)\delta J_{\alpha_n'}(\tau_n')\dots\delta J_{\alpha_1'}(\tau_1')}\Big|_{\overline{J}=J=0} \quad . \tag{2.3.29}$$

2.4 Derivation of Dyson's Equation

In this section we will derive the Dyson equation and define the self energy. By using the previously derived Feynman rules for the interacting Green function, we can derive the Feynman rules for the self-energy. Using these rules we will then derive the Hartree-Fock equations in first order perturbation theory. First we define the so called average field as the derivative of the generator of the connected Green functions

$$\begin{aligned}\varphi_\lambda &= \langle\psi_\lambda\rangle_{\overline{J},J} = -\frac{\delta}{\delta\overline{J}_\lambda}W[\overline{J},J]\,,\\ \overline{\varphi}_\lambda &= \langle\overline{\psi}_\lambda\rangle_{\overline{J},J} = -\zeta\frac{\delta}{\delta J_\alpha}W[\overline{J}_\lambda,J_\lambda]\,,\end{aligned} \tag{2.4.1}$$

and perform a Legendre transformation. Here we define the Legendre transformation in a functional sense. It should be noted, that the Legendre transformation can not be defined in the usual way, that is analog to one dimensional functions $f\left(\frac{\partial f}{\partial x}\right) = \frac{\partial f}{\partial x}x - f$. Where the standard way in physics is to let the y-axis show in the negative direction, in order to let the Legendre transformation work for convex functions rather than concave ones. Here the definition is tailor made to work with the Grassmann derivative as we shall see shortly. So we take the Legendre transformation

$$\Gamma[\overline{\varphi}_\lambda,\overline{\varphi}_\lambda] = -W[\overline{J}_\lambda,J_\lambda] - \sum_\lambda\int d\tau'\left[\overline{\varphi}_\lambda J_\lambda + \overline{J}_\lambda\varphi_\lambda\right]\,. \tag{2.4.2}$$

Note that if $W[\overline{J},J]$ is of the form $W[\overline{J},J] = \overline{u}_{w_1}u_{w_1} + \overline{g}_{w_2}g_{w_2}$ then φ_λ is of the form $\overline{g}_{w_1}u_{w_1} + \overline{u}_{w_2}g_{w_2}$. Likewise $\overline{\varphi}_\lambda$ will be of the form $\overline{\varphi}_\lambda = \overline{u}_{w_1}g_{w_1} + \overline{g}_{w_2}u_{w_2}$ therefore $\varphi_\lambda,\overline{\varphi}_\lambda \in U^-$. In order to apply the chain rule (2.1.98) it is necessary that $J,\overline{J}\in U^-$, derivating Γ with respect to φ yields.

$$\begin{aligned}\frac{\delta\Gamma[\overline{\varphi}_\lambda,\varphi_\lambda]}{\delta\overline{\varphi}_\lambda} &= -\frac{\delta W}{\delta\overline{\varphi}_\lambda} - \sum_\gamma\int d\tau'\left\{P(\overline{\varphi}_\gamma)\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{\varphi}_\gamma}{\delta\overline{\varphi}_\lambda}J_\gamma + P(\overline{J}_\gamma)\frac{\delta\varphi_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right\}\\
&= -\frac{\delta W}{\delta\overline{\varphi}_\lambda} - \sum_\gamma\int d\tau'\left\{\zeta\overline{\varphi}_\gamma\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{\varphi}_\gamma}{\delta\overline{\varphi}_\lambda}J_\gamma + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right\}\\
&= -\sum_\gamma\int d\tau'\left[\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda}\frac{\delta W}{\delta J_\gamma} + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\frac{\delta W}{\delta\overline{J}_\gamma}\right] - \sum_\gamma\int d\tau'\left\{\dots\right\}\\
&= -\sum_\gamma\int d\tau'\left[-\zeta\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda}\overline{\varphi}_\gamma - \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right] - \sum_\gamma\int d\tau'\left\{\dots\right\}\\
&= \sum_\gamma\int d\tau'\left[\zeta\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda}\overline{\varphi}_\gamma + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right] - \sum_\gamma\int d\tau'\left[\zeta\overline{\varphi}_\gamma\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{\varphi}_\gamma}{\delta\overline{\varphi}_\lambda}J_\gamma + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right]\\
&= \sum_\gamma\int d\tau'\left[\zeta\overline{\varphi}_\gamma\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right] - \sum_\gamma\int d\tau'\left[\zeta\overline{\varphi}_\gamma\frac{\delta J_\gamma}{\delta\overline{\varphi}_\lambda} + \frac{\delta\overline{\varphi}_\gamma}{\delta\overline{\varphi}_\lambda}J_\gamma + \frac{\delta\overline{J}_\gamma}{\delta\overline{\varphi}_\lambda}\varphi_\gamma\right]\\
&= -\sum_\gamma\int d\tau'\left[J_\gamma\delta_{\gamma,\lambda}\delta(\tau-\tau')\right] = -J_\lambda(\tau)\,.\end{aligned} \tag{2.4.3}$$

The counterpart can be evaluated to

$$\begin{aligned}
\frac{\delta\Gamma[\overline{\varphi}_\lambda,\varphi_\lambda]}{\delta\varphi_\lambda} &= -\frac{\delta W}{\delta\varphi_\lambda} - \sum_\gamma \int d\tau' \left\{ P(\overline{\varphi}_\gamma)\frac{\delta J_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{\varphi}_\gamma}{\delta\varphi_\lambda}J_\gamma + P(\overline{J}_\gamma)\frac{\delta\varphi_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right\} \\
&= -\frac{\delta W}{\delta\varphi_\lambda} - \sum_\gamma \int d\tau' \left\{ \zeta\varphi_\gamma\frac{\delta J_\gamma}{\delta\varphi_\lambda} + \zeta\overline{J}_\gamma\frac{\delta\varphi_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right\} \\
&= -\sum_\gamma \int d\tau' \left[\frac{\delta J_\gamma}{\delta\varphi_\lambda}\frac{\delta W}{\delta J_\gamma} + \frac{\delta\overline{J}}{\delta\varphi_\lambda}\frac{\delta W}{\delta\overline{J}_\gamma} \right] - \sum_\gamma \int d\tau' \{\ldots\} \\
&= -\sum_\gamma \int d\tau' \left[-\zeta\frac{\delta J_\gamma}{\delta\varphi_\lambda}\varphi_\gamma - \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right] - \sum_\gamma \int d\tau' \{\ldots\} \\
&= \sum_\gamma \int d\tau' \left[\zeta\frac{\delta J_\gamma}{\delta\varphi_\lambda}\varphi_\gamma + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right] - \sum_\gamma \int d\tau' \left\{ \zeta\varphi_\gamma\frac{\delta J_\gamma}{\delta\varphi_\lambda} + \zeta\overline{J}_\gamma\frac{\delta\varphi_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right\} \\
&= \sum_\gamma \int d\tau' \left[\varphi_\gamma\zeta\frac{\delta J_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right] - \sum_\gamma \int d\tau' \left\{ \zeta\varphi_\gamma\frac{\delta J_\gamma}{\delta\varphi_\lambda} + \zeta\overline{J}_\gamma\frac{\delta\varphi_\gamma}{\delta\varphi_\lambda} + \frac{\delta\overline{J}_\gamma}{\delta\varphi_\lambda}\varphi_\gamma \right\} \\
&= -\zeta\sum_\gamma \int d\tau'\overline{J}_\gamma\delta_{\gamma,\lambda}\delta(\tau-\tau') = -\zeta\overline{J}_\lambda(\tau)\ . \qquad (2.4.4)
\end{aligned}$$

So now in order to derive the Dyson equation we need the following terms

$$\begin{aligned}
\frac{\delta\varphi_{\lambda_3}(\tau_3)}{\delta\varphi_{\lambda_1}(\tau_1)} &= \frac{\delta}{\delta\varphi_{\lambda_1}}\left[-\frac{\delta W}{\delta\overline{J}_{\lambda_3}} \right] = -\sum_{\lambda_2}\int d\tau_2 \left[\frac{\delta J_{\lambda_2}}{\delta\varphi_{\lambda_1}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} + \frac{\delta\overline{J}_{\lambda_2}}{\delta\varphi_{\lambda_1}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} \right] \\
&= -\sum_{\lambda_2}\int d\tau_2 \left[-\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} - \zeta\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} \right] \\
&= \sum_{\lambda_2}\int d\tau_2 \left[\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} + \zeta\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} \right]\ . \qquad (2.4.5)
\end{aligned}$$

The next term is given by

$$\begin{aligned}
\frac{\delta\overline{\varphi}_{\lambda_3}(\tau_3)}{\delta\overline{\varphi}_{\lambda_1}(\tau_1)} &= \frac{\delta}{\delta\varphi_{\lambda_1}}\left[-\zeta\frac{\delta W}{\delta J_{\lambda_3}} \right] = -\zeta\sum_{\lambda_2}\int d\tau_2 \left[\frac{\delta\overline{J}_{\lambda_2}}{\delta\overline{\varphi}_{\lambda_1}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} + \frac{\delta J_{\lambda_2}}{\delta\overline{\varphi}_{\lambda_1}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}} \right] \\
&= -\zeta\sum_{\lambda_2}\int d\tau_2 \left[-\zeta\frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} - \frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}} \right] \\
&= \sum_{\lambda_2}\int d\tau_2 \left[\frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} + \zeta\frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}} \right]\ . \qquad (2.4.6)
\end{aligned}$$

Now we calculate

$$\begin{aligned}
\frac{\varphi_{\lambda_3}(\tau_3)}{\delta\overline{\varphi}_1(\tau_1)} &= \frac{\delta}{\delta\overline{\varphi}_1(\tau_1)}\left[-\frac{\delta W}{\delta\overline{J}_{\lambda_3}} \right] = -\sum_{\lambda_2}\int d\tau_2 \left[\frac{\delta\overline{J}_{\lambda_2}}{\delta\overline{\varphi}_{\lambda_1}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} + \frac{\delta J_{\lambda_2}}{\delta\overline{\varphi}_{\lambda_1}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} \right] \\
&= -\sum_{\lambda_2}\int d\tau_2 \left[-\zeta\frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} - \frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} \right] \\
&= \sum_{\lambda_2}\int d\tau_2 \left[\zeta\frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} + \frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} \right]\ , \qquad (2.4.7)
\end{aligned}$$

and finally

$$\begin{aligned}\frac{\overline{\varphi}_{\lambda_3}(\tau_3)}{\delta\varphi_{\lambda_1}(\tau_1)} &= \frac{\delta}{\delta\varphi_{\lambda_1}}\left[-\zeta\frac{\delta W}{\delta J_{\lambda_3}}\right] = -\zeta\sum_{\lambda_3}\int d\tau_2\left[\frac{\delta\overline{J}_{\lambda_2}}{\delta\varphi_{\lambda_1}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} + \frac{\delta J_{\lambda_2}}{\delta\varphi_{\lambda_1}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}}\right] \\ &= -\zeta\sum_{\lambda_2}\int d\tau_2\left[-\zeta\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} - \frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}}\right] \\ &= \sum_{\lambda_2}\int d\tau_2\left[\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\varphi_{\lambda_2}}\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}} + \zeta\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}}\right] . \end{aligned} \tag{2.4.8}$$

So now we can rewrite the four equations in matrix form i.e.

$$\sum_{\lambda_2}\int d\tau_2\begin{pmatrix}\frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}} & \frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\overline{\varphi}_{\lambda_2}} \\ \frac{\delta^2\Gamma}{\delta\varphi_{\lambda_1}\delta\varphi_{\lambda_2}} & \frac{\delta^2\Gamma}{\delta\overline{\varphi}_{\lambda_1}\delta\varphi_{\lambda_2}}\end{pmatrix}\begin{pmatrix}\frac{\delta^2 W}{\delta J_{\lambda_2}\delta\overline{J}_{\lambda_3}} & \zeta\frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta\overline{J}_{\lambda_3}} \\ \zeta\frac{\delta^2 W}{\delta J_{\lambda_2}\delta J_{\lambda_3}} & \frac{\delta^2 W}{\delta\overline{J}_{\lambda_2}\delta J_{\lambda_3}}\end{pmatrix} = \delta_{\lambda_3,\lambda_1}\delta(\tau_3-\tau_1)\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{2.4.9}$$

From this equation we immediately see that the matrix of the right hand side is the inverse of the matrix on the left hand side, which in itself consists of the connected Green function. With the notation

$$\Gamma_{\varphi,\varphi} = \frac{\delta^2\Gamma}{\delta\varphi\delta\varphi}, \qquad \Gamma_{\varphi,\overline{\varphi}} = \frac{\delta^2\Gamma}{\delta\varphi\delta\overline{\varphi}}, \qquad \Gamma_{\overline{\varphi},\varphi} = \frac{\delta^2\Gamma}{\delta\overline{\varphi}\delta\varphi} \quad \text{and} \quad \Gamma_{\overline{\varphi},\overline{\varphi}} = \frac{\delta^2\Gamma}{\delta\overline{\varphi}\delta\overline{\varphi}}\,, \tag{2.4.10}$$

we can rewrite the inverse matrix as

$$\begin{pmatrix}\Gamma_{\varphi,\overline{\varphi}} & \Gamma_{\overline{\varphi}\varphi} \\ \Gamma_{\varphi,\varphi} & \Gamma_{\overline{\varphi},\varphi}\end{pmatrix} = \zeta\begin{pmatrix}\langle\psi\overline{\psi}\rangle & \langle\overline{\psi\psi}\rangle \\ \langle\psi\psi\rangle & \langle\overline{\psi}\psi\rangle\end{pmatrix}^{-1} . \tag{2.4.11}$$

In the absence of symmetry breaking the Green functions which consists of an unequal number of ψ and $\overline{\psi}$ vanish and the above equations reduce to

$$\begin{aligned}\sum_{\lambda_2}\int d\tau_2 G_c^{(1)}(\lambda_3\tau_3|\lambda_2\tau_2)\Gamma_{\varphi_{\lambda_1},\overline{\varphi_{\lambda_2}}} &= \delta_{\lambda_3,\lambda_1}\delta(\tau_3-\tau_1)\,, \\ \sum_{\lambda_2}\int d\tau_2 G_c^{(1)}(\lambda_3\tau_3|\lambda_2\tau_2)\Gamma_{\overline{\varphi}_{\lambda_1},\varphi_{\lambda_2}} &= \delta_{\lambda_3,\lambda_1}\delta(\tau_3-\tau_1)\,. \end{aligned} \tag{2.4.12}$$

This gives us the inverse Green function immediately as

$$G_c^{(1)^{-1}}(\lambda_3,\lambda_2) = \Gamma_{\varphi_{\lambda_1},\overline{\varphi}_{\lambda_2}}\,. \tag{2.4.13}$$

It is now convenient to express $\Gamma_{\varphi_{\lambda_1},\overline{\varphi}_{\lambda_2}}$ in terms of the self-energy Σ, which is defined as the difference between the vertex function or inverse Green function of the interacting system and non interacting system. That is

$$\Gamma_{\varphi_{\lambda_1},\overline{\varphi}_{\lambda_2}} = \Gamma^{(0)}_{\varphi_{\lambda_1},\overline{\varphi}_{\lambda_2}} + \Sigma_{\varphi_{\lambda_1},\overline{\varphi}_{\lambda_2}}\,, \tag{2.4.14}$$

or equivalently

$$\mathbf{G}^{-1} = \mathbf{G}_0^{-1} + \mathbf{\Sigma}\,. \tag{2.4.15}$$

Now multiplying this equation by $\mathbf{G}$ from the right and $\mathbf{G}_0$ from the left, and doing so successively one obtains the Dyson equation

$$\mathbf{G} = \mathbf{G}_0 - \mathbf{G}_0\Sigma\mathbf{G} = \mathbf{G}_0 - \mathbf{G}_0\Sigma\mathbf{G}_0 + \mathbf{G}_0\Sigma\mathbf{G}_0\Sigma\mathbf{G}_0\ldots \quad . \tag{2.4.16}$$

Which has of course to be read as a matrix equation, including summation over all indices and integration over internal ones. The Dyson equation can now be expressed diagrammatically via

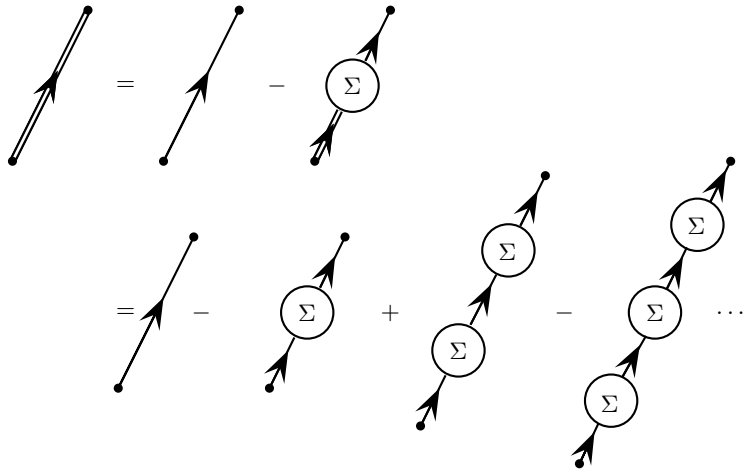


Figure 2.2: Digrammatic expression of the Dyson equation.

As can be seen in Figure 2.2, the Dyson equation is dressed. That means the whole Green function stand on both sided of the equation. In Figure 2.2 this is indicated the the double arrow. In the second line the full Green function has been inserted and only the first terms are considered. This corresponds to a perturbative description. So we can see, that if we calculate the self-energy we get the correction of the non-interacting Green function to the interacting Green function. Where the interacting Green function is now reduced to the connected Green function. Finally we want to see, how we can express the self-energy in terms of the diagrammatic perturbation theory derived for the interacting Green function. Therefore two standard definitions are required. The corrections to the connected Green function consists of all diagrams, which are connected and have, in the case of the one-particle Green function one incoming and one outgoing line. We will now define the so called amputated diagrams. A diagram is called amputated, if one removes the two external lines $\psi_\alpha(\beta)$ and $\overline{\psi}'_\alpha(\beta')$ of a connected diagram. This means the incoming and outgoing non interacting Green functions are not connected to a propagator. Therefore each external point must be connected directly to the interaction. Further a diagram is called n-particle irreducible, if it can not be disconnected into two or more disconnected pieces by separating internal propagators. Hence we are already dealing with the connected Green functions, it follows now, that the self-energy is given by all the irreducible amputated diagrams connecting the points (α_1, τ_2) and (α_2, τ_2). The Feynman rules for the self-energy therefore are given by

1 First we have to construct all unlabeled one-particle irreducible amputated diagrams consisting of the n-interaction vertices. The ingoing line is labeled by (α, β) and the outgoing line by (α', β'). All the inner vertices are connected by propagators. Two diagrams are equal if they can be transformed into each other by conserving the external legs, and the direction of the propagators.

2 For each internal time label include the propagator $g_\gamma(\tau_1 - \tau_2)$.

3 For each vertex the matrix $\langle \alpha\, \beta | \, V \, | \gamma\, \delta \rangle$ has to be added. If the external legs are connected to the same interaction vertex, the factor $\delta(\beta - \beta')$ has to be added.

4 Now one has to sum over all internal single-particle indices and integrate over all time labels τ_i, where the integrals run over $[0, \hbar\beta]$.

5 Finally one must add the pre-factor $(-1)^{n-1}\zeta^{n_c}$, where n_c is the number of closed loops.

"Do not trust arguments based on the lowest order of perturbation theory"

Steven Weinberg [49]

2.4.1 Hartree-Fock Equation

We are now in the position to derive the Hartree-Fock equation in first order perturbation theory. The first 2 diagrams given by the above Feynman rules are

(a) (b)

Figure 2.3: The Hartree (left) and Fock (right) diagrams for the self-energy.

From these diagrams we obtain the self-energy

$$\Sigma(\alpha_1\,\beta_1|\alpha_2\beta_2) = \delta(\beta_1-\beta_2)\sum_{\gamma}\Big(\langle\alpha_1\,\gamma|\,V^{(\mathrm{int})}\,|\alpha_2\,\gamma\rangle + \zeta\,\langle\alpha_1\,\gamma|\,V^{(\mathrm{int})}\,|\gamma\,\alpha_2\rangle\Big)\,n_\gamma\,. \tag{2.4.17}$$

The Hartree-Fock equation thus gives us the self-energy to a given interaction. We are now ready to calculate the self-energy for dipolar interaction. As long as we are dealing with a homogeneous system, we can transfer to the Fourier space by rewriting the Fourier transformation and simply substituting the relative positions $\mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2$. Then one integration can be carried out; in particular

$$\begin{aligned}
\langle\mathbf{k}_1\,\mathbf{k}_2|\,V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r}_2)\,|\mathbf{k}_3\,\mathbf{k}_4\rangle :&= \int\frac{d^D\mathbf{r}_1\,d^D\,\mathbf{r}_2}{V^2}\,e^{i\mathbf{r}_1\cdot(\mathbf{k}_1-\mathbf{k}_3)}V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r}_2)e^{i\mathbf{r}_2\cdot(\mathbf{k}_2-\mathbf{k}_4)}\\
&= \int\frac{d^D\mathbf{R}\,d\mathbf{r}_2}{V^2}\,V^{(\mathrm{int})}(\mathbf{R})e^{i(\mathbf{R}+\mathbf{r}_2)(\mathbf{k}_1-\mathbf{k}_3)}e^{i\mathbf{r}_2\cdot(\mathbf{k}_2-\mathbf{k}_4)}\\
&= \int\frac{d^D\mathbf{R}\,d^D\mathbf{r}_2}{V^2}\,V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_3)}e^{i\mathbf{r}_2\cdot(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)}\\
&= \int\frac{d^D\mathbf{R}}{V^2}\,V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_3)}\int\frac{d^D\mathbf{r}_2}{V}\,e^{i\mathbf{r}_2\cdot(\mathbf{k}_1+\mathbf{k}_2-\mathbf{k}_3-\mathbf{k}_4)}\\
&= \int\frac{d^D\mathbf{R}}{V}\,\delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_3+\mathbf{k}_4}\,V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_3)}\,.
\end{aligned}\tag{2.4.18}$$

Now we see that for the Hartree, term for which we have $\mathbf{k}_2 = \mathbf{k}_4$, follows that we have to evaluate $V(\mathbf{k}=0)$.

$$\begin{aligned}
&\Sigma\,(\mathbf{k}_1\beta_1|\mathbf{k}_2\beta_2) = \delta\,(\beta_1-\beta_2)\sum_{\mathbf{k}}\Big(\langle\mathbf{k}_1\mathbf{k}|\,V^{(\mathrm{int})}\,|\mathbf{k}_2\mathbf{k}\rangle + \zeta\,\langle\mathbf{k}_1\mathbf{k}|\,V^{(\mathrm{int})}\,|\mathbf{k}\mathbf{k}_2\rangle\Big)\,n_{\mathbf{k}}\\
&= \delta\,(\beta_1-\beta_2)\sum_{\mathbf{k}}\int d^D\mathbf{R}\,\Big(\delta_{\mathbf{k}_1+\mathbf{k},\mathbf{k}_2+\mathbf{k}}V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_2)} + \zeta\delta_{\mathbf{k}_1+\mathbf{k},\mathbf{k}+\mathbf{k}_2}V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k})}\Big)\,n_{\mathbf{k}}\\
&= \delta\,(\beta_1-\beta_2)\sum_{\mathbf{k}}\int\frac{d^D\mathbf{R}}{V}\,\Big(\delta_{\mathbf{k}_1,\mathbf{k}_2}V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_2)} + \zeta\delta_{\mathbf{k}_1,\mathbf{k}_2}V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k}_2)}\Big)\,n_{\mathbf{k}}\\
&= \delta\,(\beta_1-\beta_2)\sum_{\mathbf{k}}\int\frac{d^D\mathbf{R}}{V}\,\Big(V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}\,\mathbf{0}} + \zeta V^{(\mathrm{int})}(\mathbf{R})e^{i\mathbf{R}(\mathbf{k}_1-\mathbf{k})}\Big)\,n_{\mathbf{k}}\,.
\end{aligned}\tag{2.4.19}$$

Since in this form the self-energy only depends on $\mathbf{k}_1 - \mathbf{k}_2$, we can rewrite it as

$$\Sigma(\mathbf{k_1}) := \frac{1}{V} \sum_{\mathbf{k}} \left[V^{(\mathrm{int})}(\mathbf{k} = 0) + \zeta V^{(\mathrm{int})} \left(\mathbf{k}_1 - \mathbf{k} \right) \right] n_{\mathbf{k}} \, . \tag{2.4.20}$$

Chapter 3

Ultracold Fermions in a Homogeneous System

3.1 Dipolar Interaction

In the following chapter we investigate how the interaction of an ultracold quantum gas affects its properties. In order to do so we will use the classical derived interaction energies of dipole-dipole interaction and Coulomb interaction. In a real system of course all interactions are present, but depending on the chosen substance the dipolar or Coulomb interaction or other interactions, will be more dominant. The classical dipole-dipole interaction formula, which we are going to use, is in itself an approximation and it seems reasonable to recap shortly how the Coulomb potential and the dipole-dipole interaction are defined. In a 3-dimensional system the Coulomb potential is given by

$$\varphi_{\mathrm{Cou}}(\mathbf{r}) = \frac{e}{4\pi\varepsilon_0}\frac{1}{|\mathbf{r}-\mathbf{r}'|} =: K\frac{e}{|\mathbf{r}-\mathbf{r}'|}\,, \tag{3.1.1}$$

where $\mathbf{r}$ is the location of the potential and $\mathbf{r}'$ is the location of the charge and e is the charge of the particle. Here and in the following pages K will always be $\frac{1}{4\pi\varepsilon_0}$ and ε_0 is the vacuum permittivity. The Coulomb potential is given here as the solution for a point charge of the Poisson equation in three dimensions. The two dimensional Poisson equation can naturally also be solved, but is then not a representation of the real law of nature. Here we will use the three-dimensional law and restrict it to two dimensions. To describe a dipole it is easiest to create one out of two point particles of opposite charges. It is pointed out, that the formula of a dipole is defined as the result of this simple construction, and normally just identified with this formula in a multipole expansion. So if two point charges of opposite charges are given at a distance, then by simply adding the respective potentials of two point charges, we get

$$\phi = \phi_1 + \phi_2 = eK\left(\frac{1}{r_2'} - \frac{1}{r_1'}\right) = eK\left(\frac{1}{\left|\mathbf{r}-\mathbf{r}_s-\frac{\mathbf{d}}{2}\right|} - \frac{1}{\left|\mathbf{r}-\mathbf{r}_s+\frac{\mathbf{d}}{2}\right|}\right)\,, \tag{3.1.2}$$

where $\mathbf{d}$ is the distance of the two point charges. Now approximating the denominator, by assuming $2R \gg d$, for which the derived potential will only be valid, with

$$\left[1 \pm \frac{d\cos(\alpha)}{2R} + \left(\frac{d}{2R}\right)^2\right]^{-\frac{1}{2}} \approx 1 \mp \frac{d}{2R}\cos(\alpha), \tag{3.1.3}$$

where $\mathbf{R} := \mathbf{r} - \mathbf{r}_s$ and α describes the angle between d and R, one gets the classical potential of a dipole

$$\phi \approx eK\frac{\mathbf{d}\cdot\mathbf{R}}{R^3}\,. \tag{3.1.4}$$

Together with the definition for the dipole moment $\mathbf{p} = e\mathbf{d}$ we get the commonly known potential

$$\phi_{\mathrm{Dip}}(\mathbf{r}) = \frac{\mathbf{p}\cdot\mathbf{R}}{R^3} \,. \tag{3.1.5}$$

Now with the potential we can calculate the electric field of a dipole by simply taking the gradient.

$$\begin{aligned}\mathbf{E} = -\nabla\phi &= -K\left[\frac{\nabla\left(\mathbf{p}\cdot\mathbf{R}\right)}{R^3} + \left(\mathbf{p}\cdot\mathbf{R}\right)\nabla\left(\frac{1}{R^3}\right)\right] \\ &= K\frac{3\left(\mathbf{p}\cdot\mathbf{n}\right)\mathbf{n} - \mathbf{p}}{R^3} \,.\end{aligned} \tag{3.1.6}$$

where $\mathbf{n} = \frac{\mathbf{R}}{R}$ is the distance between the two point-charges.

3.1.1 Dipolar Interaction Energy

We are now calculating the interaction energy of two dipoles. In order to do so, we consider one dipole in the potential of the other. The electrostatic energy is then given by [50]

$$W = \int d^3\mathbf{r}\,\rho(\mathbf{r})\varphi(\mathbf{r}) \,. \tag{3.1.7}$$

By Taylor expansion of the external field $\varphi(\mathbf{r})$ and bringing the expansion in the right form, so that the classical dipole field (3.1.6) is recognized, one gets

$$\varphi(\mathbf{r}) = \varphi(0) - \mathbf{r}\cdot\mathbf{E}(0) - \dots \,, \tag{3.1.8}$$

where we have neglected the quadrupole moment and higher momenta. With this expression the energy is given by

$$W = e\varphi(0) - \mathbf{p}\cdot\mathbf{E}(0) + \dots \,. \tag{3.1.9}$$

Here the dipole moment is defined by $\mathbf{p} = \int \mathrm{dV}\,\rho(\mathbf{r}')\mathbf{r}'$, which is equivalent to the above definition for the special charge distribution

$$\rho(\mathbf{r}') = e\delta\left(\mathbf{r}' - \frac{\mathbf{d}}{2}\right) - e\delta\left(\mathbf{r}' + \frac{\mathbf{d}}{2}\right) \,. \tag{3.1.10}$$

The dipole-dipole interaction can now be derived by inserting the field (3.1.6) in (3.1.8). The result is

$$W_{12} = K\frac{\mathbf{p}_1\cdot\mathbf{p_2} - 3(\mathbf{p}_1\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{|\mathbf{r}_1 - \mathbf{r}_2|^3} \,. \tag{3.1.11}$$

where $\mathbf{n} = \frac{\mathbf{r}_1 - \mathbf{r}_2}{|\mathbf{r}_1 - \mathbf{r}_2|}$ denotes the direction between the two dipoles. This formula represents the dipole-dipole interaction, that we will use in this form as a two-body interaction for the rest of this work. It is customary to write V for the dipole-dipole interaction. Furthermore it will be useful to define the first and second part of the dipole-dipole interaction in the following way

$$V^{(\mathrm{int})} = V_1^{(\mathrm{int})} + V_2^{(\mathrm{int})} = K\frac{\mathbf{p}_1\cdot\mathbf{p}_2}{|\mathbf{r}_1 - \mathbf{r}_2|} + K\frac{\left(\mathbf{p}_1\cdot\mathbf{n}\right)\left(\mathbf{p}_2\cdot\mathbf{n}\right)}{|\mathbf{r}_1 - \mathbf{r}_2|} \,. \tag{3.1.12}$$

Furthermore we will often restrict ourselves to the case, that the two dipoles are parallel and restricted to the x-z plane. That is momentarily writing $\mathbf{q}$ for $\mathbf{p}_2$ $q_1 = p_1$, $q_3 = p_3$ and $q_2 = p_2 = 0$. The second part of the dipole-dipole interaction (3.1.12) then reads

$$V_2(x,y) = -3K\frac{(\mathbf{p}_2\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{r^3} = -3K\frac{x^2p_1^2}{(x^2+y^2)^{\frac{5}{2}}} \,. \tag{3.1.13}$$

In order to work with (3.1.11), we will switch to spherical coordinates or polar coordinates, respectively. To do this, we will now introduce the following angle definitions

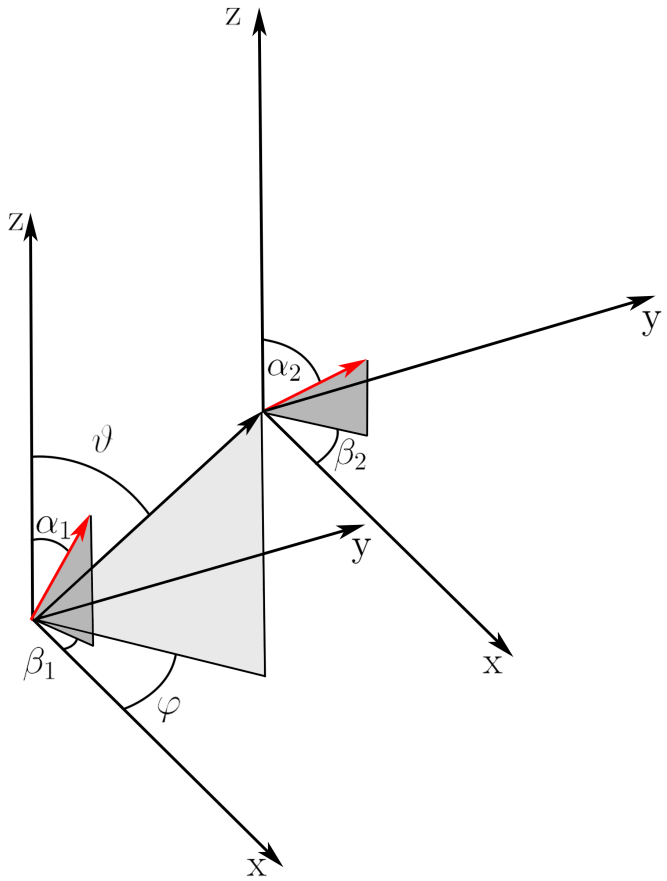


Figure 3.1: Definitions of the angles for a configuration of two dipoles.

$$\mathbf{p}_1 = p_1 \begin{pmatrix} \sin(\alpha_1)\cos(\beta_1) \\ \sin(\alpha_1)\sin(\beta_1) \\ \cos(\alpha_1) \end{pmatrix}, \qquad \mathbf{p}_2 = p_2 \begin{pmatrix} \sin(\alpha_2)\cos(\beta_2) \\ \sin(\alpha_2)\sin(\beta_2) \\ \cos(\alpha_2) \end{pmatrix}, \qquad \mathbf{r} = r \begin{pmatrix} \sin(\vartheta)\cos(\varphi) \\ \sin(\vartheta)\sin(\varphi) \\ \cos(\vartheta) \end{pmatrix}. \tag{3.1.14}$$

The dipoles $\mathbf{p}_1$ and $\mathbf{p}_2$ are now described by the angles given in (3.1.14) as illustrated in Figure 3.1. These definitions will now be used to derive the dipole-dipole interaction for the special cases of parallel dipoles in three and two dimensions respectively.

3.1.2 Dipole-Dipole Interaction for Parallel Dipoles in Three Dimensions

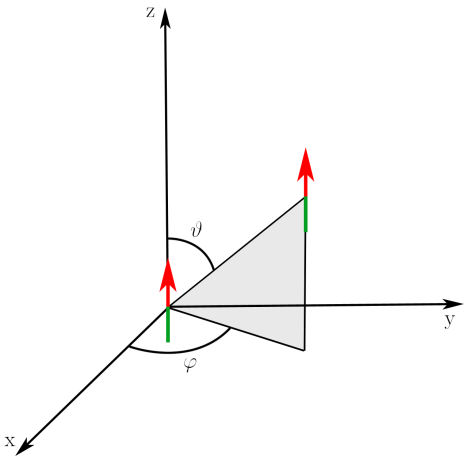


Figure 3.2: Angles ϑ and φ for two parallel dipoles in three dimensions. Since the two dipoles are always parallel, only the ϑ angle is relevant.

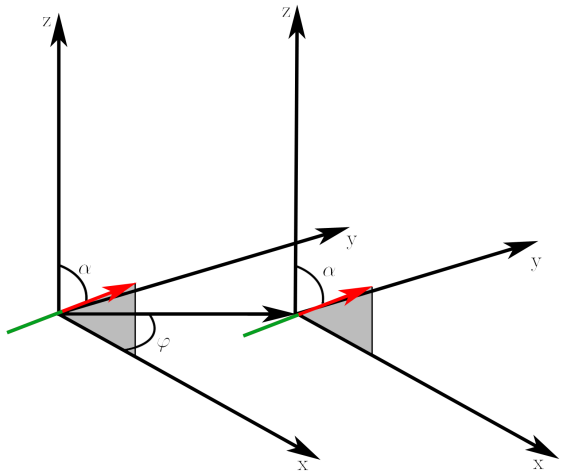


Figure 3.3: The angles for two dipoles in the two-dimensional plane. The dipoles are restricted to the x-z plane, therefore the φ angle changes the relative orientation of the two.

If we now assume that we apply an external electric field, which is strong enough to align all dipoles along it, as in Figure 3.2, we have $\mathbf{p}_1 || \mathbf{p}_2$. By denoting the angle between $\mathbf{p}_1$ and $\mathbf{n}$, according to (3.1.14) as ϑ , we get

$$\begin{aligned} V^{(\mathrm{int})}(\mathbf{r}) &= K\frac{p_1\, p_2}{r^3}\left(1-3\cos^2(\vartheta)\right) \\ &= -K\frac{2p_1\, p_2}{r^3}P_2(\cos(\vartheta)) \end{aligned} \tag{3.1.15}$$

where $P_2(x) = \frac{1}{2}\left(3x^2-1\right)$ is the second Legendre polynom. Here the electric field is directed in z-direction. The first dipole is set in the origin of a given coordinate system and the second dipole is at a distance r. Since the dipoles are parallel and always pointing in the z-direction, the system is symmetric regarding the azimuth angle φ.

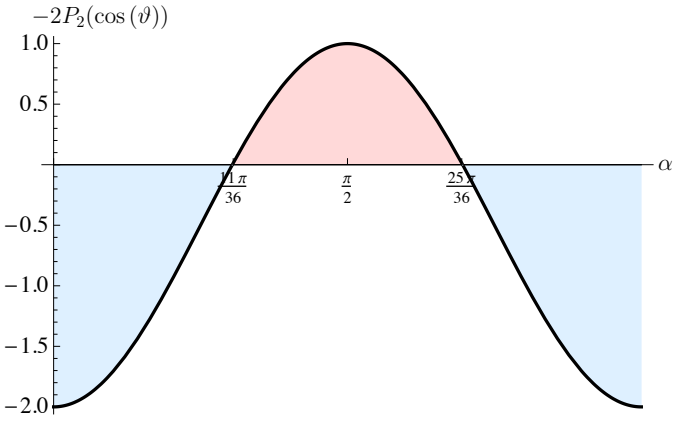


Figure 3.4: Plot of $-2P_2(\cos(\vartheta))$. The function changes from negative (attractive) to positive (repulsive).

The whole setting of these configurations is then given by the angle ϑ. For $\vartheta = \frac{\pi}{2}$ the dipoles are restricted to the x-y plane for $\vartheta = 0$, the dipoles are in front of each other, where we expect the peak of attraction. This holds true by looking at the sign change of the function as shown in Figure 3.4. The critical angle for which the interaction changes from repulsive to attractive is the magic angle $\overline{\vartheta} := \arccos\left(\frac{1}{\sqrt{3}}\right)$ which is well known from NMR [51]. As we can see from Figure 3.4, the interaction is repulsive for ϑ with

$$55^\circ = \frac{11\pi}{36} \approx \arccos\left(\frac{1}{\sqrt{3}}\right) < \vartheta < \pi - \arccos\left(\frac{1}{\sqrt{3}}\right) \approx \frac{25\pi}{36} = 125^\circ\,. \tag{3.1.16}$$

3.1.3 Dipole-Dipole Interaction for Parallel Dipoles in Two Dimensions

If we now turn to the two-dimensional system it turns out that, if we consider the dipoles parallel in the x-y plane, the angular dependencies of the dipole-dipole interaction vanishes. Therefore we consider the electric field to be tilted against the z-direction. By doing so, and starting from (3.1.14) and setting $\alpha_2 \longrightarrow \alpha_1 =: \alpha, \beta_2 \longrightarrow \beta_1$, and $\beta_1 \longrightarrow 0$ we arrive at

$$V^{(\mathrm{int})}(\mathbf{r}) = K\frac{p_1\, p_2}{r^3}\left[1 - 3\sin^2(\alpha)\cos^2(\varphi)\right] . \tag{3.1.17}$$

Now here the angle α describes the tilting of the dipole's towards the z-direction and φ describes the angle in the plane of their relative position. Because we have set $\beta = 0$ both dipoles will only move in the x-z plane, so if they are tilted they will always point in x-direction see Figure 3.3. For $\varphi = 0$ and $\alpha = \frac{\pi}{2}$ the two dipoles are aligned in the x-axis. The head of one pointing to the tail of the other. In this scenario, we have the strongest attraction. In contrast for $\alpha = \frac{\pi}{2}$ and $\varphi = \frac{\pi}{2}$, the two dipoles are lying in the x-y plane and we have repulsion. If we now consider $\alpha = 0$ the dipoles will be parallel for every φ and the interaction is the same since they are simply parallel. This can also directly be seen in (3.1.17). Obviously it does not matter if the second dipole lies left or right to the first dipole and likewise the interaction will be the same, if the second dipole lies above the first one or under the first one so the only angles we have to consider are $0 \leq \alpha, \varphi \leq \frac{\pi}{2}$. In the two dimensional case the critical angle $\overline{\varphi}$, where the interaction potential vanishes, depends on the orientation of α. Explicitly this dependency is given by

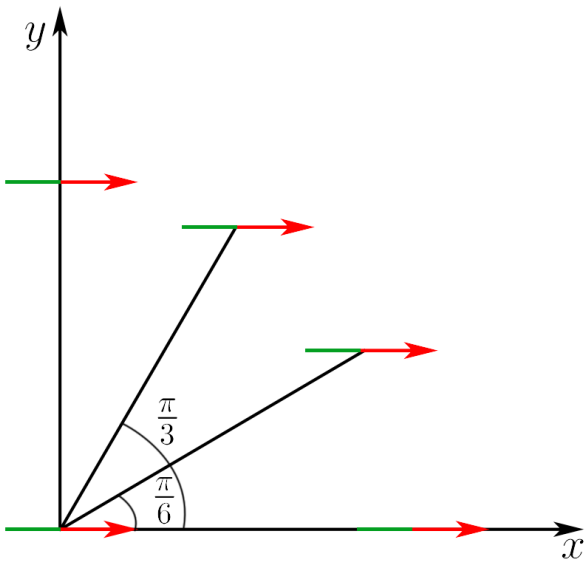


Figure 3.5: Aerial view on the x-y plane of the two-dimensional dipole-dipole configuration for the four angles $\varphi = 0, \frac{\pi}{6}, \frac{\pi}{3}, \frac{\pi}{2}$.

$$\overline{\varphi} = \arccos\left(\frac{1}{\sqrt{3\sin^2(\alpha)}}\right) . \tag{3.1.18}$$

We will later look for the 4 different angles $\alpha = 0, \frac{\pi}{6}, \frac{\pi}{3}, \frac{\pi}{2}$, which are shown in Figure 3.5 at the dispersion relation. The interaction potential changes then as shown in Figure 3.6.

3.2 Fourier Transformation for Dipole-Dipole and Coulomb Interaction

In order to solve the Hartree-Fock equation we will transform to Fourier space. This is only possible, because we have a translation invariant system. We will derive the Fourier transformation for the three and two dimensional system and compare them later.

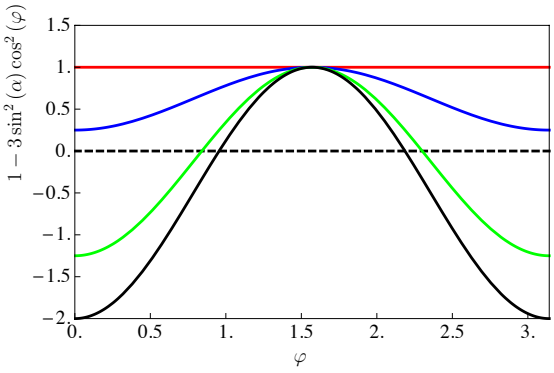


Figure 3.6: in Dipole-dipole interaction changes from attractive to repulsive for the four different positions of the orientation of the dipole to the z axis. The angles α used are 0 (red) $\frac{\pi}{6}$ (blue) $\frac{\pi}{3}$ (green) and $\frac{\pi}{2}$ (black).

3.2.1 Fourier Transformation of the Three-Dimensional Dipole-Dipole Interaction

We will now set the **k**-vector in the z-direction, so α_1 is then the angle between z and $\mathbf{p}_1$. The electric field aligns the dipoles, so that it points also in the direction of $\mathbf{p}_1$.The Fourier transformation of (3.1.11) reads in spherical coordinates

$$V_{3D}^{\text{Dipole}}(\mathbf{k}) = K\int_{\varepsilon}^{R} dr r^2 \int_0^{\vartheta} d\vartheta \sin(\vartheta)\int_0^{2\pi} d\varphi\, \frac{\mathbf{p}_1\cdot\mathbf{p}_2 - 3(\mathbf{p}_1\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{r^3} e^{-ikr\cos(\vartheta)} \tag{3.2.1}$$

$$\begin{aligned} &= Kp_1p_2\int_{\varepsilon}^{R} dr\frac{1}{r}\int_0^{\pi} d\vartheta\sin(\vartheta)\int_0^{2\pi} d\varphi\, e^{-ikr\cos(\vartheta)}\Big\{[\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2)+\cos(\alpha_1)\cos(\alpha_2)] \\ &\quad - 3\left[\cos^2(\vartheta)\cos(\alpha_1)\cos(\alpha_2)+\sin^2(\vartheta)\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\varphi)\cos(\beta_2-\varphi)\right. \\ &\quad \left.+\cos(\vartheta)\sin(\vartheta)\left[\cos(\varphi)\cos(\beta_2-\varphi)\sin(\alpha_2)+\cos(\beta_1-\varphi)\sin(\alpha_1)\cos(\alpha_2)\right]\right\}, \end{aligned}$$

where we have introduced the two cutoff parameters ε and R to be discussed at the end. The φ integration can now immediately be executed and leads to

$$\begin{aligned} V_{3D}^{\text{Dipole}}(\mathbf{k}) &= K\int_{\varepsilon}^{R} r^2\,dr\int_0^{\pi} d\vartheta\sin(\vartheta)\int_0^{2\pi} d\varphi\,\frac{\mathbf{p}_1\cdot\mathbf{p}_2-3(\mathbf{p}_1\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{r^3}e^{-ikr\cos(\vartheta)} \\ &= K\pi\int_{\varepsilon}^{R} dr\frac{1}{r}\int_0^{\pi} d\vartheta\sin(\vartheta)e^{-ikr\cos(\vartheta)} \\ &\quad\times\left\{\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2)\left[2-3\sin^2(\vartheta)\right]+\cos(\alpha_1)\cos(\alpha_2)\left[2-6\cos^2(\vartheta)\right]\right\}. \end{aligned} \tag{3.2.2}$$

Now we calculate

$$\int_0^{\pi}\sin(\vartheta)d\vartheta\left[2-3\sin^2(\vartheta)\right]e^{-ikr\cos(\vartheta)} = \int_{-1}^{1} d\eta\left[2-3(1-\eta^2)\right]e^{-ikr\eta} = \frac{4\sin(kr)}{kr}+\frac{12\cos(kr)}{(kr)^2}-12\frac{\sin(kr)}{(kr)^3}. \tag{3.2.3}$$

In quite the same way we can derive

$$\int_0^{\pi} d\vartheta\sin(\vartheta)\left[2-6\cos^2(\vartheta)\right]e^{-ikr\cos(\vartheta)} = \int_{-1}^{1} d\eta[2-6\eta^2]e^{-ikr\eta} = -\frac{8\sin(kr)}{kr}+\frac{24\sin(kr)}{(kr)^3}-\frac{24\cos(kr)}{(kr)^2}. \tag{3.2.4}$$

Combining these results we get the intermediate result the intermediate result

$$V_{\mathrm{3D}}^{\mathrm{Dipole}}(\mathbf{k}) = K\int_{\varepsilon}^{R} dr r^2 \int_0^{\vartheta} d\vartheta \sin(\vartheta)\int_0^{2\pi} d\varphi \frac{\mathbf{p}_1\cdot\mathbf{p}_2 - 3(\mathbf{p}_1\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{r^3} e^{-ikr\cos(\vartheta)} \tag{3.2.5}$$
$$= A\int_{\varepsilon}^{R}\frac{dr}{r}\left[\frac{4\sin(kr)}{kr} + \frac{12\cos(kr)}{(kr)^2} - 12\frac{\sin(kr)}{(kr)^3}\right] + B\int_{\varepsilon}^{R}\frac{dr}{r}\left[\frac{24\sin(kr)}{(kr)^3} - \frac{24\cos(kr)}{(kr)^2} - \frac{8\sin(kr)}{kr}\right],$$

where we have set

$$A := \pi p_1 p_2 \sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2), \qquad B := \pi p_1 p_2 \cos(\alpha_1)\cos(\alpha_2). \tag{3.2.6}$$

The respective $\frac{\sin(kr)}{r^\ell}$ integrals can now be brought in the following form via partial integration

$$\begin{aligned}
\int_a^b dr\frac{\sin(\alpha r)}{r^2} &= \left[\frac{\sin(\alpha a)}{a} - \frac{\sin(\alpha b)}{b}\right] + \alpha\int_a^b dr\frac{\cos(\alpha r)}{r}\\
\int_a^b dr\frac{\cos(\alpha r)}{r^3} &= \frac{1}{2}\left[\frac{\cos(\alpha a)}{a^2} - \frac{\cos(\alpha b)}{b^2}\right] - \frac{\alpha}{2}\left[\frac{\sin(\alpha a)}{a} - \frac{\sin(\alpha b)}{b}\right] - \frac{\alpha^2}{2}\int_a^b\frac{\cos(\alpha r)}{r}dr\\
\int_a^b dr\frac{\sin(\alpha r)}{r^4} &= \frac{1}{3}\left[\frac{\sin(\alpha a)}{a^3} - \frac{\sin(\alpha b)}{b^3}\right] + \frac{\alpha}{6}\left[\frac{\cos(\alpha a)}{a^2} - \frac{\cos(\alpha b)}{b^2}\right]\\
&\quad - \frac{\alpha^2}{6}\left[\frac{\sin(\alpha a)}{a} - \frac{\sin(\alpha b)}{b}\right] - \frac{\alpha^3}{6}\int_a^b dr\frac{\cos(\alpha r)}{r}.
\end{aligned} \tag{3.2.7}$$

Then the first part yields

$$\begin{aligned}
\int_{\varepsilon}^{R} dr\left[\frac{4\sin(kr)}{kr^2} + \frac{12\cos(kr)}{k^2r^3} - 12\frac{\sin(kr)}{k^3r^4}\right] &= -\frac{4\sin(k\varepsilon)}{k^3\varepsilon^3} + \frac{4\sin(kR)}{k^3R^3} + \frac{4\cos(k\varepsilon)}{k^2\varepsilon^2} - \frac{4\cos(kR)}{k^2R^2}\\
&= 4\left(\frac{j_1(kR)}{kR} - \frac{j_1(k\varepsilon)}{k\varepsilon}\right),
\end{aligned} \tag{3.2.8}$$

where j_1 denotes the spherical Bessel function

$$j_1(x) := \frac{\sin(x)}{x^2} - \frac{\cos(x)}{x}. \tag{3.2.9}$$

In the same way the second term leads

$$\int_{\varepsilon}^{R}\frac{dr}{r}\left[\frac{24\sin(kr)}{(kr)^3} - \frac{24\cos(kr)}{(kr)^2} - \frac{8\sin(kr)}{kr}\right] = 8\left(\frac{j_1(k\varepsilon)}{k\varepsilon} - \frac{j_1(kR)}{kR}\right). \tag{3.2.10}$$

The whole Fourier transformation (3.2.6) then reduces to

$$\begin{aligned}
V_{\mathrm{3D}}^{\mathrm{Dipole}}(\mathbf{k}) &= K\int_{\varepsilon}^{R} dr r^2\int_0^{\vartheta} d\vartheta\sin(\vartheta)\int_0^{2\pi} d\varphi\frac{\mathbf{p}_1\cdot\mathbf{p}_2 - 3(\mathbf{p}_1\cdot\mathbf{n})(\mathbf{p}_2\cdot\mathbf{n})}{r^3}e^{-ikr\cos(\vartheta)}\\
&= 4K\left[A\left(\frac{j_1(kR)}{kR} - \frac{j_1(k\varepsilon)}{k\varepsilon}\right) + 2B\left(\frac{j_1(k\varepsilon)}{k\varepsilon} - \frac{j_1(kR)}{kR}\right)\right]\\
&= 4\pi K p_1 p_2\left[\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2)\left(\frac{j_1(kR)}{kR} - \frac{j_1(k\varepsilon)}{k\varepsilon}\right)\right.\\
&\qquad \left. + 2\cos(\alpha_1)\cos(\alpha_2)\left(\frac{j_1(k\varepsilon)}{k\varepsilon} - \frac{j_1(kR)}{kR}\right)\right].
\end{aligned} \tag{3.2.11}$$

We now check the calculation for the case that the two dipoles are parallel, that is if $\alpha_1 = \alpha_2$ and $\beta_1 = \beta_2$. We then have

$$\begin{aligned} V_{\mathrm{3D}}^{(\mathrm{int})}(k) &= \pi K \mathbf{p}_1 \cdot \mathbf{p}_2 \Big\{ 4\sin^2(\alpha_1) \left(\frac{j_1(kR)}{kR} - \frac{j_1(k\varepsilon)}{k\varepsilon} \right) + 8\cos^2(\alpha_1) \left(\frac{j_1(k\varepsilon)}{k\varepsilon} - \frac{j_1(kR)}{kR} \right) \Big\} \\ &= 8\pi K p_1 p_2 \left(\frac{j_1(k\varepsilon)}{k\varepsilon} - \frac{j_1(kR)}{kR} \right) P_2(\cos(\alpha_1)) \,, \end{aligned} \tag{3.2.12}$$

which agrees with the result of Ref. [35].
We will now try to take the limits of both cutoff parameters. If $k > 0$ is arbitrarily given, the limits can be taken for $\varepsilon \to 0$ and $R \to \infty$ and the terms tend to $\frac{1}{3}$ and 0 accordingly. Explicitly writing down the series representation for sin and cos

$$\begin{aligned} \frac{j_1(x)}{x} &= \frac{1}{x} \left(\frac{\sin(x)}{x^2} - \frac{\cos(x)}{x} \right) = \sum_{n=0}^{\infty} (-1)^n \left[\frac{1}{(2n+1)!} - \frac{1}{(2n)!} \right] x^{2n-2} \\ &= \sum_{n=1}^{\infty} (-1)^{n+1} \underbrace{\left[\frac{2n}{(2n+1)!} \right]}_{\geq 0} x^{2n-2} \leq \sum_{n=1}^{\infty} \frac{1}{3} x^{2n-2} = \frac{-1}{3(x^2-1)} \overset{x\to\infty}{\longrightarrow} 0 \,, \end{aligned} \tag{3.2.13}$$

gives the limit for $R \to \infty$. In order to see the limit for $\varepsilon \to 0$, we simply observe that the exact sum in (3.2.13) start with $\frac{1}{3}$ and all higher terms are of positive powers of x. So the final formula in the limit $\varepsilon \to 0$ and $R \to \infty$ yields

$$V_{\mathrm{3D}}^{(\mathrm{int})}(\mathbf{k}) = \frac{8\pi K p_1 p_2}{3} P_2(\cos(\alpha_1)) \,. \tag{3.2.14}$$

3.2.2 Fourier Transformation for Two-Dimensional Dipole-Dipole Interaction

We will now consider the two-dimensional case. In order to derive the Fourier transformation in two-dimensions we have to use polar coordinates. Furthermore the dipoles are now restricted to the x-y plane, so naturally the $\mathbf{r}$ vector will also be restricted to the x-y plane, i.e. we have $\vartheta = \frac{\pi}{2}$. Thus from (3.1.14) follows directly

$$\begin{aligned} \mathbf{p}_1 \cdot \mathbf{p}_2 &= p_1 p_2 \left[\sin(\alpha_1) \sin(\alpha_2) \cos(\beta_1 - \beta_2) + \cos(\alpha_1) \cos(\alpha_2) \right] \,, \\ (\mathbf{p}_1 \cdot \mathbf{n})(\mathbf{p}_2 \cdot \mathbf{n}) &= p_1 p_2 \left[\cos(\beta_1 - \varphi) \cos(\beta_2 - \varphi) \sin(\alpha_1) \sin(\alpha_2) \right] \,. \end{aligned} \tag{3.2.15}$$

Before we will start to tackle the task of deriving the Fourier transformation it will be necessary to previously assemble some integrals and relations for Bessel functions. We start with the integral representation in [52] for the Bessel functions, which follows directly from the Poisson's integral representation

$$\int_0^{2\pi} d\varphi e^{-ix\cos(\varphi)} = 2\pi J_0(x) \quad \forall_x \, x > 0 \,. \tag{3.2.16}$$

We also need the two following recurrence relations for Bessel functions [53]

$$\frac{dJ_\nu(z)}{dz} = -J_{\nu+1}(z) + \frac{\nu}{z} J_\nu(z) \,, \tag{3.2.17a}$$

$$\frac{2\nu J_\nu(z)}{z} = J_{\nu+1}(z) + J_{\nu-1}(z) \,. \tag{3.2.17b}$$

The Bessel functions obey also the following symmetry [53]

$$J_{-\nu}(z) = (-1)^\nu J_\nu(z) \,. \tag{3.2.18}$$

In order to calculate the Fourier integral, we will need the following identities

$$\int_0^{2\pi} d\varphi \cos^2(\varphi) e^{-ikr\cos(\varphi)} = \int_0^{2\pi} d\varphi e^{-ikr\cos(\varphi)} - \int_0^{2\pi} d\varphi \sin^2(\varphi) e^{-ikr\cos(\varphi)} \,. \tag{3.2.19}$$

The second integral is now determined by differentiating twice under the integral sign and partial integration, as well as relations (3.2.17a), (3.2.18)

$$\begin{aligned}\int_0^{2\pi} \sin^2(\varphi) e^{-ikr\cos(\varphi)} &= \frac{1}{ikr}\int_0^{2\pi} d\varphi \sin(\varphi)\frac{\partial}{\partial\varphi} e^{-ikr\cos(\varphi)} = \frac{1}{ikr}\left[-i\frac{\partial}{\partial(kr)}\int_0^{2\pi} d\varphi e^{-ikr\cos(\varphi)}\right] \\ &= \frac{-1}{kr}\frac{\partial}{\partial(kr)} J_0(kr) = \frac{2\pi}{kr} J_1(kr) \,,\end{aligned} \tag{3.2.20}$$

so that we now also obtain the integral (3.2.19) by using (3.2.17b)

$$\int_0^{2\pi} d\varphi \cos^2(\varphi) e^{-ikr\cos^2(\varphi)} = 2\pi\left[J_0(kr) - \frac{J_1(kr)}{kr}\right] = 2\pi\left[\frac{J_1(kr)}{kr} - J_2(kr)\right] \,. \tag{3.2.21}$$

To integrate over r we will need the following integrals, where we have used partial integration as well as relation (3.2.17a):

$$\int_\varepsilon^R \frac{dr}{r^2} J_0(kr) = \left[\frac{1}{\varepsilon}J_0(k\varepsilon) - \frac{1}{R}J_0(kR)\right] - k\left[J_1(kR) - J_1(k\varepsilon)\right] - k\int_{k\varepsilon}^{kR} dx J_2(x) \,. \tag{3.2.22}$$

Next we observe, that by the same procedure we get the relation

$$\int_\varepsilon^R dr \frac{J_2(r)}{r^2} = \left[-\frac{1}{r}J_2(kr)\right]_\varepsilon^R + k\int_\varepsilon^R \frac{J_1(kr)}{r} dr - 2\int_\varepsilon^R \frac{J_2(kr)}{r^2} \,. \tag{3.2.23}$$

Since we have now the same integrals on both sides of the equation we can rewrite equation (3.2.23) as

$$\begin{aligned} 3\int_\varepsilon^R dr \frac{J_2(r)}{r^2} &= \left[-\frac{1}{r}J_2(kr)\right]_\varepsilon^R + k\int_\varepsilon^R \frac{J_1(kr)}{r} dr \\ &= \left[\frac{J_2(k\varepsilon)}{\varepsilon} - \frac{J_2(kR)}{R}\right] + k\left[J_1(kR) - J_1(k\varepsilon)\right] + k\int_{k\varepsilon}^{kR} J_2(x) dx \,. \end{aligned} \tag{3.2.24}$$

Finally we look at the integral, by using (3.2.21) and (3.2.20)

$$\begin{aligned} &\int_0^{2\pi} d\varphi \cos(\beta_1 - \varphi)\cos(\beta_2 - \varphi) e^{-ikr\cos(\varphi)} \\ &= \cos(\beta_1)\cos(\beta_2)\int_0^{2\pi} d\varphi \cos^2(\varphi) e^{-ikr\cos(\varphi)} + \sin(\beta_2)\sin(\beta_1)\int_0^{2\pi} d\varphi \sin^2(\varphi) e^{-ikr\cos(\varphi)} \\ &= 2\pi\left[\cos(\beta_1)\cos(\beta_2)\left(\frac{J_1(kr)}{kr} - J_2(kr)\right) + \sin(\beta_2)\sin(\beta_1)\frac{J_1(kr)}{kr}\right] \\ &= 2\pi\left[\cos(\beta_1 - \beta_2)\frac{J_1(kr)}{kr} - \cos(\beta_1)\cos(\beta_2)\frac{J_2(kr)}{kr}\right] \\ &= 2\pi\left[\cos(\beta_1 - \beta_2)\left[\frac{1}{2}J_0(kr) + \frac{1}{2}J_2(kr)\right] - \cos(\beta_1)\cos(\beta_2)\frac{J_2(kr)}{kr}\right] \\ &= 2\pi\left[\cos(\beta_1 - \beta_2)\frac{J_0(kr)}{2} + \left(\frac{\cos(\beta_1 - \beta_2)}{2} - \cos(\beta_1)\cos(\beta_2)\right)\frac{J_2(kr)}{kr}\right] \\ &= \pi\left[\cos(\beta_1 - \beta_2)J_0(kr) - \left[\cos(\beta_1)\cos(\beta_2) - \sin(\beta_1)\sin(\beta_2)\right]\frac{J_2(kr)}{kr}\right] \\ &= \pi\left[\cos(\beta_1 - \beta_2)J_0(kr) - \cos(\beta_1 + \beta_2)\frac{J_2(kr)}{kr}\right] \,. \end{aligned} \tag{3.2.25}$$

Now we are in position to derive the Fourier transformation

$$V_{2\mathrm{D}}^{\mathrm{Dipole}}(\mathbf{k}) = K\int_{\varepsilon}^{R} rdr\int_{0}^{2\pi} d\varphi V_{2D}(r,\varphi)e^{-ikr\cos(\varphi)} \tag{3.2.26}$$
$$= Kp_1p_2\int_{\varepsilon}^{R}\frac{dr}{r^2}\int_{0}^{2\pi} d\varphi\Big\{\left[\cos(\alpha_1)\cos(\alpha_2)+\cos(\beta_1-\beta_2)\sin(\alpha_1)\sin(\alpha_2)\right]e^{-ikr\cos(\varphi)}$$
$$-3\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\varphi)\cos(\beta_2-\varphi)e^{-ikr\cos(\varphi)}\Big\}\,.$$

The φ integration yields using (3.2.25)

$$V_{2\mathrm{D}}^{\mathrm{Dipole}}(\mathbf{k}) = K\int_{\varepsilon}^{R} rdr\int_{0}^{2\pi} d\varphi V_{2D}(r,\varphi)e^{-ikr\cos(\varphi)} \tag{3.2.27}$$
$$= 2\pi Kp_1p_2\int_{\varepsilon}^{R}\frac{dr}{r^2}\Big\{\left[\cos(\alpha_1)\cos(\alpha_2)+\cos(\beta_1-\beta_2)\sin(\alpha_1)\sin(\alpha_2)\right]J_0(kr)$$
$$-\frac{3}{2}\sin(\alpha_1)\sin(\alpha_2)\left(\cos(\beta_1-\beta_2)J_0(kr)-\cos(\beta_1+\beta_2)\frac{J_2(kr)}{kr}\right)\Big\}$$
$$= \pi Kp_1p_2\int_{\varepsilon}^{R}\frac{dr}{r^2}\left\{\left[2\cos(\alpha_1)\cos(\alpha_2)-\cos(\beta_1-\beta_2)\sin(\alpha_1)\sin(\alpha_2)\right]J_0(kr)\right. \tag{3.2.28}$$
$$\left.+3\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1+\beta_2)\frac{J_2(kr)}{kr}\right\}\,.$$

The r-integration can be done with the relations (3.2.22), (3.2.24)

$$V_{2\mathrm{D}}^{\mathrm{Dipole}}(\mathbf{k}) = \pi Kp_1p_2\Big\{\left[2\cos(\alpha_1)\cos(\alpha_2)-\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2)\right]\Big[\left(\frac{J_0(k\varepsilon)}{\varepsilon}-\frac{J_0(kR)}{R}\right) \tag{3.2.29}$$
$$-k\left[J_1(kR)-J_1(k\varepsilon)\right]-k\int_{k\varepsilon}^{kR}J_2(x)dx\Big]+\left[\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1+\beta_2)\right]\Big[\left(\frac{J_2(k\varepsilon)}{\varepsilon}-\frac{J_2(kR)}{R}\right)$$
$$+\;k\left[J_1(kR)-J_1(k\varepsilon)\right]+k\int_{k\varepsilon}^{kR}J_2(x)dx\Big]\Big\}$$

In the case, that the two dipoles are parallel, we have $\alpha_2=\alpha_1$ and $\beta_1=\beta_2$, and therefore

$$\left[2\cos(\alpha_1)\cos(\alpha_2)-\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1-\beta_2)\right] = 2\cos^2(\alpha_1)-\sin^2(\alpha_1)\cos(0) = 2P_2(\cos(\alpha_1))\,,$$
$$\left[\sin(\alpha_1)\sin(\alpha_2)\cos(\beta_1+\beta_2)\right] = \sin^2(\alpha_1)\cos(2\beta_1)\,. \tag{3.2.30}$$

Thus we obtain the final result

$$V_{2\mathrm{D}}^{\mathrm{Dipole}}(\mathbf{k}) = 2\pi Kp_1p_2P_2(\cos(\alpha_1))\left\{\left(\frac{J_0(k\varepsilon)}{\varepsilon}-\frac{J_0(kR)}{R}\right)-k\left[J_1(kR)-J_1(k\varepsilon)\right]-k\int_{k\varepsilon}^{kR}J_2(x)dx\right\}$$
$$+\,\pi Kp_1p_2\sin(\alpha_1)^2\cos(2\beta_1)\left\{\left(\frac{J_2(k\varepsilon)}{\varepsilon}-\frac{J_2(kR)}{R}\right)+k\left[J_1(kR)-J_1(k\varepsilon)\right]+k\int_{k\varepsilon}^{kR}J_2(x)dx\right\}\,. \tag{3.2.31}$$

This result agrees with the one given in Ref. [35]. Now due to the behaviour of the Bessel functions the only terms that remain in the limit $\varepsilon\to 0$ and $R\to\infty$ are the integrals, and the first term, which diverges. We keep the term with its $\frac{1}{\varepsilon}$ behavior and get

$$V_{2\mathrm{D}}^{\mathrm{Dipole}}(\mathbf{k}) = 2\pi Kp_1p_2P_2(\cos(\alpha_1))\left(\frac{1}{\varepsilon}-k\right)+\pi Kp_1p_2k\sin^2(\alpha_1)\cos(2\beta_1)\,. \tag{3.2.32}$$

Mandatory to calculate the integral it was necessary to introduce the ultraviolet cutoff ε. Now one runs into the problem, that the Fourier transformation diverges for $\varepsilon \to 0$. The only chance one has to obtain a final result is, if the Hartree and Fock diagrams cancel out this ultraviolet divergency. This happens in the homogeneous case, which makes it possible to carry out the calculation. We will use this obtained knowledge later in the trapped case to gain finite results.

3.2.3 Fourier Transformation for Three-Dimensional Coulomb Interaction

To calculate the Fourier transformation of the Coulomb potential

$$V(\mathbf{r}) = K\frac{1}{|\mathbf{r}-\mathbf{r}'|} = K\frac{1}{|\mathbf{R}|}\,, \tag{3.2.33}$$

we will use the Schwinger trick by rewriting the integral representation of the Gamma function as

$$\frac{1}{a^x} = \frac{1}{\Gamma(x)}\int_0^\infty d\tau \tau^{x-1}e^{-a\,x}\,. \tag{3.2.34}$$

With this we can now simply rewrite the Fourier transformation as

$$\begin{aligned} K\int d^3\mathbf{R}\frac{1}{|\mathbf{R}|}e^{-i\mathbf{k}\mathbf{R}} &= K\int d^3R\frac{1}{\sqrt{\mathbf{R}^2}}e^{-i\mathbf{k}\mathbf{R}} = K\frac{1}{\Gamma\left(\frac{1}{2}\right)}\int d^3\mathbf{R}\int_0^\infty d\tau\,\tau^{\frac{1}{2}-1}e^{-\tau\mathbf{R}^2}e^{-i\mathbf{k}\mathbf{R}} \\ &= K\frac{1}{\sqrt{\pi}}\int_0^\infty d\tau\,\tau^{-\frac{1}{2}}\int d^3\mathbf{R}e^{-(\tau\mathbf{R}^2+i\mathbf{k}\mathbf{R})}\,, \end{aligned} \tag{3.2.35}$$

completing the square now leads to

$$= K\frac{1}{\sqrt{\pi}}\int_0^\infty d\tau\,\tau^{-\frac{1}{2}}e^{\frac{k^2}{4\tau}}\int d^3\mathbf{R}e^{-\left(\sqrt{\tau}\mathbf{R}-\frac{i\mathbf{k}}{2\sqrt{\tau}}\right)^2}\,, \tag{3.2.36}$$

and with the substitution

$$\eta = \left(\sqrt{\tau}\mathbf{R}-\frac{-i\mathbf{k}}{2\sqrt{\tau}}\right)^2, \qquad \mathrm{Det}\left(\frac{\partial R}{\partial \eta}\right) = \frac{1}{\sqrt{\tau}^3}\,, \tag{3.2.37}$$

we conclude that

$$K\int d^3\mathbf{R}\frac{1}{|\mathbf{R}|}e^{-i\mathbf{k}\mathbf{R}} = K\pi\int_0^\infty d\tau\,\frac{1}{\tau^2}e^{-\frac{k^2}{4\tau}}\,. \tag{3.2.38}$$

The last integration can be performed with the substitution $u := \frac{1}{\tau}$ and we arrive at

$$K\int d^3\mathbf{R}\frac{1}{|\mathbf{R}|}e^{-i\mathbf{k}\mathbf{R}} = K\,\frac{4\pi}{k^2}\,. \tag{3.2.39}$$

3.2.4 Fourier Transformation for Two-Dimensional Coulomb Interaction

In two dimensions we can do the Fourier transformation as follows, first we note

$$K\int_0^\infty r dr\int_0^{2\pi}d\varphi\,\frac{1}{r}e^{ikr\cos(\varphi)} = K\int_0^\infty dr\int_0^{2\pi}d\varphi\,e^{ikr\cos(\varphi)} = 2\pi K\int_0^\infty dr\,J_0(kr)\,, \tag{3.2.40}$$

where we have used (3.2.16) to get the Bessel function J_0. Now in order to calculate the second integral one has to use a trick analog to the three-dimensional Yukawa trick, by introducing a converging making factor as follows

$$\begin{aligned}
\int_0^\infty dr e^{-\alpha r} J_0(kr) &= \frac{1}{2\pi}\int_0^\infty dr\, e^{-\alpha r}\int_0^{2\pi} d\varphi\, e^{-ikr\cos(\varphi)} \qquad \alpha > 0 \\
&= \frac{1}{2\pi}\int_0^{2\pi} d\varphi \int_0^\infty dr\, e^{-[\alpha + ik\cos(\varphi)]r} \\
&= \frac{1}{2\pi}\int_0^{2\pi} d\varphi \frac{-1}{\alpha + ik\cos(\varphi)} e^{-[\alpha+ik\cos(\varphi)]r}\Big|_0^\infty \\
&= \frac{1}{2\pi}\int_0^{2\pi} d\varphi \frac{1}{\alpha + ik\cos(\varphi)}\,, \\
&= \frac{1}{2\pi}\frac{2\pi}{\sqrt{\alpha^2 - (-ik)^2}} \\
&= \frac{1}{\sqrt{\alpha^2 + k^2}}
\end{aligned} \tag{3.2.41}$$

where we have used the Kepler integral. Now with $\alpha = 0$ and for $k > 0$ follows

$$V_{\mathrm{Col}}^{(\mathrm{int})}(\mathbf{k}) := K\frac{2\pi}{k}\,. \tag{3.2.42}$$

3.3 Self-Energy Derivation for a Homogeneous System within Hartree-Fock Approximation

3.3.1 For Dipole-Dipole Interaction in Three Dimensions

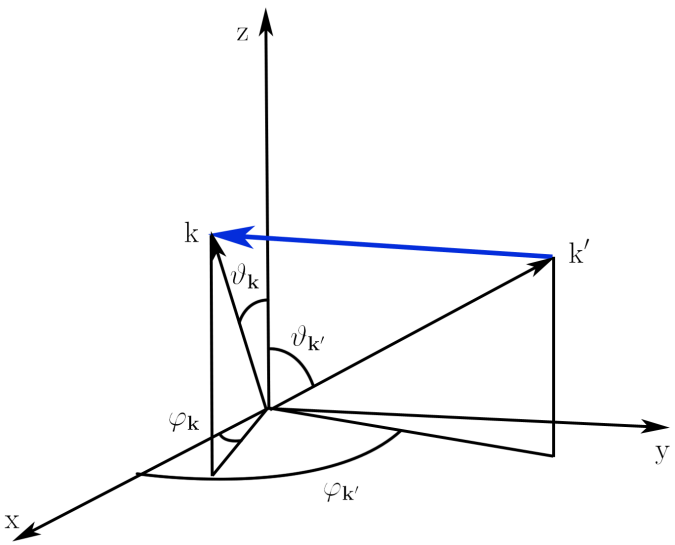


Figure 3.7: Illustration of considered angles. The figure is adapted from [35] .

If we are dealing with ultracold gases $T \approx 0$ the Fermi function tends towards the Θ-distribution and we can substitute the sum with the integral

$$\frac{1}{V}\sum_{\mathbf{k}'}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2}n_{\mathbf{k}} \longrightarrow \int \frac{d^2k'}{(2\pi)^2}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2}\,, \tag{3.3.1}$$

where the integration extends over the Fermi sphere.

Before we proceed we again stress the point, that (2.4.20) are the Hartree-Fock equation in first order perturbation theory. That is we will not solve the self-consistent Hartree Fock equation, which would change the distribution $n_{\mathbf{k}}$ in (2.4.20) and consequently deforme the Fermi sphere in the upcoming integrals. While higher perturbations have already been considered [54], we are not aware of a fully self-consistent calculation at the present time. We now calculate the Hartree-Fock self-energy for the homogeneous system. We start by inserting the Fourier transformation (3.2.14) in equation (2.4.20):

$$\begin{aligned}\Sigma^{\mathrm{HF}}_{\mathrm{3D}}(\mathbf{k}) &= \frac{1}{V}\sum_{\mathbf{k}'}\left[V_{\mathrm{3D}}(\mathbf{k}=\mathbf{0}) - V_{\mathrm{3D}}(\mathbf{k}-\mathbf{k}')\right]n_{\mathbf{k}'} \\ &= -\frac{8\pi K\mathbf{p}_1\cdot\mathbf{p}_2}{3}\sum_{\mathbf{k}'}P_2(\cos(\alpha_{k-k'}))n_{\mathbf{k}'}\,.\end{aligned} \tag{3.3.2}$$

We will now replace again the sum with the integration, as explained in (3.3.1). Then we get

$$\Sigma^{\mathrm{HF}}_{\mathrm{3D}}(\mathbf{k}) = -\frac{8\pi K\mathbf{p}_1\cdot\mathbf{p}_2}{3}\int_{\mathbf{k}'\leq\mathbf{k}_F}\frac{d^3k'}{(2\pi)^3}P_2(\cos(\alpha_{\mathbf{k}-\mathbf{k}'}))\,, \tag{3.3.3}$$

The angle $\alpha_{k-k'}$ denotes the angle between the z-axes and the vector $\mathbf{k}-\mathbf{k}'$ and can be expressed according to Figure 3.7. [1]

$$\cos(\alpha_{k-k'}) = \frac{k\cos(\vartheta_{\mathbf{k}}) - k'\cos(\vartheta_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \frac{k\cos(\vartheta_{\mathbf{k}}) - k'\cos(\vartheta'_{\mathbf{k}})}{\sqrt{k^2+k'^2-2kk'\cos(\alpha_{k-k'})}}\,, \tag{3.3.7}$$

where $\vartheta_{\mathbf{k}}$ and $\vartheta_{\mathbf{k}'}$ are the angles between the z-axis and $\mathbf{k}$, $\mathbf{k}'$ and α is the angle between $\mathbf{k}$ and $\mathbf{k}'$. If we write $\cos(\alpha_{k-k'}) = \sin(\vartheta_{\mathbf{k}})\sin(\vartheta_{\mathbf{k}'})\cos(\varphi_{\mathbf{k}}-\varphi_{\mathbf{k}'}) + \cos(\vartheta_{\mathbf{k}})\cos(\vartheta_{\mathbf{k}'})$ we get

$$\cos(\alpha_{k-k'}) = \frac{k\cos(\vartheta_{\mathbf{k}}) - k'\cos(\vartheta_{\mathbf{k}'})}{\sqrt{k^2+k^{2\prime}-2kk'\left[\sin(\vartheta_{\mathbf{k}})\sin(\vartheta_{\mathbf{k}'})\cos(\varphi_{\mathbf{k}}-\varphi_{\mathbf{k}'})+\cos(\vartheta_{\mathbf{k}})\cos(\vartheta_{\mathbf{k}'})\right]}}\,. \tag{3.3.8}$$

[1] A more pedestrian way to see this relation is

$$\mathbf{q} = q\begin{pmatrix}\sin(\alpha)\cos(\beta)\\ \sin(\alpha)\sin(\beta)\\ \cos(\alpha)\end{pmatrix} \qquad \mathbf{k} = k\begin{pmatrix}\sin(\vartheta_k)\cos(\varphi_k)\\ \sin(\vartheta_k)\cos(\varphi_{\mathbf{k}})\\ \cos(\vartheta_k)\end{pmatrix} \qquad \mathbf{k}' = k'\begin{pmatrix}\sin(\vartheta'_k)\cos(\varphi'_{\mathbf{k}})\\ \sin(\vartheta'_k)\cos(\varphi'_{\mathbf{k}})\\ \cos(\vartheta'_{\mathbf{k}})\end{pmatrix} \tag{3.3.4}$$

$$\hat{\mathbf{z}}\cdot\mathbf{q} = (\mathbf{k}-\mathbf{k}') = (k-k')\cos(\alpha) = k\cos(\vartheta_{\mathbf{k}}) - k'\cos(\vartheta'_{\mathbf{k}}) \tag{3.3.5}$$

$$\cos(\alpha_{k-k'}) = \frac{k\cos(\vartheta_{\mathbf{k}}) - \cos(\vartheta_{\mathbf{k}})}{|\mathbf{k}-\mathbf{k}'|} \tag{3.3.6}$$

Together with the definition of the Legendre polynomials, it follows

$$\Sigma^{\mathrm{HF}}_{3\mathrm{D}}(k) = -\frac{8\pi K \mathbf{p}_1\cdot\mathbf{p}_2}{3}\int_{k'\le k_F}\frac{d^3k'}{(2\pi)^3}P_2(\cos(\alpha_{k-k'})) \tag{3.3.9}$$

$$= -\frac{K\mathbf{p}_1\cdot\mathbf{p}_2}{3\pi^2}$$

$$\times\left[\underbrace{\int_{k'\le k_F}d^3k'\frac{3(k\cos(\vartheta_{\mathbf{k}})-k'\cos(\vartheta_{\mathbf{k}'}))^2}{2\left(k^2+k^{2\prime}-2kk'\left[\sin(\vartheta_{\mathbf{k}})\sin(\vartheta_{\mathbf{k}'})\cos(\varphi_{\mathbf{k}}-\varphi_{\mathbf{k}'})+\cos(\vartheta_{\mathbf{k}})\cos(\vartheta_{\mathbf{k}'})\right]\right)}}_{:=\mathrm{Int}_A}-\int_{k'\le k_F}d^3k'\frac{1}{2}\right].$$

The second integral can be evaluated immediately

$$\frac{1}{2}\int_{k'\le k_F}d^3k' = \frac{1}{2}\int d\Omega\int_0^{k_F}k'dk' = \frac{2\pi k_F^3}{3}\,. \tag{3.3.10}$$

Now lets evaluate the first integral. We first note that, due to the cylindrical symmetry, we can project the $\mathbf{k}$ vector in the k_z-k_x plane, i.e. we put $\varphi_{\mathbf{k}}=0$. Furthermore we shall define the following shorthand notations

$$\begin{aligned}A &= 3k^{\prime 2}\sin(\vartheta_{\mathbf{k}'})\left[k\cos(\vartheta_{\mathbf{k}'})-k'\cos(\vartheta_{\mathbf{k}'})\right]^2,\\ B &= 2[k^2+k^{\prime 2}-2kk'\cos(\vartheta)\cos(\vartheta_{\mathbf{k}'})],\\ C &= -4kk'\sin(\vartheta_{\mathbf{k}}),\end{aligned} \tag{3.3.11}$$

so with this notation we get

$$\mathrm{Int}_A = \int_0^{k_F}dk'\int_0^{\pi}d\vartheta_{\mathbf{k}'}\int_0^{2\pi}d\varphi_{\mathbf{k}'}\frac{A}{B+C\cos(\varphi_{\mathbf{k}'})}\,. \tag{3.3.12}$$

This is the Kepler integral, which can be solved analytically as long as the following relations (3.3.13) are fulfilled. Now we note that $0\le\vartheta_{\mathbf{k}}\le\pi$ and $0\le\vartheta_{\mathbf{k}'}\le\pi$ and $k,k'>0$. So we have

$$\left.\begin{array}{c}0\le 4(k-k')^4\le B^2\le 4(k+k')^4\\ -4kk'\le C^2\le 0\end{array}\right\}\quad\Longrightarrow\quad B^2-C^2>0\quad\forall_{k\neq k'}\forall_{\vartheta,\vartheta'\neq\pi}\,, \tag{3.3.13}$$

so we can use the following formula

$$\int_0^{2\pi}d\varphi_{\mathbf{k}'}\frac{A}{B+C\cos(\varphi_{\mathbf{k}'})} = 2A\int_0^{\pi}\frac{d\varphi_{\mathbf{k}'}}{B+C\cos(\varphi_{\mathbf{k}'})} = \frac{2A\pi}{\sqrt{B^2-C^2}}\,. \tag{3.3.14}$$

Now we can concentrate on the ϑ' integral. Again it will be necessary to introduce some new notations

$$\begin{aligned}u &= \cos(\vartheta_{\mathbf{k}}),\\ K_1 &= k^2+k^{\prime 2},\\ L_1 &= 2kk',\\ H_1 &= K_1^2-L_1^2\sin^2(\vartheta_{\mathbf{k}}),\\ H_2 &= 2K_1L_1\cos(\vartheta_{\mathbf{k}})\,.\end{aligned} \tag{3.3.15}$$

If we now return to the integral keeping in mind, that we have to change the measure $\frac{du}{d\vartheta_{\mathbf{k}'}} = -\sin(\vartheta_{\mathbf{k}'})$ and have $u(0)=1$ as well $u(\pi)=-1$, we can switch the integral immediately and use the minus sign as follows

$$\int_0^{\pi}d\vartheta_{\mathbf{k}'}\frac{3\pi k^{\prime 2}\sin(\vartheta_{\mathbf{k}'})\left[k\cos(\vartheta_{\mathbf{k}})-k'\cos(\vartheta_{\mathbf{k}'})\right]^2}{\sqrt{[k^2+k^{\prime 2}-2kk'\cos(\vartheta_{\mathbf{k}})\cos(\vartheta_{\mathbf{k}'})]^2-4k^2k^{\prime 2}\sin(\vartheta_{\mathbf{k}})^2}} = \int_{-1}^{1}du\frac{3k^{\prime 2}\pi\left[k\cos(\vartheta_{\mathbf{k}})-k'u\right]^2}{\sqrt{H_1+L_1^2u^2-H_2u}} \tag{3.3.16}$$

again introducing new notations and expanding the integrand we arrive at

$$\int_{-1}^{1} du \frac{3k'^2\pi \left[k\cos\left(\vartheta_{\mathbf{k}}\right) - k'u\right)^2}{\sqrt{H_1 + L_1^2u^2 - H_2u}} = \int_{-1}^{1} du \frac{I_1}{\sqrt{H_1 + L_1^2u^2 - H_2u}} \cdot + \int_{-1}^{1} du \frac{I_2u}{\sqrt{H_1 + L_1^2u^2 - H_2u}} + \int_{-1}^{1} du \frac{I_3u^2}{\sqrt{H_1 + L_1^2u^2 - H_2u}} \tag{3.3.17}$$

with

$$\begin{aligned} I_1 &= 3\pi k^2 k'^2 \cos\left(\vartheta_{\mathbf{k}}\right), \\ I_2 &= -6\pi k k'^3 \cos\left(\vartheta_{\mathbf{k}}\right), \\ I_3 &= 3\pi k'^4. \end{aligned} \tag{3.3.18}$$

The integrals can be solved in the following way as long as

$$4L_1^2H_1 - (-H_2)^2 = 16k^2k_1^2(k^2 - k_1^2)^2 \sin\left(\vartheta_{\mathbf{k}}\right) \overset{!}{>} 0\,, \tag{3.3.19}$$

which is the case as long as $k \neq k'$. Note that the integral can also be solved for $k = k'$. Just its form is different. Using the following integrals

$$\begin{aligned} \int \frac{dx}{\sqrt{ax^2+bx+c}} &= \frac{1}{\sqrt{a}}\text{arsinh}\left(\frac{2ax+b}{\sqrt{4ac-b^2}}\right) + C_1, \\ \int dx \frac{x}{\sqrt{ax^2+bx+c}} &= \frac{\sqrt{ax^2+bx+c}}{a} - \frac{b}{2a}\left[\frac{1}{\sqrt{a}}\text{arsinh}\left(\frac{2ax+b}{\sqrt{4ac-b^2}}\right) + C_2,\right] \\ \int dx \frac{x^2}{\sqrt{ax^2+bx+c}} &= \left(\frac{x}{2a} - \frac{3b}{4a^2}\right)\sqrt{ax^2+bx+c} + \frac{3b^2-4ac}{8a^2}\left[\frac{1}{\sqrt{a}}\text{arsinh}\left(\frac{2ax+b}{\sqrt{4ac-b^2}}\right) + C_3\right]\,, \end{aligned} \tag{3.3.20}$$

we can simplify the expression (3.3.17) to

$$\begin{aligned} &\int_{-1}^{1} du \frac{3k'^2\pi \left[k\cos\left(\vartheta_{\mathbf{k}}\right) - k'u\right]^2}{\sqrt{H_1 + L_1^2u^2 - H_2u}} \\ &= \left[\frac{I_1}{\sqrt{L_1^2}} - \frac{I_2H_2}{2L_1^2\sqrt{L_1^2}} + I_3\left(\frac{3H_2^2 - 4L_1^2H_1}{8L_1^4\sqrt{L_1^2}}\right)\right]\left[\text{arsinh}\left(\frac{2L_1^2+H_2}{\sqrt{4L_1^2H_1-H_2^2}}\right) - \text{arsinh}\left(\frac{-2L_1^2+H_2}{\sqrt{4L_1^2H_1-H_2^2}}\right)\right] \\ &+ \left[\frac{I_2}{L_1^2} - \frac{3H_2I_3}{4L_1^4}\right]\left(\sqrt{L_1^2+H_2+H_1} - \sqrt{L_1^2-H_2+H_1}\right) + \frac{I_3}{2L_1^2}\left(\sqrt{L_1^2+H_2+H_1} + \sqrt{L_1^2-H_2+H_1}\right)\,. \end{aligned} \tag{3.3.21}$$

We will first look at the argument of the arsinh in the following way

$$\frac{\pm 2L_1^2 - H_2}{\sqrt{4L_1^2H_1 - H_2^2}} =: \varphi\,, \tag{3.3.22}$$

and use the identity

$$\text{arsinh}(x) = \log\left(x + \sqrt{x^2+1}\right)\,, \tag{3.3.23}$$

with which we can deduce

$$\begin{aligned} \text{arsinh}\left(\frac{2L_1^2+H_2}{\sqrt{4L_1^2H_1-H_2^2}}\right) - \text{arsinh}\left(\frac{-2L_1^2+H_2}{\sqrt{4L_1^2H_1-H_2^2}}\right) &= \log\left[\frac{(k+k')}{(k-k')}\tan\left(\frac{\vartheta_{\mathbf{k}}}{2}\right)\right] - \log\left[\frac{(k-k')}{(k+k')}\tan\left(\frac{\vartheta_{\mathbf{k}}}{2}\right)\right] \\ &= \log\left[\frac{(k+k')^2}{(k-k')^2}\right]\,. \end{aligned} \tag{3.3.24}$$

The next step is to evaluate the square root terms. First notice

$$\sqrt{L_1^2 \pm H_2 + H_1} = \sqrt{k^2 + k'^2 \pm 2kk' \cos^2(\vartheta_{\mathbf{k}})} = k^2 + k'^2 \pm 2kk' \cos(\vartheta_{\mathbf{k}}) \,. \tag{3.3.25}$$

In the last step we could leave the square root, due to the fact that $k, k' > 0$ and $0 \leq \vartheta_{\mathbf{k}} \leq \pi$ and hence

$$\begin{aligned} k^2 + k'^2 + 2kk' \cos(\vartheta_{\mathbf{k}}) &\geq k^2 + k'^2 + 2kk' \cos(\pi) = k^2 + k'^2 + 2kk' = (k+k')^2 \geq 0 \\ k^2 + k'^2 - 2kk' \cos(\vartheta_{\mathbf{k}}) &\geq k^2 + k'^2 + 2kk' \cos(0) = k^2 + k'^2 - 2kk' = (k-k')^2 \geq 0 \,. \end{aligned} \tag{3.3.26}$$

With that we can finally write this cumbersome expression in the simple form

$$\begin{aligned} \sqrt{L_1^2 + H_2 + H_1} - \sqrt{L_1^2 - H_2 + H_1} &= -4kk' \cos(\vartheta_{\mathbf{k}}) \,, \\ \sqrt{L_1^2 + H_2 + H_1} + \sqrt{L_1^2 - H_2 + H_1} &= 2(k^2 + k'^2) \,. \end{aligned} \tag{3.3.27}$$

Next we evaluate the other terms, keeping in mind, that we are not really interested in simplifying them yet. We sort by k', and start with

$$\begin{aligned} \frac{I_1}{\sqrt{a}} - \frac{I_2 b}{2a\sqrt{a}} + I_3 \left(\frac{3b^2 - 4ac}{8a^2\sqrt{a}} \right) \Bigg] &= \frac{3k\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16} k' - \frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{8k} k'^3 \\ &\quad + \frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16k^3} k'^5 \,, \\ \left[\frac{I_2}{a} - \frac{3bI_3}{4a^2} \right] &= \frac{-15\pi \cos(\vartheta_{\mathbf{k}})}{16k} k' + \frac{9\pi \cos(\vartheta_{\mathbf{k}})}{16k^3} k'^3 \,. \end{aligned} \tag{3.3.28}$$

We already calculated the last factor, so we are ready to put it together and define new constants

$$\begin{aligned} &\int_{-1}^{1} du \frac{3k'^2 \pi \left[k\cos(\vartheta_{\mathbf{k}}) - k' u\right]^2}{\sqrt{H_1 + L_1^2 u^2 - H_2 u}} \\ &= \frac{3k\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16} k' \log\left[\frac{(k+k')^2}{(k-k')^2}\right] - \frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{8k} k'^3 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] \\ &\quad + \frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16k^3} k'^5 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] + \frac{3\pi[5\cos^2(\vartheta_{\mathbf{k}}) + 1]}{4} k'^2 - \frac{3\pi[3\cos^2(\vartheta_{\mathbf{k}}) - 1]}{4k^2} k'^4 \\ &= G_1 k' \log\frac{(k+k')^2}{(k-k')^2} + G_2 k'^3 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] + G_3 k'^5 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] + G_4 k'^2 + G_5 k'^4 \,, \end{aligned} \tag{3.3.29}$$

where we have introduced

$$\begin{aligned} G_1 &= \frac{3k\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16} & G_2 &= -\frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{8k} \\ G_3 &= \frac{3\pi \left[3\cos^2(\vartheta_{\mathbf{k}}) - 1\right]}{16k^3} & G_4 &= \frac{3\pi[5\cos^2(\vartheta_{\mathbf{k}}) + 1]}{4} \\ G_5 &= -\frac{3\pi[3\cos(\vartheta_{\mathbf{k}})^2 - 1]}{4k^2} \,. \end{aligned} \tag{3.3.30}$$

The integration over k can now be done analytically. Since the logarithm is zero at the point one, all integrals vanish at the lower boundary and we get

$$\begin{aligned} \int_0^{k_F} dk'\, k' \log\left[\frac{(k+k')^2}{(k-k')^2}\right] &= \frac{1}{2}\left(k_F^2 - k^2\right) \log\left[\frac{(k+k_F)^2}{(k-k_F)^2}\right] + 2kk_F \,, \\ \int_0^{k_F} dk'\, k'^3 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] &= \frac{1}{4}(k_F^4 - k^4) \log\left[\frac{(k+k_F)^2}{(k-k_F)^2}\right] + \frac{k}{3}k_F^3 + k^3 k_F \,, \\ \int_0^{k_F} dk'\, k'^5 \log\left[\frac{(k+k')^2}{(k-k')^2}\right] &= \frac{1}{6}(k_F^6 - k^6) \log\left[\frac{(k+k_F)^2}{(k-k_F)^2}\right] + \frac{2}{15}kk_F^5 + \frac{2}{9}k^3 k_F^3 + \frac{2}{3}k^5 k_F \,. \end{aligned} \tag{3.3.31}$$

Remembering the first integral we calculated immediately at the start (3.3.10), and also keeping in mind that it has a minus sign, we can write the integral over P_2 as

$$\begin{aligned}\int_{k'<k_F} dk' P_2(\cos(\alpha_{\mathbf{k}-\mathbf{k}'})) = &\left[\frac{3k\pi\left(3\cos(\vartheta_{\mathbf{k}})^2-1\right)}{16}\right]\left[\frac{1}{2}\left(k_F^2-k^2\right)\log\left(\frac{(k+k_F)^2}{(k-k_F)^2}\right)+2kk_F\right]\\ &-\left[\frac{3\pi\left(3\cos^2(\vartheta_{\mathbf{k}})-1\right)}{8k}\right]\left[\frac{1}{4}(k_F^4-k^4)\log\left(\frac{(k+k_F)^2}{(k-k_F)^2}\right)+\frac{k}{3}k_F^3+k^3k_F\right]\\ &+\left[\frac{3\pi\left(3\cos^2(\vartheta_{\mathbf{k}})-1\right)}{16k^3}\right]\left[\frac{1}{6}(k_F^6-k^6)\log\left(\frac{(k+k_F)^2}{(k-k_F)^2}\right)+\frac{2}{15}kk_F^5+\frac{2}{9}k^3k_F^3+\frac{2}{3}k^5k_F\right]\\ &+\left[\frac{3\pi\left(5\cos^2(\vartheta_{\mathbf{k}})+1\right)}{4}\right]\frac{1}{3}k_F^3\\ &-\left[\frac{3\pi\left(3\cos^2(\vartheta_{\mathbf{k}})-1\right)}{4k^2}\right]\frac{1}{5}k_F^5\\ &-\frac{2\pi}{3}k_F^3\,. \end{aligned} \tag{3.3.32}$$

$$\begin{aligned}\int_{\mathbf{k}'<k_F} dk' P_2(\cos(\alpha_{\mathbf{k}-\mathbf{k}'}) &= \left(3\cos^2(\vartheta_{\mathbf{k}})-1\right)\left[\frac{\pi k_F}{8k^2}(k^4-k_F^4)+\frac{\pi k_F^3}{3}-\frac{\pi}{32k^3}(k^2-k_F^2)^3\log\left(\frac{(k+k_F)^2}{(k-k_F)^2}\right)\right]\\ &= \left(3\cos^2(\vartheta_{\mathbf{k}})-1\right)\frac{\pi}{24}k_F^3\left[3\left(\frac{k}{k_F}\right)^2-3\frac{1}{\left(\frac{k}{k_F}\right)^2}+8+\frac{3\left(1-\left(\frac{k}{k_F}\right)^2\right)^3}{2\left(\frac{k}{k_F}\right)^3}\log\left(\frac{|1+\frac{k}{k_F}|}{|1-\frac{k}{k_F}|}\right)\right]\\ &= P_2(\cos(\vartheta_{\mathbf{k}}))k_F^3 I_{3\mathrm{D}}\left(\frac{k}{k_F}\right)\,, \end{aligned} \tag{3.3.33}$$

with the definition

$$I_{3\mathrm{D}}(x) := \frac{\pi}{12}\left[3x^2-3\frac{1}{x^2}+8+\frac{3\left(1-x^2\right)^3}{2x^3}\log\left(\frac{|1+x|}{|1-x|}\right)\right]\,. \tag{3.3.34}$$

The whole integral follows the same notations as introduced in [35]

$$\begin{aligned}\Sigma_{3\mathrm{D}}^{\mathrm{HF}}(\mathbf{k}) &= -k_F^3\frac{Kp_1p_2}{3\pi^2}P_2(\cos(\vartheta_{\mathbf{k}}))I_{3\mathrm{D}}\left(\frac{k}{k_F}\right)\\ &= -2\lambda\, E_{k_F}^{3D}P_2(\cos(\vartheta_{\mathbf{k}}))I_{3\mathrm{D}}\left(\frac{k}{k_F}\right)\,, \end{aligned} \tag{3.3.35}$$

with defining the dimensionless dipolar interactions

$$\lambda := \frac{Kp_1p_2mk_F}{3\pi^2\hbar^2} \qquad \text{and the Fermi energy} \qquad E_{k_F}^{3D} = \frac{\hbar^2k_F^2}{2m}\,. \tag{3.3.36}$$

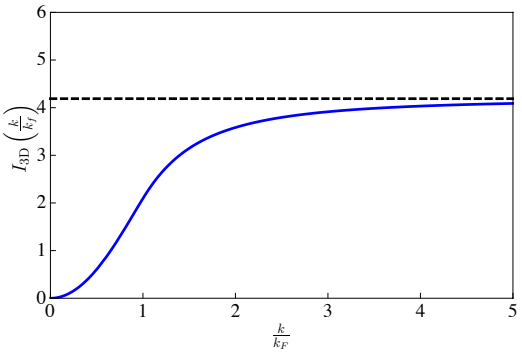


Figure 3.8: The integral I_{3D} as a function of $\frac{k}{k_F}$, converging for large k, against $\frac{4\pi}{3}$.

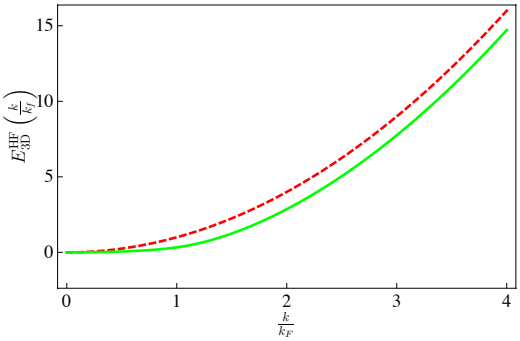


Figure 3.9: Comparison of the whole energy (green) with the free dispersion (red).

The function (3.3.34) shown in Figure 3.8 converges against $\frac{4\pi}{3}$. Therefore the self-energy (3.3.35) will be lowered by a constant factor for high momenta $\mathbf{k}$. This behaviour can also be seen in Figure 3.9. Where the whole energy dispersion is compared to the free dispersion. The convergence of (3.3.34) manifests itself in the curvature of the dispersion, which is dominated by the free dispersion. The Fermi surface in Figure 3.10 shown for $\lambda = \frac{1}{2\pi}$ is now elongated along the k_z direction. This is expected since the dipoles are directed in the z-direction. The ratio of dilatation in z-direction of $\frac{1}{2}$ is an accompanied by a compression in x-direction of approximately $\frac{1}{8}$. The strength of the deformation certainly changes with the chosen value of λ.

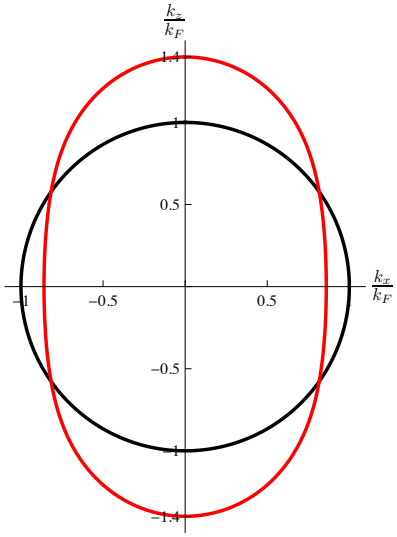


Figure 3.10: The Fermi surface in first order perturbation theory for the dipolar interaction compared to the Fermi surface with spherical symmetric interaction for $\lambda = \frac{1}{2\pi}$.

3.3.2 For Dipole-Dipole Interaction in Two Dimensions

We use the two-dimensional potential as from (3.2.32) in order to calculate the Hartree-Fock energy (2.4.20)

$$\begin{aligned}\Sigma^{\mathrm{HF}}_{2\mathrm{D}}(\mathbf{k}) &= \frac{1}{V}\sum_{\mathbf{k}'}\left[V_{2\mathrm{D}}(\mathbf{k}=0) - V_{2\mathrm{D}}(|\mathbf{k}-\mathbf{k}'|)\right] n_{\mathbf{k}'} \\ &= 2\pi K \mathbf{p}_1\cdot\mathbf{p}_2 \sum_{\mathbf{k}'} P_2(\cos(\alpha))|\mathbf{k}-\mathbf{k}'| n_{\mathbf{k}'} - \pi K \mathbf{p}_1\cdot\mathbf{p}_2 \sum_{\mathbf{k}'} |\mathbf{k}-\mathbf{k}'|\sin^2(\alpha)\cos(2\beta_{\mathbf{k}-\mathbf{k}'}) n_{\mathbf{k}'}\,.\end{aligned}$$

Again we take $\beta\to\infty$ and arrive at the integral

$$\Sigma^{\mathrm{HF}}_{2\mathrm{D}}(\mathbf{k}) = 2\pi K \mathbf{p}_1\cdot\mathbf{p}_2 \int_{k\le k_F}\frac{d^2k}{(2\pi)^2} P_2(\cos(\alpha))|\mathbf{k}-\mathbf{k}'| - \pi d^2 \int_{k\le k_F}\frac{d^2k}{(2\pi)^2}|\mathbf{k}-\mathbf{k}'|\sin^2(\alpha)\cos(2\beta_{\mathbf{k}-\mathbf{k}'})\,. \tag{3.3.37}$$

These are the integrals we want to solve, but we will start a little bit different to control the divergence for $\varepsilon\to 0$. Fortunately it will cancel due to the difference, as we shall see now. For that matter we first look at

the difference

$$V_{2\mathrm{D}}(\mathbf{k}=0) - V_{2\mathrm{D}}(|\mathbf{k}-\mathbf{k}'|) = 2\pi K \mathbf{p}_1 \cdot \mathbf{p}_2 P_2(\cos(\alpha))|\mathbf{k}-\mathbf{k}'| - \pi K \mathbf{p}_1 \cdot \mathbf{p}_2 |\mathbf{k}-\mathbf{k}'| \sin^2(\alpha) \cos(2\beta_{\mathbf{k}-\mathbf{k}'}) \,. \tag{3.3.38}$$

Now to control the $\cos(2x)$ we use the identity $\cos(2x) = 2\cos^2(x) - 1$, since we have the angle between the x-axis and the vector $\mathbf{k}-\mathbf{k}'$ the following identity holds true

$$\cos(\beta_{\mathbf{k}-\mathbf{k}'}) = \frac{k\cos(\varphi_{\mathbf{k}}) - k'\cos(\varphi_{\mathbf{k}'})}{|k-k'|} \,. \tag{3.3.39}$$

Inserting both yields to

$$\begin{aligned} &V_{2\mathrm{D}}(\mathbf{k}=0) - V_{2\mathrm{D}}(|\mathbf{k}-\mathbf{k}'|) \qquad (3.3.40)\\ &= \pi K \mathbf{p}_1 \cdot \mathbf{p}_2 \left[2P_2(\cos(\alpha)) + \sin^2(\alpha)\right] \sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})} - 2\pi K \mathbf{p}_1 \cdot \mathbf{p}_2 \sin^2(\alpha_0) \\ &\quad \times \left[k^2 \cos^2(\varphi_{\mathbf{k}}) \frac{1}{\sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})}} + k'^2 \frac{\cos^2(\varphi_{\mathbf{k}'})}{\sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})}} \right. \\ &\qquad \left. -2kk'\cos(\varphi_{\mathbf{k}}) \frac{\cos(\varphi_{\mathbf{k}'})}{\sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})}} \right] \\ &=: \mathrm{Int}_1 + \mathrm{Int}_2 \,, \qquad (3.3.41) \end{aligned}$$

where

$$\begin{aligned} \mathrm{Int}_1 &:= \pi K \mathbf{p}_1 \cdot \mathbf{p}_2 \left[2P_2(\cos(\alpha)) + \sin^2(\alpha)\right] \sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})} \\ \mathrm{Int}_2 &:= \mathrm{rest} \,. \end{aligned} \tag{3.3.42}$$

First we rewrite the integral

$$\begin{aligned} \int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{1}{|\mathbf{k}-\mathbf{k}'|} &= \int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{1}{\sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})}} = \int_{-\varphi_{\mathbf{k}}}^{2\pi - \varphi_k} d\sigma \frac{1}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} \\ &= \int_0^{2\pi} d\sigma \frac{1}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} = \frac{4}{\sqrt{(k+k')^2}} \int_0^{\frac{\pi}{2}} d\omega \frac{1}{\sqrt{1 - \frac{4kk'}{(k+k')^2}\sin^2(\omega)}} \\ &= \frac{4}{\sqrt{(k+k')^2}} K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2)}}\right) \,. \end{aligned} \tag{3.3.43}$$

Here we have introduced the elliptic integral

$$K(x) := \int_0^{\frac{\pi}{2}} d\varphi \frac{1}{\sqrt{1 - x^2 \sin^2(\varphi)}} \,, \tag{3.3.44}$$

which is also shown in Figure 3.11. Second we will evaluate the integrals over $\varphi_{\mathbf{k}'}$.

$$\int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{\cos^2(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \int_0^{2\pi} d\varphi \frac{\cos^2(\varphi_{\mathbf{k}'})}{\sqrt{k^2 + k'^2 - 2kk'\cos(\varphi_{\mathbf{k}} - \varphi'_{\mathbf{k}})}} = \int_{-\varphi_{\mathbf{k}}}^{2\pi - \varphi_{\mathbf{k}}} d\sigma \frac{\cos^2(\sigma + \varphi_{\mathbf{k}})}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} \tag{3.3.45}$$

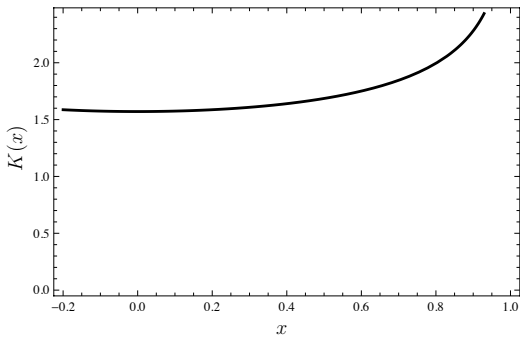


Figure 3.11: Elliptic Integral K.

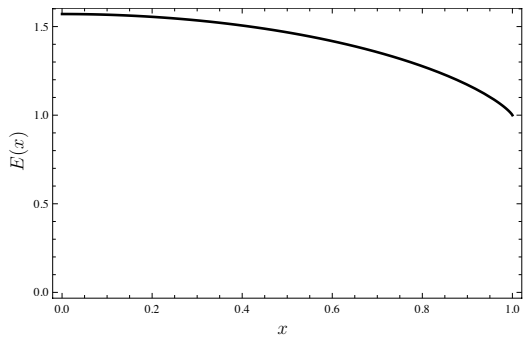


Figure 3.12: Elliptic Integral E.

Now we separate the $\cos^2(\alpha+\varphi_{\mathbf{k}})$ as follows

$$\cos^2(\sigma+\varphi_{\mathbf{k}}) = \frac{1}{2} - \frac{1}{2}\cos(2\varphi_{\mathbf{k}}) + \cos(2\varphi_{\mathbf{k}})\cos^2(\sigma) - 2\cos(\varphi_{\mathbf{k}})\sin(\varphi_{\mathbf{k}})\cos(\sigma)\sin(\sigma) \tag{3.3.46}$$

and write the first integral as

$$\begin{aligned}\int_0^{2\pi} d\varphi_{\mathbf{k}'}\frac{\cos^2(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} &= \frac{1}{2}\frac{4}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) - \frac{1}{2}\cos(2\varphi_{\mathbf{k}})\frac{4}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)\\ &+ \cos(2\varphi_{\mathbf{k}})\int_0^{2\pi} d\sigma\frac{\cos^2(\sigma)}{\sqrt{k^2+k'^2-2kk'\cos(\sigma)}}\\ &- 2\cos(\varphi_{\mathbf{k}})\sin(\varphi_{\mathbf{k}})\int_0^{2\pi} d\sigma\frac{\cos(\sigma)\sin(\sigma)}{\sqrt{k^2+k'^2-2kk'\cos(\sigma)}}\,.\end{aligned} \tag{3.3.47}$$

The last integral must be zero since the integrand is an odd function. The next integral can be written with the help of the relation for elliptic integrals

$$\int_0^{2\pi} d\sigma\frac{\cos^2(\sigma)}{\sqrt{a-b\cos(\sigma)}} = \frac{-8a(a-b)E\left(\sqrt{-\frac{2b}{a-b}}\right) + 4(2a^2+b^2)K\left(\sqrt{-\frac{2b}{a-b}}\right)}{3\sqrt{a-b}\,b^2}\,, \tag{3.3.48}$$

where we again introduced the elliptic integral

$$E(x) := \int_0^{\frac{\pi}{2}} d\varphi\sqrt{1-x^2\sin^2(\varphi)}\,, \tag{3.3.49}$$

which is also shown in Figure 3.12. Further we need the following relations

$$\begin{aligned}K(i\,\sigma) &= \frac{1}{\sqrt{1+\sigma^2}}K\left(\frac{\sigma}{\sqrt{1+\sigma^2}}\right)\,,\\ E(i\,\sigma) &= \sqrt{1+\sigma^2}E\left(\frac{\sigma}{\sqrt{1+\sigma^2}}\right)\,,\end{aligned} \tag{3.3.50}$$

so we can write the integral as:

$$\int_0^{2\pi} d\sigma\frac{\cos^2(\alpha)}{\sqrt{a-b\cos(\sigma)}} = \frac{-8a(a-b)\sqrt{1+\sigma^2}E\left(\frac{\sigma}{\sqrt{1+\sigma^2}}\right) + 4(2a^2+b^2)\frac{1}{\sqrt{1+\sigma^2}}K\left(\frac{\sigma}{\sqrt{1+\sigma^2}}\right)}{3\sqrt{a-b}\,b^2}\,. \tag{3.3.51}$$

With $\sigma = \sqrt{\frac{2b}{a-b}}$, and resubstituting $a = k^2 + k'^2$ as well as $b = 2kk'$, we can rewrite the whole integral as

$$\begin{aligned}\int_0^{2\pi} d\sigma \frac{\cos^2(\sigma)}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} \\ = \frac{-2(k^2+k'^2)\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + 2(k^4+k'^4+4k^2k'^2)\frac{1}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{3k^2k'^2} .\end{aligned} \tag{3.3.52}$$

By adding all together, we arrive at

$$\begin{aligned}\int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{\cos^2(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \frac{2}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) - \cos(2\varphi_{\mathbf{k}})\frac{2}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) \\ + \cos(2\varphi_{\mathbf{k}})\left[\frac{-2(k^2+k'^2)\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + 2(k^4+k'^4+4k^2k'^2)\frac{1}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{3k^2k'^2}\right] .\end{aligned} \tag{3.3.53}$$

Finally we have to solve the following integral

$$\int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{\cos(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \cos(\varphi_{\mathbf{k}}) \int_0^{2\pi} d\sigma \frac{\cos(\sigma)}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} - \sin(\varphi_{\mathbf{k}}) \int_0^{2\pi} d\sigma \frac{\sin(\sigma)}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} . \tag{3.3.54}$$

The second integral vanishes again, by the same argument as above, so again the function is uneven and integrated over a symmetric interval, that leaves us with:

$$\int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{\cos(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \cos(\varphi_{\mathbf{k}}) \int_0^{2\pi} d\sigma \frac{\cos(\sigma)}{\sqrt{k^2 + k'^2 - 2kk'\cos(\sigma)}} . \tag{3.3.55}$$

This time we need the following relation

$$\int_0^{2\pi} d\sigma \frac{\cos(\sigma)}{\sqrt{a - b\cos(\sigma)}} = \frac{4}{\sqrt{a-b}\,b}\left[(b-a)E\left(\sqrt{-\frac{2b}{a-b}}\right) + aK\left(\sqrt{-\frac{2b}{a-b}}\right)\right] . \tag{3.3.56}$$

Together with the relation from above we can rewrite it as So we have for this integral

$$\int_0^{2\pi} d\varphi_{\mathbf{k}'} \frac{\cos(\varphi_{\mathbf{k}'})}{|\mathbf{k}-\mathbf{k}'|} = \frac{2\cos(\varphi_{\mathbf{k}})}{kk'}\left[\frac{k^2+k'^2}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) - \sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)\right] . \tag{3.3.57}$$

Now we will rewrite the second term of the original integral

$$\begin{aligned}
\mathrm{Int}_2 = 2\pi K \mathbf{p}_1\cdot\mathbf{p}_2 \sin^2(\alpha)\Bigg[& k^2\cos^2(\varphi_{\mathbf{k}})\frac{4}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + k'^2\frac{2}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) \\
& - k'^2\cos(2\varphi_{\mathbf{k}})\frac{2}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) \\
& + k'^2\cos(2\varphi_{\mathbf{k}}) \\
& \times\left[\frac{-2(k^2+k'^2)\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + 2(k^4+k'^4+4k^2k'^2)\frac{1}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{3k^2k'^2}\right] \\
& - \frac{4\cos(\varphi_{\mathbf{k}})k^2K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{\sqrt{(k+k')^2}} - \frac{2\cos(2\varphi_{\mathbf{k}})k'^2K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{\sqrt{(k+k')^2}} - \frac{2k'^2K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{\sqrt{(k+k')^2}} \\
& + 2\cos(2\varphi_{\mathbf{k}})\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + 2\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)\Bigg] . \qquad (3.3.58)
\end{aligned}$$

The last term of (3.3.58) does not carry a $\cos(2\varphi_{\mathbf{k}})$ and we will remove it from this second anisotropic part and carry it over to Int_1 of (3.3.41). Without this last term (3.3.58) reads

$$\begin{aligned}
\mathrm{Int}_{\mathrm{ani}} &:= \mathrm{Int}_2 - 2\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) \\
&= 2\pi\sin^2(\alpha_0)\Bigg[-k'\cos(2\varphi_{\mathbf{k}})\frac{4}{\sqrt{(k+k')}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) \\
&\quad + k'\cos(2\varphi_{\mathbf{k}})\left[\frac{-2(k^2+k'^2)\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + 2(k^4+k'^4+4k^2k'^2)\frac{1}{\sqrt{(k+k')^2}}K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)}{3k^2k'^2}\right] \\
&\quad + 2\cos(2\varphi_{\mathbf{k}})\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) . \qquad (3.3.59)
\end{aligned}$$

Now, before we proceed here, let us carry the lost term to the isotropic part of the whole integral. This now reads

$$\mathrm{Int}_{\mathrm{iso}} := \mathrm{Int}_1 + 2\sqrt{(k+k')^2}E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) = 8\pi\mathbf{p}_1\cdot\mathbf{p}_2|k-k'|P_2(\cos(\alpha_0))E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) . \qquad (3.3.60)$$

Returning to the anisotropic part and simplify it a little more

$$\mathrm{Int}_{\mathrm{ani}} = 2\pi K\mathbf{p}_1\cdot\mathbf{p}_2\sin^2(\alpha_0)\cos(2\varphi_{\mathbf{k}})\sqrt{(k+k')^2}\frac{2}{3k^2}\left[\left(k-k'\right)^2K\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right) + (2k^2-k'^2)E\left(\frac{2\sqrt{kk'}}{\sqrt{(k+k')^2}}\right)\right] . \qquad (3.3.61)$$

Next we can perform the integration of the second part, keeping in mind, that we still need the k' factor from the Jacobian, so we get

$$\mathrm{I}_{\mathrm{iso}} = \frac{2}{3}k_F^3K\mathbf{p}_1\cdot\mathbf{p}_2\sin^2(\alpha_0)\cos(2\varphi_{\mathbf{k}})I_{2D}^{\mathrm{ani}}\left(\frac{k}{k_F}\right) , \qquad (3.3.62)$$

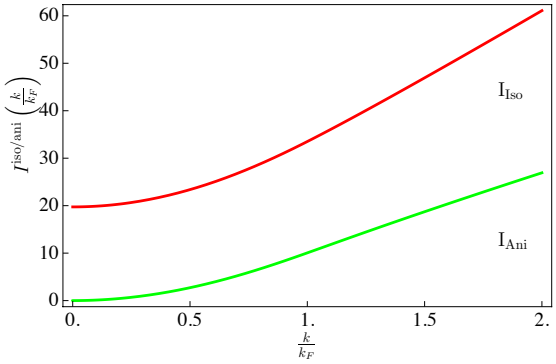


Figure 3.13: The functions $I_{2\mathrm{D}}^{\mathrm{iso}}$ and $I_{2\mathrm{D}}^{\mathrm{ani}}$.

with the definition

$$\begin{aligned} I_{2\mathrm{D}}^{\mathrm{ani}}(x) :&= 2\pi \int_0^1 dx' x' \frac{1}{x^2} \sqrt{(x+x')^2} \left[(x-x')^2 K\left(\frac{2\sqrt{xx'}}{\sqrt{(x+x')^2}} \right) + \left(2x^2 - x'^2\right) E\left(\frac{2\sqrt{xx'}}{\sqrt{(x+x')^2}} \right) \right] \\ &= 2\pi \int_0^1 dx' \frac{x'|x+x'|}{x^2} \left[(x-x')^2 K\left(\frac{2\sqrt{xx'}}{x+x'} \right) + \left(2x^2 - x'^2\right) E\left(\frac{2\sqrt{xx'}}{x+x'} \right) \right] . \end{aligned} \tag{3.3.63}$$

Now we write the isotropic part in a similar way, again keeping in mind, that we need the k' factor from the Jacobian as

$$\mathrm{Int}_{\mathrm{iso}} = \frac{2}{3} K \mathbf{p}_1 \cdot \mathbf{p}_2 P_2(\cos(\alpha_0)) k_F^3 I_{2\mathrm{D}}^{\mathrm{iso}}\left(\frac{k}{k_F}\right) , \tag{3.3.64}$$

with the definition

$$I_{2\mathrm{D}}^{\mathrm{iso}}\left(\frac{k}{k_F}\right) = 12\pi \int_0^1 dx' x' \left|x - x'\right| E\left(\frac{2\sqrt{xx'}}{x+x'} \right) . \tag{3.3.65}$$

The whole energy can now be written as, remembering the factor $\frac{1}{(2\pi)^2}$ coming out of the Fourier transformation

$$\begin{aligned} \Sigma_{2\mathrm{D}}^{\mathrm{HF}}(\mathbf{k}) &= \frac{K \mathbf{p}_1 \cdot \mathbf{p}_2 m k_F}{3\pi^2\hbar^2} \frac{\hbar^2 k_F^2}{2m} \left\{ P_2(\cos(\alpha)) I_{2\mathrm{D}}^{\mathrm{iso}}\left(\frac{k}{k_F}\right) - \sin^2(\alpha) \cos(2\varphi_{\mathbf{k}}) I_{2\mathrm{D}}^{\mathrm{ani}}\left(\frac{k}{k_F}\right) \right\} \\ &= \lambda_{3D} E_{k_F} \left\{ P_2(\cos(\alpha)) I_{2\mathrm{D}}^{\mathrm{iso}}\left(\frac{k}{k_F}\right) - \sin^2(\alpha) \cos(2\varphi_{\mathbf{k}}) I_{2\mathrm{D}}^{\mathrm{ani}}\left(\frac{k}{k_F}\right) \right\} , \end{aligned} \tag{3.3.66}$$

with the notation of

$$\begin{aligned} \lambda_{3D} &:= \frac{K \mathbf{p}_1 \cdot \mathbf{p}_2 m k_F}{3\pi^2\hbar^2} \\ E_{k_F} &:= \frac{\hbar^2 k_F^2}{2m} . \end{aligned} \tag{3.3.67}$$

As we can see the Fermi surface in two-dimensions resembles a circle for the case $\alpha = 0$. This is a direct consequence of the isotropy of the system. If the dipoles are tilted towards the critical angle $\overline{\vartheta}$ the elongation along the k_x axies reaches the maximal value. In Figure 3.13 the functions $I_{2D}^{iso}(x)$ and $I_{2D}^{ani}(x)$ are shown, hence $P_2(\cos(\alpha))$ only runs in in intervall $\left[-\frac{\pi}{2}, 1\right]$, the main contribution to the self-energy comes from the isotropic part. As we have seen the scenarios of dipole-diople interaction are quite different in two and three dimensions. The anisotropy of the dipole-dipole interaction camouflages the main contribution a little, hence the anisotropy and the more divergent potential in two-dimensions contribute to the self-energy. Therefore we will look at the Coulomb interaction in the next chapter to estimate how strong the constraining to two-dimension affects the self-energy. Before we do so, we shall look at the dispersion in more detail.

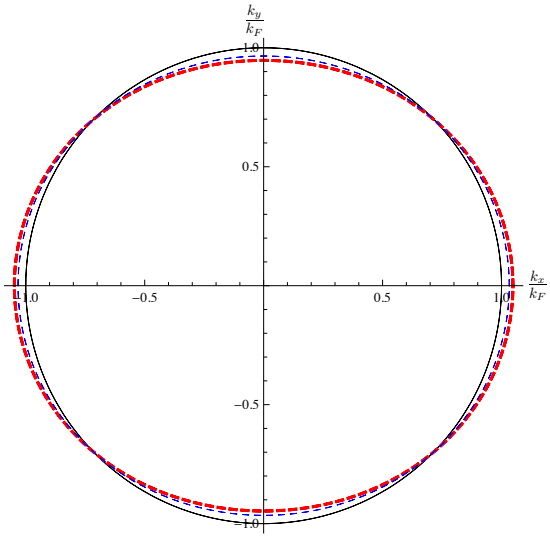
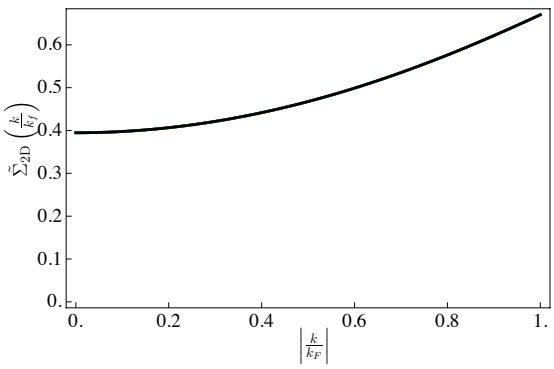
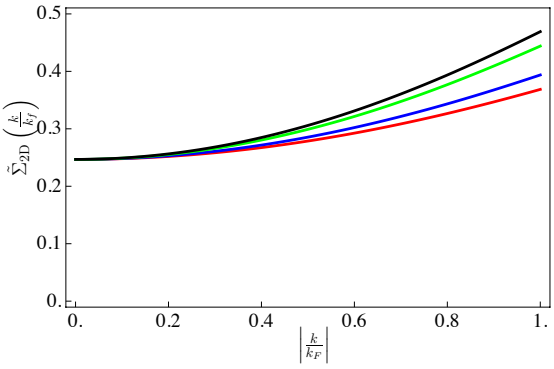


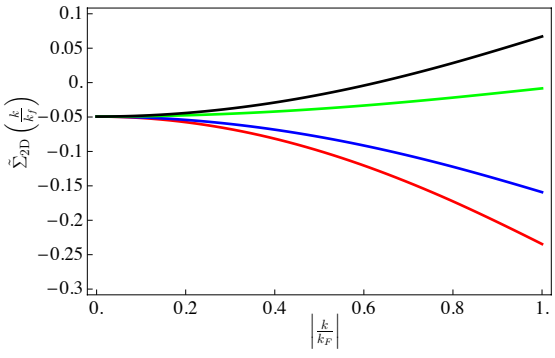
Figure 3.14: Deformed Fermi surfaces for the angles $\alpha = 0$ (black), $\alpha = \arccos\left(\frac{1}{\sqrt{3}}\right)$ (red) and the angle $\alpha = \frac{\pi}{2}$ (blue) for $lambda = 0.02$.



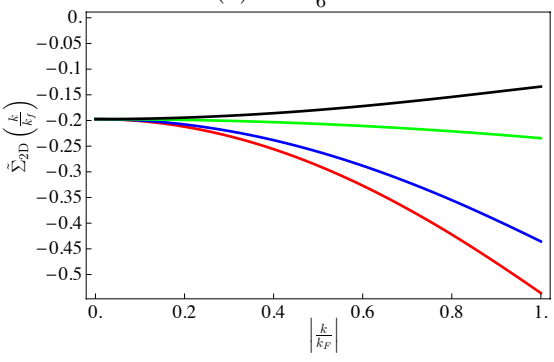
(a) $\alpha = 0$.



(b) $\alpha = \frac{\pi}{6}$.



(c) $\alpha = \frac{\pi}{3}$.



(d) $\alpha = \frac{\pi}{2}$

Figure 3.15: The self-energy for four different settings α of the dipole-dipole interaction. For each setting four different settings of $\varphi_{\mathbf{k}}$ 0 (red), $\frac{\pi}{6}$ (blue), $\frac{\pi}{3}$ (green), $\frac{\pi}{2}$ (black) are given. $\lambda = 0.02$.

In Figure 3.15 the self-energy is given for four dipole settings α. For each setting four different dispersion

directions $\varphi_{\mathbf{k}}$ are shown. In the first Figure 3.15a the configuration $\alpha = 0$ is shown. Since the dipole-dipole interaction (3.1.17) is isotropic in that case the dispersion is also the same for each value $\varphi_{\mathbf{k}}$. The next Figure 3.15b shows the dispersion relation for $\alpha = \frac{\pi}{6}$. Due to the anisotropy of the dipole-dipole interaction a splitting occurs depending on the propagation of the quasiparticle. The dipoles are restricted to the x-z plane, pointing in x-direction. As can be seen from the figure the propagation along the x-direction, that is $\varphi_{\mathbf{k}} = 0$ is lower than a propagation with a perpendicular component. The positive curvature indicates, that the dipole-dipole interaction is still repulsive and that the system is stable. The Figure 3.15c shows that once the critical angle is passed, the curvature of the dispersion relies on the angle $\varphi_{\mathbf{k}}$. This corresponds with our previous observations regarding the angle dependency (3.1.18) for the dipole-dipole interaction. For the angle $\alpha = \frac{\pi}{2}$ Figure 3.15d the change from a negative curvature to a positive one happens for greater $\varphi_{\mathbf{k}}$. This dependency also corresponds with our observations in Figure 3.6 .

3.3.3 For Coulomb interaction in Three-Dimensions

In order to get a better understanding of what happens when a three-dimensional system is restricted to a two-dimensional plane, we will also consider a Coulomb gas in three and two dimensions. At first we notice that for the Coulomb interaction the Hartree term is infinity. This is a well known problem for the Coulomb gas, which is normally bypassed by demanding the gas to be neutral of charge and adding a term of the form $\sum_{k_1,k_2} \frac{4\pi e^2}{k^2} \rho k \overline{\psi}_{k_1-k_2} \psi_k$, which neutralizes the Hartree term. This model is commonly referred to as Jellium model. We will therefore neglect the Hartree term as well. The Fourier transformation (3.2.39) yields to solve the integral

$$\begin{aligned} \int \frac{d^3k'}{(2\pi)^3} \frac{1}{|\mathbf{k}-\mathbf{k}'|^2} &= \int \frac{d^3k'}{(2\pi)^3} \frac{1}{k^2 + k'^2 - 2kk'\cos(\vartheta)} \\ &= \frac{1}{(2\pi)^2} \int_0^{k_F} dk' k'^2 \int_{-1}^{1} du \frac{1}{k^2 + k'^2 - 2kk'u} \,. \end{aligned} \tag{3.3.68}$$

We now first evaluate the u-integral, for this we make the substitutions $A := k^2 + k'^2$ and $B := 2kk'$ so we get

$$\int_{-1}^{1} \frac{du}{k^2 + k'^2 - 2kk'u} = -\frac{\log(k^2 + k'^2 - 2kk')}{2kk'} + \frac{\log(k^2 + k'^2 + 2kk')}{2kk'} \,. \tag{3.3.69}$$

Next we evaluate the integrals of the form

$$\pm \frac{1}{2k} \int_0^{k_F} dk' k' \log(k^2 + k'^2 \pm 2kk') \,, \tag{3.3.70}$$

so we will have a closer look at

$$\begin{aligned} \pm \int_0^{k_F} dk' k' \log(k^2 + k'^2 \pm 2kk') &= \pm \left[\frac{k'^2}{2} \log(k^2 + k'^2 \pm 2kk') \right]_0^{k_F} \\ &\quad \mp \int_0^{k_F} dk' \frac{k'^3}{k^2 + k'^2 \pm 2kk'} - k \int_0^{k_F} dk' \frac{k'^2}{k^2 + k'^2 \pm 2kk'} \,. \end{aligned} \tag{3.3.71}$$

Next we evaluate the two remaining integrals, we start with

$$\begin{aligned}\int_0^{k_F} dk' \frac{k'^3}{k^2+k'^2\pm 2kk'} &= \int_0^{k_F} dk' \frac{k'^3}{(k\pm k')^2} = \int_k^{k\pm k_F} d\alpha \frac{(\alpha-k)^3}{\alpha^2} \\ &= \left[\int_k^{k\pm k_F} d\alpha \frac{-k^3+3k^2\alpha-3k\alpha^2+\alpha^3}{\alpha^2}\right] \qquad (3.3.72)\\ &= \left[\mp\frac{k^2k_F}{k\pm k_F} \mp 2kk_F + \frac{k_F^2}{2} + 3k^2\log\left(\left|\frac{k\pm k_F}{k}\right|\right)\right], \qquad (3.3.73)\end{aligned}$$

and now we can do the integral

$$\begin{aligned}\int_0^{k_F} \frac{k'^2}{k^2+k'^2\pm 2kk'}dk' &= \int_0^{k_F} \frac{k'^2}{(k\pm k'^2)}dk' \\ &= \pm\int_k^{k\pm k_F} \frac{(\alpha-k)^2}{\alpha^2}d\alpha = \pm\int_k^{k\pm k_F} d\alpha\frac{\alpha^2+k^2-2\alpha k}{\alpha^2} \\ &= k_F + \frac{kk_F}{k\pm k_F} \mp 2k\log\left(\left|\frac{k\pm k_F}{k}\right|\right). \qquad (3.3.74)\end{aligned}$$

Now we can go back to our original integral with

$$\begin{aligned}\int_0^{k_F} k'\log\left(k^2+k'^2+2kk'\right) &= \frac{k_F^2}{2}\log\left(k^2+k_F^2+2kk_F^2\right) - \left[-\frac{k^2k_F}{k+k_F} - 2kk_F + \frac{k_F^2}{2} + 3k^2\log\left(\frac{k+k_F}{k}\right)\right] \\ &\quad - k\left[k_F + \frac{kk_F}{k+k_F} - 2k\log\left(\frac{k+k_F}{k}\right)\right] \\ &= \frac{k_F^2}{2}\log\left(k^2+k_F^2+2kk_F^2\right) + kk_F - \frac{k_F^2}{2} - k^2\log\left(\frac{k+k_F}{k}\right), \qquad (3.3.75)\end{aligned}$$

and

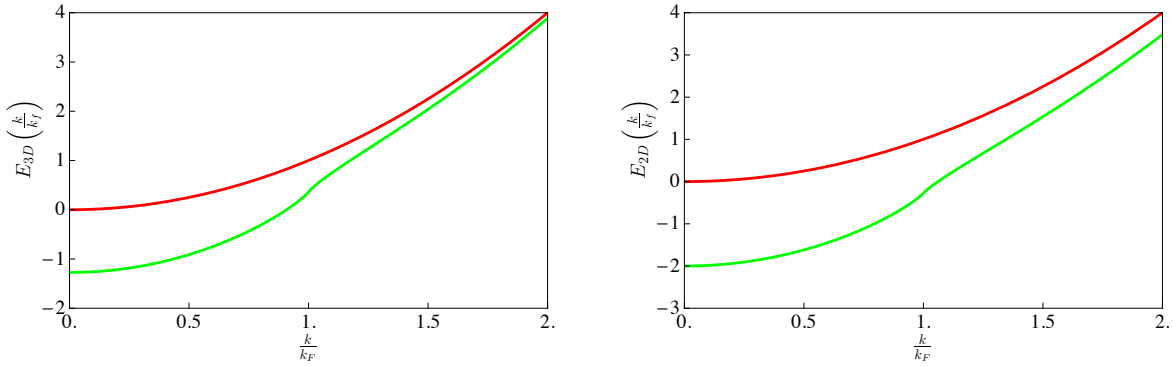
$$\begin{aligned}-\int_0^{k_F} \log\left(k^2+k'^2-2kk'\right) &= -\left[\frac{k_F^2}{2}\log\left(k^2+k_F^2-2kk_F\right)\right] + \left[\frac{k^2k_F}{k-k_F} + 2kk_F + \frac{k_F^2}{2} + 3k^2\log\left(\frac{k-k_F}{k}\right)\right] \\ &\quad - k\left[k_F + \frac{kk_F}{k-k_F} + 2k\log\left(\frac{k-k_F}{k}\right)\right] \\ &= \frac{-k_F^2}{2}\log\left(k^2+k_F^2-2kk_F\right) + kk_F + \frac{k_F^2}{2} + k^2\log\left(\left|\frac{k-k_F}{k}\right|\right). \qquad (3.3.76)\end{aligned}$$

We keep in mind, that we need the factor $\frac{1}{2k}$, so this yields to

$$\begin{aligned}\int \frac{d^3k'}{(2\pi)^3}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2} &= \frac{1}{(2\pi)^2}\left(\left[\frac{k_F^2}{4k}\log\left(k^2+k_F^2+2kk_F^2\right) + \frac{k_F}{2} - \frac{k_F^2}{4k} - \frac{k}{2}\log\left(\left|\frac{k+k_F}{k}\right|\right)\right]\right. \\ &\quad \left.+\left[-\frac{k_F^2}{4k}\log\left(k^2+k_F^2-2kk_F\right) + \frac{k_F}{2} + \frac{k_F^2}{4k} + \frac{k}{2}\log\left(\left|\frac{k-k_F}{k}\right|\right)\right]\right) \\ &= \frac{k_F}{8\pi^2}\left[2 + \frac{k_F^2-k^2}{k_F\,k}\log\left(\left|\frac{k+k_F}{k-k_F}\right|\right)\right]. \qquad (3.3.77)\end{aligned}$$

Finally we derived

$$\int \frac{d^3k'}{(2\pi)^3}\frac{1}{|\mathbf{k}-\mathbf{k}'|^2} = \frac{k_F}{8\pi^2}\left[2 + \frac{k_F^2-k^2}{k_F\,k}\log\left(\left|\frac{k+k_F}{k-k_F}\right|\right)\right], \qquad (3.3.78)$$



(a) 3D. (b) 2D.

Figure 3.16: The dispersion relation in contrast to the free electron gas in three (left) and (two) dimensions

and we define the element as

$$I^{3D}_{Cou}(x) := \frac{1}{8\pi^2}\left[2 + \frac{1}{x}\left(1-x^2\right)\log\left(\left|\frac{x+1}{x-1}\right|\right)\right] . \tag{3.3.79}$$

The Hartree-Fock energy can then be written as

$$\Sigma_{HF}(k) := \frac{\hbar^2 k^2}{2m} - 8\pi K \frac{e^2}{2a_0} I^{3D}_{Cou}\left(\frac{k}{k_F}\right) . \tag{3.3.80}$$

For the electron gas it is customary [55] to introduce the electron density ρ_0 as

$$\frac{1}{\rho_0} = \frac{4\pi}{3} a_0 r_s^3 , \tag{3.3.81}$$

where $a_0 = \frac{1}{K}\frac{\hbar^2}{me^2}$ is the Bohr radius and r_s is a dimensionless parameter. One can see from (3.3.81) that $r_s a_0$ defines the radius of a sphere which on average includes one electron or particle. The Fermi wave vector can now be expressed via the electron density as

$$k_F = \left(3\pi^2 \rho_0\right)^{\frac{1}{3}} . \tag{3.3.82}$$

Suitable units to describe the electron gas are then

$$\frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2ma_0^2}\left(\frac{k}{k_F}\right)^2 \left(\frac{1.92}{r_s}\right)^{\frac{1}{3}}, \quad e^2 k_F = \left(\frac{1.92}{r_s}\right)\frac{e^2}{a_0} \quad \text{with} \quad \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \approx 1.92 , \tag{3.3.83}$$

and since $\frac{\hbar^2}{2ma_0^2} = K\frac{e^2}{2a_0}$, we can Plot (3.3.80) in units of $\frac{\hbar^2}{2ma_0^2}$.

3.3.4 For Coulomb interaction in Two Dimensions

The integral is now very similar to the dipole case, so we keep the integration here short. We start with

$$\begin{aligned}
\int_0^{2\pi} d\varphi_{k'} \frac{1}{|\mathbf{k}-\mathbf{k}'|} &= \int_{-\varphi_k}^{2\pi-\varphi_k} d\alpha \frac{1}{\sqrt{k^2+k'^2-2kk'\cos(\alpha)}} \\
&= \int_0^{2\pi} d\alpha \frac{1}{\sqrt{(k+k')^2 - 4kk'\cos^2\left(\frac{\alpha}{2}\right)}} = \frac{4}{|k+k'|}\int_0^{\frac{\pi}{2}} d\beta \frac{1}{\sqrt{1-\frac{4kk'}{(k+k')^2}\sin^2(\beta)}} \\
&= \frac{4}{|k+k'|} K\left(\frac{2\sqrt{kk'}}{|k+k'|}\right) .
\end{aligned} \tag{3.3.84}$$

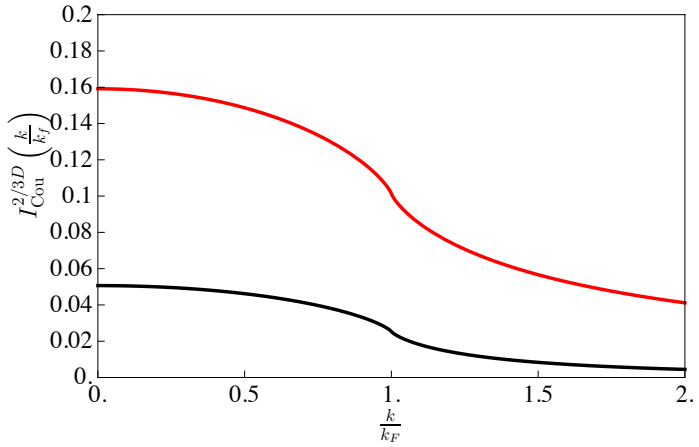


Figure 3.17: The correction function to the free electron interaction in Hartree-Fock approximation in two dimensions.

Where K is the elliptic integral (3.3.44) Now we will rewrite the k' integral as follows:

$$\begin{aligned}\int \frac{d^2k'}{(2\pi)^2}\frac{1}{|\mathbf{k}-\mathbf{k}'|} &= \frac{1}{(2\pi)^2}\int_0^{k_F} dk'\,k'\frac{4}{|k+k'|}K\left(\frac{2\sqrt{kk'}}{|k+k'|}\right)\\ &= \frac{1}{(2\pi)^2}k_F^2\int_0^1 dx'\,x'\frac{4}{k_F|x+x'|}K\left(\frac{2x\sqrt{xx'}}{x|x+x'|}\right)\\ &= \frac{k_F}{\pi^2}\int_0^1 dx'\,x'\frac{1}{|x+x'|}K\left(\frac{2\sqrt{xx'}}{|x+x'|}\right)\ . \end{aligned} \tag{3.3.85}$$

Finally we define

$$I^{(2D)}_{Cou}(x) := \frac{1}{\pi^2}\int_0^1 x'dx'\,\frac{1}{|x+x'|}K\left(\frac{2\sqrt{xx'}}{|x+x'|}\right)\ . \tag{3.3.86}$$

and we can write the Hartree-Fock energy in two dimensions as

$$\Sigma^{2D}_{Cou}(k) = \frac{\hbar^2k^2}{2m} - 4\pi K\frac{e^2}{2a_0}I^{(2D)}_{Cou}\left(\frac{k}{k_F}\right)\ . \tag{3.3.87}$$

As we can see from Figure 3.16 the difference of the self-energy in dependence of the dispersion $\frac{k}{k_F}$ is almost twice as big as the self-energy for the three-dimensional case. In contrast to the dipole-dipole interaction the Coulomb interaction is one power of r less divergent and yet the difference between two and three dimensions is significant. These observation together with the difference between the isotropic and anisotropic contributions in (3.3.66) let us conclude that the main contributions for the self-energy comes from the long range character of the dipole-dipole interaction.

Chapter 4

Two-Dimensional Fermi Gas with Dipolar Interaction within a Harmonic Trap

Until now we have considered a homogeneous systems without any external trapping potential. In any experiment of ultracold system the atoms must be trapped. For a two-dimensional system this can for example be done with a reflecting laser beam forming a standing wave and therefore forming a so called pancake trap. In reality the system is then quasi two-dimensional. That is the third dimension is highly surepressd. We will take the electronic or optical trap in the Hamiltonian in the following form

$$V^{(\mathrm{trap})}(\mathbf{x}) = \frac{m\omega^2}{2}\left(x^2+y^2\right) \ . \tag{4.0.1}$$

The H_0 Hamiltonian now reads

$$H_0 = -\frac{\hbar^2}{2m}\nabla^2 + V^{(\mathrm{trap})}(\mathbf{x}) \ . \tag{4.0.2}$$

Since this is the known one-particle Hamiltonian for the harmonic oscillator, we can give the eigenfunctions as

$$\psi_{\mathbf{n}}(\mathbf{x}) = \prod_{i=1}^{2} e^{-\frac{m\omega_i x_i^2}{2\hbar}} \frac{1}{\sqrt{2^{n_i} n_i!}} \left(\frac{m\omega_i}{\pi\hbar}\right)^{\frac{1}{4}} H_{n_i}\left(\sqrt{\frac{m\omega_i}{\hbar}}x_i\right) \ . \tag{4.0.3}$$

To calculate the self-energy according to the theory outlined above one has to evaluate the self-energy matrix in the eigenfunctions of H_0. Therefore one has to calculate (2.4.17) with the following matrix elements

$$\begin{aligned}
\langle \alpha\,\gamma|\, V^{(\mathrm{int})}\, |\delta\,\gamma\rangle &= \int d^2\mathbf{r}' d^2\mathbf{r}'' \left\langle \alpha\,\gamma|\mathbf{r}'\,\mathbf{r}''\right\rangle V^{(\mathrm{int})} \left\langle \mathbf{r}'\mathbf{r}''|\delta\,\gamma\right\rangle \\
&= \int d^2\mathbf{r}' d^2\mathbf{r}'' \overline{\psi}_\alpha(\mathbf{r}')\overline{\psi}_\gamma(\mathbf{r}'')V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\psi_\delta(\mathbf{r}')\psi_\gamma(\mathbf{r}'') \\
\langle \alpha\,\gamma|\, V^{(\mathrm{int})}\, |\gamma\,\delta\rangle &= \int d^2\mathbf{r}' d^2\mathbf{r}'' \left\langle \alpha\,\gamma|\mathbf{r}'\,\mathbf{r}''\right\rangle V^{(\mathrm{int})} \left\langle \mathbf{r}'\mathbf{r}''|\gamma\,\delta\right\rangle \\
&= \int d^2\mathbf{r}' d^2\mathbf{r}'' \overline{\psi}_\alpha(\mathbf{r}')\overline{\psi}_\gamma(\mathbf{r}'')V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\psi_\gamma(\mathbf{r}')\psi_\delta(\mathbf{r}'') \ ,
\end{aligned} \tag{4.0.4}$$

and then diagonalize the whole Hamiltonian with respect to the quantum numbers. This approach however is to cumbersome dealing with fermions, where we have to take the n_γ sum only up to the Fermi edge. In order to proceed we will therefore calculate the self-energy matrix in position space. The self-energy matrix given by the Fourier transformation of the relative coordinates and the center of mass is a quantity frequently used in the field of ultracold quantum gases [29, 56]. We will calculate the Hartree and Fock self-energy

$\Sigma(\mathbf{k},\mathbf{R})$ systematically within leading orders of the particle number N as well as within the semiclassical approximation often used in the field of ultracold quantum gases. The semiclassical approximation is well established approximation in this field, however the combination of the strong dipole-dipole interactions combined with the restriction to two-dimensions motivates us to investigate the self-energy as the simplest quantity possible to compare both approaches.

4.1 Large N Approximation for the Hartree-Fock Self-Energy

We will start with evaluating the matrix elements of (2.4.17) in position space as follows

$$\begin{aligned}
\Sigma^{\mathrm{H}}_{\gamma}(\mathbf{r}_1\,\tau_1|\mathbf{r}_2\,\tau_2) &= \delta(\tau_1-\tau_2)\,\langle\mathbf{r}_1\,\gamma|\,V^{(\mathrm{int})}\,|\mathbf{r}_2\,\gamma\rangle \\
&= \delta(\tau_1-\tau_2)\int d^2\mathbf{r}'d^2\mathbf{r}''\,\langle\mathbf{r}_1\,\gamma|\mathbf{r}'\,\mathbf{r}''\rangle\,V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\,\langle\mathbf{r}'\,\mathbf{r}''|\mathbf{r}_2\,\gamma\rangle \\
&= \delta(\tau_1-\tau_2)\int d^2\mathbf{r}'d^2\mathbf{r}''\delta(\mathbf{r}_1-\mathbf{r}')\psi_\gamma(\mathbf{r}'')V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\delta(\mathbf{r}'-\mathbf{r}_2)\psi_\gamma(\mathbf{r}'') \\
&= \delta(\tau_1-\tau_2)\int d^2\mathbf{r}''\delta(\mathbf{r}_1-\mathbf{r}_2)\psi_\gamma(\mathbf{r}'')V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r}'')\psi_\gamma(\mathbf{r}'') \\
&= \delta(\tau_1-\tau_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\int d^2\mathbf{r}\psi_\gamma(\mathbf{r})V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r})\psi_\gamma(\mathbf{r}) \qquad (4.1.1)
\end{aligned}$$

$$\begin{aligned}
\Sigma^{\mathrm{F}}_{\gamma}(\mathbf{r}_1\,\tau_1|\mathbf{r}_2\,\tau_2) &= -\delta(\tau_1-\tau_2)\,\langle\mathbf{r}_1\,\gamma|\,V^{(\mathrm{int})}\,|\gamma\,\mathbf{r}_2\rangle \\
&= -\delta(\tau_1-\tau_2)\int d^2\mathbf{r}'d^2\mathbf{r}''\,\langle\mathbf{r}_1\,\gamma|\mathbf{r}'\,\mathbf{r}''\rangle\,V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\,\langle\mathbf{r}'\,\mathbf{r}''|\gamma\,\mathbf{r}_2\rangle \\
&= -\delta(\tau_1-\tau_2)\int d^2\mathbf{r}'d^2\mathbf{r}''\delta(\mathbf{r}_1-\mathbf{r}')\overline{\psi}_\gamma(\mathbf{r}'')V^{(\mathrm{int})}(\mathbf{r}'-\mathbf{r}'')\psi_\gamma(\mathbf{r}')\delta(\mathbf{r}''-\mathbf{r}_2) \\
&= -\delta(\tau_1-\tau_2)\overline{\psi}_\gamma(\mathbf{r}_2)V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r}_2)\psi_\gamma(\mathbf{r}_1)\,. \qquad (4.1.2)
\end{aligned}$$

Since the Green functions are all evaluated at the same vertex, we can integrate out the imaginary time by using the Fourier transformation. Here ω_m are the antiperiodic Matsubara frequencies. The Fourier transformation then reads

$$\Sigma(\mathbf{k},\omega_m,\mathbf{R}) := \int_0^{\hbar\beta} d(\tau_1-\tau_2)e^{i\omega_m(\tau_1-\tau_2)}\Sigma(\mathbf{k},\mathbf{R},\tau_1-\tau_2)\,, \qquad (4.1.3)$$

and can immediately be executed for the Hartree and Fock term. Next we will perform the Fourier transformation for the relative coordinates of the Fock term. For the Hartree term, we will just need to perform the Fourier transformation of the relative coordinate. Before we proceed we introduce the relative and the center of mass coordinate

$$\begin{aligned}
\mathbf{r}_r &:= \mathbf{r}_1-\mathbf{r}_2 \qquad & \mathbf{r}_1 &= \frac{\mathbf{r}_1+\mathbf{r}_2}{2}+\frac{\mathbf{r}_1-\mathbf{r}_2}{2} = \mathbf{R}+\frac{\mathbf{r}_r}{2}\,, \\
\mathbf{R} &= \frac{\mathbf{r}_1+\mathbf{r}_2}{2} \qquad & \mathbf{r}_2 &= \frac{\mathbf{r}_1+\mathbf{r}_2}{2}-\frac{\mathbf{r}_1-\mathbf{r}_2}{2} = \mathbf{R}-\frac{\mathbf{r}_r}{2}\,. \qquad (4.1.4)
\end{aligned}$$

For the Hartree and Fock matrices (4.1.1), (4.1.2) this yields

$$\begin{aligned}
\Sigma^{\mathrm{H}}(\mathbf{k},\mathbf{R}) &= \int d^2\mathbf{r}\,\psi_\gamma\left(\mathbf{R}-\mathbf{r}\right)V^{(\mathrm{int})}(\mathbf{r})\psi_\gamma(\mathbf{R}-\mathbf{r}), \\
\Sigma^{\mathrm{F}}(\mathbf{k},\mathbf{R}) &= -\int d^2\mathbf{r}\,\psi_\gamma\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right)V^{(\mathrm{int})}(\mathbf{r})\psi_\gamma\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)e^{-i\mathbf{k}\mathbf{r}}\,. \qquad (4.1.5)
\end{aligned}$$

With these two matrix elements, we arrive at the following formula for the self-energy in the center of mass and relative momentum representation

$$\Sigma\left(\mathbf{k},\mathbf{R}\right)=\sum_{\gamma}\int d^{2}\mathbf{r}V^{(\mathrm{int})}(\mathbf{r})\left[\psi_{\gamma}\left(\mathbf{R}-\mathbf{r}\right)\psi_{\gamma}(\mathbf{R}-\mathbf{r})-\psi_{\gamma}\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right)\psi_{\gamma}\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)e^{-i\mathbf{kr}}\right]n_{\gamma}\,. \tag{4.1.6}$$

Since the dipole-dipole interaction is highly divergent at the point $r=0$, we will have to find a way to control the divergence. In order to do so we will add a zero in the following form

$$\Sigma\left(\mathbf{k},\mathbf{R}\right)=\sum_{\gamma}\int d^{2}\mathbf{r}V^{(\mathrm{int})}(\mathbf{r})\left\{(\psi_{\gamma}(\mathbf{R}-\mathbf{r})\psi_{\gamma}(\mathbf{R}-\mathbf{r})-f(\mathbf{R},\mathbf{r})]-\left[\psi_{\gamma}\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right)\psi_{\gamma}\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)e^{-i\mathbf{kr}}-f(\mathbf{R},\mathbf{r})\right]\right\}n_{\gamma}\,. \tag{4.1.7}$$

The above introduced function $f(\mathbf{R},\mathbf{r})$ has yet to be determined. Roughly speaking the function $f(\mathbf{R},\mathbf{r})$ has to be chosen in such a way that it cancels the probability density $\psi_{\gamma}(\mathbf{R}-\mathbf{r})\psi_{\gamma}(\mathbf{R}-\mathbf{r})$ and $\psi_{\gamma}\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right)\psi_{\gamma}\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)$ in the limit $\mathbf{r}\to\mathbf{0}$, respectively. In order to make the notation more clear, we will write the new Hartree and Fock contributions to the self-energy as

$$\begin{aligned}\Sigma^{\mathrm{H}\prime}(\mathbf{k},\mathbf{R})&:=\sum_{\gamma}\int d^{2}\mathbf{r}V^{(\mathrm{int})}(\mathbf{r})\left[\psi_{\gamma}\left(\mathbf{R}-\mathbf{r}\right)\psi_{\gamma}(\mathbf{R}-\mathbf{r})-f(\mathbf{R},\mathbf{r})\right]n_{\gamma}\,,\\ \Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R})&:=-\sum_{\gamma}\int d^{2}\mathbf{r}\,V^{(\mathrm{int})}(\mathbf{r})\left[\psi_{\gamma}\left(\mathbf{R}-\frac{\mathbf{r}}{2}\right)\psi_{\gamma}\left(\mathbf{R}+\frac{\mathbf{r}}{2}\right)e^{-i\mathbf{kr}}-f(\mathbf{R},\mathbf{r})\right]n_{\gamma}\,.\end{aligned} \tag{4.1.8}$$

Next we approximate the wave functions with the help of the Stirling approximation [57] for Hermite polynomes

$$\begin{aligned}\psi_{n}(x)&=\frac{1}{\sqrt{2^{n}n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}e^{-\frac{m\omega}{2\hbar}x^{2}}H_{n}\left(\sqrt{\frac{m\omega}{\hbar}}x\right)\\ &\approx\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^{n}n!}}\left(\frac{2n}{e}\right)^{\frac{n}{2}}\sqrt{2}\cos\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}x-n\frac{\pi}{2}\right)\left(1-\frac{\frac{m\omega}{\hbar}x^{2}}{2n}\right)^{-\frac{1}{4}}\,,\end{aligned} \tag{4.1.9}$$

which is valid for large quantum numbers n, that is high energies $E_{n}=\hbar\omega\left(n+\frac{1}{2}\right)$. In the following we will use in various expressions that the oscillating part of the wave function can be neglected for high energy levels when integrating over the position. We will demonstrate this approximation exemplarily within the evaluation of the normalization constant of $\psi_{n}(x)$.

$$\begin{aligned}\int dx\,|\psi_{n}(x)|^{2}&=\int_{-\sqrt{\frac{2\hbar n}{m\omega}}}^{\sqrt{\frac{2\hbar n}{m\omega}}}dx\,\overline{N}^{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\frac{1}{2^{n}n!}\left(\frac{2n}{e}\right)^{n}2\left(\frac{2n}{2n-\frac{m\omega}{\hbar}x^{2}}\right)^{\frac{1}{2}}\cos^{2}\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}x-n\frac{\pi}{2}\right)\\ &=\int_{-\sqrt{\frac{2\hbar n}{m\omega}}}^{\sqrt{\frac{2\hbar n}{m\omega}}}dx\,\overline{N}^{2}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}}\frac{1}{2^{n}n!}\left(\frac{2n}{e}\right)^{n}2\left(\frac{2n}{2n-\frac{m\omega}{\hbar}x^{2}}\right)^{\frac{1}{2}}\left[\frac{1}{2}+\frac{1}{2}\cos\left(2\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}x-n\pi\right)\right]\,.\end{aligned} \tag{4.1.10}$$

By using

$$\int_{-\sqrt{2n}}^{\sqrt{2n}}dx\sqrt{\frac{2n}{2n-x^{2}}}=\sqrt{2n}\int_{-1}^{1}dx\frac{1}{\sqrt{1-x^{2}}}\,, \tag{4.1.11}$$

and

$$\int_{-\sqrt{2n}}^{\sqrt{2n}}dx\sqrt{\frac{2n}{2n-x^{2}}}\cos\left(\sqrt{2n}x-n\frac{\pi}{2}\right)=\cos\left(n\pi\right)\sqrt{2n}\int_{-1}^{1}dx\,\frac{1}{\sqrt{1-x^{2}}}\cos\left(4nx\right)\,. \tag{4.1.12}$$

we obtain for large n that the cos integrand is highly oscillating compared to the smooth root function on the interval $[-1,1]$, so we can neglect it. The non oscillating part of the integral (4.1.10) can easily be performed and we get

$$\int_{-\sqrt{\frac{2\hbar n}{m\omega}}}^{\sqrt{\frac{2\hbar n}{m\omega}}} dx \left(\frac{2n}{2n-\frac{m\omega}{\hbar}x^2}\right)^{\frac{1}{2}} = \int_{-\sqrt{\frac{2\hbar n}{m\omega}}}^{\sqrt{\frac{2\hbar n}{m\omega}}} dx \frac{1}{\sqrt{1-\frac{m\omega}{2n\hbar}x^2}} = \sqrt{\frac{2n\hbar}{m\omega}}\int_{-1}^{1} du \frac{1}{\sqrt{1-u^2}} = \sqrt{\frac{2n\hbar}{m\omega}}\pi \,.$$

The N factor is then given by

$$\overline{N} = \sqrt{\frac{e^n n!}{\sqrt{2\pi} n^{n+\frac{1}{2}}}} \,. \tag{4.1.13}$$

With this, we arrive at the normalized wave function that we are going to use

$$\psi_n(x) = D\frac{1}{(2n-\frac{m\omega}{\hbar}x^2)^{\frac{1}{4}}}\cos\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}x - n\frac{\pi}{2}\right) \qquad \text{with} \qquad D := \left(\frac{4\,m\omega}{\pi^2\hbar}\right)^{\frac{1}{4}} \,. \tag{4.1.14}$$

These eigenfunction approximations (4.1.14) maybe recognized as the WKB wave functions of the harmonic oscillator. The wave functions certainly only consider the probability density within the harmonic trap. Naturally there exists a probability density outside of the harmonic potential which decays exponentially. Here these regions are neglected and set to zero. Note that this neglection as well as the neglection of the oscillatory terms in the wave function used further below is exact when we are interested in the leading $N \to \infty$ behaviour likewise for of the self-energy and particle number. This is mainly based on the fact, that in leading order $N \to \infty$ both quantities are diverging meaning, that in the n_γ sum (4.1.8) large quantum numbers n are most important.

4.1.1 Derivation of the Hartree Self-Energy for Large Particle Numbers

Now we will rewrite the Hartree term in two dimensions first ignoring the artificial subtraction term. Before we do so, we will use the Poisson sum formula [39], which justifies for $N \to \infty$ that the summation over the quantum numbers n can be converted to an integral.

$$\sum_{n=-\infty}^{\infty} f(m) = \sum_{\ell=-\infty}^{\infty}\int_{-\infty}^{\infty} dz f(z) e^{2\pi i \ell z} \,. \tag{4.1.15}$$

In our case this yields

$$\sum_{n=\frac{m\omega}{2\hbar}x^2}^{n_F} \frac{1}{\sqrt{2n-\frac{m\omega}{\hbar}x^2}} = \sum_{\ell=0}^{\infty}\int_{\frac{m\omega}{2\hbar}x^2}^{n_F} dz \frac{1}{\sqrt{2z-\frac{m\omega}{\hbar}x^2}} e^{i2\pi\ell z} \,. \tag{4.1.16}$$

Here we have used that the wave function is considered zero outside of the trap. Now as long as the function f in (4.1.15) does not vary much over the interval 2π, the Fourier coefficient on the right hand side will oscillate heavily and the only contribution to the sum comes from the $\ell = 0$ term. Therefore it is safe to

substitute the sum with the integral. We will put this now into action in the first part of the Hartree term.

$$\begin{aligned}
\Sigma^{\mathrm{H}}(\mathbf{k},\mathbf{R}) &= \sum_{\gamma\gamma'\leq n_F} \int dx\, dy\, V^{(\mathrm{int})}(x,y)\psi_\gamma(X-x)\psi_\gamma(X-x)\psi_{\gamma'}(Y-y)\psi_{\gamma'}(Y-y) \\
&= \frac{D^4}{2}\int_{\frac{\kappa}{2}(X-x)^2}^{n_F-\frac{\kappa}{2}(Y-y)^2} dn_1 \int_{\frac{\kappa}{2}(Y-y)^2}^{n_F-n_1} dn_2 \int dx \int dy\, V^{(\mathrm{int})}(x,y)\frac{1}{\sqrt{n_1-\frac{\kappa}{2}(X-x)^2}}\frac{1}{\sqrt{n_2-\frac{\kappa}{2}(Y-y)^2}} \\
&\qquad \times \cos^2\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n_1}\,(X-x)-n_1\frac{\pi}{2}\right)\cos^2\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n_2}\,(Y-y)-n_2\frac{\pi}{2}\right) \\
&\approx \frac{1}{4}\frac{D^4}{2}\int_{\frac{\kappa}{2}(X-x)^2}^{n_F-\frac{\kappa}{2}(Y-y)^2} dn_1 \int_{\frac{\kappa}{2}(Y-y)^2}^{n_F-n_1} dn_2 \int dx \int dy\, V^{(\mathrm{int})}(x,y)\frac{1}{\sqrt{n_1-\frac{\kappa}{2}(X-x)^2}}\frac{1}{\sqrt{n_2-\frac{\kappa}{2}(Y-y)^2}} \\
&= \frac{1}{4}D^4\int dx\int dy\int_{\frac{\kappa}{2}(X-x)^2}^{n_F-\frac{\kappa}{2}(Y-y)^2} dn_1 V^{(\mathrm{int})}(x,y)\frac{1}{\sqrt{n_1-\frac{\kappa}{2}(X-x)^2}}\int_{\frac{\kappa}{2}(Y-y)^2}^{n_F-n_1} dn_2\frac{1}{\sqrt{n_2-\frac{\kappa}{2}(Y-y)^2}} \\
&= \frac{1}{4}D^4\int dx\int dy\int_{\frac{\kappa}{2}(X-x)^2}^{n_F-\frac{\kappa}{2}(Y-y)^2} dn_1 V^{(\mathrm{int})}(x,y)\frac{\sqrt{(n_F-n_1)-\frac{\kappa}{2}(Y-y)^2}}{\sqrt{n_1-\frac{\kappa}{2}(X-x)^2}}\,. \qquad (4.1.17)
\end{aligned}$$

Where we have used the following canonical definition

$$\kappa = \frac{m\omega}{\hbar}\,, \qquad (4.1.18)$$

and wrote n_1 and n_2 for the quantum numbers γ. Next we will calculate the n_1 integral, which can also be done analytically

$$\begin{aligned}
\int_{\frac{\kappa}{2}(Y-y)^2}^{n_F-\frac{\kappa}{2}(X-x)^2} dn_1\sqrt{\frac{(n_F-n_1)-\frac{\kappa}{2}(Y-y)^2}{n_1-\frac{\kappa}{2}(X-x)^2}} &= \int_{\frac{\kappa}{2}(Y-y)^2}^{n_F-\frac{\kappa}{2}(X-x)^2} dn_1\sqrt{\frac{n_F\left[(1-\frac{n_1}{n_F})-\frac{\kappa}{2n_F}(Y-y)^2\right]}{n_F(\frac{n_1}{n_F}-\frac{\kappa}{2n_F}(X-x)^2)}} \\
&= n_F\int_{\frac{\kappa}{2n_F}(Y-y)^2}^{1-\frac{\kappa}{2n_F}(X-x)^2} du\sqrt{\frac{(1-u)-\frac{1}{2n_F}(Y-y)^2}{u-\frac{1}{2n_F}(X-x)^2}}\,. \qquad (4.1.19)
\end{aligned}$$

For $\frac{1}{2n_F}(Y-y)^2+\frac{1}{2n_F}(X-x)^2<1$ then follows

$$\begin{aligned}
\int_{\frac{1}{2n_F}(Y-y)^2}^{1-\frac{1}{2n_F}(X-x)^2} du\sqrt{\frac{(1-u)-\frac{1}{2n_F}(X-x)^2}{u-\frac{1}{2n_F}(Y-y)^2}} &= \arctan(0)-\left(\frac{1}{2n_F}(X-x)^2+\frac{1}{2n_F}(Y-y)^2-1\right)\underbrace{\arctan(\infty)}_{=\frac{\pi}{2}} \\
&= -\frac{\pi}{2}\left[\frac{\kappa}{2n_F}(Y-y)^2+\frac{\kappa}{2n_F}(X-x)^2-1\right]\,. \qquad (4.1.20)
\end{aligned}$$

Here we have executed the n integrals first. However, since we can exchange the order of integration, the previous argument about the x integration still holds and we can neglect the oscillating part. In order to proceed we will now need to look at the subtracting factor $f(\mathbf{R},\mathbf{k})$, (4.1.8) as well. To make the calculation more clear, we will at first focus on the first part (3.1.12) of the dipole-dipole interaction. The restriction of the WKB wave function to the interior of the harmonic trap gives the following integration region for the x,y-integration in (4.1.17)

$$\frac{m\omega}{\hbar}(X-x)^2+\frac{m\omega}{\hbar}(Y-y)^2\leq 2n_F\,. \qquad (4.1.21)$$

To fulfill it, we will switch to polar coordinates. We now proceed with introducing

$$\left.\begin{array}{ll}\eta = (X-x) & \\ \xi = (Y-y) & \end{array}\right. \quad \text{and} \quad \left.\begin{array}{ll}\eta = r\cos(\varphi) & \\ \xi = r\sin(\varphi) & \end{array}\right\} \Longrightarrow (X-\eta)^2 + (Y-\xi)^2 = R^2 + r^2 - 2r[X\cos(\varphi) + Y\sin(\varphi)] \, .$$

Here we have written $R = \sqrt{X^2+Y^2}$. As we can see from (4.1.17) with (4.1.20) the Hartree integral without the subtraction term is still divergent at the point $r = 0$. In order to get rid of this divergence we will now choose the function $f(\mathbf{R}, \mathbf{r})$ as

$$f(\mathbf{R}, \mathbf{r}) := \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \cos\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n_1}\,(X-x) - n_1\frac{\pi}{2}\right) \cos\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n_2}\,(Y-y) - n_2\frac{\pi}{2}\right) . \tag{4.1.22}$$

Then we can do the same approximation within the n_1 and n_2 integrals as before and obtain for the modified Hartree self-energy, were the integration boundary (4.1.21) is denoted by circle

$$\begin{aligned}
&\Sigma^{\mathrm{H}\prime(1)}(\mathbf{k}, \mathbf{R}) = \\
&\quad - \frac{KD^4 n_F \pi}{8} \mathbf{p}_1 \cdot \mathbf{p}_2 \left\{ \int_{\text{circle}} dxdy \frac{1}{(x^2+y^2)^{\frac{3}{2}}} \left[\zeta(X-x)^2 + \zeta(Y-y)^2 - 1\right] \right. \\
&\qquad\qquad \left. - \int_V dxdy \frac{1}{(x^2+y^2)^{\frac{3}{2}}} \left[\zeta X^2 + \zeta Y^2 - 1\right] \right\} \\
&\quad = -\frac{\pi K D^4 n_F \mathbf{p}_1 \cdot \mathbf{p}_2}{8} \left\{ \int_{\text{circle}} dxdy \frac{\left[\zeta(\eta^2+\xi^2) - 1\right]}{\left[(X-\eta)^2 + (Y-\xi)^2\right]^{\frac{3}{2}}} - \int_V dxdy \frac{\left[\zeta(X^2+Y^2) - 1\right]}{\left[(X-\eta)^2 + (Y-\xi)^2\right]^{\frac{3}{2}}} \right\} .
\end{aligned} \tag{4.1.23}$$

Here we have set $\zeta := \frac{\kappa}{2n_F}$ and V denotes the whole volume. Furthermore the (1) indicates that we are only dealing with the first part of the dipole-dipole interaction. By introducing a parametrization for X and Y in the form of

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \sqrt{X^2+Y^2} \begin{pmatrix} \cos(\vartheta) \\ \sin(\vartheta) \end{pmatrix} ,$$

we can further simplify the expression to

$$\begin{aligned}
\Sigma^{\mathrm{H}\prime(1)}(\mathbf{k}, \mathbf{R}) &= -\frac{KD^4 n_F \mathbf{p}_1 \cdot \mathbf{p}_2 \pi}{8} \left\{ \int_0^{\sqrt{\frac{2\hbar n_F}{m\omega}}} r dr \int_0^{2\pi} d\varphi \frac{\left(\zeta r^2 - 1\right)}{\left[R^2 + r^2 - 2Rr\cos(\varphi - \vartheta)\right]^{\frac{3}{2}}} \right. \\
&\qquad \left. - \int_0^{\infty} r dr \int_0^{2\pi} d\varphi \frac{\zeta R^2 - 1}{\left[R^2 + r^2 - 2Rr\cos(\varphi - \vartheta)\right]^{\frac{3}{2}}} \right\} \\
&= -\frac{KD^4 n_F \mathbf{p}_1 \cdot \mathbf{p}_2 \pi}{8} \left\{ \int_0^{\sqrt{\frac{2\hbar n_F}{m\omega}}} r dr \int_0^{2\pi} d\varphi \frac{\zeta(r^2 - R^2)}{\left[R^2 + r^2 - 2Rr\cos(\varphi - \vartheta)\right]^{\frac{3}{2}}} \right. \\
&\qquad \left. - \int_{\sqrt{\frac{2\hbar n_F}{m\omega}}}^{\infty} r dr \int_0^{2\pi} d\varphi \frac{\zeta R^2 - 1}{\left[R^2 + r^2 - 2Rr\cos(\varphi - \vartheta)\right]^{\frac{3}{2}}} \right\} .
\end{aligned} \tag{4.1.24}$$

In the final step the integrals have been rewritten in such a way, that the one on the left hand side is convergent at $r = R$ and the integral on the right hand side is then of course convergent on the interval $[2n_F, \infty]$.

The same procedure must now be done for the second part of the dipole-dipole interaction. Here we will restrict ourselves to the case, that the two dipoles are again parallel and restricted to the x-z plane (3.1.13). The contribution of the second part to $\Sigma^{\mathrm{H}\prime}$ yields

$$\Sigma^{\mathrm{H}\prime(2)}(\mathbf{k},\mathbf{R}) = \frac{3\pi K D^4 n_F p_1^2}{8}\left\{\int_0^{\sqrt{\frac{2\hbar n_F}{m\omega}}} rdr\int_0^{2\pi} d\varphi \frac{\zeta(X^2-2Xr\cos(\varphi)+r^2\cos^2(\varphi))(r^2-R^2)}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\right.$$
$$\left. -\int_{\sqrt{\frac{2\hbar n_F}{m\omega}}}^{\infty} rdr\int_0^{2\pi} d\varphi \frac{X^2-2Xr\cos(\varphi)+r^2\cos^2(\varphi)}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\left(\zeta R^2-1\right)\right\}. \tag{4.1.25}$$

We can now write the whole Hartree term as

$$\begin{aligned}\Sigma^{H\prime}(\mathbf{k},\mathbf{R}) = &\\ &-\frac{KD^4 n_F \mathbf{p}_1\cdot\mathbf{p}_2\pi}{8}\left\{\int_0^{\sqrt{\frac{2\hbar n_F}{m\omega}}} rdr\int_0^{2\pi} d\varphi\frac{\zeta(r^2-R^2)}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{3}{2}}}\right.\\ &\qquad\left.-\int_{\sqrt{\frac{2\hbar n_F}{m\omega}}}^{\infty} rdr\int_0^{2\pi} d\varphi\frac{\zeta R^2-1}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{3}{2}}}\right\}\\ &+\frac{3\pi K D^4 n_F p_1^2}{8}\left\{\int_0^{\sqrt{\frac{2\hbar n_F}{m\omega}}} rdr\int_0^{2\pi} d\varphi\frac{\zeta(X^2-2Xr\cos(\varphi)+r^2\cos^2(\varphi))(r^2-R^2)}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\right.\\ &\qquad\left.-\int_{\sqrt{\frac{2\hbar n_F}{m\omega}}}^{\infty} rdr\int_0^{2\pi} d\varphi\frac{X^2-2Xr\cos(\varphi)+r^2\cos^2(\varphi)}{[R^2+r^2-2Rr\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\left(\zeta R^2-1\right)\right\}.\end{aligned} \tag{4.1.26}$$

In order to calculate the Hartree contribution, these four integrals have to be solved. This can be done analytically, if the r-integration is executed first, however the result is extremely cumbersome. Below we shall show that the Fock self-energy is much larger than the Hartree self-energy for $N\to\infty$, which leads us to not show this analytical result and treat the rest numerically as it is mandatory in the Fock term. Finally to see the N dependence, we will rewrite the Hartree term with the relation

$$n_F = \sqrt{2N}\,, \tag{4.1.27}$$

where N is the particle number. The verification of (4.1.27) will be shown below, after we have derived both approximations. The final form of the Hertree self-energy now reads

$$\begin{aligned}\Sigma^{\mathrm{H}\prime}(\mathbf{k},\mathbf{R}) = &\\ &-\frac{1}{2^{\frac{5}{4}}\pi}K\mathbf{p}_1\cdot\mathbf{p}_2\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}N^{\frac{1}{4}}\left\{\int_0^1 rdr\int_0^{2\pi} d\varphi\frac{(r^2-\tilde{R}^2)}{[\tilde{R}^2+r^2-2\tilde{R}r\cos(\varphi-\vartheta)]^{\frac{3}{2}}}\right.\\ &\qquad\left.-\int_1^{\infty} rdr\int_0^{2\pi} d\varphi\frac{\tilde{R}^2-1}{[\tilde{R}^2+r^2-2\tilde{R}r\cos(\varphi-\vartheta)]^{\frac{3}{2}}}\right\}\\ &+\frac{3}{2^{\frac{5}{4}}\pi}Kp_1^2\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}N^{\frac{1}{4}}\left\{\int_0^1 rdr\int_0^{2\pi} d\varphi\frac{(\tilde{X}^2-2\tilde{X}r\cos(\varphi)+r^2\cos^2(\varphi))(r^2-\tilde{R}^2)}{[\tilde{R}^2+r^2-2\tilde{R}r\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\right.\\ &\qquad\left.-\int_1^{\infty} rdr\int_0^{2\pi} d\varphi\frac{\tilde{X}^2-2\tilde{X}r\cos(\varphi)+r^2\cos^2(\varphi)}{[\tilde{R}^2+r^2-2\tilde{R}r\cos(\varphi-\vartheta)]^{\frac{5}{2}}}\left(\tilde{R}^2-1\right)\right\}.\end{aligned} \tag{4.1.28}$$

where we have defined dimensionless quantities as follows.

$$\tilde{R} := \frac{R}{\sqrt{\frac{\hbar}{m\omega}} 2^{\frac{3}{4}} N^{\frac{1}{4}}} \qquad \text{and} \qquad \tilde{X} := \frac{X}{\sqrt{\frac{\hbar}{m\omega}} 2^{\frac{3}{4}} N^{\frac{1}{4}}} \,. \tag{4.1.29}$$

4.1.2 Derivation of the Fock Self-Energy for Large Particle Numbers

We will now look at the Fock term (4.1.8). Before we proceed, we will rewrite the appearing cosine terms in (4.1.8), and again introduce some short notations.

$$\begin{aligned}
&\cos\left(\underbrace{\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}}_{=:a_1}\left(X-\frac{x}{2}\right) - \underbrace{n\frac{\pi}{2}}_{=:b_1}\right)\cos\left(\sqrt{\frac{m\omega}{\hbar}}\sqrt{2n}\left(X+\frac{x}{2}\right) - n\frac{\pi}{2}\right) \\
&\quad =: \cos\left(a_1 X - a_1\frac{x}{2} - b_1\right)\cos\left(a_1 X + a_1\frac{x}{2} - b_1\right) \\
&\quad = \frac{1}{2}\cos(a_1 x) + \frac{1}{2}\cos(2a_1 X - 2b_1)
\end{aligned} \tag{4.1.30}$$

and similarly with a_2 and b_2. Now we multiply out

$$\begin{aligned}
&\frac{1}{4}\cos(a_1 x)\cos(a_2 y) + \frac{1}{4}\cos(a_1 x)\cos(2a_2 Y - 2b_2) + \frac{1}{4}\cos(2a_2 X - 2b_1)\cos(a_2 y) \\
&\qquad + \frac{1}{4}\cos(2a_1 X - 2b_1)\cos(2a_2 Y - 2b_2)\,,
\end{aligned} \tag{4.1.31}$$

and we are in position to rewrite the Fock term (4.1.34) as

$$\begin{aligned}
\Sigma^F(\mathbf{k},\mathbf{R}) &= D^4 \sum_{n_1 n_2} \int dx dy V^{(\mathrm{int})}(x,y) \\
&\times \Bigg\{ \frac{1}{(2n_1 - \kappa(X-\frac{x}{2})^2)^{\frac{1}{4}}} \frac{1}{(2n_1 - \kappa(X+\frac{x}{2})^2)^{\frac{1}{4}}} \frac{1}{(2n_2 - \kappa(Y-\frac{y}{2})^2)^{\frac{1}{4}}} \frac{1}{(2n_2 - \kappa(Y+\frac{y}{2})^2)^{\frac{1}{4}}} \\
&\quad \times \left(\frac{1}{2}\cos(a_1 x) + \frac{1}{2}\cos(2a_1 X - 2b_1)\right)\left(\frac{1}{2}\cos(a_2 y) + \frac{1}{2}\cos(2a_2 Y - 2b_2)\right) e^{-i(k_x x + k_y y)} \\
&\quad - \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \\
&\qquad \times \left(\frac{1}{2} + \frac{1}{2}\cos(2a_1(X-x) - 2b_1)\right)\left(\frac{1}{2} + \frac{1}{2}\cos(2a_2(Y-y) - 2b_2)\right) \Bigg\} \,.
\end{aligned} \tag{4.1.32}$$

For large quantum numbers we are again neglecting the oscillating parts of the integrals. However this time we cannot neglect the first term in (4.1.31) since this term exactly cuts the $r > 0$ divergence of the non-oscillating second term in (4.1.32). The other cosine terms in (4.1.31) can be neglected since they are again highly oscillating and will not contribute in leading order to the n-integral. For more details see Appendix A. The Fock term then reads

$$\begin{aligned}
\Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R}) &= \frac{1}{4} K D^4 \sum_{n_1 n_2} \int dx dy V^{(\mathrm{int})}(x,y) \Bigg\{ \frac{1}{(2n_1 - \kappa(X-\frac{x}{2})^2)^{\frac{1}{4}}} \frac{1}{(2n_1 - \kappa(X+\frac{x}{2})^2)^{\frac{1}{4}}} \\
&\quad \frac{1}{(2n_2 - \kappa(Y-\frac{y}{2})^2)^{\frac{1}{4}}} \frac{1}{(2n_2 - \kappa(Y+\frac{y}{2})^2)^{\frac{1}{4}}} \cos(a_1 x)\cos(a_2 y) e^{-i(k_x x + k_y y)} - \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \Bigg\} \,.
\end{aligned} \tag{4.1.33}$$

The main contribution to the integral for $N \to \infty$ comes from the integration region $\sqrt{r} \ll 1$, which leads us to the neglection of the $\mathbf{r}$-depndence of the prefactor of the first term in (4.1.33) and further on we can extend the integration region to the whole $x-y$ plane leading to

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R}) &\approx D^4 \sum_{n_1 n_2} \int dx \int dy V^{(\mathrm{int})}(x,y) \\ &\times \left\{ \frac{1}{4} \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \cos(a_1 x) \cos(a_2 y) e^{-i(k_x x + k_y y)} - \frac{1}{4} \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \right\} \\ &= \frac{1}{4} D^4 \sum_{n_1 n_2} \int dx \int dy V^{(\mathrm{int})}(x,y) \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \left[\cos(a_1 x) \cos(a_2 y) e^{-i(k_x x + k_y y)} - 1 \right] .\end{aligned} \tag{4.1.34}$$

Concentrating ourselves on the first part of the dipole-dipole interaction, we get

$$\begin{aligned}&\Sigma^{F\prime(1)}(\mathbf{k},\mathbf{R}) \\ &= K\, D^4 \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{4} \sum_{n_1 n_2} \int dx \int dy \frac{1}{(x^2+y^2)^{\frac{3}{2}}} \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \left[\cos(a_1 x) \cos(a_2 y) e^{-i(k_x x + k_y y)} - 1 \right] \\ &= K\, D^4 \frac{\mathbf{p}_1 \cdot \mathbf{p}_2}{4} \sum_{n_1 n_2} \int_0^{R_f} dr \int_0^{2\pi} d\varphi \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \\ &\quad \times \frac{1}{r^2} \left[\cos\left(a_1 r \cos(\varphi)\right) \cos\left(\cos(a_2 r \sin(\varphi)\right) e^{-i[k_x r \cos(\varphi) + k_y r \sin(\varphi)]} - 1 \right] .\end{aligned} \tag{4.1.35}$$

Together with the subtraction part the whole angle integration over φ is given by

$$\begin{aligned}&\int_0^{2\pi} d\varphi \left[\cos(a_1 r \cos(\varphi)) \cos(a_2 r \sin(\varphi)) e^{-i[k_x r \cos(\varphi) + k_y r \sin(\varphi)]} - 1 \right] \\ &= \frac{\pi}{2} \left[J_0\left(\sqrt{(a_1 - k_x)^2 + (a_2 - k_y)^2} r \right) - 1 + J_0\left(\sqrt{(a_1 - k_x)^2 + (a_2 + k_y)^2} r \right) - 1 \right. \\ &\qquad \left. + J_0\left(\sqrt{(a_1 + k_2)^2 + (a_2 - k_y)^2} r \right) - 1 + J_0\left(\sqrt{(a_1 + k_x)^2 + (a_2 + k_y)^2} r \right) - 1 \right] .\end{aligned} \tag{4.1.36}$$

We now rewrite a_1 and a_2 as $a_1 = \sqrt{\kappa}\sqrt{2n_1}$ $\;a_2 = \sqrt{\kappa}\sqrt{2n_2}$ and execute the r-integration after substituting out of the square roots, which leads to

$$\begin{aligned}\Sigma^{F\prime(1)}(\mathbf{k},\mathbf{R}) = K\, D^4 \sqrt{\kappa} \frac{\mathbf{p}_1 \cdot \mathbf{p}_2 \pi}{8} \sum_{n_1 n_2} \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \left[\sqrt{\left(\sqrt{2n_1} - \hat{k}_x\right)^2 + \left(\sqrt{2n_2} - \hat{k}_y\right)^2} \right. \\ \left. + \sqrt{\left(\sqrt{2n_1} - \hat{k}_x\right)^2 + \left(\sqrt{2n_2} + \hat{k}_y\right)^2} + \sqrt{\left(\sqrt{2n_1} + \hat{k}_x\right)^2 - \left(\sqrt{2n_2} + \hat{k}_y\right)^2} + \sqrt{\left(\sqrt{2n_1} + \hat{k}_x\right)^2 + \left(\sqrt{2n_2} + \hat{k}_y\right)^2} \right] .\end{aligned} \tag{4.1.37}$$

Here we have introduced the dimensionless wave vector components $\hat{k}_\ell = \frac{k_\ell}{\sqrt{\kappa}}$. If we now replace the sum with the integral, which is possible due to the Poisson formula approximation argued above we arrive at the integral

$$\begin{aligned}&\Sigma^{\mathrm{F}\prime(1)}(\mathbf{k},\mathbf{R}) \\ &= -K\, D^4 \sqrt{\kappa} \frac{\mathbf{p}_1 \cdot \mathbf{p}_2 \pi}{8} \int_{\frac{\kappa X^2}{2}}^{n_F} dn_1 \int_{\frac{\kappa Y^2}{2}}^{n_F - n_1} dn_2 \frac{1}{\sqrt{2n_1 - \kappa X^2}} \frac{1}{\sqrt{2n_2 - \kappa Y^2}} \left[\sqrt{(\sqrt{2n_1} - \hat{k}_x)^2 + (\sqrt{2n_2} - \hat{k}_y)^2} \right. \\ &\left. + \sqrt{(\sqrt{2n_1} - \hat{k}_x)^2 + (\sqrt{2n_2} + \hat{k}_y)^2} + \sqrt{(\sqrt{2n_1} + \hat{k}_x)^2 + (\sqrt{2n_2} - \hat{k}_y)^2} + \sqrt{(\sqrt{2n_1} + \hat{k}_x)^2 + (\sqrt{2n_2} + \hat{k}_y)^2} \right] .\end{aligned} \tag{4.1.38}$$

We will now also consider the second part of the dipole-dipole interaction. In order to do so, we will again restrict the dipoles to the condition of being parallel and lying in the x-z plane (3.1.13). Before we start, we first have to solve the integral:

$$\begin{aligned}
&\int_0^{2\pi} d\varphi \cos(2\varphi)\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi)) e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))} \qquad (4.1.39)\\
&\quad = \cos(2\vartheta)\int_0^{2\pi} d\varphi \cos(2(\varphi\pm\vartheta))\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi)) e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))}\\
&\qquad \pm \sin(\mp 2\vartheta)\int_0^{2\pi} d\varphi \sin(2(\varphi\pm\vartheta))\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi)) e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))} ,
\end{aligned}$$

where the ϑ has been introduced in accordance with four parametrizations for $a \pm \hat{k}$ as

$$\begin{aligned}
\begin{pmatrix} a_1-\hat{k}_x \\ a_2-\hat{k}_y \end{pmatrix} &= \sqrt{(a_1-\hat{k}_x)^2+(a_2-\hat{k}_y)^2}\begin{pmatrix}\cos(\vartheta_1)\\ \sin(\vartheta_1)\end{pmatrix}\\
\begin{pmatrix} a_1-\hat{k}_x \\ a_2+\hat{k}_y \end{pmatrix} &= \sqrt{(a_1-\hat{k}_x)^2+(a_2+\hat{k}_y)^2}\begin{pmatrix}\cos(\vartheta_2)\\ \sin(\vartheta_2)\end{pmatrix}\\
\begin{pmatrix} a_1+\hat{k}_x \\ a_2-\hat{k}_y \end{pmatrix} &= \sqrt{(a_1+\hat{k}_x)^2+(a_2-\hat{k}_y)^2}\begin{pmatrix}\cos(\vartheta_3)\\ \sin(\vartheta_3)\end{pmatrix}\\
\begin{pmatrix} a_1+\hat{k}_x \\ a_2+\hat{k}_y \end{pmatrix} &= \sqrt{(a_1+\hat{k}_x)^2+(a_2+\hat{k}_y)^2}\begin{pmatrix}\cos(\vartheta_4)\\ \sin(\vartheta_4)\end{pmatrix} . \qquad (4.1.40)
\end{aligned}$$

The integral can now be executed and yields

$$\begin{aligned}
&\int_0^{2\pi} d\varphi \cos(2\varphi)\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi)) e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))} \qquad (4.1.41)\\
&\quad = -\frac{\pi}{2}\left[\cos(2\vartheta_1) J_2\left(\sqrt{(a_1-\hat{k}_x)^2+(a_2-\hat{k}_y)^2}\, r\right) + \cos(2\vartheta_2) J_2\left(\sqrt{(a_1-\hat{k}_x)^2+(a_2+\hat{k}_y)^2}\, r\right)\right.\\
&\qquad \left. + \cos(2\vartheta_3) J_2\left(\sqrt{(a_1+\hat{k}_x)^2+(a_2-\hat{k}_y)^2}\, r\right) + \cos(2\vartheta_4) J_2\left(\sqrt{(a_1+\hat{k}_x)^2+(a_2+\hat{k}_y)^2}\, r\right)\right]\\
&\quad = -\frac{\pi}{2}\left[\cos(2\vartheta_1) J_2(--) + \cos(2\vartheta_2) J_2(-+) + \cos(2\vartheta_3) J_2(+-) + \cos(2\vartheta_4) J_2(++)\right]\\
&\quad = \frac{\pi}{2}\left[J_2(--) + J_2(-+) + J_2(+-) + J_2(++)\right]\\
&\qquad - \pi\left[\cos^2(\vartheta_1) J_2(--) + \cos^2(\vartheta_2) J_2(-+) + \cos^2(\vartheta_3) J_2(+-) + \cos^2(\vartheta_4) J_2(++)\right] , \qquad (4.1.42)
\end{aligned}$$

where we have introduced the notation

$$J_2(\pm;\pm) := J_2\left(\sqrt{(a_1\pm k_x)^2+(a_2\pm k_y)^2}\, r\right) . \qquad (4.1.43)$$

To solve the first φ integral of (4.1.34) we proceed as before:

$$\begin{aligned}
&\int_0^{2\pi} d\varphi \cos^2(\varphi)\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi))e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))}\\
&=\frac{1}{2}\int_0^{2\pi} d\varphi \cos(a_1 r\cos(\varphi))\cos a_2 r\sin(\varphi))e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\cos(\varphi))}\\
&\quad+\frac{1}{2}\int_0^{2\pi} d\varphi \cos(2\varphi)\cos(a_1 r\cos(\varphi)\cos(a_2 r\sin\varphi)e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\cos(\varphi))}\\
&=-\frac{\pi}{4}\left[J_0(--)+J_0(-+)+J_0(+-)+J_0(++)\right]+\frac{\pi}{4}\left[J_2(--)+J_2(-+)+J_2(+-)+J_2(++)\right]\\
&\quad-\frac{\pi}{2}\left[\cos^2(\vartheta_1)J_2(--)\cos^2(\vartheta_2)J_2(-+)+\cos(\vartheta_3)J_2(+-)+\cos^2(\vartheta_4)J_2(++)\right]\ .
\end{aligned}\tag{4.1.44}$$

For the r-integration, we again substitute the square roots out of the Bessel functions and bring the -1 of the subtracted Green function to the Bessel function J_0 in order to make it convergent. The integration over the Bessel functions of second order combined with the factor $\frac{1}{r^2}$ simply gives $\frac{1}{3}$. With that said we get:

$$\begin{aligned}
&\int_0^{\infty} dr\int_0^{2\pi} d\varphi\frac{1}{r^2}\left[\cos^2(\varphi)\cos(a_1 r\cos(\varphi))\cos(a_2 r\sin(\varphi))e^{-i(\hat{k}_x r\cos(\varphi)+\hat{k}_y r\sin(\varphi))}-\cos^2(\varphi)\right] \qquad (4.1.45)\\
&\quad=-\frac{\pi}{4}\left[\sqrt{--}+\sqrt{-+}+\sqrt{+-}+\sqrt{++}\right]\\
&\qquad+\frac{\pi}{12}\left[\sqrt{--}+\sqrt{-+}+\sqrt{+-}+\sqrt{++}\right]\\
&-\frac{\pi}{6}\left[\cos^2(\vartheta_1)\sqrt{--}+\cos^2(\vartheta_2)\sqrt{-+}+\cos^2(\vartheta_3)\sqrt{+-}+\cos^2(\vartheta_4)\sqrt{++}\right]\\
&\quad=-\frac{\pi}{6}\left[\sqrt{--}+\sqrt{-+}+\sqrt{+-}+\sqrt{++}\right]-\frac{\pi}{6}\left[\frac{(a_1-\hat{k}_x)^2}{\sqrt{--}}+\frac{(a_1-\hat{k}_x)^2}{\sqrt{-+}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{+-}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{++}}\right]
\end{aligned}$$

where we have introduced in accordance with (4.1.43) the short-hand notation

$$\sqrt{(\pm;\pm)}:=\sqrt{\left(a_1\pm\hat{k}_x\right)^2+\left(a_2\pm\hat{k}_y\right)^2}\,. \tag{4.1.46}$$

The whole second integral can now be written as:

$$\begin{aligned}
&\Sigma^{\mathrm{F}\prime(2)}(\mathbf{k},\mathbf{R})\\
&=-KD^4\frac{3p_1^2}{4}\sum_{n_1 n_2}\frac{1}{\sqrt{2n_1-\kappa X^2}}\frac{1}{\sqrt{2n_2-\kappa Y^2}}\int dxdy\frac{1}{(x^2+y^2)^{\frac{5}{2}}}\left(x^2\cos(a_1 x)\cos(a_2 y)e^{-i(\hat{k}_x x+\hat{k}_y y)}-x^2\right)\\
&=KD^4\frac{\pi p_1^2}{8}\sum_{n_1,n_2}\frac{1}{\sqrt{2n_1-\kappa X^2}}\frac{1}{\sqrt{2n_2-\kappa Y^2}}\left[\left(\sqrt{--}+\sqrt{-+}+\sqrt{+-}+\sqrt{++}\right)\right.\\
&\qquad\left.+\left(\frac{(a_1-\hat{k}_x)^2}{\sqrt{--}}+\frac{(a_1-\hat{k}_x)^2}{\sqrt{-+}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{+-}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{++}}\right)\right]\ .
\end{aligned}\tag{4.1.47}$$

We can now combine the first (4.1.38) and second (4.1.47) part of the dipole-dipole interaction to

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R}) &= -\frac{1}{4}KD^4\sum_{n_1,n_2}\int dxdyV^{(\mathrm{int})}(x,y)\frac{1}{\sqrt{2n_1-\kappa X^2}}\frac{1}{\sqrt{2n_2-\kappa Y^2}}\left(\cos(a_1x)\cos(a_2y)e^{-i(\hat{k}_xx+\hat{k}_yy)}-1\right)\\ &= KD^4\frac{\pi p_3^2}{8}\sum_{n_1,n_2}\frac{1}{\sqrt{2n_1-X^2}}\frac{1}{\sqrt{2n_2-Y^2}}\Bigg\{\left[\sqrt{--}+\sqrt{-+}+\sqrt{+-}+\sqrt{++}\right]\\ &\quad+p_1^2\left[\frac{(a_1-\hat{k}_x)^2}{\sqrt{--}}+\frac{(a_1-\hat{k}_x)^2}{\sqrt{-+}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{+-}}+\frac{(a_1+\hat{k}_x)^2}{\sqrt{++}}\right]\Bigg\}. \end{aligned}\tag{4.1.48}$$

The final form for the Fock term reads then explicitly

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R}) &= KD^4\sqrt{\kappa}\frac{\pi p_3^2}{8}\int_{\frac{\kappa X^2}{2}}^{n_F}dn_1\int_{\frac{\kappa Y^2}{2}}^{n_F-n_1}dn_2\frac{1}{\sqrt{2n_1-\kappa X^2}}\frac{1}{\sqrt{2n_2-\kappa Y^2}}\\ &\quad\times\Bigg\{p_3^2\Bigg[\sqrt{\left(\sqrt{2n_1}-\hat{k}_x\right)^2+\left(\sqrt{2n_2}-\hat{k}_y\right)^2}+\sqrt{\left(\sqrt{2n_1}-\hat{k}_x\right)^2+\left(\sqrt{2n_2}+\hat{k}_y\right)^2}\\ &\quad+\sqrt{\left(\sqrt{2n_1}+\hat{k}_x\right)^2+\left(\sqrt{2n_2}-\hat{k}_y\right)^2}+\sqrt{\left(\sqrt{2n_1}+\hat{k}_x\right)^2+\left(\sqrt{2n_2}+\hat{k}_y\right)^2}\Bigg]\\ &\quad+p_1^2\Bigg[\frac{(\sqrt{2n_1}-\hat{k}_x)^2}{\sqrt{\left(\sqrt{2n_1}-\hat{k}_x\right)^2-\left(\sqrt{2n_2}+\hat{k}_y\right)^2}}+\frac{(\sqrt{2n_1}-\hat{k}_x)^2}{\sqrt{\left(\sqrt{2n_1}-\hat{k}_x\right)^2+\left(\sqrt{2n_2}+\hat{k}_y\right)^2}}\\ &\quad+\frac{(\sqrt{2n_1}-\hat{k}_x)^2}{\sqrt{\left(\sqrt{2n_1}+\hat{k}_x\right)^2+\left(\sqrt{2n_2}-\hat{k}_y\right)^2}}+\frac{(\sqrt{2n_1}+\hat{k}_x)^2}{\sqrt{\left(\sqrt{2n_1}+\hat{k}_x\right)^2+\left(\sqrt{2n_2}+\hat{k}_y\right)^2}}\Bigg]\Bigg\}. \end{aligned}\tag{4.1.49}$$

Finally we will rewrite the Fock term in such a way that we can see the N dependence upon it. As in the case of the Hartree self-energy we use (4.1.27). The final form then reads

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k},\mathbf{R}) &= \frac{1}{2^{\frac{3}{4}}\pi}K\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}N^{\frac{3}{4}}\int_{\tilde{X}^2}^{1}dn_1\int_{\tilde{Y}^2}^{1-n_1}dn_2\frac{1}{\sqrt{n_1-\tilde{X}^2}}\frac{1}{\sqrt{n_2-\tilde{Y}^2}}\\ &\quad\times\Bigg\{p_3^2\Bigg[\sqrt{\left(\sqrt{n_1}-\tilde{k}_x\right)^2+\left(\sqrt{n_2}-\tilde{k}_y\right)^2}+\sqrt{\left(\sqrt{n_1}-\tilde{k}_x\right)^2+\left(\sqrt{n_2}+\tilde{k}_y\right)^2}\\ &\quad+\sqrt{\left(\sqrt{n_1}+\tilde{k}_x\right)^2+\left(\sqrt{n_2}-\tilde{k}_y\right)^2}+\sqrt{\left(\sqrt{n_1}+\tilde{k}_x\right)^2+\left(\sqrt{n_2}+\tilde{k}_y\right)^2}\Bigg]\\ &\quad+p_1^2\Bigg[\frac{(\sqrt{n_1}-\tilde{k}_x)^2}{\sqrt{\left(\sqrt{n_1}-\tilde{k}_x\right)^2-\left(\sqrt{n_2}+\tilde{k}_y\right)^2}}+\frac{(\sqrt{n_1}-\tilde{k}_x)^2}{\sqrt{\left(\sqrt{n_1}-\tilde{k}_x\right)^2+\left(\sqrt{n_2}+\tilde{k}_y\right)^2}}\\ &\quad+\frac{(\sqrt{n_1}-\tilde{k}_x)^2}{\sqrt{\left(\sqrt{n_1}+\tilde{k}_x\right)^2+\left(\sqrt{n_2}-\tilde{k}_y\right)^2}}+\frac{(\sqrt{n_1}+\tilde{k}_x)^2}{\sqrt{\left(\sqrt{n_1}+\tilde{k}_x\right)^2+\left(\sqrt{n_2}+\tilde{k}_y\right)^2}}\Bigg]\Bigg\}. \end{aligned}\tag{4.1.50}$$

Where we have set

$$\tilde{k}_\ell := \frac{\hat{k}_\ell}{\sqrt{\frac{\hbar}{m\omega}} 2^{\frac{3}{2}} N^{\frac{1}{4}}} \quad \text{and} \quad \tilde{X}_\ell := \frac{X_\ell}{\sqrt{\frac{\hbar}{m\omega}} 2^{\frac{3}{2}} N^{\frac{1}{4}}} \tag{4.1.51}$$

4.2 Semiclassical Approximation for the Hartree-Fock Self-Energy

The standard way to calculate the self-energy for ultracold quantum gases would be to use the semiclassical approximation. In order to do compare our results, we will now evaluate the Hartree Fock diagrams (2.3) with the semiclassical Green functions which is given for equal times by [58]

$$G\left(\mathbf{x}_1\tau|\mathbf{x}_2\tau\right) = -\int \frac{dp^2}{(2\pi\hbar)^2} e^{i\mathbf{p}(\mathbf{x}_1-\mathbf{x}_2)} \frac{1}{e^{\beta(H[\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}]-\mu)}+1} \,, \tag{4.2.1}$$

where the Hamiltionian is evaluated as follows

$$H[\mathbf{x}_1,\mathbf{x}_2;\mathbf{p}] = \frac{\mathbf{p}^2}{2m} + V^{(\mathrm{trap})}\left(\frac{\mathbf{x}_1+\mathbf{x}_2}{2}\right) - \mu \,. \tag{4.2.2}$$

We will now evaluate the Hartree-Fock equations with the semiclassical Green function. We start again with the Hartree term

$$\begin{aligned}
\Sigma^H(\mathbf{r}_1,\tau_1|\mathbf{r}_2,\tau_2) &= \zeta^{n_1}\delta(\tau_1-\tau_2)\int d^2\mathbf{r}_3 d^2\mathbf{r}_4 \left\langle \mathbf{r}_1\mathbf{r}_3\right| V \left|\mathbf{r}_2\mathbf{r}_4\right\rangle G(\mathbf{r}_4\tau|\mathbf{r}_3\tau) \\
&= -\delta(\tau_1-\tau_2)\int d^2\mathbf{r}_3 d^2\mathbf{r}_4 \delta(\mathbf{r}_1-\mathbf{r}_2)\delta(\mathbf{r}_3-\mathbf{r}_4)V(\mathbf{r}_2-\mathbf{r}_4)G(\mathbf{r}_4\tau|\mathbf{r}_3\tau) \\
&= -\delta(\tau_1-\tau_2)\,\delta(\mathbf{r}_1-\mathbf{r}_2)\int d^2\mathbf{r}\, V^{(\mathrm{int})}\left(\mathbf{r}_1-\mathbf{r}\right) G\left(\mathbf{r},\tau_1|\mathbf{r},\tau_1\right) \\
&= -\delta(\tau_1-\tau_2)\delta(\mathbf{r}_1-\mathbf{r}_2)\int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'') G\left(\mathbf{r}_1-\mathbf{r}'',\tau_1|\mathbf{r}_1-\mathbf{r}'',\tau_1\right) \\
&= -\delta(\tau_1-\tau_2)\delta(\mathbf{r}_r)\int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'') G\left(\mathbf{R}+\frac{\mathbf{r}_r}{2}-\mathbf{r}'',\tau_1\middle|\mathbf{R}+\frac{\mathbf{r}_r}{2}-\mathbf{r}'',\tau_1\right) \,.
\end{aligned} \tag{4.2.3}$$

In the same manner we get the following term for the Fock diagram

$$\begin{aligned}
\Sigma^F(\mathbf{r}_1,\tau|\mathbf{r}_2,\tau) &= \delta(\tau_1-\tau_2)\int d^2\mathbf{r}_3 d^2\mathbf{r}_4 \left\langle \mathbf{r}_1\mathbf{r}_3\right| V \left|\mathbf{r}_4\mathbf{r}_2\right\rangle G(\mathbf{r}_4\tau|\mathbf{r}_3\tau) \\
&= \delta(\tau_1-\tau_2)\int d^2\mathbf{r}_3 d^2\mathbf{r}_4 \delta(\mathbf{r}_1-\mathbf{r}_4)\delta(\mathbf{r}_3-\mathbf{r}_2)V^{(\mathrm{int})}(\mathbf{r}_4-\mathbf{r}_2)G(\mathbf{r}_4\tau|\mathbf{r}_3\tau) \\
&= \delta(\tau_1-\tau_2)V^{(\mathrm{int})}(\mathbf{r}_1-\mathbf{r}_2)G(\mathbf{r}_1,\tau_1|\mathbf{r}_2,\tau_2) \,.
\end{aligned} \tag{4.2.4}$$

and in analogy to above we again perform the Fourier transformation in time and relative space

$$\begin{aligned}
\Sigma^H(\mathbf{k}',\mathbf{R}) &= -\int d^2\mathbf{r}_r e^{-i\mathbf{k}'\cdot\mathbf{r}_r}\delta(\mathbf{r}_r)\int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'')\, G\left(\mathbf{R}+\frac{\mathbf{r}_r}{2}-\mathbf{r}'',\tau_1\middle|\mathbf{R}+\frac{\mathbf{r}_r}{2}-\mathbf{r}'',\tau_1\right) \\
&= -\int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'')\, G\left(\mathbf{R}-\mathbf{r}'',\tau_1|\mathbf{R}-\mathbf{r}'',\tau_1\right) \,.
\end{aligned} \tag{4.2.5}$$

For the Fock term we arrive at

$$\Sigma^F(\mathbf{k}',\mathbf{R}) = \delta(\tau_1-\tau_2)\int d^2\mathbf{r}_r\, e^{-i\mathbf{k}'\mathbf{r}_r} V^{(\mathrm{int})}(\mathbf{r}_r)\, G\left(\mathbf{R}+\frac{\mathbf{r}_r}{2}\middle|\mathbf{R}-\frac{\mathbf{r}_r}{2}\right) \,. \tag{4.2.6}$$

To control the singularity at $V(\mathbf{0})$ we add

$$\int d^2\mathbf{r}\, V^{(\mathrm{int})}(\mathbf{r})\, G(\mathbf{R},\mathbf{R})\ , \tag{4.2.7}$$

to the Hartree term and again subtract it from the Fock term. We will again write these terms with the prime and arrive for the Hartree term at

$$\begin{aligned}
\Sigma^{H\prime}(\mathbf{k}',\mathbf{R}) &= -\int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'')\left\{G\left(\mathbf{R}-\mathbf{r}'',\tau_1|\mathbf{R}-\mathbf{r}'',\tau_1\right)-G\left(\mathbf{R},\mathbf{R}\right)\right\} \\
&= \int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'') \\
&\quad\times\left\{\frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi_k\int_0^{\infty} k\,dk\,\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R}-\mathbf{r}'')\right)\right. \\
&\qquad\left.-\frac{1}{(2\pi)^2}\int_0^{2\pi} d\varphi_k\int_0^{\infty} kdk\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right)\right\} \\
&= \int d^2\mathbf{r}''\, V^{(\mathrm{int})}(\mathbf{r}'')\left\{\frac{m}{(2\pi)\hbar^2}\left[E_f-V(\mathbf{R}-\mathbf{r}'')\right]\Theta\left(E_F-V\left(\mathbf{R}-\mathbf{r}''\right)\right)-\frac{m}{(2\pi)\hbar^2}\left[E_f-V(\mathbf{R})\right]\right\}\ .
\end{aligned} \tag{4.2.8}$$

Where we have evaluated the Greens function for $T\approx 0$ as

$$G\left(\mathbf{R}+\frac{\mathbf{r}_r}{2}\middle|\mathbf{r}-\frac{\mathbf{r}_r}{2}\right)=\int\frac{d^2\mathbf{k}}{(2\pi)^2}e^{-i\mathbf{k}\mathbf{r}_r}\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right) \tag{4.2.9}$$

as well as

$$G\left(\mathbf{R}|\mathbf{R}\right)=\int\frac{d^2k}{(2\pi)^2}\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right)\ . \tag{4.2.10}$$

Now we subtract again the term $\int d^2\mathbf{r}_r\, V(\mathbf{r}_r)G(\mathbf{R},\mathbf{R})$ and arrive at the following Fock term

$$\begin{aligned}
\Sigma^{F\prime}(\mathbf{k}',\mathbf{R}) &= \int d^2\mathbf{r}_r\, V^{(\mathrm{int})}(\mathbf{r}_r)\left\{G\left(\mathbf{R}+\frac{\mathbf{r}_r}{2}|\mathbf{R}-\frac{\mathbf{r}_r}{2}\right)e^{-ik'\mathbf{r}_r}-G(\mathbf{R},\mathbf{R})\right\} \\
&= -\int d^2\mathbf{r}_r\, V^{(\mathrm{int})}(\mathbf{r}_r)\int\frac{d^2\mathbf{k}}{(2\pi)^2}\left\{e^{-i\mathbf{r}_r(\mathbf{k}'-\mathbf{k})}\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right)-\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right)\right\} \\
&= -\int\frac{d^2k}{(2\pi)^2}\left\{V^{(\mathrm{int})}(\mathbf{k}'-\mathbf{k})-V^{(\mathrm{int})}(\mathbf{k}=0)\right\}\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right) \\
&= \int\frac{d^2k}{(2\pi)^2}\left\{V^{(\mathrm{int})}(\mathbf{k}=0)-V^{(\mathrm{int})}(\mathbf{k}'-\mathbf{k})\right\}\Theta\left(E_f-\frac{\hbar^2k^2}{2m}-V(\mathbf{R})\right)
\end{aligned} \tag{4.2.11}$$

4.2.1 Semiclassical Derivation of the Hartree Self-Energy

Due to the Theta function the first integral of the Hartree term has to be taken over the following region

$$(X-x'')^2+(Y-y'')^2\le\frac{2E_f}{m\omega^2}. \tag{4.2.12}$$

The second integral has to be taken over the whole volume. We arrive at the following semiclassical Hartree term

$$\begin{aligned}\Sigma^{\mathrm{H}\prime}(\mathbf{k}',\mathbf{R}) &= \frac{m}{(2\pi)\hbar^2}\int_{\text{circle}} d^2\mathbf{r}'' V^{(\text{int})}(r'')\left[E_f - V(\mathbf{R}-\mathbf{r}'')\right] - \frac{m}{(2\pi)\hbar^2}\int_V d^2r'' V_1^{(\text{int})}(\mathbf{r}'')\left[E_f - V(\mathbf{r})\right] \\ &= \frac{m}{(2\pi)\hbar^2}\left\{\int_{\text{circle}} dx''dy'' V^{(\text{int})}(x,y)\left(E_f - \frac{m\omega^2}{2}\left[(X-x'')^2+(Y-y')^2\right]\right)\right. \\ &\qquad\left. - \int_V d^2x'' V^{(\text{int})}(x,y)\left[E_f - \frac{m\omega^2}{2}(X^2+Y^2)\right]\right\} \\ &= \frac{m}{(2\pi)\hbar^2}\left\{\int_{\text{circle}} d^2\eta V^{(\text{int})}(x,y)\left[E_f - \frac{m\omega^2}{2}(\eta^2+\xi^2)\right] - \int_V d^2\eta V^{(\text{int})}(x,y)\left[E_f - \frac{m\omega^2}{2}(X^2+Y^2)\right]\right\}. \end{aligned} \tag{4.2.13}$$

As we can see this integral corresponds exactly to our previous derived Hartree integral (4.1.23).

4.2.2 Semiclassical Derivation of the Fock Self-Energy

The Fock term can most easily be evaluated with the help of the previous derived Fourier transformation

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k}',\mathbf{R}) &= \int \frac{d^2k}{(2\pi)^2}\left\{V^{(\text{int})}(\mathbf{k}=0) - V^{(\text{int})}(\mathbf{k}'-\mathbf{k})\right\}\Theta\left(E_f - \frac{\hbar^2k^2}{2m} - V(\mathbf{X})\right) \\ &= \int_0^{\sqrt{\frac{2m}{\hbar}\left(E_f - V(X)\right)}} kdk \int_0^{2\pi} d\varphi_k \left\{V^{(\text{int})}(\mathbf{k}=0) - V^{(\text{int})}(\mathbf{k}'-\mathbf{k})\right\} \\ &= \Sigma_{\text{2D}}^{HF}\left(\sqrt{\frac{2m}{\hbar}\left[E_f - \frac{m\omega^2}{2}\left(X^2+Y^2\right)\right]}\right). \end{aligned} \tag{4.2.14}$$

Here we have used the solution for the homogeneous case Σ_{2D}^{HF} (3.3.66). Therefore we get for the Fock term

$$\begin{aligned}\Sigma^{\mathrm{F}\prime}(\mathbf{k}',\mathbf{R}) &= \frac{2}{3}\frac{1}{(2\pi)^2}K\mathbf{p}_1\mathbf{p}_2 2^{\frac{9}{4}}N^{\frac{3}{4}}\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}\left[1-\left(\tilde{X}^2+\tilde{Y}^2\right)\right]^{\frac{3}{2}} \\ &\quad\times\left\{P_2(\cos(\alpha)I_{\text{2D}}^{iso}\left(\frac{\tilde{k}}{\sqrt{1-\left(\tilde{X}^2+\tilde{Y}^2\right)}}\right) - \sin^2(\alpha)\cos(2\varphi_k)I_{\text{2D}}^{\text{ani}}\left(\frac{\tilde{k}}{\sqrt{1-\left(\tilde{X}^2+\tilde{Y}^2\right)}}\right)\right\}. \end{aligned} \tag{4.2.15}$$

where we have again used the dimensionless quantities (4.1.29).

4.2.3 Determination of Chemical Potential

In order to compare the results, we have to calculate the chemical potentials within the large N and semiclassical approximation independently. The particle number is defined as

$$N = \int d^2r\, n(\mathbf{r})\,. \tag{4.2.16}$$

For the large N calculation the density has to be evaluated as

$$\begin{aligned} n(\mathbf{r}) &= \sum_\gamma |\varphi_\gamma(\mathbf{r})|^2 n_\gamma = \frac{D^4}{4}\int_{\kappa\frac{x^2}{2}}^{n_F} dn_1 \int_{\kappa\frac{y^2}{2}}^{n_F-n_1} dn_2 \frac{1}{\sqrt{2n_1-\kappa x^2}}\frac{1}{\sqrt{2n_2-\kappa y^2}} \\ &= -\frac{D^4}{16}\frac{\pi m\omega}{\hbar}\left[x^2+y^2-\frac{2n_F}{\kappa}\right]\Theta\left(\frac{2n_F}{\kappa}-x^2-y^2\right). \end{aligned} \tag{4.2.17}$$

Here we have again used that the cosine terms can be neglected for the n-integration, see also Appendix A Therefore we get

$$N = \frac{D^4}{16}\frac{\pi m\omega}{\hbar}\int_0^{\sqrt{\frac{2n_F}{\kappa}}} rdr \int_0^{2\pi} d\varphi \left[r^2 - \frac{2n_F}{\kappa}\right] = \frac{n_F^2}{2}\,. \tag{4.2.18}$$

If we substitute $E_F := \hbar\omega n_F$ we get

$$N = \frac{E_F^2}{2\omega^2\hbar^2} \tag{4.2.19}$$

The same calculation can now be done for the semiclassical approximation as

$$\begin{aligned} n(\mathbf{x}) &= \int \frac{d^2k}{(2\pi)^2}\,\Theta\left(E_F - \frac{\hbar^2k^2}{2m} - V(\mathbf{x})\right) \\ &= \frac{1}{4\pi}\left[\frac{2m}{\hbar^2}\left(E_F - \frac{m\omega^2}{x}(x^2+y^2)\right)\right] \end{aligned} \tag{4.2.20}$$

So now we can calculate N for

$$N = \frac{1}{4\pi}\int_{-\sqrt{\frac{2E_F}{m\omega}}}^{\sqrt{\frac{2E_F}{m\omega^2}}} dy \int_{-\sqrt{\frac{2E_F}{n\omega}-y}}^{\sqrt{\frac{2E_F}{m\omega}-y^2}} dx \frac{2m}{\hbar^2}\left[E_F - \frac{m\omega^2}{2}(x^2+y^2)\right] = \frac{E_F^2}{2\omega^2\hbar^2} \tag{4.2.21}$$

As we can see the two probability densities (4.2.17) and (4.2.20) are the same. So the difference of the two approximations lies in the off diagonal elements of the Green function.

4.3 Discussion

In the following we use $\tilde{\Sigma}^{\mathrm{H}}$ and $\tilde{\Sigma}^{\mathrm{F}}$ as dimensionless self-energies calculated from (4.1.28) and (4.1.50) by setting $K\mathbf{p}_1 \cdot \mathbf{p}_2 \left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}} = 1$. Where we have considered parallel dipoles and calulculatd the components for each given dipole setting α. By comparing (4.1.28) with (4.1.50) in the large N approximation or (4.2.15) with (4.2.13) respectively we see that the Fock self-energy dominates over the Hartree-energy by a factor $N^{\frac{1}{2}}$ for large particle numbers. Furthermore the Hartree contribution has no k dependencies and therefore only provides a constant shift in the one-particle energy. For that matter we will consider the Hartree and Fock self-energy separately

4.3.1 Discussion of the Hartree Self-Energy

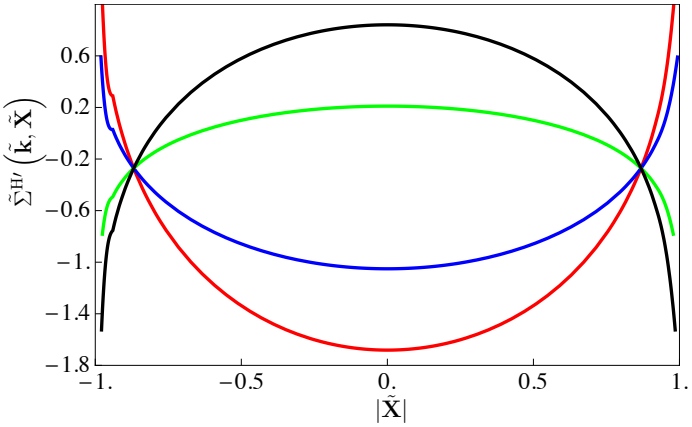


Figure 4.1: Shown are the Hartree contribution to the self-energy $\Sigma^{\mathrm{H}\prime}$ as a function of $\tilde{X}$ for $\tilde{Y} = 0$ and for the four different dipole settings $\alpha = 0$ (red), $\frac{\pi}{6}$ (blue), $\frac{\pi}{3}$ (green) and $\frac{\pi}{2}$(black).

As already mentioned the large N and the semiclassical approximation for the Hartree self-energy coincide. Due to the divergence of the Hartree and Fock self-energies separately, which has its origin in the strong dipole-dipole interaction in two dimensions, we had the freedom to choose the function $f(\mathbf{R}, \mathbf{k})$ in (4.1.8) in order to make them each finite. Similar holds true for the semiclassical approximation. For that reason the Hartree contribution to the self-energy in both approximations is equal only by construction. We note here that the so calculated semiclassical Hartree self-energy (4.2.13) includes non-local contributions to the self-energy, which exceed the local density approximation. These contributions are clearly beyond the first order gradient approximation. In Figure 4.1 we show the dimensionless Hartree self-energy as a function of $\tilde{X}$ and $\tilde{Y} = 0$ for various dipole settings. The convex-concave behaviour of the curves is independent of the chosen value of $\tilde{Y}$. We obtain from the figure, that by passing the critical angle $\overline{\vartheta}$ the curvature of the Hartree self-energy changes from concave to convex. This behaviour corresponds with the Fock self-energy given below.

4.3.2 Discussion of the Fock Self-Energy

In contrast to the Hartree self-energy the dominant Fock self-energies differ in the Large N and semiclassical approximation. First we will look at the Fock self-energy as a function of $\tilde{X}$ for $\tilde{Y}$=0 for various $\tilde{\mathbf{k}}$ directions given by $\varphi_{\mathbf{k}}$ and $|\tilde{\mathbf{k}}| = \frac{1}{\sqrt{2}}$. For this we show in Figure 4.2 $\tilde{\Sigma}^{\mathrm{F}\prime}$ for the large N approximation (left panel) and the semiclassical approximation (right panel) where each row corresponds to one dipole setting. We see from Figure 4.2 that the Fock self-energy varies for different values of φ_k. This splitting increases for larger values of α. This corresponds to the increasing instability of the dipole-dipole interaction for larger α-values.

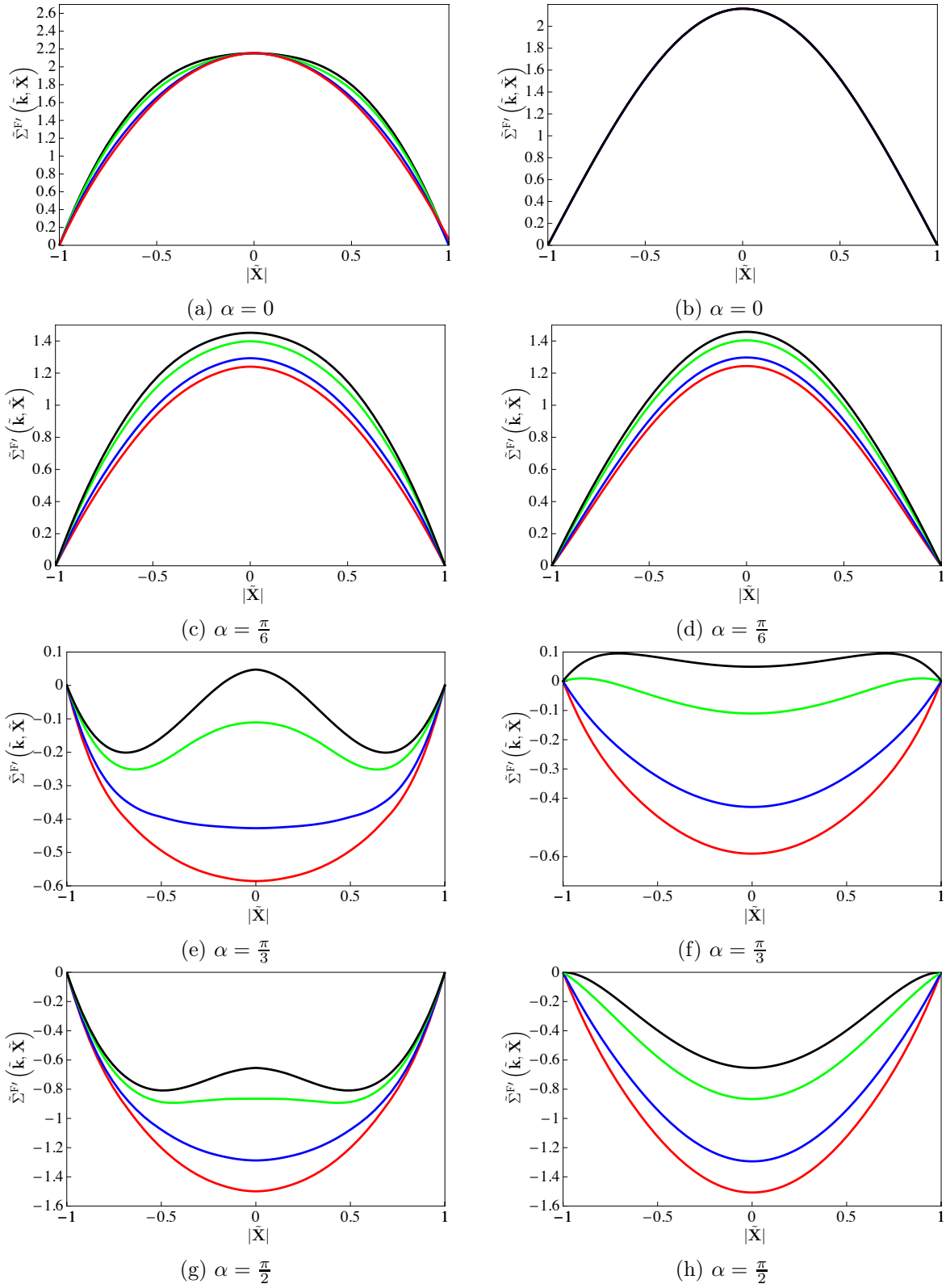
By passing the critical angle $\overline{\vartheta}$ the Fock self-energy even switches within the stable region from a concave to a convex behaviour. This general behaviour is in general independent of the chosen value of $|\tilde{\mathbf{k}}| > 0$. For $|\tilde{\mathbf{k}}| = 0$ the splitting vanishes. We obtain further from Figure 4.2 that the two approximations to the Fock self-energy coincide at $\tilde{X} = 0$. This is true in general independent of the chosen values for $\alpha, \tilde{\mathbf{k}}$ at the origin $\tilde{\mathbf{R}} = 0$. In Figure 4.3 we show $\tilde{\Sigma}^{\mathrm{F}\prime}$ for exemplary selected (α, φ_k) configurations for $\tilde{Y} = 0$ and $|\tilde{\mathbf{k}}| = \frac{1}{\sqrt{2}}$. Here both approximations to the self-energy are shown in one plot. We obtain from the figure that for increasing α-values the difference between the large N and the semiclassical approximation increases. In the instability region of the dipole-dipole interaction the differences between both approximations increase drastically.

Within the Thomas-Fermi picture, we interpret the calculated local self-energy $\Sigma^{H\prime}(\mathbf{R}, \mathbf{k}) + \Sigma^{F\prime}(\mathbf{R}, \mathbf{k})$ together with the free energy as the energy of a quasiparticle added to the system at position $\mathbf{R}$ with momentum $\mathbf{k}$. The whole Green function within the gradient expansion is in general given by $G^{-1}(\mathbf{k}, \mathbf{R}) = G_0^{-1}(\mathbf{k}, \mathbf{R}) + \Sigma(\mathbf{k}, \mathbf{R})$. This relation is not to be confused with the matrix equation (2.4.15) and is only valid within the gradient expansion. For details we refer to [59]. Within the semiclassical approximation the G_0^{-1} is given by $\left(\omega - \frac{\hbar^2\mathbf{k}^2}{2m} - V(\mathbf{R})\right)$. The spatial spectrum is then given by $E(\mathbf{k}, \mathbf{R}) = \frac{\hbar^2\mathbf{k}^2}{2m} - \Sigma(\mathbf{k}, \mathbf{R}) + V(\mathbf{R})$. In oder to give the same interpretation using the large N approximation one would also have to evaluate G_0^{-1}. However this interpretation only becomes interesting once the spatial self-energy is experimentally accessible.

We show in Figure 4.4 the Fock self-energy $\tilde{\Sigma}^{F\prime}(\mathbf{R}, \mathbf{k})$ as a function of $|\tilde{\mathbf{k}}|$ for $\tilde{\mathbf{R}} = 0$ for various α and $\varphi_{\mathbf{k}}$ settings within both approximations. In correspondence with the discussion above we obtain a larger dispersion splitting as a function of $\varphi_{\mathbf{k}}$ for increasing values of α. The curvature of the self-energy even becomes negative in the instability regions of the dipole-dipole interaction. This behaviour then corresponds to the dispersion behaviour of the homogeneous system already discussed in (3.3.2). We obtain furthermore from the figure no deviations of the Fock self-energy within the large N and the semiclassical approximation. This behaviour is only exactly fulfilled at the center of the trap, where the trap potential varies least. In Figure 4.5 we now show the Fock energy dispersion away from the center of the trap, for $\tilde{X} = \frac{1}{\sqrt{2}}$ and $\tilde{Y} = 0$ for both approximation. Corresponding to the previous discussion, concerning the dispersion behaviour in the stable and unstable regions of the dipole-dipole interaction, we obtain here a similar behaviour. We furthermore obtain from the figure, that now even in the stable configurations of the interaction the deviations of the semiclassical and large N approximations are significant.

We note here, that the assumption of large particle numbers $N \gg 1$ is in general fulfilled in ultracold trapped Fermi systems. This means that our large N approximation for the self-energy is almost exact within the Hartree-Fock approximation. This is not fulfilled for the semiclassical approximation of the Hartree-Fock self-energy, which uses a short-time short-distance, approximation for the non-interacting Green function. This approximation even neglects leading terms in $\hbar$ being important for high energy levels. One well known example that this neglection can be substantial is known from the semiclassical approach to quantum chaos [39], where this short-time, short-distance approximation to the Green function leads only to the classical smeared contribution to the density of states. In fact the true density of states for high energy levels in quantum systems is largely affected by approximations going beyond short-time, short-distance for the Green function.

Finally we like to address the possibility to access the spatial self-energy experimentally. To our knowledge it is not yet possible to measure the one-particle excitation spectrum experimentally. Experiments, which have be carried out in this direction use Raman-Bragg spectroscopy [60] and photon emission spectroscopy [61]. For the Bragg experiments in a homogeneous system the structure factor is directly correlated with the spectrum of the system [62]. Within the local density approximation the local structure factor can be determined. The local structure is then weighted by the local particle number in order to obtain the global experimentally accessible structure factor. In that sense the local excitation spectrum can be determined. This is a rather rough approximation where the differences between the self-energy calculated in semiclassical and large N approximation should not be seen. The situation certainly changes once, as proposed in [61], the spatial energy spectrum is accessible.



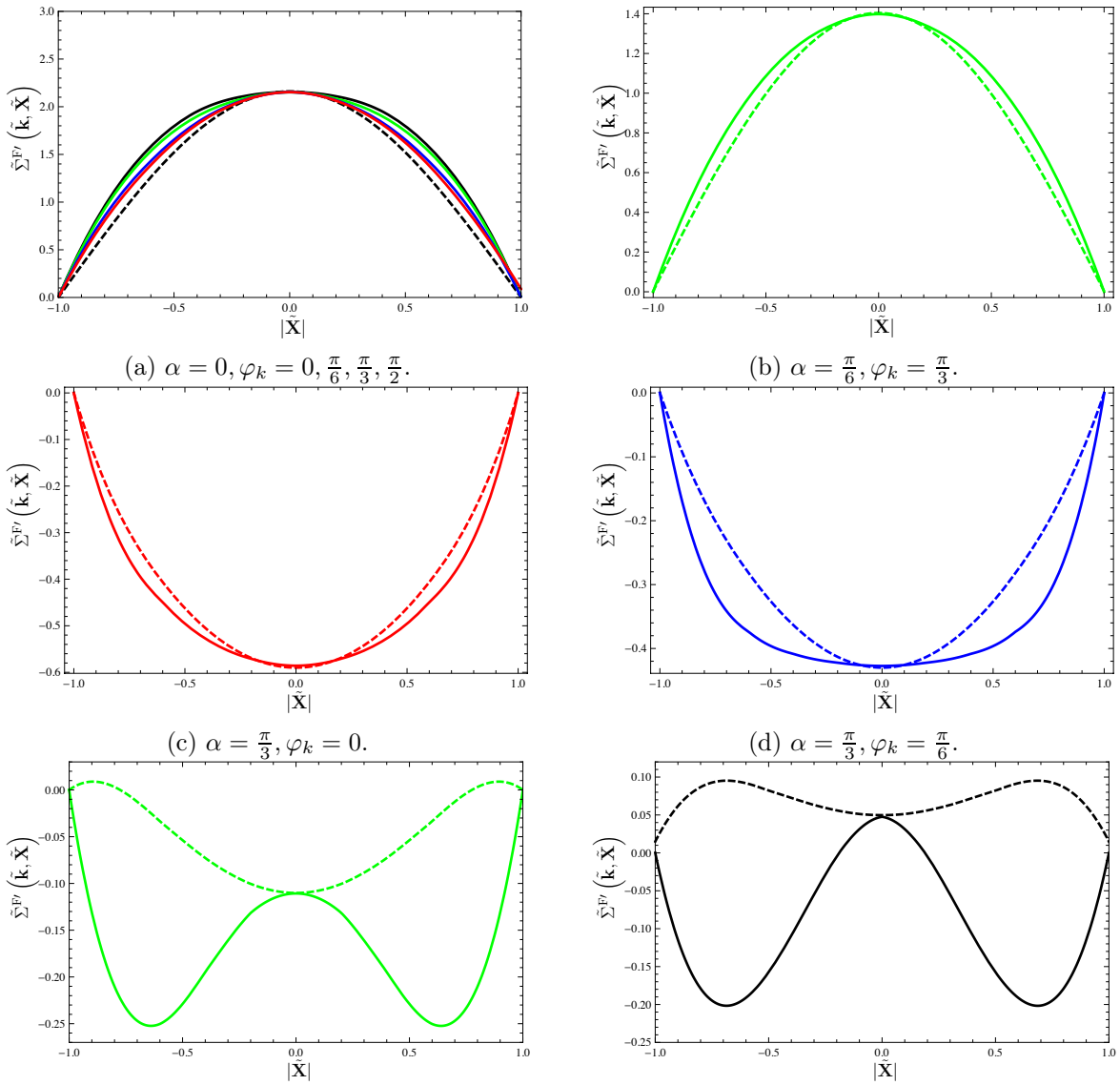
(a) $\alpha = 0$ (b) $\alpha = 0$

(c) $\alpha = \frac{\pi}{6}$ (d) $\alpha = \frac{\pi}{6}$

(e) $\alpha = \frac{\pi}{3}$ (f) $\alpha = \frac{\pi}{3}$

(g) $\alpha = \frac{\pi}{2}$ (h) $\alpha = \frac{\pi}{2}$

Figure 4.2: Center of Mass dependency of Σ^{Fl} for the large N (left column) and semiclassical (right column) approximation. Each row corresponds to one dipole setting (form top to botom) $\alpha = 0, \frac{\pi}{6}, \frac{\pi}{3}, \frac{\pi}{2}$. For each α and $|\mathbf{k}| = \frac{1}{\sqrt{2}}$ four different dispersion directions are shown φ_k with 0 (red), $\frac{\pi}{6}$ (blue) and $\frac{\pi}{3}$ (green) $\frac{\pi}{2}$ (black).



(a) $\alpha = 0, \varphi_k = 0, \frac{\pi}{6}, \frac{\pi}{3}, \frac{\pi}{2}$.

(b) $\alpha = \frac{\pi}{6}, \varphi_k = \frac{\pi}{3}$.

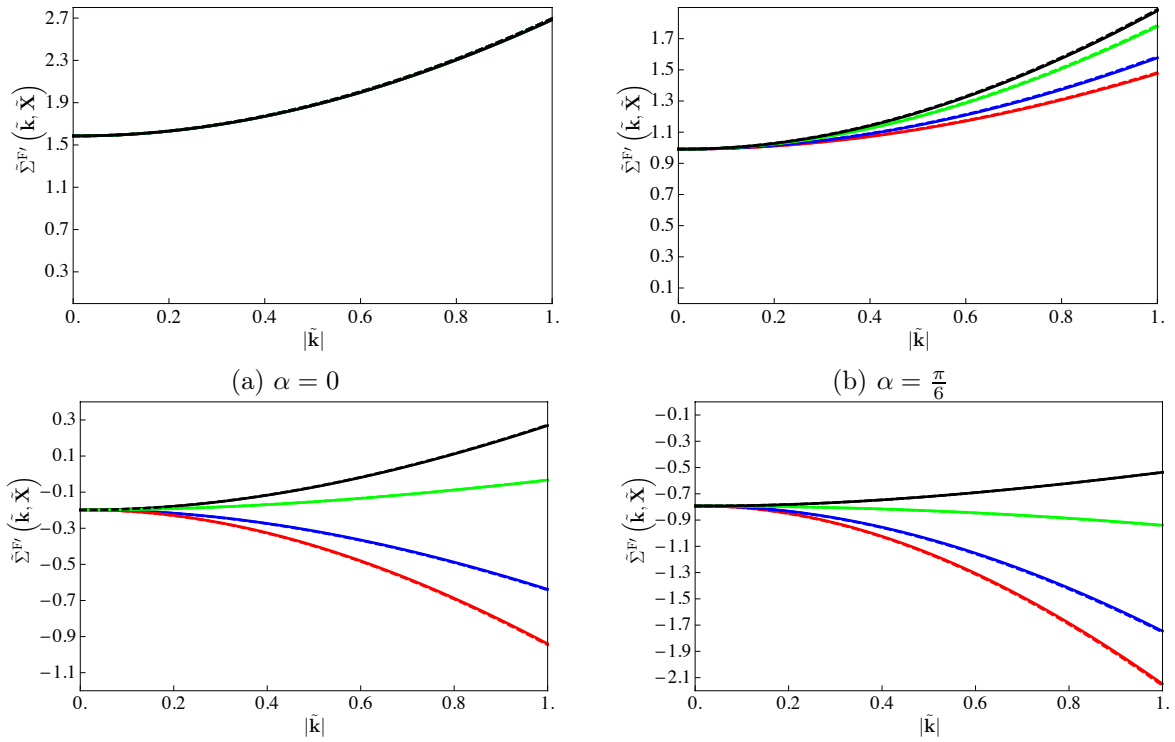
(c) $\alpha = \frac{\pi}{3}, \varphi_k = 0$.

(d) $\alpha = \frac{\pi}{3}, \varphi_k = \frac{\pi}{6}$.

(e) $\alpha = \frac{\pi}{3}, \varphi_k = \frac{\pi}{3}$.

(f) $\alpha = \frac{\pi}{2}, \varphi_k = \frac{\pi}{3}$.

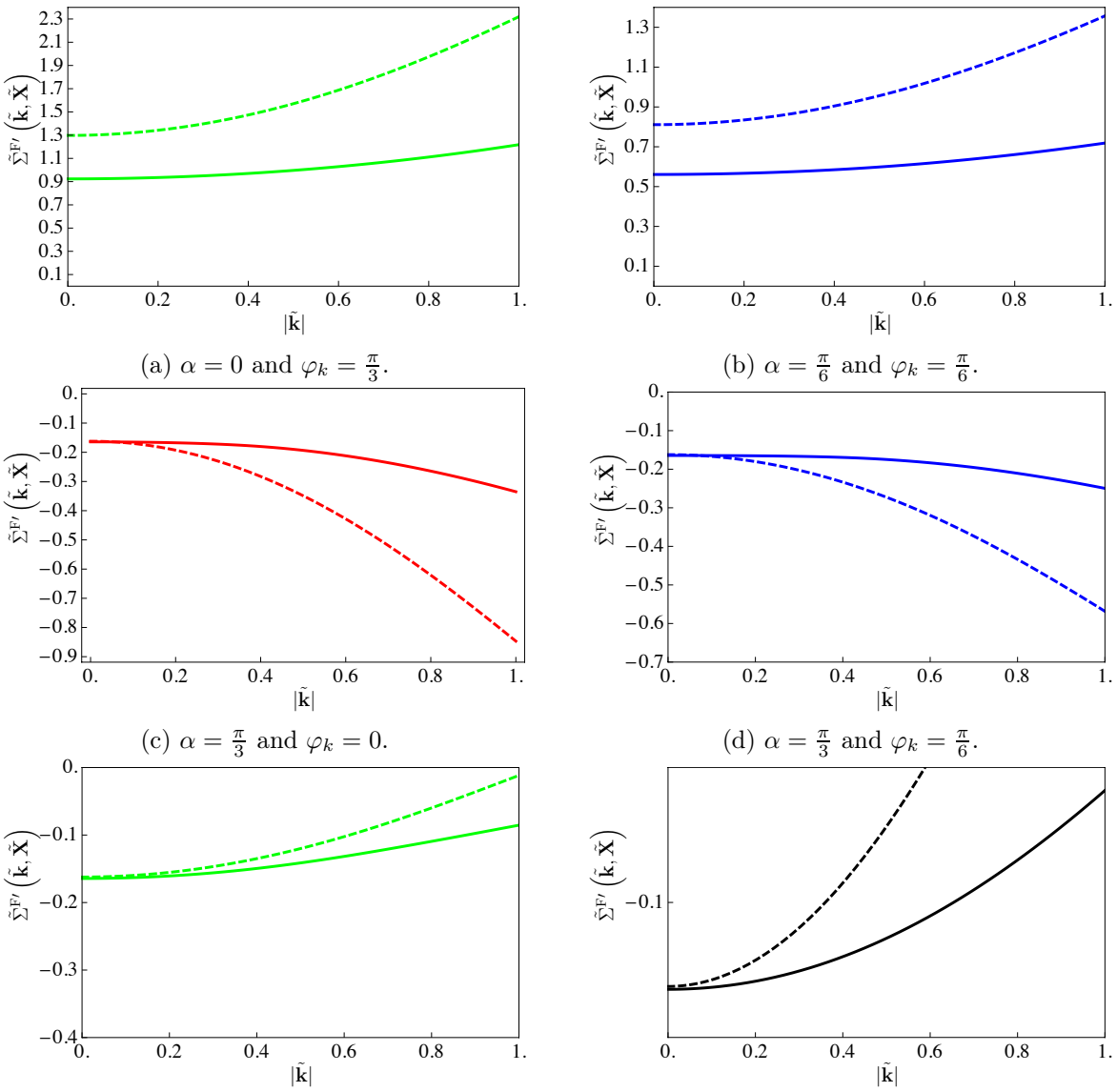
Figure 4.3: Comparison of the large N approximation (solid) and semiclassical (dashed) approximation. Shown are exemplary selected plots from Figure 4.2 with $|\tilde{\mathbf{k}}| = \frac{1}{\sqrt{2}}$.



(a) $\alpha = 0$ (b) $\alpha = \frac{\pi}{6}$

(c) $\alpha = \frac{\pi}{3}$ (d) $\alpha = \frac{\pi}{2}$

Figure 4.4: Dispersion relation for $\tilde{X} = 0$ and $\tilde{Y} = 0$ shown for both the large N (solid) and semiclassical (dashed) approximation for four different diople settings α and for four different directions of φ_k= 0 (red), $\frac{\pi}{6}$ (blue) and $\frac{\pi}{3}$ (green) $\frac{\pi}{2}$ (black).



(a) $\alpha = 0$ and $\varphi_k = \frac{\pi}{3}$.

(b) $\alpha = \frac{\pi}{6}$ and $\varphi_k = \frac{\pi}{6}$.

(c) $\alpha = \frac{\pi}{3}$ and $\varphi_k = 0$.

(d) $\alpha = \frac{\pi}{3}$ and $\varphi_k = \frac{\pi}{6}$.

(e) $\alpha = \frac{\pi}{3}$ and $\varphi_k = \frac{\pi}{3}$.

(f) $\alpha = \frac{\pi}{3}$ and $\varphi_k = \frac{\pi}{2}$.

Figure 4.5: Expemplarly selected dispersion relation for $X = \frac{1}{2}$, $Y = 0$ and $|\tilde{\mathbf{k}}| = 1$ and for different dipole settings as well as different φ_k dependencies.

Chapter 5

Summary and Outlook

5.1 Summary

The description of Many-Body quantum systems from first principles is only possible by taking into account several approximations. One approximation often made in the field of ultracold quantum gases is the assumption that one deals with dilute weak interacting systems. Further accounting for the fact that a low-dimensional system such as the here considered dipolar interaction within two dimensions increases the ultraviolet divergence, it is worth to recapitulate if standard assumptions are still valid. For that matter we started by deriving the fermionic coherent state path integral, which is often just carried on the side of the bosonic coherent state path integral [34, 46, 48], not really outlining the Grassmann character of the theory. Therefore, we made an extra effort and started by deriving all needed calculation rules for the underlying Grassmann algebra. Beyond some standard rules the main goals of this part were to derive the product as well as the chain rule for Grassmann functions (2.1.29), (2.1.31), (2.1.37) and functionals (2.1.86), (2.1.91), (2.1.98). For the product rule the order of the derivated and non-derivated terms now matter. The same holds true for the chain rule, were the order of the inner and outer derivative is now important. We registered, that one has to distinguish between the chaining of the analytic functions with Grassmann functions (2.1.31) or functionals (2.1.91), respectively, and the chaining of Grassmann functions/functionals with Grassmann functions/functionals (2.1.37), (2.1.98). As it turned out for Grassmann functions and functionals the chain rule only holds true for certain functions. For details see (2.1.31), (2.1.37) and (2.1.91), (2.1.98). The chain-rule for Grassmann functions was later used to derive the Wick theorem (2.3.9). The product rule and chain rule for Grassmann functionals were needed to derive the Dyson equation (2.4.16) from which we then derived our main Hartree-Fock equations (2.4.17). Once the Grassmann algebra rules were assembled, the fermionic coherent states could be constructed (2.1.113) and their overcompletness (2.1.121) was proven. Equipped with the necessary tools we derived the fermionic coherent state path integral (2.2.15) and derived expressions such as the partition function (2.2.23) and the imaginary-time Green function (2.2.66). For the free system we derived the Fermi-Dirac statistic (2.2.73) and the free imaginary Green function (2.2.74). While the free system can be threated analytically, the situation changes when interactions come into play. In order to consider interactions, we used perturbation theory. Using the path integral (2.2.23) and the Wick theorem (2.3.9), we could establish the Feynman rules for the partition function (2.3.1), which then again were used to derive the Feynman rules for the interacting Green function (2.3.2). By deriving the Dyson equation (2.4.16) and further reducing the Feynman graphs by only considering the connected Green function (2.3.29), we could finally develop the Feynman rules for the self-energy (2.4). Taking the first-order Feynman graphs, we arrived at the Hartree-Fock equation for the self-energy (2.4.17) in first order perturbation theory.

The second part starts by taking a closer look at the dipole-dipole interaction (3.1.11). We derived the special cases for parallel dipoles in three dimensions (3.1.15) and parallel dipoles in two-dimensions (3.1.17). Considering parallel dipoles was motivated by the assumption, that one considers a system with an external

electric field, which polarizes the dipoles. The anisotropy of the interaction causes the existence of stable and unstable regions depending on the angle between the dipoles and the external electric field. While in three-dimensions the change from stable to unstable systems is characterized by the critical angle $\overline{\vartheta}$ in (3.1.16), the two-dimensional stability depends not only on the orientation of the dipoles to the electric field, but also on the orientation between the two dipoles Figure 3.6 . Having discussed the dipole-dipole interaction, we next calculated the Hartree-Fock equations for the self-energy in first order perturbation theory for a homogeneous Fermi gas at $T \approx 0$ (2.4.20). Due to the translational invariance of the system, the self-energy can be derived using Fourier transformation. As it turned out the Fourier transformation for the dipole-dipole interaction in three-dimensions is well defined (3.2.14), while the Fourier transformation for the dipole-dipole interaction in two-dimensions contains an ultraviolet divergence (3.2.32). This divergence originates in the $\frac{1}{r^3}$ dependence of the dipole-dipole interaction and is not present in the Fourier transformation of the two-dimensional Coulomb interaction (3.2.42). The Coulomb interaction was mainly considered to compare the two interactions in two and three dimensions. Using the Fourier transformation we calculated the self-energy for the three and two-dimensional system. The calculation for the three-dimensional system leads to the solution (3.3.35). The anisotropic character of the self-energy only depends on the orientation of the dipoles and the dispersion is independent of the azimuth angle. Compared to the three-dimensional system the two-dimensional calculation inherits the subtlety that, as mentioned before, the Fourier transformation is divergent in two dimensions. However, since the divergence turns out to appear in the Hartree and Fock term it canceled out in (2.4.20) and the final result is finite. The result was then given in (3.3.66). As already mentioned, the repulsive or attractive interaction depends not only on the orientation of the dipoles towards the electric field, but also on the orientation of the dipoles to each other. This behaviour manifests itself in the calculated quasiparticle dispersions, which changes from a positive (stable) to negative (unstable) curvature as can be seen in Figure 3.15. We then shortly proceeded in calculating the self-energy for the Coulomb interaction as well (3.3.87). As can be seen in Figure 3.16, the self-energy to free-energy ratio is significantly larger in two dimensions than in three. The same holds true for the dipole-dipole interaction, where the ratio is even larger, as can be seen from Figure 3.13. We also mention that we cannot say that the difference between the $\frac{1}{r^3}$ dependence of the dipole-dipole interaction compared to the $\frac{1}{r^2}$ dependence of the Coulomb interaction causes the divergence, as the Hartree term is divergent in the case of the Coulomb interaction and the self-energy was only derived by assuming there exists an equally large background field, due to charge neutrality, so the negative divergent Hartree term cancels with this positive background field.

In the next chapter we investigated an ultracold Fermi gas within an electric trapping potential in two-dimensions (4.0.1). Starting from the Hartree-Fock equations (2.4.17) we evaluate them in position space, before transforming to relative and center-of-mass coordinates, so we arrived at the self-energy expression for $\Sigma(\mathbf{k}, \mathbf{R})$. As observed in the homogeneous case (3.3.66), while the Hartree and Fock terms are divergent separately, they converge together. By introducing the function $f(\mathbf{R}, \mathbf{k})$ (4.1.22) we were able to make the Hartree and Fock term convergent separately. We approximated the exact Green function systematically in leading order of large particle numbers N and derived expressions for the Hartree (4.1.28) and Fock self-energy (4.1.50). Next we took the semiclassical Green function (4.2.1), and calculated the Hartree and Fock diagrams (2.3) by making them convergent using the same technique as in the large N approximation. It turns out the Hartree terms are the same in both approximations, however due to the freedom of choosing $f(\mathbf{R}, \mathbf{k})$, they are equal only by construction. In contrast to the Hartree term, the Fock term in the large N and semiclassical approximation are different. Finally we compared the results for both approximations starting with the Fock self-energy dependence of $\tilde{X}$ for the value $\tilde{Y} = 0$ and $|\tilde{\mathbf{k}}| = \frac{1}{\sqrt{2}}$. We saw that both approximations reveal a characteristic $\varphi_{\mathbf{k}}$ dependence of the self-energy. This $\varphi_{\mathbf{k}}$ dependence splitting increases for larger values of α, that is the more the dipoles are tilted towards the plane. This behaviour is in correspondence with the stability behaviour of the dipole-dipole interaction. The self-energy even switches from a concave behaviour (stable) to a convex (unstable) behaviour according to Figure (4.2). Independent of the chosen values of α and $|\tilde{\mathbf{k}}|$ the two approximations coincide at the center of the trap $\tilde{\mathbf{R}} = 0$. In accordance with this we saw that the

dispersion relation within the center of the trap is identical for the large N and semiclassical approximation Figure 4.4. This behaviour only holds true for the center of the trap and away from the center of mass we saw significant differences Figure (4.2) within the dispersion relation. As noted before the large particle number assumption $N \gg 1$ is in general fulfilled in ultracold systems making our large N approximation almost exact within the Hartree-Fock approximation. We also pointed out, that this does not hold in general for the semiclassical Green function, which uses a short-time short-distance approximation.

5.2 Outlook

The investigation of degenerated Fermi systems in two dimensions represents a relatively fresh research field just on the boundary of experimental breakthrough. Therefore, the theoretical descriptions for real systems become more interesting. Descriptions of ultracold Fermi systems are either made in the collisonless or hydrodynamic limit. A more accurate description considers the regime in between of these two extreme cases. Here the self-energy has a significant contribution. However we have to say that already the calculation of the local self-energy lies on the boundary of what is possible analytically, so it is questionable if the large N approximation can be used further in this form. However it would be interesting trying to calculate the real spectrum within the large N approximation. Also it would be interesting to calculate the large N approximation in three-dimensions and again compare the two approximations.

Chapter 6

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Chapter 7

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Appendices

Appendix A

Saddle Point Approximation for n Integration

So far we have just stated that the cosine terms vanish when the integration over the quantum numbers n is executed. To see that the $\cos\left(\sqrt{2n}x - n\frac{\pi}{2}\right)$ can indeed be neglect for the n-integration, we will now demonstrate, that exemplary in one dimension. For that matter we look at the integral:

$$\int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{2n-x^2}} \cos^2\left(\sqrt{2n}x - n\frac{\pi}{2}\right) = \frac{1}{2}\int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{2n-x^2}} + \frac{1}{2}\int_{\frac{x^2}{2}}^{n_F} dn \frac{\cos(2\sqrt{2n}x - n\pi)}{\sqrt{2n-x^2}}\,. \tag{A.0.1}$$

The integral we are interested in is

$$\int_{\frac{x^2}{2}}^{n_F} dn \frac{\cos(2\sqrt{2n}x - n\pi)}{\sqrt{2n-x^2}} = \frac{1}{2}\int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{2n-x^2}} \left(e^{-i(2\sqrt{2n}x - n\pi)} + e^{-i(2\sqrt{2n}x - n\pi)}\right)\,. \tag{A.0.2}$$

The suppressions away from the saddle point is then the same as for the n-integration (4.1.12). So the only integration regime remaining to discuss is around the saddle point. If we define the function

$$a(x) = 2\sqrt{2n}x - n\pi. \tag{A.0.3}$$

We can make a saddle point approximation around n_s where $a'(n_s) = 0$.

$$\begin{aligned}
a'(n) &= \frac{1}{\sqrt{2n}}x - \pi \\
a''(n) &= \frac{x}{\sqrt{2n}n^{\frac{3}{2}}} \\
a'(n_s) = 0 &\Longrightarrow n_s = \frac{2n^2}{\pi^2} \\
a(n-n_s) &= a(n-n_s) + a'(n_s)\Delta n^2 = \frac{2x^2}{\pi} - \frac{\pi^3}{8x^2}\Delta n^2,
\end{aligned} \tag{A.0.4}$$

where $\Delta n := n - n_2$. We now just look on one of the integrals (A.0.2) $n_F \gg 1$

$$\sim \int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{2n_s - x^2}} e^{i\frac{2x^2}{\pi} - i\frac{\pi^3}{8x^2\Delta n^2}} = \int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{x^2(\frac{4}{\pi^2} - 1)}} e^{i\frac{2x^2}{\pi} - i\frac{\pi^3}{8x^2 n_s^2}}$$

$$= e^{i\frac{2x^2}{\pi}} \int_{\frac{x^2}{2}}^{n_F} dn \frac{1}{\sqrt{x^2(\frac{4}{\pi^2} - 1)}} e^{i\frac{2x^2}{\pi}} e^{-i\frac{\pi^3}{8x^2 n_s^2}} \tag{A.0.5}$$

$$= e^{\frac{i2x^2}{\pi}} \sqrt{\frac{8}{(4-\pi^2)\pi}} \int_{\frac{\pi^{\frac{3}{2}}}{4\sqrt{2}x}}^{\frac{\pi^{\frac{3}{2}}}{\sqrt{8x^2}}} d\eta \, e^{-i\eta^2} \, . \tag{A.0.6}$$

The integral (A.0.6) is finite. Therefore the contribution to (A.0.1) is neglectable compared to the leading divergent terms.

Appendix B

Baker-Campbell-Hausdorff Formula

The Baker-Campbell-Hausdorff formula is used various times throughout this text. For a proof we refer to [39]. Here we want to show how to use the linear map $\mathrm{ad}_x[y]$ in (2.1.44) to arrive at the relation (2.1.46) from the integral representation.

$$e^x e^y = e^z \tag{B.0.1}$$

$$Z = X + \int_0^1 \mathrm{d}t g\left(e^{\mathrm{ad}_x} e^{t\,\mathrm{ad}_y}\right)[y] \quad \text{mit} \quad g(z) = \frac{z\log(z)}{z-1}\,. \tag{B.0.2}$$

First we use the following series representation for the logarithm

$$\log(z) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)}(z-1)^{n+1}\,. \tag{B.0.3}$$

Now we can write

$$\begin{aligned}
g(z) &= \frac{z}{z-1}\log(z) = \frac{z}{z-1}\sum_{n=0}^{\infty}\frac{(-1)^n}{(n+1)}(z-1)^{n+1} \\
&= \frac{z}{z-1}\left[(z-1) - \frac{1}{2}(z-1)^2 + \frac{1}{3}(z-1)^3 - \frac{1}{4}(z-1)^4 + \frac{1}{5}(z-1)^5 - \dots\right] \\
&= \frac{1}{z-1}[1+(z-1)]\left[(z-1) - \frac{(z-1)^2}{2} + \frac{(z-1)^3}{3} - \frac{(z-1)^4}{4} + \frac{(z-1)^5}{5} - \dots\right] \\
&= \frac{1}{z-1}\left((z-1) - \frac{(z-1)^2}{2} + \frac{(z-1)^3}{3} - \frac{(z-1)^4}{4} + \frac{(z-1)^5}{5} - \dots\right. \\
&\qquad\qquad \left. +(z-1)^2 - \frac{(z-1)^3}{2} + \frac{(z-1)^4}{3} - \frac{(z-1)^5}{4} + \frac{(z-1)^6}{6} - \dots\right) \\
&= \left(1 - \frac{(z-1)}{2} + \frac{(z-1)^2}{3} - \frac{(z-1)^3}{4} + \frac{(z-1)^4}{5} - \dots\right. \\
&\qquad\qquad \left. +(z-1) - \frac{(z-1)^2}{2} + \frac{(z-1)^3}{3} - \frac{(z-1)^4}{4} + \frac{(z-1)^5}{6} - \dots\right) \\
&= 1 + (z-1)\left(1-\frac{1}{2}\right) + (z-1)^2\left(\frac{1}{3}-\frac{1}{2}\right) + (z-1)^3\left(\frac{1}{3}-\frac{1}{4}\right) + (z-1)^4\left(\frac{1}{5}-\frac{1}{4}\right) + \dots \\
&= 1 + (z-1)\left(\frac{1}{1}-\frac{1}{2}\right) - (z-1)^2\left(\frac{1}{2}-\frac{1}{3}\right) + (z-1)^3\left(\frac{1}{3}-\frac{1}{4}\right) - (z-1)^4\left(\frac{1}{4}-\frac{1}{5}\right) + \dots
\end{aligned} \tag{B.0.4}$$

and with $\left(\frac{1}{m}-\frac{1}{m+1}\right)=\frac{m+1}{m(m+1)}-\frac{m}{m(m+1)}=\frac{1}{m(m+1)}$ we get

$$g(z)=1+\sum_{m=1}^{\infty}\frac{1}{m(m+1)}(-1)^{m+1}(z-1)^m\,. \tag{B.0.5}$$

Then we expand the expression

$$\begin{aligned}
e^{\mathrm{ad}_x}e^{t\,\mathrm{ad}_y} &= \left(\sum_{n=0}^{\infty}\frac{(\mathrm{ad}_x)^n}{n!}\right)\left(\sum_{k=0}^{\infty}\frac{t\,(\mathrm{ad}_y)^k}{k!}\right)\\
&= \left(1+\frac{(\mathrm{ad}_x)}{1!}+\frac{(\mathrm{ad}_x)^2}{2!}+\frac{(\mathrm{ad}_x)^3}{3!}+\dots\right)\left(1+\frac{t\,(\mathrm{ad}_y)}{1!}+\frac{t^2\,(\mathrm{ad}_y)^2}{2!}+\frac{t^3\,(\mathrm{ad}_y)^3}{3!}+\dots\right)\\
&= 1+\frac{(\mathrm{ad}_x)}{1!}+\frac{(\mathrm{ad}_x)^2}{2!}+\frac{(\mathrm{ad}_x)^3}{3!}+\frac{t\,(\mathrm{ad}_y)}{1!}+\frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!}+\frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!}+\frac{t\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)}{3!1!}\\
&\quad+\frac{t^2\,(\mathrm{ad}_y)^2}{2!}+\frac{t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!2!}+\frac{t^2\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{2!2!}+\frac{t^3\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)^3}{2!3!}\\
&\quad+\frac{t^3\,(\mathrm{ad}_y)^3}{3!}+\frac{t^3\,(\mathrm{ad}_x)(\mathrm{ad}_y)^3}{1!3!}+\frac{t^3\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)^3}{2!3!}+\frac{t^3\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)^3}{3!3!}\\
&= 1+\frac{\mathrm{ad}_x}{1!}+\frac{t\,(\mathrm{ad}_y)}{1!}+\frac{(\mathrm{ad}_x)^2}{2!}+\frac{t^2\,(\mathrm{ad}_y)^2}{2!}+\frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!}+\\
&\quad+\frac{(\mathrm{ad}_x)^3}{3!}+\frac{t^3\,(\mathrm{ad}_y)^3}{3!}+\frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!}+\frac{t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!2!}+\dots
\end{aligned} \tag{B.0.6}$$

and now consider

$$\begin{aligned}
(z-1) &= \left(e^{\mathrm{ad}_x}e^{t\mathrm{ad}_x}-1\right)\\
&= \left(\frac{\mathrm{ad}_x}{1!}+\frac{t\,\mathrm{ad}_y}{1!}+\frac{(\mathrm{ad}_x)^2}{2!}+\frac{t^2\,(\mathrm{ad}_y)^2}{2!}+\frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!}\right.\\
&\qquad\left.+\frac{(\mathrm{ad}_x)^3}{3!}+\frac{t^3\,(\mathrm{ad}_y)^3}{3!}+\frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!}+\frac{t^2\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{1!2!}+\dots\right)
\end{aligned} \tag{B.0.7}$$

The second term is then given by

$$
\begin{aligned}
&\left(e^{\mathrm{ad}_x} e^{t\mathrm{ad}_y} - 1\right)^2 \\
&= \Bigg(\frac{\mathrm{ad}_x^2}{1!1!} + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!} + \frac{(\mathrm{ad}_x)^3}{2!} + \frac{t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!2!} + \frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{1!1!1!} \\
&\quad + \frac{(\mathrm{ad}_x)^4}{1!3!} + \frac{t^3\,(\mathrm{ad}_x)(\mathrm{ad}_y)^3}{1!3!} + \frac{t\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)}{1!2!1!} + \frac{t^2\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)^2}{1!1!2!} + \dots \\
&\quad + \frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)}{1!1!} + \frac{t^2(\mathrm{ad}_y)^2}{1!1!} + \frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{1!2!} \\
&\quad + \frac{t^3(\mathrm{ad}_y)^3}{1!2!} + \frac{t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!1!} + \frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)^3}{1!3!} \\
&\quad + \frac{t^4(\mathrm{ad}_y)^4}{1!3!} + \frac{t^2(\mathrm{ad}_y)(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{1!2!1!} + \frac{t^3(\mathrm{ad}_y)(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{1!1!2!} + \dots \\
&\quad + \frac{(\mathrm{ad}_x)^3}{2!1!} + \frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!} + \frac{(\mathrm{ad}_x)^4}{2!2!} + \frac{t^2(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{2!2!} \\
&\quad + \frac{t\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)}{2!1!1!} + \frac{(\mathrm{ad}_x)^5}{2!3!} \\
&\quad + \frac{t^3(\mathrm{ad}_x)^2(\mathrm{ad}_y)^3}{2!3} + \frac{t\,(\mathrm{ad}_x)^4(\mathrm{ad}_y)}{2!2!1!} + \frac{t^2\,(\mathrm{ad}_x)^4(\mathrm{ad}_y)^2}{2!1!2!} + \dots \\
&\quad + \frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)}{2!1!} + \frac{t^3(\mathrm{ad}_y)^3}{2!1!} + \frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)^2}{2!2!} + \frac{t^4(\mathrm{ad}_y)^4}{2!2!} + \frac{t^3(\mathrm{ad}_y)^2(\mathrm{ad}_x)(\mathrm{ad}_y)}{2!1!1!} \\
&\quad + \frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)^3}{2!3!} + \frac{t^5(\mathrm{ad}_y)^5}{2!3!} + \frac{t^3(\mathrm{ad}_y)^2(\mathrm{ad}_x)(\mathrm{ad}_y)}{2!2!1!} + \frac{t^4(\mathrm{ad}_y)^2(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{2!1!2!} + \dots \\
&\quad + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)}{1!1!1!} + \frac{t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!1!1!} + \frac{t\,(\mathrm{ad}_x)^4(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{1!1!2!} + \frac{t^3(\mathrm{ad}_x)(\mathrm{ad}_y)^3}{1!1!2!} \\
&\quad + \frac{t^2(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!1!1!} + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)^3}{1!1!3!} + \frac{t^4\,(\mathrm{ad}_x)(\mathrm{ad}_y)^4}{1!1!3!} \\
&\quad + \frac{t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{1!1!2!1!} + \frac{t^3\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{1!1!1!2!} + \dots \Bigg) \,.
\end{aligned}
\tag{B.0.8}
$$

Now we will have a look at the third term

$$
\begin{aligned}
&\left[\mathrm{ad}_x + t\mathrm{ad}_y + \frac{(\mathrm{ad}_x)^2}{2!} + \dots\right]\left[\mathrm{ad}_x + t\mathrm{ad}_y \frac{(\mathrm{ad}_x)^2}{2!} + \dots\right] \\
&= \mathrm{ad}_x^2 + t\,(\mathrm{ad}_x)(\mathrm{ad}_y) + \frac{(\mathrm{ad}_x)^3}{2!} + t(\mathrm{ad}_y)(\mathrm{ad}_x) + t^2(\mathrm{ad}_y)^2 + \frac{t\,(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{2!} \\
&\quad + \frac{(\mathrm{ad}_x)^3}{2!} + \frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!} + \frac{(\mathrm{ad}_x)^4}{2!2!} + \dots
\end{aligned}
\tag{B.0.9}
$$

$$
\begin{aligned}
&\left[\mathrm{ad}_x + t\,\mathrm{ad}_y + \frac{(\mathrm{ad}_x)^2}{2!}\right]^3 \\
&= \mathrm{ad}_x^3 + t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y) + \frac{(\mathrm{ad}_x)^4}{2!} + t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x) + t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2 + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{2!} \\
&+ \frac{(\mathrm{ad}_x)^4}{2!} + \frac{t\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)}{2!} + \frac{(\mathrm{ad}_x)^5}{2!2!} \\
&+ t(\mathrm{ad}_y)(\mathrm{ad}_x)^2 + t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y) + \frac{t\,(\mathrm{ad}_y)(\mathrm{ad}_x)^3}{2!} \\
&+ t^2\,(\mathrm{ad}_y)^2(\mathrm{ad}_x) + t^3\,(\mathrm{ad}_y)^3 + \frac{t^2\,(\mathrm{ad}_y)^2(\mathrm{ad}_x)^2}{2!} + \frac{t\,(\mathrm{ad}_y)(\mathrm{ad}_x)^3}{2!} + \frac{t^2\,(\mathrm{ad}_y)(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!} \\
&+ \frac{t\,(\mathrm{ad}_y)(\mathrm{ad}_x)^4}{2!2!} + \frac{(\mathrm{ad}_x)^4}{2!} + \frac{t\,(\mathrm{ad}_x)^3(\mathrm{ad}_y)}{2!} + \frac{(\mathrm{ad}_x)^5}{2!2!} + \frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)(\mathrm{ad}_x}{2!} \\
&+ t^2\frac{(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{2!} + t\frac{(\mathrm{ad}_x)^2\mathrm{ad}_y(\mathrm{ad}_x)^2}{2!2!} + \frac{(\mathrm{ad}_x)^5}{2!2!} + t\frac{(\mathrm{ad}_x)^4(\mathrm{ad}_y)}{2!2!} + \frac{(\mathrm{ad}_x)^6}{2!2!2!}
\end{aligned}
\tag{B.0.10}
$$

Then we can write g as

$$
\begin{aligned}
g\left(e^{\mathrm{ad}_x}e^{t\mathrm{ad}_y}\right) = 1 &+ \frac{1}{2}\left[\frac{\mathrm{ad}_x}{1!} + \frac{t(\mathrm{ad}_y)}{1!} + \frac{(\mathrm{ad}_x)^2}{2!} + \frac{t^2(\mathrm{ad}_y)^2}{2!} + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!}\right. \\
&\left. + \frac{(\mathrm{ad}_x)^3}{3!} + \frac{t^3(\mathrm{ad}_y)^3}{3!} + \frac{t\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!} + \frac{t^2\,(\mathrm{ad}_x)^2(\mathrm{ad}_y)^2}{1!2!} + \ldots\right] \\
&- \frac{1}{6}\left[(\mathrm{ad}_x)^2 + \frac{t(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!} + \frac{(\mathrm{ad}_x)^3}{2!} + \frac{t^2(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!2!} + \frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{1!1!1!}\right. \\
&\quad + \frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)}{1!1!} + \frac{t^2(\mathrm{ad}_y)^2}{1!1!} + \frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{2!1!} + \frac{t^3(\mathrm{ad}_y)^3}{2!1!} + \frac{t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)}{1!1!1!} \\
&\quad + \frac{(\mathrm{ad}_x)^3}{2!1!} + \frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{2!1!} \\
&\quad \left. + \frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)}{2!1!} + \frac{t^3(\mathrm{ad}_y)^3}{2!1!} + \frac{t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)}{1!1!1!} + \frac{t^2(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{1!1!1!} + \ldots\right] \\
&+ \frac{1}{12}\left[(\mathrm{ad}_x)^3 + t\,(\mathrm{ad}_x)^2\mathrm{ad}_y + t\,(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x) + t^2\,(\mathrm{ad}_x)(\mathrm{ad}_y)^2 + t\,(\mathrm{ad}_y)(\mathrm{ad}_x)^2\right. \\
&\quad \left. + t^2\,(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y) + t^2\,(\mathrm{ad}_y)^2(\mathrm{ad}_x) + t^3\,(\mathrm{ad}_y)^3 + \ldots\right]
\end{aligned}
\tag{B.0.11}
$$

$$
\begin{aligned}
g\left(e^{\mathrm{ad}_x}e^{t\mathrm{ad}_y}\right) &= 1+\frac{1}{2}\mathrm{ad}_x+t\mathrm{ad}_y \\
&+\frac{(\mathrm{ad}_x)^2}{4}+\frac{t^2(\mathrm{ad}_y)^2}{4}+\frac{t(\mathrm{ad}_x)(\mathrm{ad}_y)}{2}-\frac{(\mathrm{ad}_x)^2}{6}-\frac{t(\mathrm{ad}_x)(\mathrm{ad}_y)}{6}-\frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)}{6}-\frac{t^2(\mathrm{ad}_y)^2}{6} \\
&+\frac{(\mathrm{ad}_x)^3}{12}+\frac{t^3(\mathrm{ad}_y)^3}{12}+\frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{4}-\frac{(\mathrm{ad}_x)^3}{12}-\frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{6} \\
&-\frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{12}-\frac{t^3(\mathrm{ad}_y)^3}{12}-\frac{t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)}{6}-\frac{(\mathrm{ad}_x)^3}{12}-\frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{12} \\
&-\frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)}{12}-\frac{t^3(\mathrm{ad}_y)^3}{12}-\frac{t(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)}{6}-\frac{t^2(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{6} \\
&+\frac{(\mathrm{ad}_x)^3}{12}+\frac{t(\mathrm{ad}_x)^2(\mathrm{ad}_y)}{12}+\frac{t(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)}{12}+\frac{t^2(\mathrm{ad}_x)(\mathrm{ad}_y)^2}{12}+\frac{t(\mathrm{ad}_y)(\mathrm{ad}_x)^2}{12} \\
&+\frac{t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)}{12}+\frac{t^2(\mathrm{ad}_y)^2(\mathrm{ad}_x)}{12}+\frac{t^3(\mathrm{ad}_y)^3}{12}+\dots \\
&= 1+\frac{\mathrm{ad}_x}{2}+\frac{t}{2}\mathrm{ad}_y \\
&+\frac{1}{12}(\mathrm{ad}_x)^2+\frac{1}{12}t^2(\mathrm{ad}_x)^2+\frac{1}{3}t(\mathrm{ad}_x)(\mathrm{ad}_y)-\frac{1}{6}t(\mathrm{ad}_y)(\mathrm{ad}_x) \\
&+\frac{1}{12}t(\mathrm{ad}_x)^2\mathrm{ad}_y+\frac{1}{4}t^2(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)-\frac{1}{12}t(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)-\frac{1}{12}t^2(\mathrm{ad}_x)(\mathrm{ad}_y)^2\,. \qquad \text{(B.0.12)}
\end{aligned}
$$

The integration now yields

$$
\begin{aligned}
\int_0^1 \mathrm{d}t g\left(e^{\mathrm{ad}_x}e^{t\mathrm{ad}_y}\right) &= 1+\frac{\mathrm{ad}_x}{2}+\frac{\mathrm{ad}_y}{4} \\
&+\frac{1}{12}(\mathrm{ad}_x)^2+\frac{1}{36}(\mathrm{ad}_y)^2+\frac{1}{6}(\mathrm{ad}_x)(\mathrm{ad}_y)-\frac{1}{12}(\mathrm{ad}_y)(\mathrm{ad}_x) \\
&+\frac{1}{24}(\mathrm{ad}_x)^2\mathrm{ad}_y+\frac{1}{12}(\mathrm{ad}_y)(\mathrm{ad}_x)(\mathrm{ad}_y)-\frac{1}{24}(\mathrm{ad}_x)(\mathrm{ad}_y)(\mathrm{ad}_x)-\frac{1}{36}(\mathrm{ad}_x)(\mathrm{ad}_y)^2+\dots
\end{aligned} \qquad \text{(B.0.13)}
$$

$$
\begin{aligned}
\int_0^1 dtg\left(e^{\mathrm{ad}_x}e^{t\,\mathrm{ad}_y}\right)[y] &= y+\frac{1}{2}[x,y]+[y,y]+\frac{1}{12}[x,[x,y]]+\frac{1}{36}[y,[y,y]] \\
&+\frac{1}{6}[x,[y,y]]-\frac{1}{12}[y,[x,y]] \\
&+\frac{1}{24}[x,[x,[y,y]]]+\frac{1}{12}[y,[x,[y,y]]] \\
&-\frac{1}{24}[x,[y,[x,y]]]-\frac{1}{36}[x,[y,[y,y]]] \\
&= y+\frac{1}{2}[x,y]+\frac{1}{12}[x,[x,y]]-\frac{1}{12}[y[x,y]] \\
&-\frac{1}{24}[x,[y,[x,y]]]+\dots\,. \qquad \text{(B.0.14)}
\end{aligned}
$$

And so we finally get

$$
\begin{aligned}
z = x+\int_0^1 \mathrm{d}t g\left(e^{\mathrm{ad}_x}e^{t\mathrm{ad}_y}\right)[y] = \\
x+y+\frac{1}{2}[x,y]+\frac{1}{12}\left([x,[x,y]]-[y,[x,y]]\right)-\frac{1}{24}[x,[y,[x,y]]]+\dots\,. \qquad \text{(B.0.15)}
\end{aligned}
$$

Appendix C

Gauss Integrals

Gauss Integrals

While dealing with the path integral the use of Gaussian integrals is unavoidable, here we shortly assemble the most needed properties: We start with the standard Gauss integral, as it is well known, the derivation start by taking the square and switching to polar coordinates. The result reads

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi}. \tag{C.0.1}$$

The next step to take is making a simple substitution, which leads to

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \int_{-\infty}^{\infty} dx\, e^{-(\sqrt{a}x)^2} = \frac{1}{\sqrt{a}} \int_{-\infty}^{\infty} d\eta\, e^{-\eta^2} = \sqrt{\frac{\pi}{a}}. \tag{C.0.2}$$

The next step is to take a linear term into account. The formula can then be brought to the standard form (C.0.1) by a quadratic expansion.

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2+bx} = \int_{-\infty}^{\infty} dx\, e^{-(\sqrt{a}x-\frac{b}{2\sqrt{a}})^2+\frac{b^2}{4a}} = \sqrt{\frac{\pi}{a}} e^{\frac{b^2}{4a}} \qquad \mathrm{Re}(a) > 0. \tag{C.0.3}$$

Complex Gauss integrals are defined as

$$\int d(\overline{z}, z)\, e^{-\overline{z}wz} := \int_{-\infty}^{\infty} \mathrm{Re}(z) \int_{-\infty}^{\infty} \mathrm{Im}(z)\, e^{-\overline{z}wz}. \tag{C.0.4}$$

By rewriting the complex numbers with the their real and imaginary part as $z = z_x + iz_y$ and $w = w_x + iw_y$

$$(z_x - iz_y)(w_x + iw_y)(z_x + iz_y) = (w_x + iw_y)z_x^2 + (w_x + iw_y)z_y^2 = wz_x^2 + wz_y^2 \tag{C.0.5}$$

the complex Gauss integral (C.0.4) can be solved with the help of (C.0.1)

$$\int d(\overline{z}, z)\, e^{-\overline{z}wz} = \int_{-\infty}^{\infty} dz_x \int_{-\infty}^{\infty} dz_y e^{-(wz_x^2+wz_y^2)} = \sqrt{\frac{\pi}{w}} \int_{-\infty}^{\infty} dz_x e^{-wz_x^2} = \frac{\pi}{w} \quad \mathrm{Re}(w) > 0\,. \tag{C.0.6}$$

In the same way we can can solve

$$\begin{aligned} \int d(\overline{z}, z) e^{-\overline{z}wz+\overline{u}z+\overline{z}v} &= \int_{-\infty}^{\infty} dz_x e^{-wz_x^2+(\overline{u}+v)z_x} \int_{-\infty}^{\infty} dz_y\, e^{-wz_y^2+i(\overline{u}-v)z_y} \\ &= \frac{\pi}{w} e^{\frac{(\overline{u}+v)^2-(\overline{u}-v)^2}{4w}} = \frac{\pi}{w} e^{\frac{(\overline{u}^2+v^2+2\overline{u}v-\overline{u}^2-v^2+2\overline{u}v}{4w}} \\ &= \frac{\pi}{w} e^{\frac{\overline{u}v}{w}} \quad \mathrm{Re}(w) > 0\,. \end{aligned} \tag{C.0.7}$$

Multidimensional Gauss integrals

Based on the above expressions we can now go over to the really needed multidimensional Gauss integrals. For simplicity we assume a real Matrix $\mathbf{A}$ which is symmetric and positive. Then there exits an orthogonal transforamtion $\mathbf{D}$ with $\mathbf{D}^T\mathbf{D} = \mathbf{D}^T\mathbf{D} = \mathbb{1}$ and $\mathbf{D}^T A\mathbf{D} = \mathrm{diag}(\lambda_1, \lambda_2, ..., \lambda_n) =: \mathbf{B}$. With this we can now solve the integral

$$\begin{aligned}\int d\mathbf{v} e^{-\mathbf{v}^T\mathbf{A}\mathbf{v}} &= \int d\mathbf{v} e^{-\mathbf{v}^T(\mathbf{D}\mathbf{D}^T)\mathbf{A}(\mathbf{D}\mathbf{D}^T)\mathbf{v}} = \int d\mathbf{v} e^{-(\mathbf{v}^T\mathbf{D})\mathbf{D}^T\mathbf{A}\mathbf{D}(\mathbf{D}^T\mathbf{v})} \\ &= \int d\mathbf{u} e^{-\mathbf{u}^T\mathbf{B}\mathbf{u}} = \prod_{n=1}^{N}\left[\int dx_n e^{-\lambda_n u_n^2}\right] \\ &= \prod_{n=1}^{N}\left[\sqrt{\frac{\pi}{\lambda_n}}\right] = \pi^{\frac{N}{2}}\prod_{n=1}^{N}\frac{1}{\sqrt{\lambda_n}} = \pi^{\frac{N}{2}}\frac{1}{\sqrt{\prod_{n=1}^{N}\lambda_n}} \\ &= \pi^{\frac{N}{2}}\frac{1}{\sqrt{\det(\mathbf{A})}}\,. \end{aligned} \tag{C.0.8}$$

The n-dimensional analogue to (C.0.3) can be solved by considering the following matrix transformations $\mathbf{u} = \mathbf{v} + \mathbf{A}^{-1}\mathbf{j} \Rightarrow \mathbf{v} = \mathbf{u} - \mathbf{A}^{-1}\mathbf{j} \Rightarrow \mathbf{v}^T = \mathbf{u}^T - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T$,

$$\begin{aligned}-\mathbf{v}^T\mathbf{A}\mathbf{v} - 2\mathbf{j}^T\mathbf{v} &= -\left[\mathbf{u}^T - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\right]\mathbf{A}\left[\mathbf{u} - \mathbf{A}^{-1}\mathbf{j}\right] - 2\left[\mathbf{j}^T\mathbf{u} - \mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right] \\ &= -\mathbf{u}^T\mathbf{A}\mathbf{u} + \mathbf{u}^T\mathbf{A}\mathbf{A}^{-1}\mathbf{j} + \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{u} - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{A}^{-1}\mathbf{j} - 2\mathbf{j}^T\mathbf{u} + 2\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right] \\ &= -\mathbf{u}^T\mathbf{A}\mathbf{u} + \mathbf{u}^T\mathbf{j} + \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{u} - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{j} - 2\mathbf{j}^T\mathbf{u} + 2\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right]\,. \end{aligned} \tag{C.0.9}$$

Due to the fact, tat the inverse of a symmetric matrix is again symmetric, we can write $\left(\mathbf{A}^{-1}\right)^T = \mathbf{A}^{-1}$, with which follows:

$$\begin{aligned}-\mathbf{v}^T\mathbf{A}\mathbf{v} - 2\mathbf{j}^T\mathbf{v} &= -\left[\mathbf{u}^T - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\right]\mathbf{A}\left[\mathbf{u} - \mathbf{A}^{-1}\mathbf{j}\right] - 2\left[\mathbf{j}^T\mathbf{u} - \mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right] \\ &= -\mathbf{u}^T\mathbf{A}\mathbf{u} + \mathbf{u}^T\mathbf{A}\mathbf{A}^{-1}\mathbf{j} + \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{u} - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{A}^{-1}\mathbf{j} - 2\mathbf{j}^T\mathbf{u} + 2\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right] \\ &= -\mathbf{u}^T\mathbf{A}\mathbf{u} + \mathbf{u}^T\mathbf{j} + \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{A}\mathbf{u} - \mathbf{j}^T\left(\mathbf{A}^{-1}\right)^T\mathbf{j} - 2\mathbf{j}^T\mathbf{u} + 2\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}\right]\,. \end{aligned} \tag{C.0.10}$$

With this considerations we can solve the following Gauss integral

$$\int d\mathbf{v} e^{-\mathbf{v}^T\mathbf{A}\mathbf{v} - 2\mathbf{j}^T\mathbf{v}} = e^{\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}}\int d\mathbf{u} e^{-\mathbf{u}^T\mathbf{A}\mathbf{u}} = \pi^{\frac{N}{2}}\frac{1}{\sqrt{\det(\mathbf{A})}}e^{\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}}\,. \tag{C.0.11}$$

Other forms of writing the last expressions are

$$\int d\mathbf{v} e^{-\mathbf{v}^T\mathbf{A}\mathbf{v} \pm 2\mathbf{j}^T\mathbf{v}} = \pi^{\frac{N}{2}}\frac{1}{\sqrt{\det(\mathbf{A})}}e^{\mathbf{j}^T\mathbf{A}^{-1}\mathbf{j}}\,. \tag{C.0.12}$$

Next we look at the n-dimensional complex Gauss integral. In this case we consider a hermetic Matrix $\mathbf{A}$, that is $\mathbf{A} = \mathbf{A}^\dagger$, then there exists a unitary transformation $\mathbf{U}$ with $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbb{1}$, such that $\mathbf{U}^\dagger\mathbf{A}\mathbf{U} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots \lambda_N) =: \mathbf{B}$ where $\lambda_i \in \mathbb{C}$ are the eigenvalues of the matrix $\mathbf{A}$. Then the following

complex Gauss integral can be solved

$$\begin{aligned}\int d(\mathbf{v},\mathbf{v}^\dagger)\, e^{-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}} &= \int d(\mathbf{v},\mathbf{v}^\dagger)\, e^{-\mathbf{v}^\dagger(\mathbf{U}\mathbf{U}^\dagger)\mathbf{A}(\mathbf{U}\mathbf{U}^\dagger)\mathbf{v}} = \int d(\mathbf{v},\mathbf{v}^\dagger)\, e^{-(\mathbf{v}^\dagger\mathbf{U})\mathbf{U}^\dagger\mathbf{A}\mathbf{U}(\mathbf{U}^\dagger\mathbf{v})} \\ &= \int d(\mathbf{a},\mathbf{a}^\dagger)\, e^{-\mathbf{a}^\dagger\mathbf{B}\mathbf{a}} = \prod_i^N \int d(\mathbf{a},\overline{\mathbf{a}})\, e^{-\overline{a}_i\lambda_i a_i} \\ &= \prod_i^N \frac{\pi}{\lambda_i} = \pi^N \frac{1}{\prod_i \lambda_i} \\ &= \pi^N \frac{1}{\det(\mathbf{A})}\,. \end{aligned} \tag{C.0.13}$$

By considering the transformation

$$\mathbf{v}^\dagger = \mathbf{u}^\dagger + \mathbf{w}^\dagger\mathbf{A}^{-1} \qquad\qquad \mathbf{v} = \mathbf{u} + \mathbf{A}^{-1}\mathbf{w}'\,,$$

we can conclude

$$\begin{aligned}-\mathbf{v}^\dagger\mathbf{A}\mathbf{v} + \mathbf{w}^\dagger\mathbf{v} + \mathbf{v}^\dagger\mathbf{w}' &= -\left[\mathbf{u}^\dagger + \mathbf{w}^\dagger\mathbf{A}^{-1}\right]\mathbf{A}\left[\mathbf{u} + \mathbf{A}^{-1}\mathbf{w}'\right] + \mathbf{w}^\dagger\left[\mathbf{u} + \mathbf{A}^{-1}\mathbf{w}'\right] + \left[\mathbf{u}^\dagger + \mathbf{w}^\dagger\mathbf{A}^{-1}\right]\mathbf{w}' \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u} - \mathbf{u}^\dagger\mathbf{A}\mathbf{A}^{-1}\mathbf{w}' - \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{A}\mathbf{u} - \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{A}\mathbf{A}^{-1}\mathbf{w}' + \mathbf{w}^\dagger\mathbf{u} \\ &\qquad + \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}' + \mathbf{u}^\dagger\mathbf{w}' + \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}' \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u} - \mathbf{u}^\dagger\mathbf{w}' - \mathbf{w}^\dagger\mathbf{u} - \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}' + \mathbf{w}^\dagger\mathbf{u} + \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}' + \mathbf{u}^\dagger\mathbf{w}' + \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}' \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u} + \mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}'\,, \end{aligned} \tag{C.0.14}$$

and finally solve the following n-dimensional complex Gauss integral

$$\begin{aligned}\int d(\mathbf{v},\mathbf{v}^\dagger) = e^{-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}+\mathbf{w}^\dagger\mathbf{v}+\mathbf{v}^\dagger\mathbf{w}'} &= \int \mathrm{d}(\mathbf{u},\mathbf{u}^\dagger) e^{-\mathbf{u}^\dagger\mathbf{A}\mathbf{u}+\mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}'} \\ &= e^{\mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}'} \int d(\mathbf{u},\mathbf{u}^\dagger) e^{-\mathbf{u}^\dagger\mathbf{A}\mathbf{u}} \\ &= \pi^N \frac{1}{\det(\mathbf{A})} e^{\mathbf{w}^\dagger\mathbf{A}^{-1}\mathbf{w}'}\,. \end{aligned} \tag{C.0.15}$$

Finally we have to consider the Grassmann Gauss integral.

$$\int d\overline{\eta} \int d\eta\, e^{-\overline{\eta}a\eta}\,. \tag{C.0.16}$$

According to to our convention (2.1.57(and the fact that we can expand the expontental function due to Baker-Campbell-Hausdorff formula (2.1.44), we can immediately solve the simple Gauss integral

$$\int d\overline{\eta} \int d\eta\,(1 - \overline{\eta}a\,\eta) = -a\int d\overline{\eta} \int d\eta\,\overline{\eta}\,\eta = a\int d\overline{\eta} \int d\eta\,\eta\,\overline{\eta} = a\int d\overline{\eta}\eta = a$$

Next we use a hermetic transformation $\mathbf{U}\mathbf{U}^\dagger = \mathbf{U}^\dagger\mathbf{U} = \mathbb{1}$ so that $\mathbf{U}$ diagonalizes the matrix $\mathbf{A}$, that is $\mathbf{U}^\dagger\mathbf{A}\mathbf{U} = \mathrm{diag}(\lambda_1,\lambda_2,\ldots\lambda_N) =: \mathbf{B}$. Now we can solve the Grassmann Gauss integral the same way as the

complex Gauss integral

$$\begin{aligned}\int d(\mathbf{v}^\dagger,\mathbf{v})e^{-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}} &= \int d(\mathbf{v}^\dagger,\mathbf{v})e^{\mathbf{v}^\dagger\mathbf{A}\mathbf{v}} = \int d(\mathbf{v},\mathbf{v}^\dagger)e^{\mathbf{v}^\dagger(\mathbf{U}\mathbf{U}^\dagger)\mathbf{A}(\mathbf{U}^\dagger\mathbf{U})\mathbf{v}} \\ &= \int d(\mathbf{v}^\dagger,\mathbf{v})e^{\overline{\mathbf{v}}^\dagger(\mathbf{U}\mathbf{U}^\dagger)\mathbf{A}(\mathbf{U}^\dagger\mathbf{U})\mathbf{v}} \\ &= \int d(\mathbf{v}^\dagger,\mathbf{v})e^{\overline{\mathbf{v}}^\dagger\mathbf{U}(\mathbf{U}^\dagger\mathbf{A}\mathbf{U})\mathbf{U}^\dagger\mathbf{v}} \\ &= \prod_{i=1}^{N}\int d\overline{u}_i\, du_i\, e^{\overline{u}_i\lambda_i u_i} \\ &= \prod_{i=1}^{N}\int d\overline{u}_i\, du_i\, (1-\lambda_i\overline{u}_i u_i) \\ &= \prod_{i=1}^{N}\lambda_i = \det(\mathbf{A})\ . \end{aligned} \tag{C.0.17}$$

Next we consider the integral

$$\int d(\mathbf{v}^\dagger,\mathbf{v})e^{-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}+\rho^\dagger\mathbf{v}+\mathbf{v}^\dagger\rho} = \prod_{i=1}^{N}\int d\overline{v}_i dv_i\, e^{-\overline{v}_i A_{i\,j}v_j+\overline{\rho}_i v_i+\overline{v}_i\rho_i} \qquad \overline{v},v,\overline{\rho},\rho\in\text{Grassmann} \quad A \text{ hermetic}\ , \tag{C.0.18}$$

and make the substitution

$$\begin{aligned}\mathbf{u} = \mathbf{v}-\mathbf{A}^{-1}\rho \quad &\Leftrightarrow \quad \mathbf{v} = \mathbf{u}+\mathbf{A}^{-1}\rho \qquad \text{or} \quad v_i = u_i + A^{-1}_{ij}\rho_j \\ \mathbf{u}^\dagger = \mathbf{v}^\dagger-\mathbf{A}^{-1}\rho^\dagger \quad &\Leftrightarrow \quad \mathbf{v}^\dagger = \mathbf{u}+\mathbf{A}^{-1}\rho \qquad \text{or} \quad \overline{v}_i = \overline{u}_i + \overline{A}_{ij}{}^{-1}\rho_j\ . \end{aligned} \tag{C.0.19}$$

With this substitution we are in position to rewrite the exponent as

$$\begin{aligned}-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}+\rho^\dagger\mathbf{v}+\mathbf{v}^\dagger\rho &= \left[\mathbf{u}^\dagger+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\right]\mathbf{A}\left[\mathbf{u}+\mathbf{A}^{-1}\rho\right]+\rho^\dagger\left(\mathbf{u}+\mathbf{A}^{-1}\rho\right)+\left(\mathbf{u}^\dagger+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\right)\rho \\ &= -\left[\mathbf{u}^\dagger\mathbf{A}\mathbf{u}+\mathbf{u}^\dagger\mathbf{A}\mathbf{A}^{-1}\rho+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\mathbf{A}\mathbf{u}+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\mathbf{A}\mathbf{A}^{-1}\rho\right] \\ &\qquad +\rho^\dagger\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho+\mathbf{u}^\dagger\rho+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\rho \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u}-\mathbf{u}^\dagger\rho-\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\mathbf{A}\mathbf{u}-\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\rho+\rho^\dagger\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho+\mathbf{u}^\dagger\rho+\rho^\dagger\left(\mathbf{A}^{-1}\right)^\dagger\rho \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u}-\mathbf{u}^\dagger\rho-\rho^\dagger\mathbf{A}^{-1}\mathbf{A}\mathbf{u}-\rho^\dagger\mathbf{A}^{-1}\rho+\rho^\dagger\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho+\mathbf{u}^\dagger\rho+\rho^\dagger\mathbf{A}^{-1}\rho \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u}-\rho^\dagger\mathbf{u}+\rho^\dagger\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho \\ &= -\mathbf{u}^\dagger\mathbf{A}\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho\ . \end{aligned} \tag{C.0.20}$$

Now we are able to solve the Grassmann Gauss integral as follows

$$\begin{aligned}\int d(\mathbf{v}^\dagger,\mathbf{v})e^{-\mathbf{v}^\dagger\mathbf{A}\mathbf{v}+\rho^\dagger\mathbf{v}+\mathbf{v}^\dagger\rho} &= \int d(\mathbf{v}^\dagger,\mathbf{v})e^{-\mathbf{u}^\dagger\mathbf{A}\mathbf{u}+\rho^\dagger\mathbf{A}^{-1}\rho} \\ &= e^{\rho^\dagger\mathbf{A}^{-1}\rho}\int d(\mathbf{v}^\dagger,\mathbf{v})e^{-\mathbf{u}^\dagger\mathbf{A}\mathbf{u}} \\ &= e^{\rho^\dagger\mathbf{A}^{-1}\rho}\det(\mathbf{A})\ . \end{aligned} \tag{C.0.21}$$

Appendix D

Solving Differential Equation for Free Green Function

We have derived the expression for the Green function using the path integral. Thereby it was crucial to analyse what happens at equal times. It is instructive to see how one can derive the Green function immediately, if the subtlety of equal times is not given. For completeness this derivation is shown here. We can also solve the differential equation

$$(\hbar\partial_\tau + \varepsilon_\lambda - \mu)\, G\left(\lambda\ \tau|\lambda\tau'\right) = \delta(\tau - \tau')\,, \tag{D.0.1}$$

with the boundary condition

$$G\left(\lambda\hbar\beta|\lambda\tau'\right) = \zeta G\left(\lambda\, 0|\lambda\tau'\right) \tag{D.0.2}$$

First we set $a = \varepsilon_\lambda - \mu$ and $y := \tau - \tau' \Rightarrow \frac{\partial f}{\partial \tau} = \frac{\partial f}{\partial y}$ and solve the homogenious part

$$\begin{aligned} &(\hbar\partial_y + a)\, G(y) = 0 \\ &\Rightarrow G(y) = \underbrace{G(0)}_{=:K} e^{-\frac{a}{\hbar}y} = K e^{-\frac{a}{\hbar}y}\,. \end{aligned} \tag{D.0.3}$$

To solve the inhomogenious part, we use the Fourier transformation, therefore we start with

$$\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega g(\omega) e^{-i\omega y} \qquad \text{and} \qquad \delta(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega y}\,, \tag{D.0.4}$$

so one gets

$$(\hbar\partial_y + a)\,\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega g(\omega) e^{-i\omega y} = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega e^{-i\omega y} \quad \Rightarrow \quad g(\omega) = \frac{1}{a - i\hbar\omega}\,. \tag{D.0.5}$$

Now we have to solve the integral

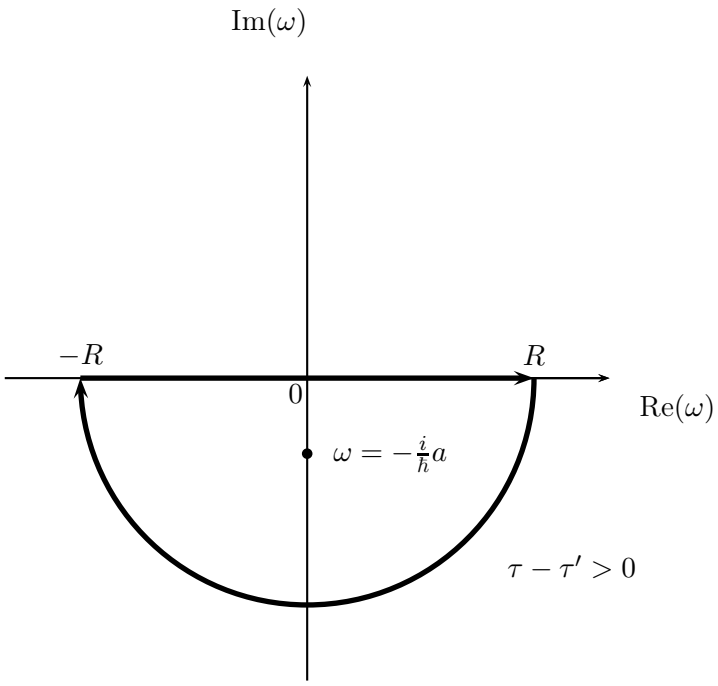
$$\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \frac{1}{a-i\hbar\omega}e^{-i\omega y} \qquad a>0\,. \tag{D.0.6}$$

For that look at

$$\frac{1}{2\pi}\int_{-R}^{R} \frac{1}{a-i\hbar\omega}e^{-i\omega y}d\omega \tag{D.0.7}$$

and for the lower contour we have

$$\begin{aligned}\gamma(t) &= Re^{-it} \quad 0\le t\le 0\\ \gamma'(t) &= -Re^{-it}\end{aligned} \tag{D.0.8}$$



Now we can make the estimation

$$\begin{aligned}&\left|\frac{1}{2\pi}\int_\gamma \mathrm{d}\omega \frac{1}{a-i\hbar\omega}e^{-i\omega y}\right| = \left|\frac{1}{2\pi}\int_0^\pi \mathrm{dt}\,\frac{1}{a-i\hbar Re^{-it}}e^{-iyRe^{-it}}\left(-Rie^{-it}\right)\right|\\ &\le \frac{1}{2\pi}\int_0^\pi \mathrm{dt}\,\left|\frac{e^{iyR(\cos(t)-i\sin(t))}}{a-i\hbar Re^{-it}}R\right| = \frac{1}{2\pi}\int_0^\pi \mathrm{dt}\,\frac{Re^{-Ry\sin(t)}}{|a-i\hbar Re^{-it}|}\\ &\overset{2}{\le} \frac{1}{2\pi}\int_0^{2\pi}\mathrm{dt}\,\frac{R\,e^{-Ry\sin(t)}}{R\,\hbar} = \frac{1}{2\pi\hbar}\int_0^{2\pi}\mathrm{dt}\,e^{-Ry\sin(t)}\\ &= \frac{1}{2\pi\hbar}2\int_0^{\frac{\pi}{2}}\mathrm{dt}\;\; e^{-Ry\sin(t)} = \frac{1}{\pi\hbar}\int_0^{\frac{\pi}{2}}\mathrm{dt}\,e^{-Ry\sin(t)}\\ &\overset{3}{\le} \frac{1}{2\pi\hbar}\int_0^{\frac{\pi}{2}}\mathrm{dt}\,e^{-Ry\frac{2}{\pi}t}\\ &= \frac{1}{\pi\hbar}\frac{\pi(1-e^{-yR})}{2R} = \frac{1}{2\hbar}\frac{(1-e^{-yR})}{R}\overset{R\to\infty}{\longrightarrow}0\,. \quad {}^{1}\end{aligned} \tag{D.0.9}$$

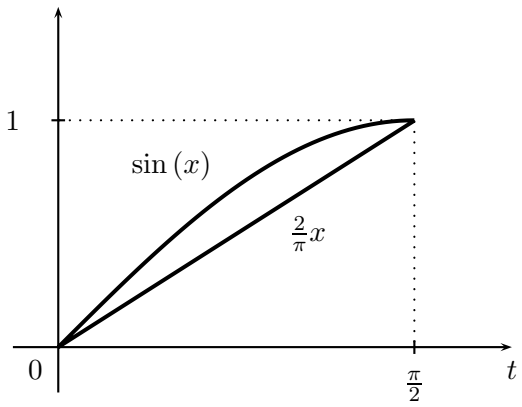
Where we have used

$$|a-i\hbar Re^{-it}| = |(-1)\left(-a+i\hbar Re^{-it}\right)| = |i\hbar Re^{-it}-a| \ge |\hbar R-a| \ge \hbar R \tag{D.0.11}$$

[1] For any $\varepsilon>0$ there exists an R_0 such that $\frac{1}{2}R_0\varepsilon>1 \Leftrightarrow \frac{2}{R_0}<\varepsilon$

$$\left|\frac{1-e^{-R}}{R}\right| \le \frac{1+e^{-yR}}{R} \le \frac{2}{R} < \varepsilon \qquad \forall_{R>R_0} \tag{D.0.10}$$

$$\sin(t) \geq \frac{2}{\pi} t \qquad \text{with} \qquad 0 \leq t \leq \pi \tag{D.0.12}$$



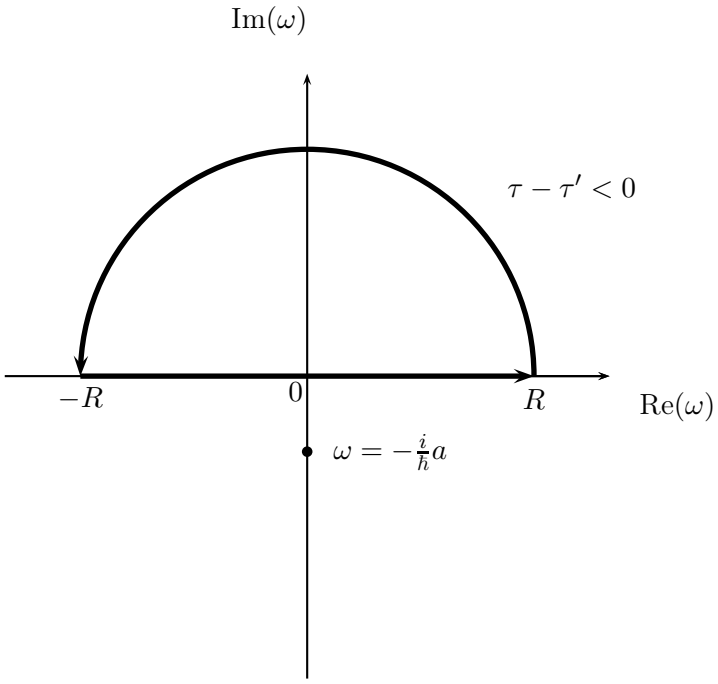
So we have

$$\begin{aligned}
\int_{-\infty}^{\infty} \mathrm{dt} \frac{1}{a - i\hbar\omega} e^{-i\omega y} &= \lim_{R\to\infty} \int_{-R}^{R} \frac{dt1}{a - i\hbar\omega} e^{-i\omega y} = 2\pi i \,\mathrm{Res}(\omega; -\frac{i}{\hbar}a) \\
\mathrm{Res}(\omega; -\frac{i}{\hbar}a) &= \lim_{\omega\to -\frac{i}{\hbar}a} \left(\omega - (-\frac{i}{\hbar}a)\right) \frac{1}{a - i\hbar\omega} e^{-i\omega y} \\
&= \lim_{\omega\to -\frac{i}{\hbar}a} \frac{1}{(-i\hbar)} e^{-i\omega y} = \frac{1}{-i\hbar} e^{-\frac{1}{\hbar}ay}
\end{aligned} \tag{D.0.13}$$

Therefore we get

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}\omega \frac{1}{a - i\hbar\omega} e^{-i\omega y} = -\frac{2\pi i}{2\pi} \left(\frac{1}{-i\hbar} e^{-\frac{1}{\hbar}ay}\right) = \frac{1}{\hbar} e^{-\frac{1}{\hbar}ay} \tag{D.0.14}$$

For $y < 0$ we take the upper contour



And the integral leads

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{1}{1-i\hbar\omega} e^{-i\omega y} = 0 \quad \text{(D.0.15)}$$

For the upper contour we have

$$\begin{aligned} \gamma(t) &= Re^{it} \quad 0 \le t \le 0 \\ \gamma'(t) &= Re^{it} \qquad\qquad \text{(D.0.16)} \end{aligned}$$

For the upper contour we have the curve. We now write for $y < 0$

$$y < 0 \quad -iy \quad \rightarrow \quad i|y| \qquad \text{(D.0.17)}$$

So we can make the estimation

$$\begin{aligned} &\left| \frac{1}{2\pi} \int_\gamma \mathrm{d}\omega \frac{1}{a-i\hbar\omega} e^{i\omega|y|} \right| = \left| \frac{1}{2\pi} \int_0^\pi \mathrm{dt}\, \frac{1}{a-i\hbar Re^{it}} e^{i|y|Re^{it}} \left(Rie^{it}\right) \right| \\ &\le \frac{1}{2\pi} \int_0^\pi \mathrm{dt} \left| \frac{e^{i|y|R(\cos(t)+i\sin(t))}}{a-i\hbar Re^{it}} R \right| = \frac{1}{2\pi} \int_0^\pi \mathrm{dt}\, \frac{Re^{-R|y|\sin(t)}}{|a-i\hbar Re^{it}|} \\ &\overset{2}{\le} \frac{1}{2\pi} \int_0^{2\pi} \mathrm{dt}\, \frac{R\, e^{-R|y|\sin(t)}}{R\,\hbar} = \frac{1}{2\pi\hbar} \int_0^{2\pi} \mathrm{dt}\, e^{-R|y|\sin(t)} \\ &= \frac{1}{2\pi\hbar} 2 \int_0^{\frac{\pi}{2}} \mathrm{dt}\ \ e^{-R|y|\sin(t)} = \frac{1}{\pi\hbar} \int_0^{\frac{\pi}{2}} \mathrm{dt}\, e^{-R|y|\sin(t)} \\ &\overset{3}{\le} \frac{1}{2\pi\hbar} \int_0^{\frac{\pi}{2}} \mathrm{dt}\, e^{-R|y|\frac{2}{\pi}t} \\ &= \frac{1}{\pi\hbar} \frac{\pi(1-e^{-|y|R})}{2R} = \frac{1}{2\hbar} \frac{(1-e^{-|y|R})}{R} \overset{R\to\infty}{\longrightarrow} 0 \quad {}^{1} \end{aligned} \qquad \text{(D.0.18)}$$

The general solution reads

$$G(y) = Ke^{-\frac{a}{\hbar}y} + \frac{1}{\hbar} e^{-\frac{1}{\hbar}ay}\, \theta(y) \qquad \text{(D.0.19)}$$

or

$$G(\lambda\tau|\lambda\tau') = Ke^{-\frac{1}{\hbar}(\varepsilon_\lambda-\mu)(\tau-\tau')} + \frac{1}{\hbar} e^{-\frac{1}{\hbar}(\varepsilon_\lambda-\mu)(\tau-\tau')}\, \theta(\tau-\tau')\,. \qquad \text{(D.0.20)}$$

From the boundary condition, we now get for K

$$K = \frac{\zeta e^{-a\beta}\theta(\hbar\beta - \tau') - \theta(-\tau')}{\hbar(1-\zeta e^{-a\beta})}. \tag{D.0.21}$$

Inserting now back to

$$G(\tau-\tau') = \frac{1}{\hbar} e^{\frac{-a(\tau-\tau')}{\hbar}} \left[\frac{\zeta e^{-a\beta}\theta(\hbar\beta-\tau') - \theta(-\tau')}{(1-\zeta e^{-a\beta})} \,.+ \theta(\tau-\tau') \right] \tag{D.0.22}$$

Now it is $0 < \tau' < \hbar\beta$

$$[\ldots] = \frac{1}{\hbar} e^{-a\frac{(\tau-\tau')}{\hbar}} \left[\frac{\zeta e^{-a\beta}}{(1-\zeta e^{-a\beta})} + \theta(\tau-\tau') \right]$$

$$[\ldots] = 1 + \frac{\zeta}{e^{a\beta}-\zeta} \quad \tau > \tau' \qquad \text{and} \qquad [\ldots] = \frac{\zeta}{e^{a\beta}-\zeta} \quad \tau' > \tau \,. \tag{D.0.23}$$

The result we can combine to

$$G(\lambda\tau|\lambda\tau') = \frac{1}{\hbar} e^{-\frac{1}{\hbar}(\varepsilon_\lambda - \mu)(\tau-\tau')} \left[(1+\zeta n_\lambda)\,\theta(\tau-\tau') + \zeta n_\lambda \theta(\tau'-\tau) \right] \,. \tag{D.0.24}$$