Master's thesis

NTNU
Norwegian University of Science and Technology

Stine Ekrheim and Marthe Elise Fiskerstrand Roheim

# Ginzburg-Landau Theory for Charge Density Waves and Superconductivity

Master's thesis in Applied Physics and Mathematics
Supervisor: Asle Sudbø
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# Abstract

Motivated by the recent interest in Cuprates high-temperature superconductors we study the interplay between two of its symmetry-breaking phases, superconductivity and charge density wave. Starting with a microscopic theory, we derived an effective bosonic action by integrating over the fermionic degrees of freedom. By using the functional integral formalism we derived self-consistent equations for the order parameters and extrapolated the theory to include fluctuations around its normal state. This resulted in a Ginzburg-Landau theory describing a system with charge density waves and superconductivity. There are three main points in our results. Firstly, the phases do not co-exist in the model we have used. Secondly, our calculations showed that charge density waves are more resistant to spacial fluctuations than superconductivity. Lastly, the coefficients in the Ginzburg-Landau theory were mostly the same for the bare charge density wave terms and the bare superconductivity terms.

# Sammendrag

Motivert av den økende interessen for Cuprate-høytemperatur-superledere, tar denne oppgaven for seg samspillet mellom to av dens symmetribrytende faser, superledning og ladningstetthetsbølger. Fra en mikroskopisk teori utledet vi en effektiv bosonisk teori ved å integrere ut de fermioniske frihetsgradene. Ved å bruke funksjonal-integral-metoder har vi utledet selvkonsistente ligninger for ordensparameterne og deretter utvidet teorien til å inkludere fluktuasjoner. Dette resulterte i en Ginzburg-Landau-teori som beskriver et system med ladningstetthetsbølger og superledning. Oppgavens resultater kan oppsummeres i tre hovedpoeng. For det første er det ingen koeksistens av fasene i modellen vi har undersøkt. For det andre viser våre beregninger at ladningstetthetsbølger er mer motstandsdyktige mot romlige fluktuasjoner, sammenlignet med superledning. Avslutnignsvis fant vi ut at koeffisientene i Ginzburg-Landau-teorien deler den samme strukturen for ladningstetthetsbølge-ordensparameteren og superlednings-ordensparameteren.

# Preface

This master's thesis is written in the last semester of a five-year integrated Master's degree program in Applied Physics and Mathematics at the Norwegian University of Science and Technology (NTNU). Firstly, we want to give a big thanks to our supervisor Asle Sudbø for his time, expertise, and his guidance throughout this thesis. This has truly been more than we have hoped for. In addition to this, we want to thank our fellow students at QuSpin who made this year so much better both socially and educationally. We also want to thank our boyfriends for their support throughout this year. Next, we want to give thanks to two of the Ph.D. students at QuSpin, Niels Henrik Aase and Christian Svingen Johnsen, for their help and discussion. We also want to thank the QuSpin coordinator, Karen-Elisabeth Sødahl, for many nice talks over a coffee. A special thanks must also be given to our brilliant fellow master's student Sondre Duna Lundemo for sharing his specialization project and knowledge with us, giving us the opportunity to write a master thesis about functional integral formalism without having any pre-knowledge about this specific theory. Lastly, we want to thank each other for the incredible cooperation and friendship we developed through the years.

Stine Ekrheim — Marthe Roheim

Stine Ekrheim — Marthe Elise F. Roheim

Trondheim, Norway, June 2023

# Contents

# Chapter 1

# Introduction

## 1.1 Background

In 1955, Peierls' theoretical work showed that the instability of a half-filled one-dimensional chain induces a charge density wave (CDW) [1]. Since then, the CDW phase has been an active field of research. In terms of applications, researchers have studied bulk layered CDW materials, which are useful in super-capacitors [2], oscillators [3], sensors [4], and spin-electronic devices [5]. The CDW state is also interesting due to its interplay with other phases, such as superconductivity. [1]

Superconductivity (SC) was discovered in 1911 by a Dutch physicist, Heike Kamerlingh Onnes [7]. Onnes's research showed a sudden drop in resistivity when cooling Mercury to $\sim 4$ K. It took 22 years before another important property of superconductivity was discovered, the Meissner effect [8]. The effect is that a superconductor will repel a magnetic field. Superconductors are useful in high-power transmission lines [9], MR [10], quantum computers [11], and spintronics [12].

Materials that can host the CDW and SC state are usually characterized by reduced dimensionality of their electronic and structural properties. Such materials include copper-oxide (cuprate) high-temperature superconductors [13], one-dimensional organic chains [14], single-element actinide $\alpha$ uranium [15] and layered transition-metal chalcogenides [16–19]. In 2013 Geim stated that different materials can be used as building blocks to make new materials with desired properties [20]. Recently, new fields of applications for layered systems (2D), such as transition-metal dichalcogenides, have been discovered [21]. Another highly interesting material is the cuprate high-temperature superconductors, discovered by Bednorz and Müller in 1986 [22, 23]. The properties of these materials have been heavily researched in the last decades [24–28]. They are susceptible to different types of ordering; superconductivity, charge density waves, spin density waves, anti-ferromagnetism, and a pseudo-gap phase [25, 29]. According to da Silva Neto et al. [30], understanding the mechanism of superconductivity and its interplay with other possible spin or charge orderings in high–transition temperature ($T_{\mathrm{C}}$) cuprate superconductors remains one of the greatest challenges in condensed matter physics. The interplay that

[1] Some of the introduction is from the Specialization project by Roheim and Ekrheim [6]

we are interested in here, is the one between CDWs and SC. They both are symmetry-breaking phases where their order parameters also describe their energy gaps [24, 31, 32]. Several experimental and theoretical results show that they are competing phases [33, 34]. However, several papers show evidence for co-existence between CDWs and SC [35–40]

We will derive a theory for the interplay between these phases using the functional field integral method. In the 1970s, non-perturbative problems received more and more attention, and the need for a new way to solve them arose. Up until then, many problems in condensed matter physics were solved in a perturbative manner, which means adding small perturbations to solvable systems. The functional integral method gave the researchers new theoretical insight into problems beyond perturbation theory. This method was originally developed for high-energy physics but was also applicable in condensed matter physics. Non-perturbative problems are present in various contexts, for example in strongly correlated electron systems, quantum magnetism, and phase transitions. A common factor for these systems is that they exhibit emergent phenomena and that they have a collective behavior that can not be described by perturbative methods alone.

By using the strength of the functional field integrals we can develop a Ginzburg-Landau theory from a stationary point of the order parameters in our system. The Ginzburg-Landau theory was proposed by Ginzburg in 1950 [41] for superconductivity. The theory was based on the work of Landau for superfluidity from 1941 [42]. Some years later, the microscopic theory for superconductivity by Bardeen, Cooper, and Schrieffer (BCS) (1957) was published [43], which gave the physicist a better understanding of the superconducting phase.

## 1.2 Structure of the thesis

The following section will introduce the essential building blocks of the theory that will be used throughout the thesis. This includes the formalism of the functional integral, with its most important underlying derivations. Following this theory, we will in section 3 use the functional integral formalism to describe the CDW state. During the section, we will derive its mean-field equation and the critical temperature of the phase transition from a microscopic model. Finally, from this, we will derive a Ginzburg-Landau theory describing the CDW state. The thesis's next section will answer the question of whether CDWs and SC can co-exist in the system we are looking at. In order to answer this question, we will derive a Ginzburg-Landau theory for a system with CDWs and SC. Following the main part of the thesis is the summary and outlook, where we will summarize our results.

# Chapter 2

# Preliminaries

In this chapter, we will establish the foundation of a theory that will answer the question of whether charge density waves and superconductivity can coexist in the presented model. The theory in the preliminaries' is built upon the following books, *Condensed matter field theory* by Altlands and Simons' [44], *Quantum Many-Particle Systems* by Negele and Orland [45], and the unpublished lecture notes from the course *Functional Integral Methods in Condensed Matter Physics* by professor Asle Sudbø at NTNU [46].

## 2.1 Conventions

First, we want to establish some of the notations and conventions that will be used throughout this thesis. Firstly, we use bold font to write vectors, $\mathbf{k}$, and $\hat{k}$ for the unit vector. Later on, we will use a four-vector, which we will write as $k = (\mathbf{k}, \omega)$. For an operator, we will use hat-notations, where the reader will be able to distinguish the operator from the unit vector by context. Plancks constant $\hbar$, and the Boltzmann constant $k_B$, will be set to unity throughout the thesis. The convention we use for the Fourier transformation is

$$f(k) = \frac{1}{\sqrt{N}} \int_{-\infty}^{\infty} \mathrm{e}^{-i\mathbf{kr}} f(\mathbf{r}) \tag{2.1.1}$$

where N is the number of lattice sites.

## 2.2 Second quantization

In many-body quantum theory for identical particles, the operators can be defined as a matrix element in a $N$-dimensional Hilbert space, which is the direct product of the one-particle Hilbert space

$$\mathcal{H}^N \equiv \underbrace{\mathcal{H} \otimes \cdots \otimes \mathcal{H}}_{N \text{ copies}}. \tag{2.2.1}$$

We are interested in the subset $\mathcal{F}^N \subset \mathcal{H}^N$ which defines the physical $N$-body Hilbert space[1]. By describing the system of particles in the occupation number representation,

[1] Alexander Altland and Ben Simons *Condensed Matter Field Theory* p.42 (2010) [44]

every state can be represented by $|n_1, n_2, ...\rangle$, where $n_i$ is the occupation number of particle $i$ in the state. From this, we have that every state in $\mathcal{F}^N$ can be represented by a state vector $|\Psi\rangle$ on the form

$$|\Psi\rangle = \sum_{n_1,n_2,...} c_{n_1,n_2,...}|n_1, n_2, ...\rangle, \tag{2.2.2}$$

where $c_{n_1,n_2,...}$ are complex coefficients. In order to have a theory that can be used in the Grand Canonical ensemble, with an unknown number of particles, we define the relevant Fock space as

$$\mathcal{F} = \bigoplus_{N=0}^{\infty} \mathcal{F}^N. \tag{2.2.3}$$

Here, $\mathcal{F}$ defines the principal arena of quantum many-body theory. The vacuum space, $\mathcal{F}^0$, has one normalized basis state, the vacuum state $|0\rangle$, which contains no particles. By introducing the operator $a_i^\dagger : \mathcal{F} \to \mathcal{F}$, which raises the occupation number for particle $i$ by one, we have the tools needed to construct every state from the vacuum state

$$|n_1, n_2, ...\rangle = \prod_i \frac{1}{(n_i!)^{1/2}} (a_i^\dagger)^{n_i}|0\rangle. \tag{2.2.4}$$

To complete the picture we also need the opposite operator, the annihilation operator $a_i$. This operator decreases the occupation number for particle $i$ by one. The commutation relations for the annihilation and creation operators for bosons are

$$[a_i, a_j^\dagger] = \delta_{ij}, \quad [a_i, a_j] = 0, \quad [a_i^\dagger, a_j^\dagger] = 0, \tag{2.2.5}$$

where the commutator is defined as $[A, B] = AB - BA$. For fermions we have that

$$\{a_i, a_j^\dagger\} = \delta_{ij}, \quad \{a_i, a_j\} = 0, \quad \{a_i^\dagger, a_j^\dagger\} = 0, \tag{2.2.6}$$

where the anti-commutator is defined as $\{A, B\} = AB + BA$. The difference is due to the Pauli principle for fermions, which says that there can only be one fermion per state. For bosons, there are no limitations on the number of particles per state.

## 2.3 Coherent states

The following section will state some of the most important results in chapter 4.1 of the book *Condensed matter field theory* [44]. The aim is to continue the derivation of a theory for many-body Hamiltonians. Motivated by the section about second quantization, the next step is to present the eigenstates for the annihilation operator, called *coherent states*. The coherent state representation is an elegant formalism that makes it possible to establish a general structure for both fermions and bosons. This might be surprising since there are, as we will see, significant differences in their algebraic structure. By the Pauli principle, we know that the eigenvalues for fermions need to anticommute. In order to fulfill this condition we need to introduce something called Grassmann numbers[2]. First, we will present the coherent states for bosons where the eigenvalues can be represented by complex numbers.

[2]Named after the German mathematician Hermann Günther Grassmann (1809-1877). Credited with inventing what is now called exterior algebra.

### 2.3.1 Bosons

We want to look at the eigenstates of the bosonic Fock-space, and as we have just seen in equation (2.2.4), every state can be expressed by using creation operators on the vacuum state. One could therefore think that it would have been possible to find an eigenstate to this operator. However, the creation operator *increases the minimum* number of particles with one, and therefore can not have an eigenstate. The annihilation operator on the other hand, *decreases the maximum* number of particles in the state by one, which makes it possible to have an eigenstate. Moving forward, let us assume that we have been able to find an eigenstate $|\phi\rangle$ for the annihilation operator, with a consisting eigenvalue $\phi_i$. This gives us the eigenvalue equation

$$a_i|\phi\rangle = \phi_i|\phi\rangle, \tag{2.3.1}$$

which is true for all $i$. The eigenstates $|\phi\rangle$ are called bosonic coherent states and can be expressed as

$$|\phi\rangle \equiv \exp\Big(\sum_i \phi_i a_i^\dagger\Big)|0\rangle, \tag{2.3.2}$$

where $\phi = \{\phi_i\}$ is a set of complex numbers. By taking the hermitian conjugate of the eigenvalue equation (2.3.1) we get the left eigenstates of the creation operators

$$\langle\phi|a_i^\dagger = \langle\phi|\bar{\phi}_i, \tag{2.3.3}$$

where $\langle\phi| = \langle 0|\exp(\sum_i \bar{\phi}_i a_i)$ and $\bar{\phi}$ is the complex conjugate of $\phi$. From equation (2.3.2), we can see that the derivative, of the eigenstate $|\phi\rangle$, with respect to the eigenvalue gives the creation operator acting on the eigenstate. The same argument applies to the left eigenstate of the annihilation operator,

$$a_i^\dagger|\phi\rangle = \partial_{\phi_i}|\phi\rangle, \quad \langle\phi|a_i = \partial_{\bar{\phi}_i}\langle\phi|. \tag{2.3.4}$$

The next step is to find the overlap between two coherent states. We have that $\langle\phi|\theta\rangle = \langle 0|\mathrm{e}^{\sum_i \bar{\phi}_i a_i}|\theta\rangle = \mathrm{e}^{\sum_i \bar{\phi}_i\theta_i}\langle 0|\theta\rangle$. This allows us to write the overlap and the norm of a state as

$$\langle\phi|\theta\rangle = \exp\Big(\sum_i \bar{\phi}_i\theta_i\Big), \quad \langle\phi|\phi\rangle = \exp\Big(\sum_i \bar{\phi}_i\phi_i\Big), \tag{2.3.5}$$

respectively. The coherent states form an overcomplete set of states in Fock space and the unity operator $\mathbf{1}_{\mathcal{F}}$ is

$$\mathbf{1}_{\mathcal{F}} = \int \prod_i \frac{d\bar{\phi}_i d\phi_i}{2\pi i}\mathrm{e}^{-\sum \bar{\phi}_i\phi_i}|\phi\rangle\langle\phi|, \tag{2.3.6}$$

where $d\bar{\phi}_i d\phi_i = d\mathrm{Re}\phi_i d\mathrm{Im}\phi_i$. This finishes the coherent states for bosons, and next up we will present the coherent states of fermions.

### 2.3.2 Fermions

As pointed out earlier, the eigenvalues of the fermionic operators must anticommute. Hence, before proceeding, we need to introduce "numbers" that anti-commute, Grassmann numbers.

A complete treatment of **Grassmann algebra** is given in *The method of second quantization* by Berezin [47], we will only introduce the properties needed to present the theory of the coherent state for fermions. Grassmann algebra is defined by a set of generators $\{\xi_\alpha\}$ where $\alpha = 1, ..., n$. The first thing to note is that Grassmann numbers anti-commute

$$\xi_\alpha \xi_\beta = -\xi_\beta \xi_\alpha, \tag{2.3.7}$$

which is the desired property. This property essentially gives us that $\xi_\alpha^2 = 0$. Due to the anti-commutation, functions of Grassmann numbers can be defined by their Taylor expansion with a finite number of terms

$$f(\xi_1, \ldots, \xi_k) = \sum_{n=0}^{\infty} \sum_{i_1,\ldots,i_n=1}^{k} \frac{1}{n!} \frac{\partial^n f}{\partial \xi_{i_1} \cdots \partial \xi_{i_n}} \bigg|_{\xi=0} \xi_{i_n} \cdots \xi_{i_1}, \tag{2.3.8}$$

where $\xi_1, \ldots, \xi_k$ are Grassmann numbers. Any function which depends on only one variable can be written as

$$f(\xi) = f(0) + f'(\xi)\big|_{\xi=0} \xi. \tag{2.3.9}$$

Due to the properties of Grassmann numbers, both derivatives and integration are different from what we are used to from real and complex numbers. For Grassmann numbers these operations are defined as

$$\frac{\partial}{\partial \xi} \xi = 1, \quad \int d\xi 1 = 0, \quad \int d\xi \xi = 1. \tag{2.3.10}$$

This shows us that the integration and derivation of Grassmann variables are essentially the same. For instance, the integration of a function of one Grassmann variable gives

$$\int d\xi f(\xi) = \int d\xi \left[ f(0) + f'(\xi)\big|_{\xi=0} \xi \right] = f'(\xi)\big|_{\xi=0}, \tag{2.3.11}$$

which is the same answer as for derivation, $\partial_\xi f(\xi) = f'(\xi)\big|_{\xi=0}$. Now, being more familiar with Grassmann numbers, we are ready to proceed to the derivation of coherent states for fermions.

To create coherent states for fermions we need to expand the relevant Fock-space. We introduce a generator $\xi_\alpha$ to every annihilation operator $a_\alpha$ and another generator $\bar{\xi}_\alpha$ to every creation operator, $a_\alpha^\dagger$. This allows us to expand every vector in this general Fock-space

$$|\psi\rangle = \sum_\alpha \xi_\alpha |\xi_\alpha\rangle, \tag{2.3.12}$$

where the generators, $\xi_\alpha$ are Grassmann numbers and $|\xi_\alpha\rangle$ are vectors in the Fock space. We will later see that these are the eigenvalues and eigenvectors of the annihilation operator. The anti-commutation relations between the operators and their generators are defined as

$$\{\xi, a\} = 0, \quad \{\bar{\xi}, a^\dagger\} = 0. \tag{2.3.13}$$

The next important definition is the effect of a dagger, $(\xi a)^\dagger = \bar{\xi} a^\dagger$. The significant difference from the bosonic case is that $\xi$ and $\bar{\xi}$ *are independent* of each other. Moreover, despite the sign-change in the exponent, we can write the fermion coherent state in the same way as for the bosonic case

$$|\xi\rangle = \exp\big(-\sum_\alpha \xi_\alpha a_\alpha^\dagger\big)|0\rangle, \tag{2.3.14}$$

where the minus is due to the eigenvalue-equation

$$a_\alpha|\xi\rangle = \xi_\alpha|\xi\rangle. \tag{2.3.15}$$

The proof for this is shown in appendix A. Due to the similarities to the structure of the bosonic coherent states, we will only list the results

$$\langle\xi| = \langle 0|\exp\big(\sum_\alpha \bar{\xi}_\alpha a_\alpha\big), \quad \langle\xi|a_\alpha^\dagger = \langle\xi|\bar{\xi}_\alpha, \tag{2.3.16}$$

$$a_\alpha^\dagger|\xi\rangle = -\partial_{\xi_\alpha}|\xi\rangle, \quad \langle\xi|a_\alpha = \partial_{\bar{\xi}_\alpha}\langle\xi|. \tag{2.3.17}$$

From this, we can find that the overlap between two coherent states is

$$\langle\xi|\eta\rangle = \langle 0|\mathrm{e}^{\sum_\alpha \bar{\xi}_\alpha a_\alpha}\mathrm{e}^{-\sum_\alpha \eta_\alpha a_\alpha^\dagger}|0\rangle = \langle 0|\prod_\alpha(1+\bar{\xi}_\alpha a_\alpha)(1-\eta_\alpha a_\alpha^\dagger)|0\rangle \tag{2.3.18}$$

$$= \prod_\alpha(1+\bar{\xi}_\alpha\eta_\alpha) = \mathrm{e}^{\sum_\alpha \bar{\xi}_\alpha\eta_\alpha}. \tag{2.3.19}$$

From this, we can find the unit operator in the fermionic Fock space

$$\mathbf{1}_{\mathcal{F}} = \int\prod_\alpha d\bar{\xi}_\alpha d\xi_\alpha \mathrm{e}^{-\sum_\alpha \bar{\xi}_\alpha\xi_\alpha}|\xi\rangle\langle\xi|. \tag{2.3.20}$$

Finally, we define a Grassmann coherent state representation

$$|\psi\rangle = \int\prod_\alpha d\bar{\xi}_\alpha d\xi_\alpha \mathrm{e}^{-\sum_\alpha \bar{\xi}_\alpha\xi_\alpha}\psi(\bar{\xi})|\xi\rangle, \tag{2.3.21}$$

where $\psi(\bar{\xi}) = \langle\xi|\psi\rangle$.

Before moving on we want to state some of the mathematical and physical differences between fermionic and bosonic coherent states. Mathematically there are two notably important differences besides some sign changes. Firstly, as we have already mentioned, the Grassmann numbers $\xi$ and $\bar{\xi}$ are completely independent of each other. Secondly,

**Summary of the coherent states for bosons and fermions**

| | |
|---|---|
| Eigenstate | $\lvert\xi\rangle = \exp\big(\zeta \sum_\alpha \xi_\alpha a^\dagger_\alpha\big)\lvert 0\rangle$ |
| Annihilation operator | $a_\alpha\lvert\xi\rangle = \xi_\alpha\lvert\xi\rangle, \quad \langle\xi\rvert a_\alpha = \frac{\partial}{\partial\bar{\xi}_\alpha}\langle\xi\rvert$ |
| Creation operator | $a^\dagger_\alpha\lvert\xi\rangle = \zeta\frac{\partial}{\partial\xi_\alpha}\lvert\xi\rangle, \quad \langle\xi\rvert a^\dagger_\alpha = \langle\xi\rvert\bar{\xi}_\alpha$ |
| Matrix Element | $\langle\xi\rvert A(a^\dagger_\alpha, a_\alpha)\lvert\xi'\rangle = \exp\big(\sum_\alpha \bar{\xi}_\alpha\xi'_\alpha\big)A(\bar{\xi}_\alpha, \xi_\alpha)$ |
| Resolution of identity | $\mathbf{1}_{\mathcal{F}} = \int \mathcal{D}\xi \exp\big(-\sum_\alpha \bar{\xi}_\alpha\xi_\alpha\big)\lvert\xi\rangle\langle\xi\rvert$ |
| Trace | $\mathrm{trA} = \int \mathcal{D}\xi \exp\big(-\sum_\alpha \bar{\xi}_\alpha\xi_\alpha\big)\langle\zeta\xi\rvert A\lvert\xi\rangle$ |
| Vector in Fock Space | $\lvert\psi\rangle = \int \mathcal{D}\xi \exp\big(-\sum_\alpha \bar{\xi}_\alpha\xi_\alpha\big)\psi(\bar{\xi}_\alpha)\lvert\xi\rangle$ |
| Coherent state representation | $\psi(\bar{\xi}) = \langle\xi\vert\psi\rangle$ |
| Matrix element of creation op. | $\langle\xi\rvert a^\dagger_\alpha\lvert\psi\rangle = \bar{\xi}_\alpha\psi(\bar{\xi})$ |
| Matrix element of annihilation op. | $\langle\xi\rvert a_\alpha\lvert\psi\rangle = \frac{\partial}{\partial\bar{\xi}_\alpha}\psi(\bar{\xi})$ |

$$\mathcal{D}\xi = \frac{1}{\mathcal{N}}\prod_\alpha d\bar{\xi}_\alpha d\xi_\alpha, \quad \mathcal{N} = \begin{cases} 2\pi i & \text{for bosons} \\ 1 & \text{for fermions} \end{cases}$$

Table 2.1: Summary of the coherent states for bosons ($\zeta = 1$) and fermions ($\zeta = -1$)

unlike the integral over complex numbers, the Grassmann version of the Gaussian integral does not involve the factor $2\pi i$. The structure of the coherent states for fermions and bosons is summarized in table 2.1. The coherent states of fermions are not physical states but are useful in formulating many-fermion and many-boson theories. Due to the termination of the series expansion of Grassmann variables, every function will be linear, and the stationary point equation makes no sense for coherent fermionic states. A way to solve this is to integrate over the fermionic degree of freedom to get an effective theory. On the other hand, coherent states for bosons are physical states. For example, a classical electromagnetic field can be viewed as a coherent state of photons.

## 2.4 Gaussian integrals

In the formulation of the functional integral method, it is useful to establish a set of Gaussian integrals that will help us with the derivation of the formalism. We start out by presenting multiple Gaussian integrals over complex variables, which we will use in the formulation of functional integrals for **bosons**. The integral we want to evaluate is

$$I_{\text{boson}} = \prod_k \int \frac{d\bar{x}_k dx_k}{2\pi i} \mathrm{e}^{-\bar{x}_i A_{ij} x_j + x_j \bar{\mathcal{J}}_j + \bar{x}_i \mathcal{J}_i} \tag{2.4.1}$$

where we sum over repeated indices. We have that $A_{ij}$ is a positive definite, symmetric matrix with $\det(A) > 0$ and $x_i$ and $\mathcal{J}_i$ are vectors. It is shown in appendix B.1 that by performing the integrals we get

$$I_{\text{boson}} = \frac{1}{\det(A)} \mathrm{e}^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j}. \tag{2.4.2}$$

For **fermions**, the integration variables $\xi_k$, are Grassmann variables. As we have seen in section 2.3, the integration over Grassmann variables is different. Hence, the integral we want to look at now is

$$I_{\text{fermion}} = \prod_k \int d\bar{\xi}_k d\xi_k \mathrm{e}^{-\bar{\xi}_i A_{ij} \xi_j + \xi_i \bar{\mathcal{J}}_i + \bar{\xi}_j \mathcal{J}_j}, \tag{2.4.3}$$

where the $\mathcal{J}$'s are vectors of Grassmann-variables, and $A_{ij}$ must fulfull the same contiditions as for bosons. As shown in appendix B.2, this integral also has an elegant answer

$$I_{\text{fermion}} = \det(A) \mathrm{e}^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j} = \mathrm{e}^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j + \operatorname{tr} \ln(A)}, \tag{2.4.4}$$

where the last transition follows from the identity, $\det \mathbf{A} = \mathrm{e}^{\operatorname{tr} \ln \mathbf{A}}$. We can see that the determinant is now in the numerator compared to equation (2.4.2), where it was in the denominator. This is due to the expansion of the exponential function, which will terminate after only two terms. Physically this corresponds to the restriction of the Pauli principle. The last integral is specifically useful because it will allow us to integrate over the fermionic degrees of freedom. This means that we can work with an effective bosonic theory where it is possible to look for expansions from a stationary value of the free energy.

In this thesis, we will also work with bigger systems, where we structure parts of the system in a matrix with four indices $A_{i,j} \rightarrow A^{i,j}_{k,k'}$. The integral we need to calculate is

$$\tilde{I}_{\text{fermion}} = \prod_n \int d\bar{\xi}_n d\xi_n \mathrm{e}^{-\sum_{k,k'} \sum_{i,j} \bar{\xi}^i_k A^{ij}_{kk'} \xi^j_{k'} + \xi^i_k \bar{\mathcal{J}}^i_k + \bar{\xi}^j_k \mathcal{J}^j_k}. \tag{2.4.5}$$

By generalizing the result from appendix B.2, we get

$$\tilde{I}_{\text{fermion}} = \mathrm{e}^{\sum_k \xi^i_k \bar{\mathcal{J}}^i_k + \bar{\xi}^j_k \mathcal{J}^j_k} \mathrm{e}^{\operatorname{Tr} \log[A]} \tag{2.4.6}$$

where the trace with a capital T is defined as

$$\operatorname{Tr}[A] = \sum_k \operatorname{tr}[A]_{kk} = \sum_k \sum_i A^{ii}_{kk}, \tag{2.4.7}$$

where Tr is the trace in both upper and lower indices and tr is only for one of them.

## 2.5 Feynman path integral

The goal of this section is to formulate the many-particle partition function in the coherent state basis. To make the derivation clearer we will first introduce the Feynman path integral to express the partition function for a single particle in the position basis. To start off we consider the matrix element of the evolution operator of the system

$$\mathcal{U}(x_f, t_f; x_i, t_i) = \langle x_f | \mathrm{e}^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} | x_i \rangle, \tag{2.5.1}$$

where $|x_i\rangle$ and $\langle x_f|$ are the initial and final eigenstates of the position operator respectively, and $\hat{H}$ is the Hamiltonian of the system. In this expression, we have kept $\hbar$ to show the structure of the evolution operator, but will further set it to 1. In general, precise calculations of a physical system over a finite time interval are often not possible. However, we can divide the time interval $(t_i, t_f)$ into $M$ numbers of infinitesimal time intervals. This makes it possible to evaluate each interval separately, where each interval is characterized by a stepsize $\epsilon = \frac{t_f - t_i}{M}$. By applying this approach, we can express the matrix element $\mathcal{U}(x_f, t_f; x_i, t_i)$ as follows

$$\mathcal{U}(x_f, t_f; x_i, t_i) = \langle x_f | \big(\mathrm{e}^{-i\hat{H}\epsilon}\big)^M | x_i \rangle. \tag{2.5.2}$$

The way to solve this is to divide the matrix element into separate elements for each timestep. In order to do this we insert the completeness relation for $x_i$, $1 = \int dx_i |x_i\rangle\langle x_i|$, $M-1$ times between each factor $\mathrm{e}^{-iH\epsilon}$. Using this, the evolution operator is

$$\begin{aligned}\mathcal{U}(x_f, t_f; x_i, t_i) = \int \prod_{k=1}^{M-1} dx_k \langle x_M | \mathrm{e}^{i\epsilon\hat{H}} | x_{M-1}\rangle\langle x_{M-1} | \mathrm{e}^{i\epsilon\hat{H}} | x_{M-2}\rangle\langle x_{M-2}| \\ \times \cdots \mathrm{e}^{i\epsilon\hat{H}} | x_1\rangle\langle x_1 | \mathrm{e}^{i\epsilon\hat{H}} | x_0\rangle,\end{aligned} \tag{2.5.3}$$

where we renamed $x_i$ to $x_0$ and $x_f$ to $x_M$ to make it consistent with the notation of the inserted states. The current formulation of the matrix element $\mathcal{U}$, makes it clear that it is a summation over the entire ensemble of possible paths that a particle may take, originating from the initial position $x_0$ and terminating at the end-point $x_M$. That is why it is called a path integral.

Up to this point, the obtained result remains exact. However, in order to proceed, it is necessary to make approximations to the matrix element. We start out by evaluating a single matrix element

$$\langle x_k | \mathrm{e}^{-i\epsilon\hat{H}} | x_{k-1}\rangle = \int dp_k \langle x_k | p_k\rangle\langle p_k | e^{-i\epsilon\hat{H}} | x_{k-1}\rangle, \tag{2.5.4}$$

where we inserted the completeness relation for $p_k$. To be able to proceed with the matrix element $\langle p_k | e^{-i\epsilon H(p,x)} | x_{k-1}\rangle$ we need to arrange the position operators to the right of all the momentum operators, which is called normal ordering. It can be shown that the exponential can be expressed as a series expansion, where the first term contains the normal ordered Hamiltonian[3]

$$\mathrm{e}^{-i\epsilon H(\hat{p},\hat{x})} =: \mathrm{e}^{-i\epsilon H(\hat{p},\hat{x})} : -(\epsilon)^2 \sum_{n=0}^{\infty} \frac{(-i\epsilon)^n}{(n+2)!}\Big(H(\hat{p},\hat{x})^{n+2} - : [H(\hat{p},\hat{x})]^{n+2} : \Big), \tag{2.5.5}$$

[3]Negele, *Quantum Many-Particle Systems*, 1988, page 59 [45]

where the notation : $A$ : is the normal ordering of $A$. The first approximation is to let $M \to \infty$, which makes the step size small $\epsilon \ll 1$. Expanding to first order in $\epsilon$ gives

$$\mathrm{e}^{i\epsilon H(\hat{p},\hat{x})} \approx : \mathrm{e}^{i\epsilon H(\hat{p},\hat{x})} : . \tag{2.5.6}$$

To make the derivation clearer, we will specify the Hamiltonian to be a single particle in a potential, $\hat{H}(\hat{p},\hat{x}) = \frac{\hat{p}^2}{2m} + V(\hat{x})$. Using this, plus the fact that $\langle x_k|p_k\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{ip_kx_k}$ and $\langle p_k|x_{k-1}\rangle = \frac{1}{\sqrt{2\pi}}\mathrm{e}^{-ip_kx_{k-1}}$, we obtain

$$\begin{aligned}\langle x_k|\mathrm{e}^{-i\epsilon\hat{H}}|x_{k-1}\rangle &= \int dp_k \frac{1}{\sqrt{2\pi}}\mathrm{e}^{ip_kx_k}\mathrm{e}^{-i\epsilon H(p_k,x_{k-1})}\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-ip_kx_{k-1}} + \mathcal{O}(\epsilon^2)\\ &= \sqrt{\frac{m}{2\pi i\epsilon}}\mathrm{e}^{i\epsilon[\frac{m}{2\epsilon^2}(x_k-x_{k-1})^2 - V(x_{k-1})]} + \mathcal{O}(\epsilon^2).\end{aligned} \tag{2.5.7}$$

Next, we introduce the following

$$\lim_{\epsilon\to 0}\frac{x_k - x_{k-1}}{\epsilon} \to \frac{dx}{dt}, \quad \lim_{M\to\infty}\epsilon\sum_{k=1}^{M-1} \to \int_{t_i}^{t_f},$$
$$\lim_{M\to\infty}\int\left(\prod_{k=1}^{M-1} dx_k\sqrt{\frac{m}{2\pi i\epsilon}}\right) \to \int_{x_i,t_i}^{x_f,t_f}\mathcal{D}[x(t)].$$

By using these approximations the expression for $\mathcal{U}$ is simplified

$$\mathcal{U}(x_ft_f, x_it_i) = \int_{x_i,t_i}^{x_f,t_f}\mathcal{D}[x(t)]\mathrm{e}^{i\mathcal{S}[x(t)]}, \tag{2.5.8}$$

where the action $\mathcal{S}[x(t)]$ and the Lagrangian $L[x(t)]$ is

$$\mathcal{S}[x(t)] = \int_{t_i}^{t_f} L[x(t)], \quad L[x(t)] = \frac{1}{2}m\Big(\frac{dx}{dt}\Big)^2 - V(x(t)). \tag{2.5.9}$$

In this calculation, we have assumed a one-dimensional system. Still, it can also easily be generalized to $n$ dimension by writing $\lim_{M\to\infty}\int\Big(\prod_{k=1}^{M-1} dx_k(\frac{m}{2\pi i\epsilon})^{\frac{n}{2}}\Big) \to \int_{x_i,t_i}^{x_f,t_f}\mathcal{D}[x(t)]$.

**Partition function** Next, we will use this to find an expression for the partition function for a general Hamiltonian. From statistical mechanics, we know that we can write the partition function as

$$Z = \mathrm{tr}(\mathrm{e}^{-\beta\hat{H}}) = \int dx\langle x|\mathrm{e}^{-\beta\hat{H}}|x\rangle. \tag{2.5.10}$$

The integrand has the same form as the evolution operator, where $x_i = x_f = x$ and $\beta = i(t_f - t_i)$. By introducing the imaginary time $\tau \equiv it$, we have that

$$dt = -id\tau, \quad \frac{d}{dt} = i\frac{d}{d\tau}, \quad x(t) \to x(\tau), \tag{2.5.11}$$

which allows us to use the results from earlier. This gives the partition function formulated as a path integral

$$Z = \int dx\langle x|\mathrm{e}^{-\beta\hat{H}}|x\rangle = \int_{x(0)=x(\beta)}\mathcal{D}[x(\tau)]\mathrm{e}^{-\int_0^\beta d\tau H[x(\tau)]}. \tag{2.5.12}$$

Furthermore, it can be generalized to a many-particle system.

## 2.6 Functional integral over coherent states

For a single-particle Hamiltonian, it is convenient to express the eigenstates in the position or momentum basis, but for a many-particle system, the Hamiltonian is typically expressed by annihilation and creation operators. Consequently, we want to express the partition function for the many-particle system in the eigenstates of the annihilation operator, which were introduced in section 2.3. The derivation has the same starting point as for the path integral for a single particle, but now in the coherent state basis

$$\mathcal{U}(\bar{\phi}_{\alpha,f}t_f,\phi_{\alpha,f}t_i)=\langle\phi_f|\mathrm{e}^{-i\hat{H}(t_f-t_i)}|\phi_i\rangle. \tag{2.6.1}$$

Here, we have that $|\phi_i\rangle$ is the initial coherent state with components $\phi_{\alpha,i}$ and $\langle\phi_f|$ is the final state with components $\bar{\phi}_{\alpha,f}$. We use the same technique as in the section above and divide the finite time interval $(t_i,t_f)$ into $M$ infinitesimal time intervals, $\epsilon=\frac{t_f-t_i}{M}$. Next, we insert the resolution of identity from table 2.1 between each factor

$$\begin{aligned}&\mathcal{U}(\bar{\phi}_{\alpha,f}t_f,\phi_{\alpha,f}t_i)\\ =&\lim_{M\to\infty}\int\prod_{k=1}^{M-1}\prod_{\alpha}\frac{d\bar{\phi}_{\alpha,k}d\phi_{\alpha,k}}{\mathcal{N}}\mathrm{e}^{-\sum_{k=1}^{M-1}\sum_\alpha\bar{\phi}_{\alpha,k}\phi_{\alpha,k}}\prod_{k=1}^{M}\langle\phi_k|:\mathrm{e}^{-i\epsilon H(a^\dagger_\alpha,a_\alpha)}:+\mathcal{O}(\epsilon^2)|\phi_{k-1}\rangle,\end{aligned} \tag{2.6.2}$$

where $\mathcal{N}=1$ for fermions and $\mathcal{N}=2\pi i$ for bosons. Note that there is an additional exponential factor due to the closure relation of coherent states. It can be shown that

$$\langle\phi_k|:\mathrm{e}^{-i\epsilon H(a^\dagger_\alpha,a_\alpha)}:|\phi_{k-1}\rangle=\mathrm{e}^{\sum_\alpha\bar{\phi}_{\alpha,k}\phi_{\alpha,k-1}-i\epsilon H(\bar{\phi}_{\alpha,k},\phi_{\alpha,k})}. \tag{2.6.3}$$

Now, $\mathcal{U}$ is

$$\lim_{M\to\infty}\int\prod_{k=1}^{M-1}\prod_{\alpha}\frac{d\bar{\phi}_{\alpha,k}d\phi_{\alpha,k}}{\mathcal{N}}\mathrm{e}^{-\sum_{k=1}^{M-1}\sum_\alpha\bar{\phi}_{\alpha,k}\phi_{\alpha,k}}\mathrm{e}^{\sum_{k=1}^{M}(\sum_\alpha\bar{\phi}_{\alpha,k}\phi_{\alpha,k-1}-i\epsilon H(\bar{\phi}_{\alpha,k},\phi_{\alpha,k})}. \tag{2.6.4}$$

Next, we introduce a trajectory $\phi_\alpha(t)$ to represent the set $\{\phi_{\alpha,1},\phi_{\alpha,2},...,\phi_{\alpha,M}\}$ and let $\epsilon\to0$ which gives us

$$\lim_{\epsilon\to0}\left(\bar{\phi}_{\alpha,k}\frac{\phi_{\alpha,k}-\phi_{\alpha,k-1}}{\epsilon}\right)\equiv\bar{\phi}_\alpha(t)\partial_t\phi_\alpha(t). \tag{2.6.5}$$

Using this notation, the Hamiltonian can be written as

$$H(\bar{\phi}_{\alpha,k},\phi_{\alpha,k})\equiv H\big(\bar{\phi}_\alpha(t),\phi_\alpha(t)\big). \tag{2.6.6}$$

Finally, the expression for $\mathcal{U}$ is

$$\mathcal{U}(\bar{\phi}_{\alpha,f},t_f;\phi_{\alpha,i},t_i)=\int_{\phi_\alpha(t_i)}^{\bar{\phi}_\alpha(t_f)}\mathcal{D}[\bar{\phi}_\alpha(t),\phi_\alpha(t)]\mathrm{e}^{\sum_\alpha\bar{\phi}_\alpha(t_f)\phi_\alpha(t_i)+i\int_{t_i}^{t_f}dtL[\bar{\phi}_\alpha(t),\phi_\alpha(t)]}, \tag{2.6.7}$$

where $L$ is the Lagrangrian

$$L[\bar{\phi}_\alpha(t), \phi_\alpha(t)] = \sum_\alpha i\bar{\phi}_\alpha(t)\partial_t\phi_\alpha(t) - H\left(\bar{\phi}_\alpha(t), \phi_\alpha(t)\right) \tag{2.6.8}$$

and

$$\mathcal{D}[\bar{\phi}_\alpha(t), \phi_\alpha(t)] = \lim_{M\to\infty} \prod_{k=1}^{M-1} \prod_\alpha \frac{d\bar{\phi}_{\alpha,k} d\phi_{\alpha,k}}{\mathcal{N}}. \tag{2.6.9}$$

Having found the formulation of the evolution operator in the coherent state basis, we proceed to the partition function.

### Partition function in the coherent state basis

By following the same approach as for the single particle Hamiltonian, we start out with the partition function. The difference is that we will take the trace in the coherent state basis, and that our Hamiltonian is a many-particle Hamiltonian formulated by annihilation and creation operators

$$Z = \mathrm{tr}\left[\mathrm{e}^{-\beta(H-\mu N)}\right] = \int \prod_\alpha \frac{d\bar{\phi}_\alpha d\phi_\alpha}{\mathcal{N}} \mathrm{e}^{-\sum_\alpha \bar{\phi}_\alpha\phi_\alpha} \langle\zeta\phi|\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}|\phi\rangle, \tag{2.6.10}$$

where $\zeta = 1$ for bosons and $\zeta = -1$ for fermions. As for the position basis, we can use the result for the evolution operator to rewrite the partition function. By doing so we have that

$$\begin{gathered} \phi_{\alpha,i} = \phi_\alpha, \quad \bar{\phi}_{\alpha,f} = \zeta\bar{\phi}_\alpha, \quad i(t_f - t_i) = \beta, \\ \tau = \beta, \quad dt = -id\tau, \quad \phi(t) \to \phi(\tau), \end{gathered}$$

where we again introduced $\tau$ as an imaginary time. The partition function can now be written as

$$Z = \int_{\phi_\alpha(\beta)=\zeta\phi_\alpha(0)} \mathcal{D}[\bar{\phi}_\alpha(\tau), \phi_\alpha(\tau)]\mathrm{e}^{-S(\bar{\phi}_\alpha,\phi_\alpha)}, \tag{2.6.11}$$

where the integral limits are different for bosons and fermions. For bosons the limits are periodic, but for fermions they are anti-periodic. The action in the exponent is

$$S(\bar{\phi}_\alpha, \phi_\alpha) = \int_0^\beta d\tau \left[\sum_\alpha \bar{\phi}_\alpha(\tau)\left(\partial_\tau - \mu\right)\phi_\alpha(\tau) + H\big(\bar{\phi}_\alpha(\tau), \phi_\alpha(\tau)\big)\right], \tag{2.6.12}$$

which is the action in the time representation. To get rid of the derivative in the exponent, the Fourier conjugate representation of $\phi_\alpha(\tau)$ is introduced,

$$\phi(\tau) = \frac{1}{\sqrt{\beta}} \sum_{\omega_n} \phi_n \mathrm{e}^{-i\omega_n\tau}, \quad \omega_n = \begin{cases} 2n\pi T & \text{bosons} \\ (2n+1)\pi T & \text{fermions} \end{cases}, \quad n \in \mathbb{Z}. \tag{2.6.13}$$

where $\omega_n$ are called **Matsubara frequencies**. Using this gives us the action

$$S(\bar{\phi}_\alpha, \phi_\alpha) = \sum_n \left[\sum_\alpha \bar{\phi}_{\alpha,n}\Big(-i\omega_n - \mu\Big)\phi_{\alpha,n} + H\big(\bar{\phi}_{\alpha,n}, \phi_{\alpha,n}\big)\right]. \tag{2.6.14}$$

This is the frequency representation of the action, and the representation we will use throughout this thesis.

## 2.7 Hubbard-Stratonovich decoupling

In this thesis, we will make use of actions with a non-interacting part $S_0$ and an interacting part $S_{\text{int}}$

$$S = S_0 + S_{\text{int}}. \tag{2.7.1}$$

The aim of this section is to derive the decoupling of the interaction term. The decoupling results in integrals that are quadratic in the fermionic field variables. Hence, the integrals can be solved using the theory from section 2.4 about Gaussian integrals. Consider an interaction operator for two fermions

$$S_{\text{int}} = V_{\alpha\beta\gamma\delta}\bar{\psi}_\alpha\psi_\beta\bar{\psi}_\gamma\psi_\delta \tag{2.7.2}$$

where $\bar{\psi}$ and $\psi$ are fermionic field variables. The indices $\alpha, \beta, \gamma, \delta$ refer to an undefined set of quantum numbers, Matsubara frequencies, etc. The interaction matrix element is $V_{\alpha\beta,\gamma\delta}$. Introducing composite operators $\hat{\rho}_{\alpha\beta} \equiv \bar{\psi}_\alpha\psi_\beta$, one can rewrite the action as $\hat{\rho}_m V_{mn}\hat{\rho}_n$, where $m = (\alpha, \beta)$ and $n = (\gamma, \delta)$. To reduce the action to be quadratic in $\psi$'s, we introduce the auxiliary bosonic field $\phi$ and insert unity for the new field. We can now write

$$\mathrm{e}^{\hat{\rho}_m V_{mn}\hat{\rho}_n} = \int D\phi \mathrm{e}^{-\frac{1}{4}\phi_m V^{-1}_{mn}\phi_n}\mathrm{e}^{-\hat{\rho}_m V_{mn}\hat{\rho}_n}. \tag{2.7.3}$$

Next, we shift the bosonic fields ($\phi_m \to \phi_m + 2iV_{mn}\hat{\rho}_n$) to decouple the interaction term

$$\mathrm{e}^{\hat{\rho}_m V_{mn}\hat{\rho}_n} = \int D\phi \mathrm{e}^{-\frac{1}{4}\phi_m V^{-1}_{mn}\phi_n}\mathrm{e}^{-i\phi_m\hat{\rho}_m}. \tag{2.7.4}$$

We have now traded the quartic term in $\psi$'s interaction term with a bilinear term coupled with an auxiliary bosonic field, which is called Hubbard-Stratonovich decoupling. This might seem more complicated, but the reason why we do this is that we can integrate over the quadratic fermionic term to get an effective bosonic theory. From this, we can find the stationary point conditions. Expanding from this we can find a Ginzburg Landau theory for the fluctuating fields. Above we decoupled in the direct channel, other choices for the decoupling are in the exchange channel and in the Cooper channel, shown in figure 2.1. The calculation remains exact regardless of the decoupling channel. However, once we approximate the integral in any way, the choice of the decoupling channel becomes crucial. To make the decoupling in the different channels clearer, we will look at the electron-electron interaction

$$S_{\text{int}} = \frac{1}{2}\sum_{\sigma,\sigma'}\int d\tau \int d^d r d^d r' \bar{\psi}_\sigma(\mathbf{r},\tau)\psi_\sigma(\mathbf{r}',\tau)V_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')\bar{\psi}_{\sigma'}(\mathbf{r}',\tau)\psi_{\sigma'}(\mathbf{r},\tau) \tag{2.7.5}$$

where $\alpha = \beta = (\mathbf{r}, \tau, \sigma)$ and $\gamma = \delta = (\mathbf{r}', \tau, \sigma')$. Next, we consider the interaction term in momentum-space

$$S_{\text{int}}[\bar{\psi}, \psi] = \frac{1}{2}\sum_{\sigma,\sigma'}\sum_{k_1,\ldots,k_4}\bar{\psi}_{\sigma,k_1}\bar{\psi}_{\sigma',k_3}V(\mathbf{k}_1-\mathbf{k}_2)\psi_{\sigma',k_4}\psi_{\sigma,k_2}\delta_{k_1-k_2+k_3-k_4}, \tag{2.7.6}$$

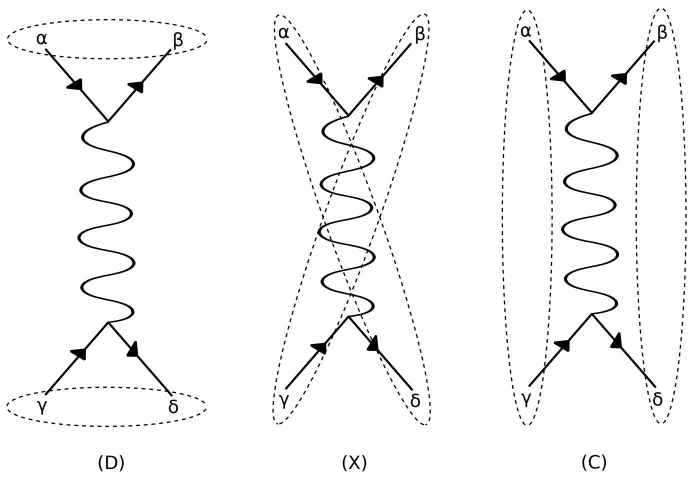



Figure 2.1: Decoupling of the interaction term where $\alpha, \beta, \gamma, \delta$ refer to an unspecified set of quantum numbers, Matsubara frequencies, etc. The decoupling is in the direct channel (D), the exchange channel (X), and the Cooper channel (C)

where $k_i = (\mathbf{k}_i, \omega_i)$ are four-momentum consisting of the spacial momentum and the Matsubara frequencies. The summation over the four-momentum includes the sum over Matsubara frequencies and the spacial momentum, $\sum_k = \sum_{n\in Z}\sum_{\mathbf{k}}$. As stated in *Condensed matter field theory*[44], the physics that tends to be the most interesting, typically arises from processes in which one of the three unbounded momenta involved in the interaction vertex is small. Consequently, we break down the full momentum summation to a restricted summation over the small-momenta ($q$) sublayers

$$S_{\text{int}}[\bar{\psi}, \psi] \cong \frac{1}{2}\sum_{k,k',q}\big( - \bar{\psi}_{\sigma,k}\psi_{\sigma',k+q}V(\mathbf{k}' - \mathbf{k})\bar{\psi}_{\sigma',k'+q}\psi_{\sigma,k'}$$

$$+\bar{\psi}_{\sigma,k}\psi_{\sigma,k+q}V(\mathbf{q})\bar{\psi}_{\sigma',k'}\psi_{\sigma',k'-q} - \bar{\psi}_{\sigma,k}\bar{\psi}_{\sigma',-k+q}V(\mathbf{k}' - \mathbf{k})\psi_{\sigma,k'}\psi_{\sigma',-k'+q}\big), \tag{2.7.7}$$

where $|q| \ll |k|, |k'|$. It is now clearer that the decoupling in the different channels is

$$\hat{\rho}_{D,q} \sim \sum_k \bar{\psi}_\sigma(k)\psi_\sigma(k+q) \quad \text{The Direct Channel (D) ,} \tag{2.7.8}$$

$$\hat{\rho}_{X,\sigma,\sigma',q} \sim \sum_k \bar{\psi}_\sigma(k)\psi_{\sigma'}(k+q) \quad \text{The Exchange Channel (X),} \tag{2.7.9}$$

$$\hat{\rho}_{C,\sigma,\sigma',q} \sim \sum_k \bar{\psi}_\sigma(k)\bar{\psi}_{\sigma'}(-k+q) \quad \text{The Cooper Channel (C).} \tag{2.7.10}$$

In chapter 3 we will look at an action to describe the charge density wave. This describes modulations of the charge density in the system. Hence, we want to decouple in the particle-hole channel, also called the direct channel. In chapter 4 we will include superconductivity in the system. This is described by a particle-pair, therefore, we need the decoupling to be in the particle-particle channel, the Cooper channel.

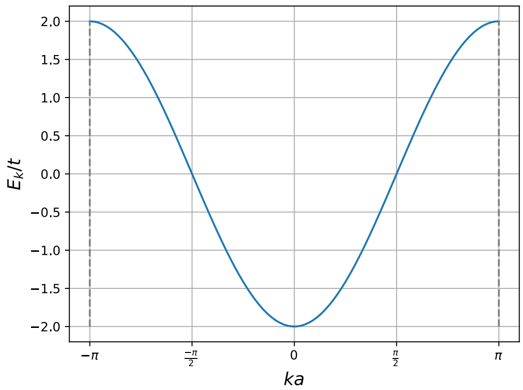



Figure 2.2: Electron energy with equally spaced ions at half-filling, where $t = 1$ is used as the energy-scale. The energies of the electrons is here defined as $\epsilon_k = -2t\cos(ka)$

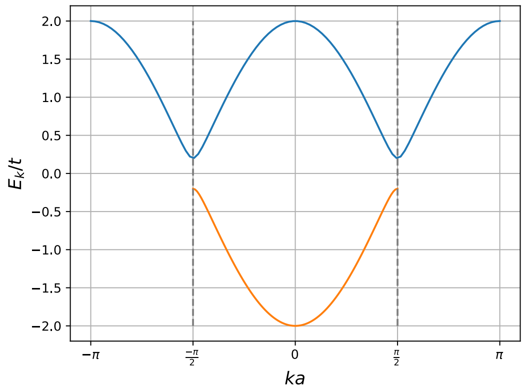



Figure 2.3: Electron energy when every second ion is displaced by the same amount in the same direction. A gap is induced at $ka = \pm\frac{\pi}{2}$.

## 2.8 Peierls instablity

Before starting on the main part of this thesis we want to establish a theory for CDWs in one dimension. In 1955 a German-British theoretical physicist Rudolf E. Peierls [1] derived the first known theory of this phenomenon. He stated that in a partially filled one-dimensional metal, the regular chain can never be stable. Assuming half-filling ($2k_F = \pi/a$), the argument goes as follows: by translating every second atom the same amount in the same direction, a new periodicity in the chain is introduced, $a \to 2a$, and the Brillouin zone is reduced to $-\frac{\pi}{2a} < k < \frac{\pi}{2a}$. This induces an energy gap at the new zone boundaries, $k_F = \frac{\pi}{2a}$ as shown in figure 2.3, which lowers the energy of each occupied state. In one dimension the decrease in electron energy is always smaller than the energy the ions gain by the distortion. This is why a $2k_F$ distortion occurs in the positions of the ions, which also induces a static charge density wave with the same periodicity. According to Pouget, the argument that Peierls gave for a half-filled band can easily be generalized to other fillings [48].

# Chapter 3

# Charge Density Waves in the Functional Integral Approach

In this chapter, the goal is to derive a Ginzburg-Landau theory for a system exhibiting a CDW phase. The theory will be derived using the formalism introduced in the preliminaries and follows the structure of Lundemo's specialization thesis[49]. Firstly, we will find an expression for the effective, bosonic action. Secondly, we will do a stationary phase analysis to find the mean-field state. As a next step, we will calculate the critical temperature of the system. Lastly, we will look at fluctuations around the mean field to derive a Ginzburg-Landau theory of the free energy for the system.

## 3.1 Effective action

We will start by introducing a general many-body Hamiltonian with a two-body interaction term. The Hamiltonian reads

$$H = \sum_{i,\sigma} (\epsilon_i - \mu) c^\dagger_{i,\sigma} c_{i,\sigma} + \frac{1}{4} \sum_{\alpha,\beta} \sum_{i,j} V^{\alpha,\beta}_{i,j} n_{i,\alpha} n_{j,\beta}, \tag{3.1.1}$$

where $n_{i,\alpha} \equiv c^\dagger_{i,\alpha} c_{i,\alpha}$ is the number operator for fermions at position $\mathbf{r}_i$ and with spin $\alpha$. The kinetic energy for a fermion at position $\mathbf{r}_i$ is denoted as $\epsilon_i$, and $\mu$ is the chemical potential in the system. The potential $V^{\alpha,\beta}_{i,j}$ describes the interaction between two fermions where one of them is at position $\mathbf{r}_i$ with spin $\alpha$, and the other one at $\mathbf{r}_j$ with spin $\beta$. We will assume that this potential is spin-independent, $V^{\alpha,\beta}_{i,j} = V_{i,j}$. Moving on, we will express the Hamiltonian in Fourier space. In section 2.7 we stated that the physics of the CDW is best described with a decoupling of the interaction term in the particle-hole channel. Following the theory from this section, we rewrite the Hamiltonian in momentum space in the following way

$$H = \sum_{\mathbf{k},\sigma} (\epsilon_{\mathbf{k}} - \mu) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{4} \sum_{\substack{\mathbf{k},\mathbf{k}',\mathbf{q} \\ \sigma,\sigma'}} V(\mathbf{q}) c^\dagger_{\mathbf{k}+\mathbf{q}/2,\sigma} c_{\mathbf{k}-\mathbf{q}/2,\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q}/2,\sigma'} c_{\mathbf{k}'+\mathbf{q}/2,\sigma'} \tag{3.1.2}$$

where $\mathbf{k} - \mathbf{q}/2$ is the inertial momentum of the first fermion, $\mathbf{k}' + \mathbf{q}/2$ is the inertial momentum of the second fermion and $\mathbf{q}$ is the exchanged momentum of the interaction.

The interaction term is shown in terms of a Feynmann diagram in figure 3.1. The full calculation of the Fourier transformation is shown in appendix C. Continuing, we will

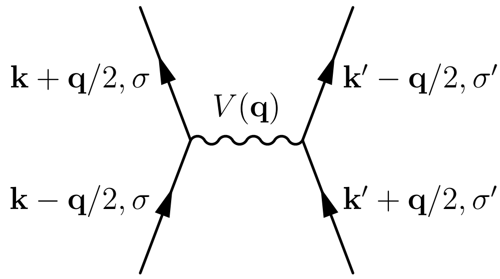



Figure 3.1: The interaction term illustrated by a Feynmann-diagram

need the action of the system

$$S[\bar{\psi},\psi]=\sum_{k,\sigma}\bar{\psi}_{k,\sigma}[-i\omega_n+\xi_{\mathbf{k}}]\psi_{k,\sigma}-\frac{1}{4}\sum_{\sigma,\sigma'}\sum_{q,k,k'}V(q)\bar{\psi}_{k+q/2,\sigma}\psi_{k-q/2,\sigma}\bar{\psi}_{k'-q/2,\sigma'}\psi_{k'+q/2,\sigma'}, \tag{3.1.3}$$

where $\psi$ is a Grassmann field, $\omega_n$ the Matsubara frequency and $\xi_k = \epsilon_k - \mu$ is the kinetic energy minus the chemical potential. The spatial momentum and the Matsubara frequency are written in terms of the compact notation, $k = (\mathbf{k}, \omega_n)$. The next step is to use the theory we introduced in the preliminaries and express the partition function as a functional integral,

$$Z=\int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-S[\bar{\psi},\psi]}. \tag{3.1.4}$$

Proceeding, we will decouple the interaction term in equation (3.1.3). In order to do this, we introduce the auxiliary field, $\kappa$. The first thing to note is that we assume that $\kappa$ is only dependent on the relative momentum $q$ in the interaction term[1]. Secondly, we assume $\kappa$ to be a real field. It can be shown that by starting with a complex auxiliary field, the result will effectively be a real field coupled to the fermionic field operators. The field $\kappa$ is in fact the order parameter of the charge density wave phase transition. According to the phenomenological theory by Landau [50] we have that an order parameter for a phase transition is defined as a quantity that vanishes in the disordered phase and is non-zero in the ordered phase. Hence, the order parameter is a quantity that measures ordering in a system below its critical temperature. Having established the properties of the order parameter $\kappa$, we introduce the measure

$$\mathbb{1}=\int \mathcal{D}\kappa \exp\left(-\sum_q \frac{\kappa(q)\kappa(-q)}{V(q)}\right). \tag{3.1.5}$$

[1]By starting with a field dependent on both the relative momentum and the center of mass momentum, $\phi(k,q)$, it can be shown that the center of mass momentum can be summed over, $\kappa(q) = \sum_k \phi(k,q)$. Thus, we are left with a field only dependent on the relative momentum, $\kappa(q)$.

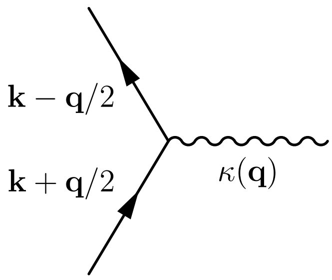



Figure 3.2: The incoming fermion with momentum $\mathbf{k}+\mathbf{q}/2$ and outgoing $\mathbf{k}-\mathbf{q}/2$ and an auxiliary field $\kappa(q)$ which decouples quartic the interaction.

Since $\kappa$ is real, it can also be shown that it is symmetric around zero in momentum space, $\kappa(-q) = \kappa(q)$. We will keep the signs in the bosonic term to shift the fields in such a way, that the quartic term in the action cancels. The shift is as follows

$$\kappa(q) \to \tilde{\kappa}(q) \equiv \kappa(q) - \frac{1}{2}V(q)\sum_{k,\sigma}\bar{\psi}_{k+q/2,\sigma}\psi_{k-q/2,\sigma}. \tag{3.1.6}$$

Inserting the shifted measure into equation (3.1.4) gives the partition function with the decoupled action

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \int \mathcal{D}[\kappa]e^{-\tilde{S}[\bar{\psi},\psi,\kappa]}, \tag{3.1.7}$$

where the decoupled action $\tilde{S}$ reads

$$\tilde{S}[\bar{\psi},\psi,\kappa] = \sum_{k,\sigma}\bar{\psi}_{k,\sigma}[-\mathcal{G}_0^{-1}(k)]\psi_{k,\sigma} + \sum_q \frac{\kappa(q)\kappa(q)}{V(q)} - \sum_{k,q,\sigma}\kappa(q)\bar{\psi}_{k-q/2,\sigma}\psi_{k+q/2,\sigma}. \tag{3.1.8}$$

The action contains three different terms. The first term is the non-interacting energy for the fermions, where we have defined the bare Greens function $\mathcal{G}_0^{-1}(k) \equiv i\omega_n - \xi_k$. The second term is the non-interacting boson energy, and the last term is fermionic fields coupled to a bosonic field, which is illustrated with a Feynmann diagram in figure 3.2. The next step is to integrate over the fermionic fields. This is calculated in equation (2.4.4) in the preliminaries. Thus, we first want to structure the fermionic action as,

$$S_f[\bar{\psi},\psi,\kappa] = \sum_\sigma\sum_{k_1,k_2}\bar{\psi}_{k_1,\sigma}[-(\hat{\mathcal{G}}^{-1})_{k_1,k_2}]\psi_{k_2,\sigma}, \tag{3.1.9}$$

where we defined the dressed Greens function as $\hat{\mathcal{G}}^{-1} = \hat{\mathcal{G}}_0^{-1} + \hat{\kappa}$. Note that $\hat{\mathcal{G}}^{-1}, \hat{\mathcal{G}}_0^{-1}$ and $\hat{\kappa}$ are now defined as operators in momentum space. The bare Green function $\mathcal{G}_0^{-1}$ is diagonal in momentum space, and the elements are defined as $(\hat{\mathcal{G}}_0)_{k,k'} \equiv \mathcal{G}_0(k)\delta_{k,k'}$. Whereas, the elements of the bosonic field operator are off-diagonal and defined as $(\hat{\kappa})_{k,k'} \equiv \kappa(k'-k)$ and we have that $\kappa(0) = 0$. Moving on, we integrate over the fermionic fields

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi e^{-\sum_{k,q,\sigma}\bar{\psi}_{k-q/2,\sigma}[-(\hat{\mathcal{G}}^{-1})_{k-q/2,k+q/2}]\psi_{k+q/2,\sigma}} = \det(-\hat{\mathcal{G}}^{-1}). \tag{3.1.10}$$

The effective action can be written as

$$S_{\text{eff}}[\kappa] = \sum_q \frac{\kappa(q)\kappa(q)}{V(q)} - \operatorname{tr}\ln(-\beta\hat{\mathcal{G}}^{-1}), \tag{3.1.11}$$

where we used the identity introduced in preliminaries, $\det \mathbf{A} = e^{\operatorname{tr}\ln \mathbf{A}}$. Note that we have multiplied the dressed Greens function with $\beta$ to make the argument in the trace-log dimensionless. Another thing to note is that the trace is in the momentum space *and* spin space. We have now found an expression for the effective action and are ready to proceed to the stationary phase analysis.

## 3.2 Stationary phase analysis

In this section, we want to derive a self-consistent equation for the mean field of $\hat{\kappa}$. Peierls stated in 1955 [1] that charge density waves in one dimension are expected to arise at $\mathbf{q} = 2\mathbf{k}_F$. In higher dimensions, one of the theories for CDWs is given by Fermi surface nesting [51]. These are also characterized by $\mathbf{q} = 2\mathbf{k}_F$. Hong Yao et. al. [52] studied a quasi-two-dimensional system with $\mathbf{q} = (2\mathbf{k}_F, 2\mathbf{k}_F)$, which described CDWs formed as stripes. In light of this, we fix the momentum at $2\mathbf{k}_F$ to find an equation for the mean field of the CDW order parameter. In this analysis, we are not interested in the dynamics of the order parameter and therefore set the respective Matsuabara frequency to zero, $\omega_v = 0$. To find a self-consistent equation for the mean field, we differentiate the action with respect to $\kappa(2k_F)$. We introduce the four-vector $2k_F \equiv (2\mathbf{k}_F, 0)$ to simplify the notation. The equation for the mean field is

$$0 \stackrel{!}{=} \frac{\delta S_{\text{eff}}}{\delta\kappa(2k_F)} = 2V^{-1}(2k_F)\kappa(2k_F) - \frac{\delta}{\delta\kappa(2k_F)}\operatorname{tr}\ln(-\beta\hat{\mathcal{G}}^{-1}), \tag{3.2.1}$$

where $\delta_{\kappa(2\mathbf{k}_F)}S_{\text{eff}}$ is the functional differentiation of the effective action. Moving on, we will look closer at the last term. Due to the trace, we can treat the operator as a function when differentiating[2]. This allows us to write the last term as

$$\frac{\delta}{\delta\kappa(2k_F)}\operatorname{tr}\ln(-\beta\hat{\mathcal{G}}^{-1}) = \operatorname{tr}\Big[\hat{\mathcal{G}}\frac{\delta\hat{\mathcal{G}}^{-1}}{\delta\kappa(2k_F)}\Big]. \tag{3.2.2}$$

Calculating the trace gives us

$$\operatorname{tr}\Big[\hat{\mathcal{G}}\frac{\delta\hat{\mathcal{G}}^{-1}}{\delta\kappa(2k_F)}\Big] = 2\sum_k \Big[\hat{\mathcal{G}}\frac{\delta\hat{\mathcal{G}}^{-1}}{\delta\kappa(2k_F)}\Big]_{k,k} = 2\sum_{k,k_1}\hat{\mathcal{G}}_{k,k_1}\Big[\frac{\delta\hat{\kappa}}{\delta\kappa(2k_F)}\Big]_{k_1,k}, \tag{3.2.3}$$

[2]Having an operator $\hat{A}(x)$ depending on a parameter $x$ and an arbitrary function $f(\hat{A})$ we can write

$$\delta_x \operatorname{tr}[f(\hat{A})] = \delta_x \sum_n \frac{f^{(n)}(0)}{n!}\operatorname{tr}(\hat{A}^n) = \sum_n \frac{f(n)(0)}{n!}\operatorname{tr}[(\delta_x\hat{A})\hat{A}^{n-1} + \hat{A}(\delta_x\hat{A})\hat{A}^{n-2} + ... + \hat{A}^{n-1}\delta_x\hat{A}]$$
$$= \sum_n \frac{n}{n!}f^{(n)}(0)\operatorname{tr}[\hat{A}^{(n-1)}(\delta_x\hat{A})] = \operatorname{tr}[f'(\hat{A})\delta_x\hat{A}]$$

where the factor 2 comes from the spin-summation in the trace. Before proceeding, we want to emphasize how the differentiation of $\hat{\kappa}$ is done. The first thing to note is that $\hat{\kappa}$ is an operator which can be written as a matrix. The matrix elements of $\kappa$ are $(\hat{\kappa})_{k,k'} = \kappa(k'-k)$, as defined earlier. Therefore, the derivative with respect to $\kappa(2k_F)$ will give a matrix with 1 wherever $k'-k = 2k_F$, and zero otherwise. Hence, we have that $\left[\frac{\delta\hat{\kappa}}{\delta\kappa(2\mathbf{k}_F,\omega_v=0)}\right]_{k_1,k} = \delta_{2\mathbf{k}_F,\mathbf{k}-\mathbf{k}_1}\delta_{\omega_n,\omega_{n_1}}$. This gives

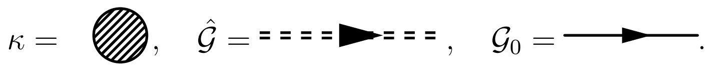
$$\mathrm{tr}\Big[\hat{\mathcal{G}}\frac{\delta\hat{\mathcal{G}}^{-1}}{\delta\kappa(2k_F)}\Big] = 2\sum_{k,k_1}\hat{\mathcal{G}}_{k,k_1}\delta_{2k_F,k-k_1} = 2\sum_{\mathbf{k}}\sum_{\omega_n}\hat{\mathcal{G}}_{k,k-2k_F}. \tag{3.2.4}$$

The stationary phase condition for $\hat{\kappa}$ can be found by plugging this back into equation (3.2.1)

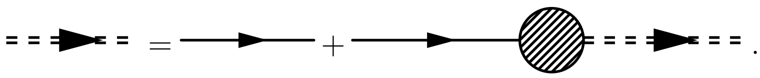
$$2\kappa(2k_F) = 2V(2k_F)\sum_k \hat{\mathcal{G}}_{k,k-2k_F}. \tag{3.2.5}$$

One solution to the equation is that $\kappa(2k_F) = 0$, because we have that $\hat{\mathcal{G}}^{-1} = [\hat{\mathcal{G}}_0^{-1} + \hat{\kappa}]^{-1}$, and $\mathcal{G}_0$ is diagonal in momentum space. Next, we are interested to look at solutions for $\Delta(2k_F) \neq 0$ to equation (3.2.5).

From the definition of $\hat{\mathcal{G}}$ we can derive a Dyson-like equation. We can use Feynmann diagrams to illustrate the equation, with the following symbols




The Dyson-like equation for the dressed Greens-function is



(3.2.6)

**Critical temperature** In addition to the mean field, we can derive the critical temperature from the stationary phase equation (3.2.5). Before we explain how the critical temperature is defined we will expand the dressed Greens function in $\kappa$. This is due to the fact that close to the critical temperature, we assume that the order parameter is approaching zero. The expansion to first order reads

$$\hat{\mathcal{G}}_{k,k-2k_F} = \big([1+\hat{\mathcal{G}}_0\hat{\kappa}]^{-1}\hat{\mathcal{G}}_0\big)_{k,k-2k_F} = (\hat{\mathcal{G}}_0)_{k,k-2k_F} - [\hat{\mathcal{G}}_0\hat{\kappa}\hat{\mathcal{G}}_0]_{k,k-2k_F} + \mathcal{O}\big(\hat{\kappa}^3\big). \tag{3.2.7}$$

Since $\hat{\mathcal{G}}_0$ is diagonal in $k$, the first term is zero, and we have that

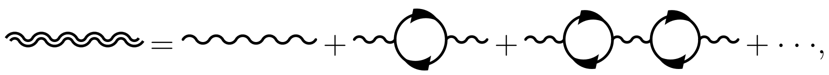
$$\kappa(2k_F) = -V(2k_F)\sum_k \mathcal{G}_0(k)\kappa(2k_F)\mathcal{G}_0(k-2k_F) + \mathcal{O}(\kappa^3). \tag{3.2.8}$$

Dividing by $\kappa(2k_F)$ gives

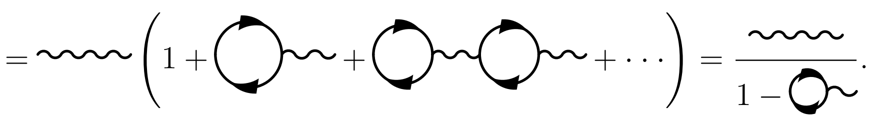
$$1 = -V(2k_F)\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F) + \mathcal{O}(\kappa^2). \tag{3.2.9}$$

From this equation, we can find an expression for the critical temperature. It is defined as the temperature which makes the charge density (Lindhard) susceptibility diverge. The susceptibility for particle-hole fluctuations is proportional to $[1+V(2k_F)\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F)]^{-1}$.

**Remark** By including particle-hole fluctuations we can find an expression for an effective potential. This potential is defined as $V_{eff} = \chi V_0$, where $\chi$ is defined as the susceptibility. To find an expression for $\chi$, we can illustrate the effective potential in terms of a series of Feynmann diagrams


(3.2.10)

where the double wiggly line is the effective potential $V_{\text{eff}}$, the single wiggly line is the bare potential $V$ and the bubble is particle-hole bubble $K$. We have focused on only the simple bubbles, which is an approximation but will quantitatively give the correct result. Pulling out a factor of the bare potential we can see that it is a geometric series, which can be expressed as


(3.2.11)

From this, we can identify an expression for how easy pair fluctuations can arise. This known as the susceptibility, $\chi_{ph} = [1 - VK]^{-1}$.

For this system, we have that $\chi_{ph} \propto [1+V(2k_F)\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F)]^{-1}$. To derive an expression for the critical temperature we will perform the $k$-summations over the bare Greens functions. The sum can be written as

$$\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F) = \sum_k \frac{1}{(i\omega_n - \xi_{\mathbf{k}})} \frac{1}{(i\omega_n - \xi_{\mathbf{k}-2\mathbf{k}_F})} \tag{3.2.12}$$

Rewriting this, and summing over the Matsubara frequencies, we get

$$\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F) = \sum_{\mathbf{k}} \frac{1}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}-2\mathbf{k}_F}} \sum_n \left[\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n - \xi_{\mathbf{k}-2\mathbf{k}_F}}\right] \tag{3.2.13}$$

$$= \beta \sum_{\mathbf{k}} \frac{1}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}-2\mathbf{k}_F}} \left[\frac{1}{1+\mathrm{e}^{\beta\xi_{\mathbf{k}}}} - \frac{1}{1+\mathrm{e}^{\beta\xi_{\mathbf{k}-2\mathbf{k}_F}}}\right]. \tag{3.2.14}$$

The calculation of the sum over the Matsubara frequencies is shown in appendix D. To proceed, we will linearize the energies

$$\epsilon_{\mathbf{k}} = \epsilon_F + \mathbf{v}_F(\mathbf{k} - \mathbf{k}_F) + \mathcal{O}(\mathbf{k}^2). \tag{3.2.15}$$

Using this we can find the linearization of $\xi_{\mathbf{k}}$ and $\xi_{\mathbf{k}-2\mathbf{k}_F}$

$$\xi_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu \approx v_F(\mathbf{k} - \mathbf{k}_F) \tag{3.2.16}$$
$$\xi_{\mathbf{k}-2\mathbf{k}_F} = \epsilon_{\mathbf{k}} - \mu + 2\epsilon_F - 2v_F\mathbf{k} \approx -v_F(\mathbf{k} - \mathbf{k}_F) \approx -\xi_{\mathbf{k}}, \tag{3.2.17}$$

where we can see that $\xi_{\mathbf{k}-2\mathbf{k}_F} \approx -\xi_{\mathbf{k}}$. Before proceeding, we must emphasize that the last transition in equation (3.2.17) is only valid for the energies close to the fermi level, which is ensured by a cut-off of the integral. Inserting this back into the expression for the particle-hole bubble (3.2.14), we get

$$\begin{aligned}\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F) &\approx \beta \sum_{\mathbf{k}} \frac{1}{2\xi_k}\left[\frac{1}{1+\mathrm{e}^{\beta\xi_k}} - \frac{1}{1+\mathrm{e}^{-\beta\xi_k}}\right] \\ &\approx -2\beta D_F \int_0^{\omega_c} d\xi \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{2\xi},\end{aligned} \tag{3.2.18}$$

where $\omega_C$ is the upper limit for where the linearization is valid. We have approximated the $\mathbf{k}$-summation to an energy integral. In the transition to an energy integral, we have used that $\sum_{\mathbf{k}} f(\xi_k) = \int d\xi D(\xi) f(\xi)$. The density of states is defined as $D(\xi) = \frac{1}{V_{sys}}\sum_k \delta(\xi - \xi_k)$, where $V_{sys}$ is the volume of the system. By using this, the calculation will still be exact, but we will approximate the density of states by its value on the fermi-surface, $D(\xi) \approx D_F$. This gives

$$1 = V(2k_F)\beta D_F \int_0^{\omega_c} d\xi \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi}. \tag{3.2.19}$$

We will write the $\beta$- and $N$-dependence in the potential explicitly and define the potential at $2k_F$ as $V(2k_F) = (N\beta)^{-1}V_{2k_F}$. The factor $(N\beta)^{-1}$ comes from Fourier transforms. In order to make the equation explicitly independent of the system size, we can write the density of states as $D_F = N_F/V$. This gives

$$1 = V_{2k_F} N_F \int_0^{\omega_c} d\xi \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi}. \tag{3.2.20}$$

We can observe that this is the same equation as for the critical temperature for the BCS superconductor. This might be surprising as they are critical phenomena in two different channels. CDWs happen in the particle-hole channel and SC in the particle-particle channel. Proceeding, we will assume that the critical temperature is small. Hence, the integral will be

$$\int_0^{\omega_c} d\xi \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi} = \int_0^{\frac{\beta\omega_c}{2}} d\xi \frac{\tanh(x)}{x} \approx \ln\left(\frac{\beta\omega_C}{2C}\right), \tag{3.2.21}$$

where $C = \frac{\pi}{4}\mathrm{e}^{-\gamma}$ and $\gamma$ is the Euler-Mascheroni constant[3]. The critical temperature can be expressed as

$$k_B T_C = \frac{2\omega_C}{\pi}\mathrm{e}^{\gamma} e^{-\frac{1}{\lambda}}, \tag{3.2.22}$$

[3]Euler-Mascheroni constant, $\gamma = \lim_{n\to\infty}\sum_{k=1}^{n}\left(\frac{1}{k} - \ln n\right) \approx 0.577215\ldots$

where $\lambda = V(2k_F)\beta D_F$. From this, we can observe that with a positive potential, the critical temperature converges logarithmic to zero when the magnitude of the potential increases. The expression for the critical temperature has the same form as in the BCS theory. According to Plakida, this points to a purely Coloumb nature of the particle-hole interaction [53].

## 3.3 Ginzburg-Landau theory for fluctuations

Next, we want to look at how the system behaves for small fluctuations around the mean field. The idea is that there is a static charge density wave at $\mathbf{q} = 2\mathbf{k}_F$, and in addition to this, there is now a slowly varying field. Therefore, we define $\kappa(q)$ as the sum of the mean field plus a fluctuating field. Hence, we have that

$$\kappa(2k_F - q) = \kappa_{\mathrm{MF}}(2k_F) + \eta(2k_F - q) \overset{T\to T_C}{=} \eta(q'), \tag{3.3.1}$$

where we defined $q' = (2\mathbf{k}_F - \mathbf{q}, 0)$ as the argument in $\eta$. We have used that the mean-field value approaches zero as $T \to T_C$ from below. Note that we are aiming for a time-independent theory, and therefore only look at fluctuations in the spacial momentum. The main principle of the Ginzburg-Landau theory is to expand the free energy around the system's normal state. Following this theory, this system's free energy can be modeled as

$$\beta F[\eta] - \beta F_{MF} = \int d^d r \left[\alpha_1|\eta|^2 + \gamma|\nabla\eta|^2 + \alpha_2|\eta|^4 + \cdots\right], \tag{3.3.2}$$

where $\alpha_i$ and $\gamma$ are phenomenological constants, and $\eta$ is the order parameter. In this section, we assume that the spatial fluctuations are small, and therefore neglect higher-order gradient terms. The phenomenological constants contain information about the system, and for this reason, the main goal of this section is to give an explicit expression for $\alpha_1, \alpha_2$, and $\gamma$. In general, we could have odd powers of the order parameter in the free energy. This would mean that $F[\eta] \neq F[-\eta]$, which in turn indicates that a spatial translation of the charge density wave would change the free energy. In addition to this argument, we will later show that this also holds mathematically. At the end of this section, we will show that the higher-order terms are negligible.

The partition function can generally[4] be written as $Z = \sum_n \mathrm{e}^{-\beta F_n}$, where we sum over all possible states $n$. By comparing this with the partition function expressed in terms of the action, we can write

$$S_{\text{eff}} = S_{\mathrm{MF}} + \beta F[\eta]. \tag{3.3.3}$$

The mean-field action will be $S_{\mathrm{MF}} \equiv -\mathrm{tr}\ln\left[-\beta\hat{\mathcal{G}}_0^{-1}\right]$, and does not provide any relevant information for us in this consideration. This is because we are only interested in the physics of the fluctuating fields. To separate the mean-field action from the terms that we are interested in, we make use of the fact that $\mathrm{tr}\ln[-\beta(\hat{\mathcal{G}}_0^{-1} + \hat{\eta})] = \mathrm{tr}\ln[-\beta\hat{\mathcal{G}}_0^{-1}] +$

[4] From thermodynamics we have that the partition function can be written as $Z_g = e^{\beta pV}$. We also have that $pV = G - F = \mu N - F$, which for our case will be $pV = F$.

$\operatorname{tr}\ln[\mathbb{1}+\hat{\mathcal{G}}_0\hat{\eta}]$. This gives us that the free energy for $\eta$ is

$$\beta F[\eta] = \sum_{q'} V^{-1}(q')\eta(q')\eta(q') - \operatorname{tr}\Big[\ln\big(\mathbb{1}+\hat{\mathcal{G}}_0\hat{\eta}\big)\Big] \tag{3.3.4}$$

using the action from equation (3.1.11). To proceed, we will use the assumption that $\eta$ is sufficiently small. This allows us to expand the last term using the following expansion

$$\ln(1+x) = -\sum_{k=1}^{\infty}\frac{(-1)^k}{k}x^k \text{ for } |x|<1. \tag{3.3.5}$$

Using this, the expansion of the trace-log can be written as

$$-\operatorname{tr}\left[-\sum_{k=1}^{\infty}\frac{(-1)^k}{k}\Big(\hat{\mathcal{G}}_0\hat{\eta}\Big)^k\right] = -\operatorname{tr}[\hat{\mathcal{G}}_0\hat{\eta}] + \frac{1}{2}\operatorname{tr}[\hat{\mathcal{G}}_0\hat{\eta}\hat{\mathcal{G}}_0\hat{\eta}] + \mathcal{O}(\eta^3). \tag{3.3.6}$$

### 3.3.1 First order

Starting off with the first-order term, we have that

$$-\operatorname{tr}[\hat{\mathcal{G}}_0\hat{\eta}] = -\sum_{k}[\hat{\mathcal{G}}_0\hat{\eta}]_{k,k} = -\sum_{k,k_1}(\hat{\mathcal{G}}_0)_{k,k_1}(\hat{\eta})_{k_1,k} = 0 \tag{3.3.7}$$

Using that $\hat{\mathcal{G}}_0$ is a diagonal matrix and that $\eta$ only contains off-diagonal matrix elements, we see that this term is zero.

### 3.3.2 Second order

For the second-order term, we will do a similar calculation

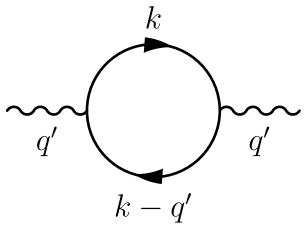
$$\begin{aligned}\frac{1}{2}\operatorname{tr}[\hat{\mathcal{G}}_0\hat{\eta}\hat{\mathcal{G}}_0\hat{\eta}] &= \frac{1}{2}\sum_{\substack{k_1,k_2\\k_3,k_4}}(\hat{\mathcal{G}}_0)_{k_1,k_2}(\hat{\eta})_{k_2,k_3}(\hat{\mathcal{G}}_0)_{k_3,k_4}(\hat{\eta})_{k_4,k_1}\\ &= \frac{1}{2}\sum_{k,q'}\mathcal{G}_0(k)\eta(q')\mathcal{G}_0(k-q')\eta(q'). \end{aligned} \tag{3.3.8}$$

Here, we used that $(\hat{\mathcal{G}}_0)_{k,k'} = \mathcal{G}_0(k)\delta_{k,k'}$, $\hat{\eta}_{k,k'} = \eta(k'-k)$, and renamed the summation momenta to be on the desired form. This gives us the expression for the free energy to second order in $\eta$

$$\beta F[\eta] = \sum_{q'} V^{-1}(q')\eta(q')\eta(q') + \sum_{k,q'}\mathcal{G}_0(k)\eta(q')\mathcal{G}_0(k-q')\eta(q'). \tag{3.3.9}$$

For each $q$ we can express the last term with a Feynmann diagram

$$\sum_k \mathcal{G}_0(k)\eta(q')\mathcal{G}_0(k-q')\eta(q') = \tag{3.3.10}$$




where the wiggly line represents the bosonic field, and the straight line the bare Greens function. The bubble is commonly referred to as a particle-hole-bubble, where we can see that it transfers the momentum $q'$. We want to remind the reader that the momentum $q'$ is the momentum of the static CDW minus a small momentum $q$. To proceed with our calculation we will assume that $q$ is small, which means that we only have long-waved fluctuations deviating from the static CDW.

### Expansion in $q$

To derive an expression for the phenomenological constant we will do an expansion of the bare Greens function. Since the theory is time-independent, we only expand in the spatial part. We have that $q' = (2\mathbf{k}_F - \mathbf{q}, 0)$, and the expansion will therefore be in $\mathbf{q}$. Expanding $\xi_{\mathbf{k}-\mathbf{q}'}$, gives

$$\xi_{\mathbf{k}-\mathbf{q}'} = \xi_{\mathbf{k}-2\mathbf{k}_F+\mathbf{q}} = \xi_{\mathbf{k}-2\mathbf{k}_F} + \frac{2(\mathbf{k}-2\mathbf{k}_F)\mathbf{q}}{2m^*} + \mathcal{O}(\mathbf{q}^2) \approx -\xi_{\mathbf{k}} + \tilde{\mathbf{v}}\cdot\mathbf{q}, \tag{3.3.11}$$

where $\tilde{\mathbf{v}} = \frac{\mathbf{k}}{m^*} - 2\mathbf{v}_F$, $m^*$ is an effective mass and we used the linearization from equation (3.2.17). We emphasize that the last transition is only valid as long as the linearization of the energy $\epsilon_{\mathbf{k}}$ is valid. To derive the expression for the coefficients $\alpha_1$ and $\gamma$ we start by rewriting the following expression

$$\begin{aligned}\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F+q) &= \sum_k \left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}}\right)\left(\frac{1}{i\omega_n + \xi_{\mathbf{k}} - \tilde{\mathbf{v}}\cdot\mathbf{q}}\right) \\ &= \sum_k \frac{1}{2\xi_{\mathbf{k}} - \tilde{\mathbf{v}}\cdot\mathbf{q}}\left[\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + \xi_{\mathbf{k}} - \tilde{\mathbf{v}}\cdot\mathbf{q}}\right].\end{aligned} \tag{3.3.12}$$

Expanding the Greens functions to second order in $\tilde{\mathbf{v}}\cdot\mathbf{q}$, gives

$$\begin{aligned}\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F+q) \approx \sum_k \Bigg\{ &\frac{1}{2\xi_{\mathbf{k}}}\left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + \xi_{\mathbf{k}}}\right) \\ &+\tilde{\mathbf{v}}\cdot\mathbf{q}\left[\frac{1}{4\xi_{\mathbf{k}}^2}\left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + \xi_{\mathbf{k}}}\right) - \frac{1}{2\xi_{\mathbf{k}}}\frac{1}{(i\omega_n + \xi_{\mathbf{k}})^2}\right] \\ +(\tilde{\mathbf{v}}\cdot\mathbf{q})^2 &\left[\frac{1}{8\xi_{\mathbf{k}}^3}\left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + \xi_{\mathbf{k}}}\right) - \frac{1}{4\xi_{\mathbf{k}}^2}\frac{1}{(i\omega_n + \xi_{\mathbf{k}})^2} - \frac{1}{2\xi_{\mathbf{k}}}\frac{1}{(i\omega_n + \xi_{\mathbf{k}})^3}\right]\Bigg\}.\end{aligned} \tag{3.3.13}$$

Moving on, we will calculate the Matsubara frequency sums. An elegant formula for calculating the sum over $(i\omega_n - \xi)^{-m}$ for fermions is given in appendix D. The formula is

$$\sum_{n\in\mathcal{Z}} \frac{1}{(i\omega_n - \xi)^m} = \frac{\beta}{(m-1)!}\partial_\xi^{m-1} f(\xi), \tag{3.3.14}$$

where $f(\xi) = \frac{1}{\exp(\beta\xi)+1}$ is the Fermi-Dirac distribution. The Matsubara sums we need are

$$\sum_n \frac{1}{i\omega_n \pm \xi_{\mathbf{k}}} = \frac{\beta}{e^{\mp\beta\xi_{\mathbf{k}}}+1}, \tag{3.3.15}$$

$$\sum_n \frac{1}{(i\omega_n + \xi_{\mathbf{k}})^2} = \frac{\beta}{1!}\partial_\xi f(-\xi) = -\frac{\beta^2}{4}\text{sech}^2(\frac{\beta\xi_{\mathbf{k}}}{2}), \tag{3.3.16}$$

$$\sum_n \frac{1}{(i\omega_n + \xi_{\mathbf{k}})^3} = -\frac{\beta^3}{8}\tanh(\frac{\beta\xi_{\mathbf{k}}}{2})\text{sech}^2(\frac{\beta\xi_{\mathbf{k}}}{2}). \tag{3.3.17}$$

Proceeding, we will first evaluate the term that is independent of $\mathbf{q}$. This is in fact the same integral as we had in equation (3.2.18) in the stationary phase analysis. Hence,

$$\begin{aligned}\alpha_1 &= \sum_k \frac{1}{2\xi_k}\left[\frac{1}{i\omega_n - \xi_k} - \frac{1}{i\omega_n + \xi_k}\right] = \sum_{\mathbf{k}} \frac{\beta}{2\xi_{\mathbf{k}}}\left[\frac{1}{e^{\beta\xi_{\mathbf{k}}}+1} - \frac{1}{e^{-\beta\xi_{\mathbf{k}}}+1}\right] \\ &= -\sum_{\mathbf{k}} \frac{\beta}{2\xi_{\mathbf{k}}}\tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) = -D_F\beta\int_0^{\omega_C}\frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi}. \end{aligned}\tag{3.3.18}$$

The next term we want to calculate is the term linear in $\mathbf{q}$. This needs a bit more consideration due to the dot product. First, we calculate the Matsubara sum,

$$\begin{aligned}&\sum_k \frac{\tilde{\mathbf{v}}\cdot\mathbf{q}}{2\xi_k}\left[\frac{-1}{(i\omega_n+\xi_k)^2} + \frac{1}{2\xi_k}\left[\frac{1}{i\omega_n - \xi_k} - \frac{1}{i\omega_n+\xi_k}\right]\right] \\ &= \sum_{\mathbf{k}} \frac{\tilde{\mathbf{v}}\cdot\mathbf{q}}{2\xi_{\mathbf{k}}}\left[-\frac{\beta^2}{4}\text{sech}^2\left(\frac{\xi_{\mathbf{k}}}{2}\right) + \frac{\beta}{2\xi_{\mathbf{k}}}\tanh\left(\frac{\xi_{\mathbf{k}}}{2}\right)\right]. \end{aligned}\tag{3.3.19}$$

Next, we want to change the $k$-sum to an energy integral. Before doing so, we will need to perform the angular integral over $\hat{k}$. We have that $\tilde{\mathbf{v}} = \frac{\mathbf{k}}{2m^*} - 2\mathbf{v}_F$. We therefore only integrate over $\hat{k}$, which gives $q_i k_i \int \frac{d\Omega}{4\pi}\hat{k}_i = 0$. Hence, equation (3.3.19) is now

$$\frac{D_F\beta\mathbf{k}_F\cdot\mathbf{q}}{8m^*}\int_{-\omega_C}^{\omega_C} d\xi\frac{-\xi\beta + \sinh(\xi)}{\xi^2}\text{sech}^2\left(\frac{\xi}{2}\right) = 0, \tag{3.3.20}$$

which is zero because of the anti-symmetric integrand.

The next term will be the quadratic them in $\mathbf{q}$. Using the Matsubara sums (3.3.15), (3.3.16) and (3.3.17) we get the following result

$$\begin{aligned}&\sum_k \frac{(\tilde{\mathbf{v}}\cdot\mathbf{q})^2}{2\xi_{\mathbf{k}}}\left[\frac{1}{4\xi_{\mathbf{k}}^2}\left(\frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n+\xi_{\mathbf{k}}}\right) - \frac{1}{2\xi_{\mathbf{k}}}\frac{1}{(i\omega_n+\xi_{\mathbf{k}})^2} - \frac{1}{(i\omega_n+\xi_{\mathbf{k}})^3}\right] \\ &= \sum_{\mathbf{k}} \beta\frac{(\tilde{\mathbf{v}}\cdot\mathbf{q})^2}{16\xi_{\mathbf{k}}^3}\left[-\sinh(\beta\xi_{\mathbf{k}}) + \beta\xi_{\mathbf{k}} + \beta^2\xi_{\mathbf{k}}^2\tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right)\right]\text{sech}^2\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right). \end{aligned}\tag{3.3.21}$$

The angular integral over $k$ reads,

$$\int \frac{d\Omega}{4\pi}\big((\mathbf{k}-2\mathbf{k}_F)\cdot\mathbf{q}\big)^2 = k_i k_j q_i q_j \int \frac{d\Omega}{4\pi}\hat{k}_i\hat{k}_j + 4\mathbf{k}_F^2\mathbf{q}^2 = \frac{1}{3}\delta_{i,j}q_i q_j k_i k_j + 4\mathbf{k}_F^2\mathbf{q}^2, \quad (3.3.22)$$

where the cross-term will be zero when doing the angular integral. This gives

$$\mathbf{q}^2\frac{\beta D_F}{16(m^*)^2}\int_{-\omega_c}^{\omega_c} d\xi \left(\frac{\mathbf{k}^2}{3}+4\mathbf{k}_F^2\right)\frac{1}{\xi^3}\left[-\sinh\left(\beta\xi\right)+\beta\xi+\beta^2\xi^2\tanh\left(\frac{\beta\xi}{2}\right)\right]\operatorname{sech}^2\left(\frac{\beta\xi}{2}\right). \quad (3.3.23)$$

We will now look closer at the expression

$$\frac{1}{16(m^*)^2}\left(\frac{\mathbf{k}^2}{3}+4\mathbf{k}_F^2\right) = \frac{1}{24m^*}(\xi_{\mathbf{k}}+\mu)+\frac{v_F^2}{4} = \frac{1}{24m^*}\xi_{\mathbf{k}}+\frac{13}{48}v_F^2. \quad (3.3.24)$$

The term multiplied by $\xi_{\mathbf{k}}$ is zero due to the anti-symmetry of the total integrand. We are then left with

$$\mathbf{q}^2 v_F^2 D_F\beta\frac{13}{48}\int_{-\omega_c}^{\omega_c} d\xi\frac{1}{\xi^3}\left[-\sinh\left(\beta\xi\right)+\beta\xi+\beta^2\xi^2\tanh\left(\frac{\beta\xi}{2}\right)\right]\operatorname{sech}^2\left(\frac{\beta\xi}{2}\right). \quad (3.3.25)$$

The integral is not possible to solve analytically, but numerically we can see that it is positive. The expression for the free energy to second order in $\eta$ is

$$\beta F[\eta] \approx \sum_{\mathbf{q}} \alpha_1\eta(2\mathbf{k}_F-\mathbf{q})\eta(2\mathbf{k}_F-\mathbf{q})+\gamma\mathbf{q}^2\eta(2\mathbf{k}_F-\mathbf{q})\eta(2\mathbf{k}_F-\mathbf{q}), \quad (3.3.26)$$

where the coefficients $\alpha_1$ and $\gamma$ are given by

$$\alpha_1 = \frac{N\beta}{V_{2\mathbf{k}_F}} - D_F\beta\int_0^{\omega_C} d\xi\frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi} \quad (3.3.27)$$

$$\gamma = v_F^2 D_F\beta\frac{13}{24}\int_0^{\omega_c} d\xi\frac{1}{\xi^3}\left[-\sinh\left(\beta\xi_k\right)+\beta\xi+\beta^2\xi^2\tanh\left(\frac{\beta\xi}{2}\right)\right]\operatorname{sech}^2\left(\frac{\beta\xi}{2}\right). \quad (3.3.28)$$

We have used the fact that the potential is a constant for small $\mathbf{q}$, $V(2\mathbf{k}_F-\mathbf{q}) \approx (N\beta)^{-1}V_{2\mathbf{k}_F}$. Note that we can evaluate the integrals in the coefficients at low temperatures. This is already done for $\alpha_1$ in the section 3.2, about the stationary phase analysis. For $\gamma$, we will let $\omega_C \to \infty$ and solve the two integrals separately [49]

$$\gamma_1 = \int_0^\infty \frac{d\xi}{\xi^3}\left[\beta\xi-\sinh\left(\beta\xi_k\right)\right]\operatorname{sech}^2\left(\frac{\beta\xi}{2}\right) = -\frac{\beta^2}{2\pi^2}\zeta(3,1/2) \quad (3.3.29)$$

$$\gamma_2 = \int_0^\infty \frac{d\xi}{\xi}\tanh\left(\frac{\beta\xi}{2}\right)\operatorname{sech}^2\left(\frac{\beta\xi}{2}\right) = \frac{7}{\pi^2}\zeta(3), \quad (3.3.30)$$

where $\zeta$ is the Riemann Zeta function[54]. The resulting coefficient we will get for $\gamma$ is

$$\gamma = v_F^2 D_F\beta^3\frac{13}{48\pi^2}\zeta(3,1/2). \quad (3.3.31)$$

This tells us that at low temperatures $\gamma$ is proportional to $T^{-3}$. Furthermore, we can see that at the critical temperature, $\alpha_1$ will change sign. We can therefore solve the equation $\alpha_1 = 0$ to find this temperature, which will be the same equation as we found for $T_C$ in the stationary phase analysis. The potential can be expressed in terms of the critical temperature using equation (3.2.22). Inserting this into $\alpha_1$, we get

$$\begin{aligned}\alpha_1 &= N\beta N_F \int_0^{\omega_C} \frac{d\xi}{\xi} \tanh\left(\frac{\beta_C \xi}{2}\right) - D_F\beta \int_0^{\omega_C} \frac{d\xi}{\xi} \tanh\left(\frac{\beta\xi}{2}\right) \\ &= \beta D_F \int_0^{\omega_C} \frac{d\xi}{\xi} \text{sech}\left(\frac{\beta_C\xi}{2}\right) \text{sech}\left(\frac{\beta\xi}{2}\right) \sinh\left(\frac{\beta_C - \beta}{2}\xi\right) \end{aligned} \tag{3.3.32}$$

We will next assume that $T$ is close to the critical temperature $T_C$

$$\begin{aligned}\alpha_1 &= \beta D_F \int_0^{\omega_C} d\xi \text{sech}^2\left(\frac{\beta_C\xi}{2}\right) \frac{\beta_C - \beta}{2} \\ &= D_F \frac{\beta}{\beta_C}(\beta_C - \beta) \tanh\left(\frac{\beta_C \omega_C}{2}\right) \propto (T - T_C) \end{aligned} \tag{3.3.33}$$

We will therefore write $\alpha_1 = \alpha_1'(T - T_C)$. Whenever $T < T_C$, $\alpha_1$ is negative, and it is favorable to create CDWs in the system. Hence, we have an unstable system. To ensure stability below $T_C$, we need to include higher-order terms.

### 3.3.3 Third order

The third order of the expansion will be

$$\begin{aligned} &-\frac{1}{3}\text{tr}[\mathcal{G}_0\eta\mathcal{G}_0\eta\mathcal{G}_0\eta] \\ = -\frac{1}{3}\sum_{k_1,k_2,k_3} &\mathcal{G}_0(k_1)\eta(-(2k_F - q_1))\mathcal{G}_0(k_1 - 2k_F + q_1)\eta(2k_F - q_2) \\ &\mathcal{G}_0(k_1 + q_1 - q_2)\eta(2k_F + k_1 + q_2). \end{aligned} \tag{3.3.34}$$

We will assume that $q_i \ll k$, and the Greens functions will just depend on $k$. The coefficient of the third-order term is

$$\sum_k (\mathcal{G}_0(k))^2 \mathcal{G}_0(k - 2k_F) = \sum_k \frac{1}{(i\omega_n - \xi_\mathbf{k})^2} \frac{1}{i\omega_n + \xi_\mathbf{k}}. \tag{3.3.35}$$

When doing the $k$-summation, it can be shown that it will be zero due to the symmetry of the Green function.

### 3.3.4 Fourth order

The calculation of the trace is done in the same manner as for the second and third order. Thus, we will just state the result

$$\begin{aligned}\frac{1}{4}\text{tr}[(\hat{\mathcal{G}}_0\hat{\eta})^4] = \frac{1}{2}\sum_k \sum_{\substack{q_1,q_2\\q_3,q_4}} &\mathcal{G}_0(k)\mathcal{G}_0(k - 2k_F + q_1)\mathcal{G}_0(k + q_1 - q_2)\mathcal{G}_0(k - 2k_F - q_4) \\ &\eta_{2k_F - q_1}\eta_{2k_F - q_2}\eta_{2k_F - q_3}\eta_{2k_F - q_4}\delta_{q_1 - q_2 + q_3 - q_4, 0}, \end{aligned} \tag{3.3.36}$$

where we have used that $\eta$ is symmetric in its argument. Since $q$ is assumed to be small compared to $\mathbf{k}$ and $\mathbf{k}_F$, we have that $\mathcal{G}_0(k-2k_F-q_i) \approx \mathcal{G}_0(k-2k_F)$. The fourth-order term is

$$\approx \frac{1}{2}\sum_k \sum_{\substack{q_1',q_2'\\q_3',q_4'}} (\mathcal{G}_0(k))^2(\mathcal{G}_0(k-2k_F))^2 \eta_{q_1'}\eta_{q_2'}\eta_{q_3'}\eta_{q_4'}\delta_{q_1-q_2+q_3-q_4},$$

where we changed back to the $q'$ notation, $q' = (2\mathbf{k}_F - q, 0)$, to make the equations more compact. Moving on, we will approximate $\xi_{\mathbf{k}-2\mathbf{k}_F}$ in the same way as we did for the second-order term, which gives the

$$\sum_k (\mathcal{G}_0(k))^2(\mathcal{G}_0(k-2k_F))^2 = \sum_k \frac{1}{(i\omega_n-\xi_\mathbf{k})^2}\frac{1}{(i\omega_n-\xi_{\mathbf{k}-2\mathbf{k}_F})^2} \approx \sum_k \frac{1}{(i\omega_n-\xi_\mathbf{k})^2}\frac{1}{(i\omega_n+\xi_\mathbf{k})^2}$$
$$= \sum_k \frac{1}{4\xi_\mathbf{k}^3}\left[\frac{1}{i\omega_n+\xi_\mathbf{k}} - \frac{1}{i\omega_n-\xi_\mathbf{k}}\right] + \sum_k \frac{1}{4\xi_\mathbf{k}^2}\left[\frac{1}{(i\omega_n+\xi_\mathbf{k})^2} + \frac{1}{(i\omega_n-\xi_\mathbf{k})^2}\right]. \tag{3.3.37}$$

Summing over the Matsubara frequencies

$$= \sum_\mathbf{k} \frac{\beta}{4(\xi_\mathbf{k})^3}\tanh\left(\beta\frac{\xi_\mathbf{k}}{2}\right) - \sum_\mathbf{k}\frac{1}{4\xi_\mathbf{k}^2}\frac{\beta^2}{4}\left[\text{sech}^2\left(\frac{\beta\xi_\mathbf{k}}{2}\right) + \text{sech}^2\left(\frac{\beta\xi_\mathbf{k}}{2}\right)\right]$$
$$= \frac{\beta}{8}D_F\int_{-\omega_C}^{\omega_C}\frac{d\xi}{\xi^3}(\sinh(\beta\xi) - \beta\xi)\text{sech}^2\left(\frac{\beta\xi}{2}\right) \tag{3.3.38}$$

where we have used that $\sum_n [i\omega_n - \xi_\mathbf{k}]^2 = -\frac{\beta^2}{4}\text{sech}^2\left(\frac{\beta\xi_\mathbf{k}}{2}\right)$. This gives that the coefficient $\alpha_2$ is

$$\alpha_2 = \frac{\beta}{8}D_F\int_0^{\omega_C}\frac{d\xi}{\xi^3}(\sinh(\beta\xi) - \beta\xi)\text{sech}^2\left(\frac{\beta\xi}{2}\right), \tag{3.3.39}$$

This can not be solved analytically, but it can be shown that it is positive. We can notice, that this is the same integral as calculated in (3.3.29), which means that the low-temperature limit is

$$\alpha_2 = \frac{\beta^3}{8\pi^2}D_F\zeta(3, 1/2) \tag{3.3.40}$$

Due to the positive coefficient, the fourth-order term counterbalances the second-order term and ensures the stability of the system, as long as the higher-order terms are sufficiently small or positive.

### 3.3.5 Higher order

Following the same arguments as for the first and third-order terms, it follows that all odd terms will be zero. However, for the even terms, the $2l$th-power term is given as,

$$\text{tr}\left[\frac{(-1)^{2l}}{2l}\left(\hat{\mathcal{G}}_0\hat{\eta}\right)^{2l}\right] = 2\frac{1}{2l}\sum_k (\mathcal{G}_0(k))^l(\mathcal{G}_0(k-2k_F))^l \prod_{i=1}^{2l}\left(\sum_{q_i'}\eta_{q_i'}\right)\delta_{\sum_i(-1)^i q_i,0}$$
$$= \alpha_l \prod_{i=1}^{2l}\left(\sum_{q_i'}\eta_{q_i'}\right)\delta_{\sum_i(-1)^i q_i,0}, \tag{3.3.41}$$

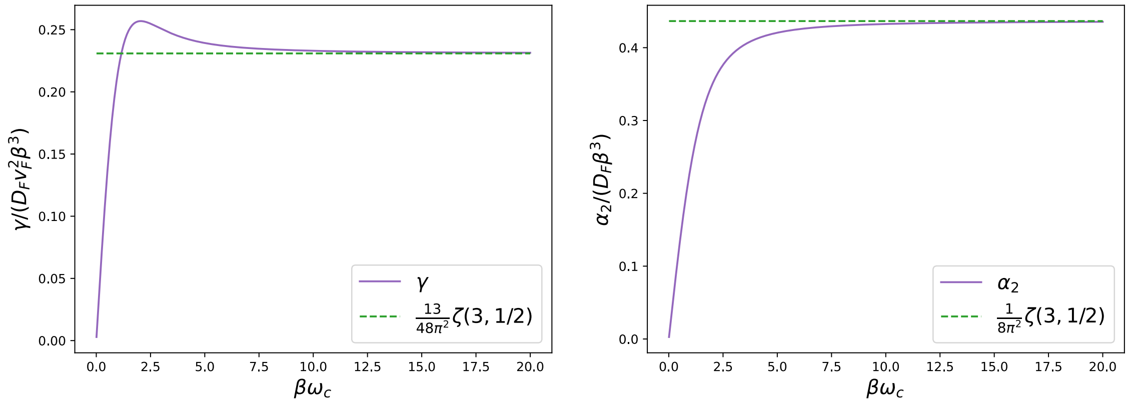



Figure 3.3: The coefficients, $\gamma$ (left) and $\alpha_2$ (right) (solid line), for the gradient term and the fourth order term, respectively, in the Ginzburg-Landau free energy for CDWs, with the low-temperature limit (dotted line)

The coefficients $\alpha_l$ are

$$\alpha_l = l^{-1} \sum_k (\mathcal{G}_0(k))^l (\mathcal{G}_0(k - 2k_F))^l = l^{-1} \sum_k \frac{1}{(i\omega_n - \xi_k)^l} \frac{1}{(i\omega_n + \xi_k)^l}. \tag{3.3.42}$$

We can see that the coefficients will decrease in magnitude for higher values of $l$. Since the first term converges, the subsequent terms will also converge and become smaller due to the increasing power of the denominator, as $l$ increases. By knowing this, combined with the fact that the fourth-order term ensures the stability of the system, it is enough to only consider the two first coefficients, $\alpha_1$ and $\alpha_2$.

### 3.3.6 Summary of the Ginzburg-Landau theory

In our derivation of the Ginzburg-Landau theory, we found expressions for the phenomenological constants in equation (3.3.2). The coefficients, together with their low-temperature limits are shown in figure 3.3. We found the critical temperature for the CDW by solving $\alpha_1 = 0$, which coincides with the results from section 3.2. Below this temperature, it is favorable to create CDWs and we need the fourth-order term to be positive, $\alpha_2 > 0$, to ensure the stability of the system. Above this critical temperature, it will be energetically costly to make CDWs, and the system will be stable. The positive coefficient in front of the gradient term tells us that spatial fluctuations of the CDWs are not favorable. Moreover, we can see that this coefficient is in line with what we would expect from a classical Ginzburg-Landau theory, $\gamma \sim v_F^2/T^3$ [44]. As a final consideration, we want to look at the system without spatial fluctuations, setting the gradient term to zero. By finding the extremum of the free energy we have that $\eta(2\alpha_1 + 4\alpha_2\eta^2) = 0$. From this, we can see that above $T_C$ there is only one solution, $\eta = 0$. Below $T_C$ the mean-field order parameter can be written as $\eta = \sqrt{-\frac{\alpha_1}{2\alpha_2}} = \sqrt{\frac{\alpha_1'}{2\alpha_2}}\sqrt{T_C - T}$. This dependence of $T_C - T$ is exactly what we would have expected for a mean-field order parameter.

# Chapter 4

# Charge Density Waves and Superconductivity in the Functional Integral Approach

In this chapter, we want to study the interplay between SC and CDWs. It is particularly interesting to see if it is energetically favorable to have a coexistence of the two phases.

## 4.1 Effective action

The structure of the derivation will be similar to what we did in chapter 3. In addition to the Hamiltonian we had in equation (3.1.1), we will add the potential $V_{\sigma,\bar{\sigma}}$, which couples fermions of different spins. This will be the potential that can give rise to a SC state in our system. The Hamiltonian that we will add to the CDW system, will be

$$H_{SC} = \frac{1}{2}\sum_{\sigma}\sum_{i,j} V_{\sigma,\bar{\sigma}}(\mathbf{r}_i - \mathbf{r}_j) c^{\dagger}_{i,\sigma} c_{i,\sigma} c^{\dagger}_{j,\bar{\sigma}} c_{j,\bar{\sigma}}. \tag{4.1.1}$$

By applying a Fourier transformation to the SC interaction term, and adding the terms from equation 3.1.1, we have that the total Hamiltonian in momentum space is

$$\begin{aligned} H = \sum_{k,\sigma} \xi_{\mathbf{k}} c^{\dagger}_{k,\sigma} c_{k,\sigma} + \frac{1}{4}\sum_{\sigma,\sigma'}\sum_{k,k',q} V(q) c^{\dagger}_{k+q/2,\sigma} c_{k-q/2,\sigma} c^{\dagger}_{k'-q/2,\sigma'} c_{k'+q/2,\sigma'} \\ + \sum_{k,k',q} \lambda(k'-k) c^{\dagger}_{k+q/2,\uparrow} c_{k'+q/2,\uparrow} c^{\dagger}_{-k+q/2,\downarrow} c_{-k'+q/2,\downarrow}, \end{aligned} \tag{4.1.2}$$

where we have defined the spin-independent potential $\lambda(k'-k) \equiv V_{\sigma,\bar{\sigma}}(k'-k)$. The Fourier transformation of the interaction term is found in appendix C. From the Hamiltonian, we can find the action of the system

$$\begin{aligned} S = \sum_{k,\sigma} \bar{\psi}_{k,\sigma}[-i\omega_n + \xi_{\mathbf{k}}]\psi_{k,\sigma} - \frac{1}{4}\sum_{\sigma,\sigma'}\sum_{k,k',q} V(q) \bar{\psi}_{k+q/2,\sigma}\psi_{k-q/2,\sigma}\bar{\psi}_{k'-q/2,\sigma'}\psi_{k'+q/2,\sigma'} \\ + \sum_{k,k',q} \lambda(k'-k)\bar{\psi}_{k+q/2,\uparrow}\bar{\psi}_{-k+q/2,\downarrow}\psi_{k'+q/2,\uparrow}\psi_{-k'+q/2,\downarrow}. \end{aligned} \tag{4.1.3}$$

Furthermore, we will decouple the interaction terms and rearrange the fields in such a way that we can integrate over the fermionic fields. Firstly, we will decouple the quartic fermion terms. The decoupling of the CDW term will be the same as in chapter 3. For the SC interaction term, we introduce the auxiliary fields $\Delta$ and its complex conjugate $\bar{\Delta}$. The combined measure for the CDWs and the SC decoupling is

$$\mathbb{1} = \int \mathcal{D}[\kappa, \bar{\Delta}, \Delta] \exp\left( -\sum_{q} \frac{\kappa(q)\kappa(-q)}{V(q)} - \sum_{q,k,k'} \frac{\bar{\Delta}(k',q)\Delta(k,q)}{\lambda(k'-k)} \right), \tag{4.1.4}$$

where we have used that the SC decoupling field is complex. From section 2.7 we stated that the SC interaction term is supposed to be decoupled in the particle-particle channel, while the CDWs decouples in the particle-hole channel. This can be written in terms of the following shifts

$$\Delta(k,q) \to \Delta(k,q) - \sum_{k'} \lambda(k'-k)\psi_{k'+q/2,\uparrow}\psi_{-k'+q/2,\downarrow}, \tag{4.1.5a}$$

$$\bar{\Delta}(k,q) \to \bar{\Delta}(k,q) - \sum_{k'} \lambda(k'-k)\bar{\psi}_{-k'+q/2,\downarrow}\bar{\psi}_{k'+q/2,\uparrow}, \tag{4.1.5b}$$

$$\kappa(q) \to \kappa(q) - \frac{1}{2}V(q)\sum_{k,\sigma} \bar{\psi}_{k+q/2,\sigma}\psi_{k-q/2,\sigma}. \tag{4.1.5c}$$

Next, we insert these shifts into the measure (4.1.4), and use that $\sum_{k'} \lambda^{-1}(k-k')\lambda(k'-k'') = \delta_{k,k''}$. When doing so, we trade the interaction terms with quadratic fermion terms coupled to bosonic auxiliary fields. The partition function reads

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \int \mathcal{D}[\kappa, \bar{\Delta}, \Delta] e^{-\tilde{S}[\bar{\psi},\psi,\kappa,\bar{\Delta},\Delta]}, \tag{4.1.6}$$

with the decoupled action

$$\tilde{S}[\bar{\psi},\psi,\kappa,\bar{\Delta},\Delta] = \sum_{q} \frac{\kappa(q)\kappa(q)}{V(q)} + \sum_{k,k',q} \frac{\bar{\Delta}(k',q)\Delta(k,q)}{\lambda(k'-k)} \tag{4.1.7a}$$

$$+ \sum_{k,\sigma} \bar{\psi}_{k,\sigma}[-\mathcal{G}_0^{-1}(k)]\psi_{k,\sigma} - \sum_{k,q,\sigma} \kappa(q)\bar{\psi}_{k-q/2,\sigma}\psi_{k+q/2,\sigma} \tag{4.1.7b}$$

$$- \sum_{k,q} \left[ \bar{\Delta}(k,q)\psi_{k+q/2,\uparrow}\psi_{-k+q/2,\downarrow} + \Delta(k,q)\bar{\psi}_{-k+q/2,\downarrow}\bar{\psi}_{k+q/2,\uparrow} \right]. \tag{4.1.7c}$$

The next step is to structure the interaction terms in a matrix such that we can integrate over the fermionic fields. To do this, we introduce the Nambu spinors

$$\bar{\Psi}_k = \begin{bmatrix} \bar{\psi}_{k,\uparrow} & \bar{\psi}_{k,\downarrow} & \psi_{-k,\uparrow} & \psi_{-k,\downarrow} \end{bmatrix}, \quad \Psi_k = \begin{bmatrix} \psi_{k,\uparrow} \\ \psi_{k,\downarrow} \\ \bar{\psi}_{-k,\uparrow} \\ \bar{\psi}_{-k,\downarrow} \end{bmatrix}. \tag{4.1.8}$$

Using these spinors and rearranging the fermionic action, we can write the total action as

$$\tilde{S}[\bar{\psi}, \psi, \kappa, \bar{\Delta}, \Delta]$$
$$= \sum_{q} \frac{\kappa(q)\kappa(-q)}{V(q)} + \sum_{k,k',q} \frac{\bar{\Delta}(k',q)\Delta(k,q)}{\lambda(k'-k)} + \sum_{k_1,k_2} \bar{\Psi}_{k_1}[-\frac{1}{2}\hat{\mathcal{F}}^{-1}_{k_1,k_2}]\Psi_{k_2},, \tag{4.1.9}$$

where we simplified the notation by relabeling the momenta as $k_1 = k - q/2$ and $k_2 = k + q/2$. Following this, we have that $\hat{\mathcal{F}}^{-1}$ is

$$\hat{\mathcal{F}}^{-1} = \hat{\mathcal{F}}_0^{-1} + \hat{\mathcal{B}}$$
$$= \begin{bmatrix} [\hat{\mathcal{G}}_0^{(p)}]^{-1} & 0 & 0 & 0 \\ 0 & [\hat{\mathcal{G}}_0^{(p)}]^{-1} & 0 & 0 \\ 0 & 0 & -[\hat{\mathcal{G}}_0^{(h)}]^{-1} & 0 \\ 0 & 0 & 0 & -[\hat{\mathcal{G}}_0^{(h)}]^{-1} \end{bmatrix} + \begin{bmatrix} \hat{\kappa} & 0 & 0 & -\hat{\Delta} \\ 0 & \hat{\kappa} & \hat{\Delta} & 0 \\ 0 & \hat{\bar{\Delta}} & -\hat{\kappa} & 0 \\ -\hat{\bar{\Delta}} & 0 & 0 & -\hat{\kappa} \end{bmatrix},$$

where the matrix-elements in $\hat{\mathcal{F}}^{-1}$ are operators in momentum space. Owing to the discreteness of the momentum, these can be structured as matrices, and their matrix elements are defined as

$$[\hat{\mathcal{G}}_0^{(p)}]^{-1}_{k,k'} = \mathcal{G}_0^{-1}(k)\delta_{k,k'}, \quad [\hat{\mathcal{G}}_0^{(h)}]^{-1}_{k,k'} = \mathcal{G}_0^{-1}(-k)\delta_{k,k'}, \tag{4.1.10}$$
$$(\hat{\kappa})_{k,k'} = \kappa(k'-k), \tag{4.1.11}$$
$$(\hat{\Delta})_{k,k'} = \Delta\left(\frac{k+k'}{2}, k-k'\right), \quad (\hat{\bar{\Delta}})_{k,k'} = \bar{\Delta}\left(\frac{k+k'}{2}, k'-k\right), \tag{4.1.12}$$

where $[\hat{\mathcal{G}}_0^{(p)}]^{-1}$ and $[\hat{\mathcal{G}}_0^{(h)}]^{-1}$ are the non-interacting Greens functions of the particle and hole, respectively [44]. In the rearrangement of the operators, we assumed that $\Delta$ and $\bar{\Delta}$ are even in their relative momenta, $k$. Integrating over the fermion fields yields

$$S_{\text{eff}} = \sum_{q} \frac{\kappa(q)\kappa(q)}{V(q)} + \sum_{k,k',q} \frac{\bar{\Delta}(k',q)\Delta(k,q)}{\lambda(k'-k)} - \frac{1}{2}\mathrm{Tr}\ln\left(-\beta\hat{\mathcal{F}}^{-1}\right). \tag{4.1.13}$$

This is the effective bosonic action of the theory. The next step is to find the mean-field configuration of the bosonic field through a stationary phase analysis.

## 4.2 Stationary phase analysis

Before developing a Ginzburg-Landau theory of the system, we want to do a stationary phase analysis to derive the mean-field configurations of $\kappa$ and $\Delta$. In order to derive this we will assume that the small momentum[1] of $\Delta$, will be set to zero, $\Delta(k,0) \to \Delta(k)$. Following the same procedure as in chapter 3, we will therefore differentiate the effective action (4.1.13) with respect to $\kappa(2k_F)$ and $\bar{\Delta}(k)$.

[1]See section 2.7 on the Hubbard-Stratonovich decoupling

### 4.2.1 Charge density waves

Starting with the order parameter for CDW, we will differentiate the effective action with respect to $\kappa(2k_F)$

$$0 \stackrel{!}{=} \frac{\delta S_{\text{eff}}}{\delta\kappa(2k_F)} = 2V^{-1}(2k_F)\kappa(2k_F) - \frac{1}{2}\text{Tr}\Big(\hat{\mathcal{F}}\frac{\delta\hat{\mathcal{F}}^{-1}}{\delta\kappa(2k_F)}\Big), \tag{4.2.1}$$

following the same steps as in section 3.2. To proceed, we need to calculate the inverse of $\hat{\mathcal{F}}^{-1}$ and differentiate $\mathcal{F}^{-1}$ with respect to the CDW order parameter. These are

$$\hat{\mathcal{F}} = \hat{\mathcal{D}}^{-1}\begin{bmatrix} [\hat{\mathcal{G}}_0^{(h)}]^{-1}+\hat{\kappa} & 0 & 0 & -\hat{\Delta} \\ 0 & [\hat{\mathcal{G}}_0^{(h)}]^{-1}+\hat{\kappa} & \hat{\Delta} & 0 \\ 0 & \hat{\bar{\Delta}} & -[\hat{\mathcal{G}}_0^{(p)}]^{-1}-\hat{\kappa} & 0 \\ -\hat{\bar{\Delta}} & 0 & 0 & -[\hat{\mathcal{G}}_0^{(p)}]^{-1}-\hat{\kappa} \end{bmatrix}, \tag{4.2.2}$$

$$\frac{\delta\hat{\mathcal{F}}^{-1}}{\delta\kappa(2k_F)} = \text{diag}(1,1,-1,-1)\frac{\delta\hat{\kappa}}{\delta\kappa(2k_F)}, \tag{4.2.3}$$

where we defined the common denominator $\hat{\mathcal{D}} = \left([\hat{\mathcal{G}}_0^{(p)}]^{-1}+\hat{\kappa}\right)\left([\hat{\mathcal{G}}_0^{(h)}]^{-1}+\hat{\kappa}\right)+\hat{\bar{\Delta}}\hat{\Delta}$. The last term of equation (4.2.1) will be

$$\text{Tr}\left[\hat{\mathcal{F}}\frac{\delta\hat{\mathcal{F}}^{-1}}{\delta\kappa(2k_F)}\right] =$$

$$\text{Tr}\left(\hat{\mathcal{D}}^{-1}\begin{bmatrix} [\hat{\mathcal{G}}_0^{(h)}]^{-1}+\hat{\kappa} & 0 & 0 & -\hat{\Delta} \\ 0 & [\hat{\mathcal{G}}_0^{(h)}]^{-1}+\hat{\kappa} & \hat{\Delta} & 0 \\ 0 & \hat{\bar{\Delta}} & [\hat{\mathcal{G}}_0^{(p)}]^{-1}+\hat{\kappa} & 0 \\ -\hat{\bar{\Delta}} & 0 & 0 & [\hat{\mathcal{G}}_0^{(p)}]^{-1}+\hat{\kappa} \end{bmatrix}\frac{\delta\hat{\kappa}}{\delta\kappa(2k_F)}\right). \tag{4.2.4}$$

Moving on, we take the trace in Nambu and momentum space,

$$\text{Tr}\Big(\hat{\mathcal{F}}\frac{\delta\hat{\mathcal{F}}^{-1}}{\delta\kappa(2k_F)}\Big) = 2\sum_{k_1,k_2}\left[\hat{\mathcal{D}}^{-1}(2\hat{\kappa}+[\hat{\mathcal{G}}_0^{(p)}]^{-1}+[\hat{\mathcal{G}}_0^{(h)}]^{-1})\right]_{k_1,k_2}\left[\frac{\delta\hat{\kappa}}{\delta\kappa(2k_F)}\right]_{k_2,k_1}. \tag{4.2.5}$$

When differentiating $\hat{\kappa}$, we used that $\left[\frac{\delta\hat{\kappa}}{\delta\kappa(2k_F)}\right]_{k_2,k_1} = \delta_{k_1-k_2,2k_F}$. Thus, the stationary phase condition is

$$\kappa(2k_F) = V(2k_F)\sum_k(\hat{\mathbf{G}})_{k,k-2k_F}, \tag{4.2.6}$$

where we defined $\hat{\mathbf{G}} = \left[\hat{\mathcal{D}}^{-1}(\hat{\kappa}+\frac{1}{2}[\hat{\mathcal{G}}_0^{(p)}]^{-1}+\frac{1}{2}[\hat{\mathcal{G}}_0^{(h)}]^{-1})\right]$ as the propagator.

To confirm that this result is in line with the result we found for the system in section 3.2, we set $\Delta = 0$ and assume $\kappa \ll 1$

$$1 = -V(2k_F)\sum_k\mathcal{G}_0(k)\mathcal{G}_0(k-2k_F). \tag{4.2.7}$$

### 4.2.2 Superconductivity

To derive the self-consistent equation for the mean-field order parameter for SC, we will differentiate the effective action with respect to $\bar{\Delta}(k)$

$$0 \stackrel{!}{=} \frac{\delta S_{\text{eff}}}{\delta \bar{\Delta}(k)} = \sum_{k'} \Delta(k')\lambda^{-1}(k-k') - \frac{\delta}{\delta \bar{\Delta}(k)} \left( \frac{1}{2} \text{Tr} \ln \left[ -\beta \hat{\mathcal{F}}^{-1} \right] \right). \tag{4.2.8}$$

By performing the differentiating in the same way as for the CDW case, we get

$$\text{Tr} \left( \hat{\mathcal{F}} \frac{\delta \hat{\mathcal{F}}^{-1}}{\delta \bar{\Delta}(k)} \right) = \text{Tr} \left( \hat{\mathcal{D}}^{-1} \begin{bmatrix} \hat{\Delta} & 0 & 0 & 0 \\ 0 & \hat{\Delta} & 0 & 0 \\ 0 & -[\hat{\mathcal{G}}_0^{(p)}]^{-1} - \hat{\kappa} & 0 & 0 \\ [\hat{\mathcal{G}}_0^{(p)}]^{-1} + \hat{\kappa} & 0 & 0 & 0 \end{bmatrix} \frac{\delta \hat{\bar{\Delta}}}{\delta \bar{\Delta}(k)} \right). \tag{4.2.9}$$

The next step is to take the trace in Nambu and momentum space

$$\text{Tr} \left( \hat{\mathcal{F}} \frac{\delta \hat{\mathcal{F}}^{-1}}{\delta \bar{\Delta}(k)} \right) = 2 \sum_{k_1,k_2} \left( \hat{\mathcal{D}}^{-1} \hat{\Delta} \right)_{k_1,k_2} \left( \frac{\delta \hat{\bar{\Delta}}}{\delta \bar{\Delta}(k)} \right)_{k_2,k_1}, \tag{4.2.10}$$

where we have that $\left( \frac{\delta \hat{\bar{\Delta}}}{\delta \bar{\Delta}(k)} \right)_{k_2,k_1} = \delta_{k_1,k_2}$. Inserting this back into equation (4.2.8), gives

$$\sum_{k'} \Delta(k')\lambda^{-1}(k-k') = \left( \hat{\mathcal{D}}^{-1} \hat{\Delta} \right)_{k,k}. \tag{4.2.11}$$

Eventually, we want an expression for $\Delta(k)$. To achieve that, we will multiply by the potential $\lambda(k''-k)$ and sum over $k$ on both sides

$$\sum_{k'} \sum_{k} \Delta(k')\lambda(k''-k)\lambda^{-1}(k-k') = \sum_{k} \lambda(k''-k) \left( \hat{\mathcal{D}}^{-1} \hat{\Delta} \right)_{k,k}. \tag{4.2.12}$$

By using that $\sum_k \lambda(k''-k)\lambda^{-1}(k-k') = \delta_{k',k''}$, we get the stationary phase equation for the SC order parameter

$$\Delta(k) = \sum_{k'} \lambda(k-k')(\hat{\mathbf{F}})_{k',k'}, \tag{4.2.13}$$

with the propagator

$$\hat{\mathbf{F}}_{k,k} = (\hat{\mathcal{D}}^{-1}\hat{\Delta})_{k,k} = \left[ \left( [\hat{\mathcal{G}}_0^{(p)}]^{-1} + \hat{\kappa} \right) \left( [\hat{\mathcal{G}}_0^{(h)}]^{-1} + \hat{\kappa} \right) + \hat{\Delta}\hat{\bar{\Delta}} \right]^{-1}_{k,k} \Delta(k) \tag{4.2.14}$$

and we assumed that $\hat{\Delta}$ is diagonal in $k$-space in this consideration. Further, we will focus on the solution where $\Delta(k) \neq 0$.

To check if our calculations are consistent with the existing theory, we will set $\hat{\kappa} = 0$, and assume $\Delta$ and $\bar{\Delta}$ to be small. The right-hand side of equation (4.2.13) can be written as

$$\sum_{k'} \lambda(k-k') \left[ [\hat{\mathcal{G}}_0^{(p)}]^{-1} [\hat{\mathcal{G}}_0^{(h)}]^{-1} + \hat{\Delta}\hat{\bar{\Delta}} \right]^{-1}_{k',k'} \Delta(k')$$
$$\approx \sum_{k'} \lambda(k-k') \mathcal{G}_0(k') \mathcal{G}_0(-k') \Delta(k'). \tag{4.2.15}$$

Next, we put the expansion back into equation (4.2.13), and get the following expression

$$\Delta(k) = \sum_{k'} \lambda(k-k') \mathcal{G}_0(k') \mathcal{G}_0(-k') \Delta(k'), \tag{4.2.16}$$

which is the linearized gap equation. In the following equations, we assume a s-wave SC, $\lambda(k-k') = \frac{\lambda}{N\beta}$. By assuming that $\Delta(k)$ is independent of the Matsubara frequency, we can perform this frequency summation

$$\Delta(\mathbf{k}) = \frac{1}{N} \sum_{\mathbf{k}'} \frac{\lambda}{2\xi_{\mathbf{k}'}} \tanh\left( \frac{\beta \xi_{\mathbf{k}'}}{2} \right) \Delta(\mathbf{k}'). \tag{4.2.17}$$

This equation has the same structure as the gap equation in the BCS model [43]. Proceeding, we will assume that $\Delta$ is a constant and use the general form of the potential

$$\Delta_0 = \sum_{k'} \lambda(k-k') \mathcal{G}_0(k') \mathcal{G}_0(-k') \Delta_0, \tag{4.2.18}$$

$$1 = \sum_{k'} \lambda(k-k') \mathcal{G}_0(k') \mathcal{G}_0(-k'). \tag{4.2.19}$$

From this, we can derive an equation for the critical temperature, and it can be shown that it will be the same as for the BCS case. The pair-susceptibility is $\chi_{pp} \propto [1 - \sum_{k'} \lambda(k-k') \mathcal{G}_0(k') \mathcal{G}_0(-k')]^{-1}$. Hence, the critical temperature will lead to a divergence in the susceptibility and we can therefore conclude that $\Delta$ is indeed a suitable order parameter for the SC phase transition.

### 4.2.3 Mean-field equations

In the stationary phase analysis, we have found the mean-field equations for the order parameters. To summarize, we found that both of the order parameters can be written as their respective potential multiplied by a propagator. The mean-field equations are

$$\Delta(k) = \sum_{k'} \lambda(k-k') (\hat{\mathbf{F}})_{k',k'}, \tag{4.2.20}$$

$$2\kappa(2k_F) = V(2k_F) \sum_{k} (\hat{\mathbf{G}})_{k,k-2k_F}, \tag{4.2.21}$$

where the propagators are

$$\hat{\mathbf{F}} = \left[\left([\hat{\mathcal{G}}_0^{(p)}]^{-1} + \hat{\kappa}\right)\left([\hat{\mathcal{G}}_0^{(h)}]^{-1} + \hat{\kappa}\right) + \hat{\bar{\Delta}}\hat{\Delta}\right]^{-1}\hat{\Delta}, \tag{4.2.22}$$

$$\hat{\mathbf{G}} = \left[\left([\hat{\mathcal{G}}_0^{(p)}]^{-1} + \hat{\kappa}\right)\left([\hat{\mathcal{G}}_0^{(h)}]^{-1} + \hat{\kappa}\right) + \hat{\bar{\Delta}}\hat{\Delta}\right]^{-1}\left(2\hat{\kappa} + [\hat{\mathcal{G}}_0^{(p)}]^{-1} + [\hat{\mathcal{G}}_0^{(h)}]^{-1}\right). \tag{4.2.23}$$

This finishes the stationary phase analysis and the next step is to derive a Ginzburg-Landau theory of the system.

## 4.3 Ginzburg-Landau theory for fluctuations

The following section involves the derivation of a Ginzburg-Landau theory to describe the interplay between superconductivity and charge density waves. Eventually, we want to derive the phenomenological constant for the coupled term between SC and CDWs to see if it is energetically favorable for them to coexist. Just as for the system with only CDWs, we want to look at small fluctuations around the mean-field value

$$\hat{\kappa} = \hat{\kappa}_{MF} + \hat{\eta} = \hat{\eta}, \quad \hat{\Delta} = \hat{\Delta}_{MF} + \hat{\nu} = \hat{\nu}, \quad \hat{\bar{\Delta}} = \hat{\bar{\Delta}}_{MF} + \hat{\bar{\nu}} = \hat{\bar{\nu}}. \tag{4.3.1}$$

From section 3.3 we have that the effective action can be written as $S_{\text{eff}} = S_{MF} + \beta F$. The mean-field action of this system will be $S_{\text{MF}} = \beta \mathcal{F}_0^{-1}$. We expect the free energy to be

$$F = F_{\text{C}} + F_{\text{S}} + F_{\text{C,S}}, \tag{4.3.2}$$

$$F_{\text{C}} = \int d^d r \left(\alpha_1 \left(\eta(r)\right)^2 + \gamma_{\text{C}} \left(\nabla\eta(r)\right)^2 + \alpha_2 \left(\eta(r)\right)^4 + \ldots\right), \tag{4.3.3}$$

$$F_{\text{S}} = \int d^d r \left(\beta_1 |\nu(r)|^2 + \gamma_{\text{S}} |\nabla\nu(r)|^2 + \beta_2 |\nu(r)|^4 + \ldots\right), \tag{4.3.4}$$

$$F_{\text{C,S}} = \int d^d r \left(\rho \left(\eta(r)\right)^2 |\nu(r)|^2 + \ldots\right), \tag{4.3.5}$$

where $F_{\text{C}}$ is the free energy only for the CDW order parameter, $F_{\text{S}}$ for the SC order parameter, and $F_{\text{C,S}}$ for the interplay between them. The coefficient that we are most interested in is the coupling coefficient $\rho$. This coefficient will tell us if it is energetically favorable to have the states coexisting or if they are competing states. To be able to calculate the coefficient in the Ginzburg-Landau theory we must first find an expression for the expansion of $\text{Tr}\ln(\mathbb{1} + \hat{\mathcal{F}}_0\hat{\mathcal{B}})$, from the action in equation (4.1.13). We have that the total free energy $F$ is

$$\beta F = \sum_q \frac{\eta(q)\eta(q)}{V(q)} + \sum_{k,k',q} \frac{\bar{\nu}(k',q)\nu(k,q)}{\lambda(k'-k)} - \frac{1}{2}\text{Tr}\ln(\mathbb{1} + \hat{\mathcal{F}}_0\hat{\mathcal{B}}). \tag{4.3.6}$$

We assume that the fluctuations are small, and we can expand the last term as

$$-\frac{1}{2}\text{Tr}\ln(\mathbb{1} + \hat{\mathcal{F}}_0\hat{\mathcal{B}}) = \frac{1}{2}\text{Tr}\left(\sum_k \frac{(-1)^k}{k}(\hat{\mathcal{F}}_0\hat{\mathcal{B}})^k\right). \tag{4.3.7}$$

The next step is to calculate the coefficients for the different orders of the expansion, to find an expression for the coefficients $\alpha_1$, $\alpha_2$, $\beta_1$, $\beta_2$, $\gamma_{\text{S}}$, $\gamma_{\text{C}}$ and $\rho$.

### 4.3.1 First order

The first term of the expansion in the equation (4.3.7) is

$$-\frac{1}{2}\mathrm{Tr}(\hat{\mathcal{F}}_0\hat{\mathcal{B}}) = -\frac{1}{2}\mathrm{Tr}\begin{bmatrix} \hat{\mathcal{G}}_0^{(p)}\hat{\eta} & 0 & 0 & -\hat{\mathcal{G}}_0^{(p)}\hat{\nu} \\ 0 & \hat{\mathcal{G}}_0^{(p)}\hat{\eta} & \hat{\mathcal{G}}_0^{(p)}\hat{\nu} & 0 \\ 0 & -\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}} & \hat{\mathcal{G}}_0^{(h)}\hat{\eta} & 0 \\ \hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}} & 0 & 0 & \hat{\mathcal{G}}_0^{(h)}\hat{\eta} \end{bmatrix}$$
$$= -\sum_k \left[\hat{\mathcal{G}}_0^{(p)}\hat{\eta}\right]_{k,k} - \sum_k \left[\hat{\mathcal{G}}_0^{(h)}\hat{\eta}\right]_{k,k} \tag{4.3.8}$$

We have that $\mathcal{G}_0$ is diagonal in $k$-space and $\hat{\eta}$ has only off-diagonal elements, leading to the term being zero.

### 4.3.2 Second order

Furthermore, we can derive the coefficients for the second-order term

$$\frac{1}{2}\mathrm{Tr}\left(\frac{1}{2}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\right) = \sum_k \left[\hat{\mathcal{G}}_0^{(p)}\hat{\eta}\hat{\mathcal{G}}_0^{(p)}\hat{\eta} - \hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k}$$
$$= \sum_{k,q} \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F+q)\eta(2k_F-q)\eta(2k_F-q)$$
$$- \sum_{k,q} \mathcal{G}(k+q/2)\mathcal{G}(-k+q/2)\nu(k,-q)\bar{\nu}(k,q). \tag{4.3.9}$$

We will start by deriving an expression for the SC second-order term. In order to derive expressions for the coefficients, we have to assume that the fluctuation of the superconductive order parameter is independent of $k$ (relative momentum), $\nu(k,q) \to \nu(q)$. The $k$-summation over the Greens functions can be written as

$$\sum_k \mathcal{G}_0(k+q/2)\mathcal{G}_0(q/2-k) \approx \sum_{k,q} \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \mathbf{q}/2\cdot\mathbf{v}} \frac{1}{-i\omega_n - \xi_{\mathbf{k}} + \mathbf{q}/2\cdot\mathbf{v}}$$
$$= \sum_k \frac{1}{2\xi_{\mathbf{k}}}\left[\frac{1}{i\omega_n + \xi_{\mathbf{k}} - \mathbf{q}/2\cdot\mathbf{v}} - \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \mathbf{q}/2\cdot\mathbf{v}}\right]. \tag{4.3.10}$$

To proceed, we expand the expression for $q \ll 1$

$$\sum_k \mathcal{G}_0(k+q/2)\mathcal{G}_0(q/2-k) \approx \frac{1}{2}\sum_k \frac{1}{\xi_{\mathbf{k}}}\Bigg\{\frac{1}{i\omega+\xi_{\mathbf{k}}} - \frac{1}{i\omega-\xi_{\mathbf{k}}}$$
$$+\frac{\mathbf{q}\cdot\mathbf{v}}{2}\Big[\frac{1}{(i\omega+\xi_{\mathbf{k}})^2} - \frac{1}{(i\omega-\xi_{\mathbf{k}})^2}\Big] + \frac{(\mathbf{q}\cdot\mathbf{v})^2}{4}\Big[\frac{1}{(i\omega+\xi_{\mathbf{k}})^3} - \frac{1}{(i\omega-\xi_{\mathbf{k}})^3}\Big]\Bigg\} \tag{4.3.11}$$

As earlier, we start by performing the Matsuabara frequency sums using the results from appendix D. The sums we need are

$$\sum_n \frac{1}{i\omega_n \pm \xi_{\mathbf{k}}} = \frac{\beta}{e^{\mp\beta\xi_{\mathbf{k}}}+1}, \tag{4.3.12}$$

$$\sum_n \frac{1}{(i\omega_n \pm \xi_{\mathbf{k}})^2} = -\frac{\beta^2}{4}\text{sech}^2(\frac{\beta\xi_{\mathbf{k}}}{2}), \tag{4.3.13}$$

$$\sum_n \frac{1}{(i\omega_n \pm \xi_{\mathbf{k}})^3} = \mp\frac{\beta^3}{8}\tanh(\frac{\beta\xi_{\mathbf{k}}}{2})\text{sech}^2(\frac{\beta\xi_{\mathbf{k}}}{2}). \tag{4.3.14}$$

From this, we see that the linear term in $q$ will be zero. Moving on, we will first look at the term independent of $q$

$$\begin{aligned}\sum_{\mathbf{k}} \frac{\beta}{2\xi_{\mathbf{k}}}\left[\frac{1}{e^{-\beta\xi_{\mathbf{k}}}+1} - \frac{1}{e^{\beta\xi_{\mathbf{k}}}+1}\right] &= \sum_{\mathbf{k}} \frac{\beta}{2\xi_{\mathbf{k}}}\tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) \\ &= \frac{\beta D(\xi_F)}{2}\int_{-\omega_c}^{\omega_c}\frac{d\xi}{\xi}\tanh\left(\frac{\beta\xi}{2}\right).\end{aligned} \tag{4.3.15}$$

This integral is not possible to solve analytically, but it can be shown that it is positive. Next, we look at the term that is quadratic in $\mathbf{q}$,

$$\gamma_{\text{S}} = \sum_{\mathbf{k}} \frac{(\mathbf{q}\cdot\mathbf{v})^2}{4}\frac{\beta^2}{8\xi_{\mathbf{k}}}\left[\tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right)\text{sech}^2\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right)\right]$$

$$= \mathbf{q}^2\frac{\beta^3 D(\xi_F)}{96m^*}\int_{-\omega_c}^{\omega_c}\frac{d\xi}{\xi}(\xi+\mu)\tanh\left(\frac{\beta\xi}{2}\right)\text{sech}^2\left(\frac{\beta\xi}{2}\right) \tag{4.3.16}$$

$$= \mathbf{q}^2\mu\frac{\beta^3 D(\xi_F)}{48m^*}\int_{0}^{\omega_c}\frac{d\xi}{\xi}\tanh\left(\frac{\beta\xi}{2}\right)\text{sech}^2\left(\frac{\beta\xi}{2}\right). \tag{4.3.17}$$

In equation (4.3.16) the $\xi$-term in the parenthesis will be zero due to the anti-symmetry of the total integrand. Like in the previous case, the integral can be shown to be positive, but it is not possible to solve it analytically. Having derived an expression for the integrals for the second-order coefficients for SC, we can write the free energy to second order as

$$\begin{aligned}\beta F[\eta,\nu,\bar{\nu}] \approx \sum_{\mathbf{q}} &\alpha_1\eta(2\mathbf{k}_F-\mathbf{q})\eta(2\mathbf{k}_F-\mathbf{q}) + \beta_1\nu(\mathbf{q})\bar{\nu}(\mathbf{q}) + \\ &\gamma_{\text{C}}\mathbf{q}^2\eta(2\mathbf{k}_F-\mathbf{q})\eta(2\mathbf{k}_F-\mathbf{q}) + \gamma_{\text{S}}\mathbf{q}^2\nu(\mathbf{q})\bar{\nu}(\mathbf{q}).\end{aligned} \tag{4.3.18}$$

The coefficients in front of the CDW order parameter, $\alpha_1$ and $\gamma_{\mathrm{C}}$, are the same as in equation (3.3.27) and (3.3.28). All of the coefficients are listed under

$$\alpha_1 = \frac{N\beta}{V_{2\mathbf{k}_F}} - \beta D_F \int_0^{\omega_C} d\xi \frac{\tanh\left(\frac{\beta\xi}{2}\right)}{\xi}, \tag{4.3.19}$$

$$\beta_1 = \frac{N\beta}{\lambda} - \beta D_F \int_0^{\omega_c} \frac{d\xi}{\xi} \tanh\left(\frac{\beta\xi}{2}\right), \tag{4.3.20}$$

$$\gamma_{\mathrm{C}} = v_F^2 \frac{13}{24} \beta D_F \int_0^{\omega_c} d\xi \frac{1}{\xi^3} \left[-\sinh\left(\beta\xi_k\right) + \beta\xi + \beta^2\xi^2 \tanh\left(\frac{\beta\xi}{2}\right)\right] \operatorname{sech}^2\left(\frac{\beta\xi}{2}\right), \tag{4.3.21}$$

$$\gamma_{\mathrm{S}} = v_F^2 \frac{\beta^3}{96} D_F \int_0^{\omega_c} \frac{d\xi}{\xi} \tanh\left(\frac{\beta\xi}{2}\right) \operatorname{sech}^2\left(\frac{\beta\xi}{2}\right). \tag{4.3.22}$$

We can observe that the second-order terms in $\alpha_1$ and $\beta_1$ are the same, but they have different potentials in their first terms. Hence, the critical temperatures of the two states will be different. By following the same scheme as in section 3.3, we can write the coefficient $\beta_1$ in terms of the deviation from the critical temperature for the SC state. Hence, the two coefficients in terms of their critical temperature are

$$\alpha_1 \approx \alpha_1'(T - T_C^{\mathrm{CDW}}), \tag{4.3.23}$$

$$\beta_1 \approx \beta_1'(T - T_C^{\mathrm{SC}}). \tag{4.3.24}$$

Note that, in this approximation $\alpha_1' = \beta_1'$.

Considering the low-temperature limit in $\gamma_{\mathrm{S}}$, the integral in the equation (4.3.22) may be evaluated analytically. Note that it will be the same as $\gamma_1$ in equation (3.3.30). Thus, in the low-temperature limit, the coefficient for the gradient term in SC is

$$\gamma_S = v_F^2 \frac{\beta^3}{96} D_F \frac{1}{\pi^2} \zeta(3, 1/2). \tag{4.3.25}$$

### 4.3.3 Third order

The terms for the third-order expansion are

$$(\hat{\mathcal{G}}_0^{(p)}\hat{\eta})^3, \quad (\hat{\mathcal{G}}_0^{(p)}\bar{\hat{\eta}})^3, \quad \hat{\mathcal{G}}_0^{(p)}\hat{\eta}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}, \quad \hat{\mathcal{G}}_0^{(h)}\hat{\eta}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}. \tag{4.3.26}$$

It can be shown that the coefficients of these terms will be zero. This is due to the anti-symmetric integrands in the energy integrals when calculating $\sum_k \left[\mathcal{G}_0^{(p/h)}\right]^3$.

### 4.3.4 Fourth order

The fourth-order terms consist of three different types of terms, the bare CDW term, the bare SC term, and the cross-term. We will derive the coefficients for these terms. The derivation starts with multiplying the matrices together and taking the traces

$$\frac{1}{2}\mathrm{Tr}\left(\frac{1}{4}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\right)$$
$$= \sum_k \Big\{ \frac{1}{4}\left[(\hat{\mathcal{G}}_0^{(p)}\hat{\eta})^4\right]_{k,k} + \frac{1}{4}\left[(\hat{\mathcal{G}}_0^{(h)}\hat{\eta})^4\right]_{k,k} + \frac{1}{2}\left[\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k}$$
$$- \left[(\hat{\mathcal{G}}_0^{(p)}\hat{\eta})^2\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k} - \left[(\hat{\mathcal{G}}_0^{(h)}\hat{\eta})^2\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\right]_{k,k} - \left[\hat{\mathcal{G}}_0^{(p)}\hat{\eta}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\eta}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k} \Big\}.$$

For the fourth-order terms, we will assume that $q \ll k$ so that the bare Greens function is only dependent on $k$. The first two terms are equivalent, which can be seen by letting $-k \to k$ in the sums. These terms will be the same as the fourth-order terms in section 3.3. Hence we will just state the result

$$\frac{1}{2}\sum_k \left[(\hat{\mathcal{G}}_0^{(p)}\hat{\eta})^4\right]_{k,k} \approx \alpha_2 \sum_{\substack{q_1,q_2\\q_3,q_4}} \eta_{q_1'}\eta_{q_2'}\eta_{q_3'}\eta_{q_4'}\delta_{q_1-q_2+q_3-q_4}, \tag{4.3.27}$$

$$\alpha_2 = \frac{\beta}{8}D_F \int_0^{\omega_C} \frac{d\xi}{\xi^3}(\sinh(\beta\xi) - \beta\xi)\mathrm{sech}^2\left(\beta\frac{\xi}{2}\right), \tag{4.3.28}$$

where we know from the section about CDWs that $\alpha_2$ in equation (3.3.39), is positive.

The next term is the quartic term for the SC order parameter

$$\frac{1}{2}\sum_k \left[\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k} \approx \beta_2 \sum_{\substack{q_1,q_2\\q_3,q_4}} \nu_{q_1}\bar{\nu}_{q_2}\nu_{q_3}\bar{\nu}_{q_4}\delta_{q_1+q_2+q_3+q_4,0}, \tag{4.3.29}$$

where $\nu_q \equiv \nu(-q)$ and $\bar{\nu}_q \equiv \bar{\nu}(q)$. This coefficient will be exactly as the coefficient for the quartic CDW term, $\alpha_2$ (3.3.39). Hence, we have that

$$\beta_2 = \frac{1}{2}\sum_k (\mathcal{G}_0(k))^2(\mathcal{G}_0(-k))^2 \approx \frac{\beta}{8}D_F \int_0^{\omega_c} \frac{d\xi}{\xi^3}\,(\sinh(\beta\xi) - \beta\xi)\,\mathrm{sech}^2(\frac{\beta\xi}{2}), \tag{4.3.30}$$

which we know is positive.

Having established the fourth-order terms for the bare SC and CDW terms, we will move on to the cross-terms. The first term to evaluate is

$$-\sum_k \left[(\hat{\mathcal{G}}_0^{(p)}\hat{\eta})^2\hat{\mathcal{G}}_0^{(p)}\hat{\nu}\hat{\mathcal{G}}_0^{(h)}\hat{\bar{\nu}}\right]_{k,k} \approx \rho_1 \sum_{\substack{q_1,q_2\\q_3,q_4}} \eta_{q_1}\eta_{q_2}\nu_{q_3}\bar{\nu}_{q_4}\delta_{q_1+q_2+q_3+q_4,0} \tag{4.3.31}$$

where

$$\rho_1 = -\sum_k \mathcal{G}_0(k)\mathcal{G}_0(k-2k_F)\mathcal{G}_0(k)\mathcal{G}_0(-k) \approx \sum_k \frac{1}{(i\omega_n - \xi_{\mathbf{k}})^2}\frac{1}{(i\omega_n + \xi_{\mathbf{k}})^2}. \tag{4.3.32}$$

In the last transition, we linearized the kinetic energy, as we did in section 3.3. We can see that this is the same integral as in the coefficient calculated for the quartic CDW term

(3.3.39), which gives us the relation $\rho_1 = 2\alpha_2$ .

For the next cross-term we see that by letting $-k \to k$ in the summation, we end up with the same coefficient as for the first cross-term

$$-\sum_k \left[ (\hat{\mathcal{G}}_0^{(h)} \hat{\eta})^2 \hat{\mathcal{G}}_0^{(h)} \hat{\bar{\nu}} \hat{\mathcal{G}}_0^{(p)} \hat{\nu} \right]_{k,k} \approx \rho_1 \sum_{\substack{q_1,q_2 \\ q_3,q_4}} \eta_{q_1} \eta_{q_2} \nu_{q_3} \bar{\nu}_{q_4} \delta_{q_1+q_2+q_3+q_4,0}. \tag{4.3.33}$$

By taking the traces of the last cross-term, we get

$$\begin{aligned} &-\sum_k \left[ \hat{\mathcal{G}}_0^{(p)} \hat{\eta} \hat{\mathcal{G}}_0^{(p)} \hat{\nu} \hat{\mathcal{G}}_0^{(h)} \hat{\eta} \hat{\mathcal{G}}_0^{(h)} \hat{\bar{\nu}} \right]_{k,k} \\ \approx &-\sum_k \mathcal{G}_0(k) \mathcal{G}_0(k-2k_F) (\mathcal{G}_0(-k))^2 \sum_{\substack{q_1,q_2 \\ q_3,q_4}} \eta_{q_1} \eta_{q_2} \nu_{q_3} \bar{\nu}_{q_4} \delta_{q_1+q_2+q_3+q_4,0} \\ &= \rho_2 \sum_{\substack{q_1,q_2 \\ q_3,q_4}} \eta_{q_1} \eta_{q_2} \nu_{q_3} \bar{\nu}_{q_4} \delta_{q_1+q_2+q_3+q_4,0}, \end{aligned} \tag{4.3.34}$$

where the last cross-term coefficient is

$$\rho_2 = -\sum_k \mathcal{G}_0(k) \mathcal{G}_0(k-2k_F) (\mathcal{G}_0(-k))^2 \approx -\sum_k \frac{1}{i\omega_n - \xi_{\mathbf{k}}} \frac{1}{(i\omega_n + \xi_{\mathbf{k}})^3}. \tag{4.3.35}$$

We will follow the same procedure as for the previous coefficients, and first rewrite the expression and do the matsubara summations

$$\begin{aligned} \rho_2 &= \sum_k \left[ \frac{1}{8\xi_{\mathbf{k}}^3} \left( \frac{1}{i\omega_n - \xi_{\mathbf{k}}} - \frac{1}{i\omega_n + \xi_{\mathbf{k}}} \right) - \frac{1}{4\xi_{\mathbf{k}}^2} \frac{1}{(i\omega_n - \xi_{\mathbf{k}})^2} + \frac{1}{2\xi_{\mathbf{k}}} \frac{1}{(i\omega_n - \xi_{\mathbf{k}})^3} \right] \\ &= \sum_{\mathbf{k}} \frac{\beta}{8\xi_{\mathbf{k}}^3} \left[ -\tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) + \frac{\beta\xi_{\mathbf{k}}}{2} \text{sech}^2\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) + \frac{\beta^2\xi_{\mathbf{k}}}{2} \tanh\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right) \text{sech}^2\left(\frac{\beta\xi_{\mathbf{k}}}{2}\right). \right] \end{aligned} \tag{4.3.36}$$

This gives us the last part of the cross-term coefficient, which will be

$$\rho_2 = \frac{\beta}{8} D_F \int_0^{\omega_C} \frac{d\xi}{\xi^3} \left[ -\sinh(\beta\xi) + \beta\xi + (\beta\xi)^2 \tanh\left(\frac{\beta\xi}{2}\right) \right] \text{sech}^2\left(\frac{\beta\xi}{2}\right). \tag{4.3.37}$$

By adding the three cross-terms together we can see that the total coefficient is

$$\rho = 2\rho_1 + \rho_2 = \frac{\beta}{16} D_F \int_{-\omega_C}^{\omega_C} \frac{d\xi}{\xi^3} \left[ 3\sinh(\beta\xi) - 3\beta\xi + (\beta\xi)^2 \tanh\left(\frac{\beta\xi}{2}\right) \right] \text{sech}^2\left(\frac{\beta\xi}{2}\right). \tag{4.3.38}$$

This gives us that the total coefficient for the cross-term $\rho$ is positive. Hence, the co-existence between CDWs and SC is not energetically favorable. Like with the other coefficients, it is possible to find a solution to the integral in the low-temperature regime. By using the calculation we did in section 3.3, we see that the cross-term coefficient is $\rho = \frac{\beta D_F}{8}(-3\gamma_1 + \beta\gamma_2) = \beta^3 D_F \frac{5}{16\pi^2} \zeta(3, 1/2)$.

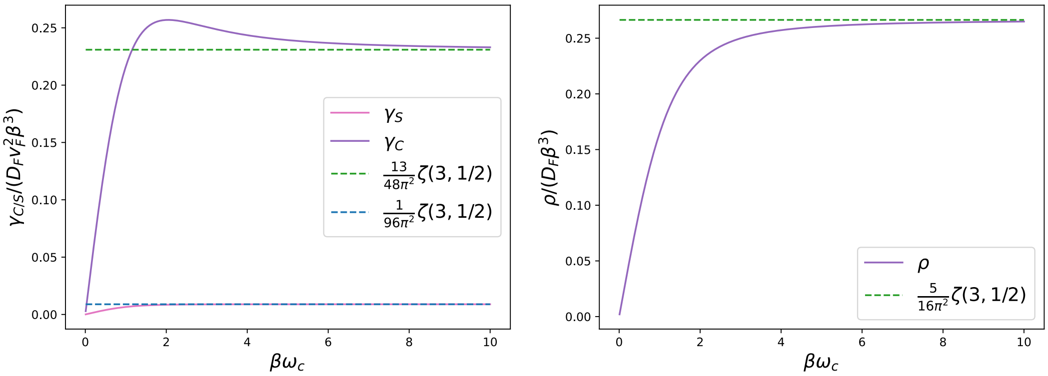



Figure 4.1: The left plot shows the gradient-square term coefficients in the Ginzburg-Landau theory (solid), with its low-temperature limits (dotted). The right plot shows the cross-term coefficient between CDWs and SC (solid) and the low-temperature limit (dotted) of this coefficient.

The total fourth-order term is

$$\frac{1}{8}\mathrm{Tr}\sum_k \left(\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\hat{\mathcal{F}}_0\hat{\mathcal{B}}\right)$$

$$\approx \alpha_2 \sum_{\substack{q_1,q_2\\q_3,q_4}} \eta_{q_1}\eta_{q_2}\eta_{q_3}\eta_{q_4}\delta_{q_1+q_2+q_3+q_4,0} + \beta_2 \sum_{\substack{q_1,q_2\\q_3,q_4}} \nu_{q_1}\bar{\nu}_{q_2}\nu_{q_3}\bar{\nu}_{q_4}\delta_{q_1+q_2+q_3+q_4,0}$$

$$+\rho \sum_{\substack{q_1,q_2\\q_3,q_4}} \eta_{q_1}\nu_{q_2}\eta_{q_3}\bar{\nu}_{q_4}\delta_{q_1+q_2+q_3+q_4,0}, \tag{4.3.39}$$

where

$$\alpha_2 = \beta_2 = \frac{\beta}{8}D_F\int_0^{\omega_c}\frac{d\xi}{\xi^3}\left(\sinh(\beta\xi) - \beta\xi\right)\mathrm{sech}^2(\frac{\beta\xi}{2}) \tag{4.3.40}$$

$$\rho = \frac{\beta}{8}D_F\int_0^{\omega_C}\frac{d\xi}{\xi^3}\left[3\sinh(\beta\xi) - 3\beta\xi + (\beta\xi)^2\tanh\left(\frac{\beta\xi}{2}\right)\right]\mathrm{sech}^2\left(\frac{\beta\xi}{2}\right) \tag{4.3.41}$$

We get that all the coefficients are positive, which ensures the stability of the system as long as the higher-order coefficients are small, positive, or both.

### 4.3.5 Higher order

We can use the same arguments as we did in subsection 3.3.5. Namely, by assuming that the bare Greens function does not depend on the momentum $q$, eventually, the same arguments apply to these coefficients.

### 4.3.6 Summary of the Ginzburg-Landau theory

In this section, we have derived expressions for the coefficients in the Ginzburg-Landau theory for CDWs and SC. We have included terms up to the fourth order and the quadratic order of the gradient term. Remarkably, most of the coefficients turn out to be very similar for the CDW terms and the SC terms, but with a few exceptions. We can note that in the quadratic terms, the difference lies in the different potentials. Assuming that these potentials are not the same, this will give two different critical temperatures for the two states, as we would expect for two different phases. By doing the same low-temperature analysis as in 3.3.6, we have that $\eta = C\sqrt{T_{C_{\text{CDW}}} - T}$ and $|\nu| = C\sqrt{T_{C_{\text{SC}}} - T}$, with the same constant $C$. The second thing to note is the difference in the gradient term. It turns out that the ratio between the gradient term for the CDWs and SC is 26, which can be seen on the left plot in figure 4.1. This tells us that the CDW state is more resistant to spacial deformations than the SC state. Regardless of the difference in magnitude, also the SC gradient coefficient is proportional to $v_F\beta^3$, just like it is in the case for CDWs. The last thing to note is that we have a positive coefficient in the cross-term between the two states. This tells us that it is not energetically favorable to have co-existence in the system. The coefficient together with the low-temperature limit is shown on the right in figure 4.1.

# Chapter 5

# Summary and Outlook

In this thesis, our primary goal was to develop a Ginzburg-Landau theory for a system that could exhibit both CDWs and SC. We were particularly interested in the interplay between these phases. The preliminaries, chapter 2, contain an overview of the main concepts of the functional integral method. In chapter 3, we started with a microscopic theory that could describe a system with CDWs. From this, we derived an effective bosonic theory from which we could do a stationary phase analysis. This analysis resulted in a mean-field equation for the order parameter and an expression for the critical temperature. The critical temperature for CDWs had the same structure as $T_C$ in the BCS theory for a superconductor [43]. This points to a purely Coloumb-driven potential in the interaction [53]. In addition to this, we derived an expression for the Lindhard susceptibility and showed its divergence at $T_C$.

From this, we extrapolated the theory from the normal state, such that it included a small, fluctuating field. This resulted in a Ginzburg-Landau theory of the system. The theory exhibited a familiar structure [44], where the second-order coefficient changes sign at the critical temperature, and the gradient term and the fourth-order term are positive for all $T$, ensuring the stability of the system. Moreover, we also showed that the temperature dependence was in line with the existing theory [43]. We also stated that the higher-order terms are negligible.

In chapter 4 we added a potential that couples fermions of different spins, to the total action. This resulted in a system exhibiting both CDWs and SC. Furthermore, we did a stationary phase analysis for this system, where we derived self-consistent equations of the mean-field configurations for the two order parameters. Deriving the equations for the critical temperatures, we saw that they behave similarly, where the only difference lies in the potentials of the interactions. Moreover, we derived an expression for the pair susceptibility and showed its divergence at the critical temperature.

The last part of the thesis contained a derivation of a Ginzburg-Landau theory for the system with CDWs and SC. The model exhibited some interesting results. Firstly, the second-order terms were almost identical for the CDW and SC terms. The only difference was in the potentials (critical temperature) for the two interactions. Secondly, we derived an expression for the modulus of the order parameter in the low-temperature limit. We showed for both phases it was proportional to $\sqrt{T - T_C}$. The coefficients for the gradient terms showed that the CDW state was 26 times more resistant to spatial deformations than the SC state. These results are intriguing due to the contrasting nature of the phases. Specifically, the superconductor breaks the electromagnetic gauge symmetry, while the CDW (charge density wave) state breaks translational symmetry. However, it is noteworthy that they exhibit the same structure in the Ginzburg-Landau coefficients. Lastly, we showed that the coexistence between SC and CDWs is not favorable in this model.

For a deeper understanding of the system, a natural next step would be to use the renormalization group theory on the Ginzburg-Landau model we constructed within the framework of this thesis. This will give an insight into how the system behaves around a critical point. Additionally, this will make the model more capable to be experimentally validated.

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# Appendix A

# Coherent State for Fermions

To prove that the state

$$|\xi\rangle = \exp\big(-\sum_\alpha \xi_\alpha a_\alpha^\dagger\big)|0\rangle \tag{A.0.1}$$

fulfills the eigenvalue equation

$$a_\alpha|\xi\rangle = \xi_\alpha|\xi\rangle, \tag{A.0.2}$$

we note that

$$a_\alpha e^{-\xi_\alpha a_\alpha^\dagger}|0\rangle = a_\alpha(1-\xi_\alpha a_\alpha^\dagger)|0\rangle \tag{A.0.3}$$

because of the anti-commutation of Grassmann numbers the Taylor expansion terminates after two terms. Next, we use the commutation rules for $\xi_\alpha$ and $a_\alpha$

$$= \xi_\alpha a_\alpha a_\alpha^\dagger|0\rangle = \xi_\alpha|0\rangle. \tag{A.0.4}$$

Further, we note that $\xi_\alpha^2 = 0$, which allows us to write

$$= \xi_\alpha(1-\xi_\alpha a_\alpha^\dagger)|0\rangle = \xi_\alpha e^{-\xi_\alpha a_\alpha^\dagger}|0\rangle \tag{A.0.5}$$

and we get that the fermionic coherent state fulfills the eigenvalue-equation. This is easier to prove than for the bosons due to the termination of the Taylor expansion.

# Appendix B

# Gaussian Integrals

In this section, we will first calculate a Gaussian integral for complex variables and then for Grassmann variables.

## B.1 Complex variables

We start out with a multiple integral over complex numbers

$$I_{\text{boson}} = \prod_k \int \mathcal{D}\bar{x}\mathcal{D}x e^{-\bar{x}_i A_{ij} x_j + x_j \bar{\mathcal{J}}_j + \bar{x}_i \mathcal{J}_i}, \tag{B.1.1}$$

where we sum over repeated indices, $A_{ij}$ is a symmetric matrix with $\det(A) > 0$, $x_i$ and $\mathcal{J}_i$ are vectors. We have also defined, $\mathcal{D}\bar{x}\mathcal{D}x = \frac{d\bar{x}_k dx_k}{2\pi i}$. First, we look closer at the exponent and want to re-write it as a square of a new variable, depended on $x$

$$-\bar{x}_i A_{ij} x_j + x_j \bar{\mathcal{J}}_j + \bar{x}_i \mathcal{J}_i = (\bar{x}_i - A^{-1}_{ij} \bar{\mathcal{J}}_j) A_{ij} (x_j - A^{-1}_{ji} \mathcal{J}_i) + \bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j. \tag{B.1.2}$$

Next, we introduce $z_i = x_i - A^{-1}_{ij} \mathcal{J}_j$ anduse that $\mathcal{D}\bar{z}\mathcal{D}z = \mathcal{D}\bar{x}\mathcal{D}x$ to write

$$I_{\text{boson}} = \int \mathcal{D}\bar{z}\mathcal{D}z e^{-\bar{z}_i A_{ij} z_j + \bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j}. \tag{B.1.3}$$

By introducing a new basis we can diagonalize the system by a unitary transformation

$$I_{\text{boson}} = e^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j} \int \mathcal{D}\bar{\tilde{z}}\mathcal{D}\tilde{z} e^{-\sum_n \lambda_n \bar{\tilde{z}}_n \tilde{z}_n}, \tag{B.1.4}$$

where $\lambda_n$ is the eigenvalues for the matrix $\mathbf{A}$. Further, we write $\tilde{z} = \sqrt{u^2 + v^2} e^{i\theta}$ and

$$\mathcal{D}\bar{\tilde{z}}\mathcal{D}\tilde{z} = \prod_k \frac{d\bar{\tilde{z}} d\tilde{z}}{2\pi i} = \prod_n \frac{du dv}{\pi} = \mathcal{D}v\mathcal{D}u, \tag{B.1.5}$$

where the change in the denominator is due to the change from complex to real integration variables.

$$I_{\text{boson}} = e^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j} \int \mathcal{D}v\mathcal{D}u e^{-\sum_n \lambda_n (u^2 + v^2)}, \tag{B.1.6}$$

which is

$$I_{\text{boson}} = \frac{1}{\det(A)} e^{\bar{\mathcal{J}}_i A^{-1}_{ij} \mathcal{J}_j} \tag{B.1.7}$$

## B.2 Grassmann variables

In this appendix, we will calculate the Gaussian integral over Grassmann variables. This corresponds to integrating over the fermionic degree of freedom. We start out with a similar integral

$$I_{\text{fermion}} = \int \mathcal{D}\bar{\xi}\mathcal{D}\xi e^{-\bar{\xi}_i A_{ij}\xi_j + \xi_i \bar{\mathcal{J}}_i + \bar{\xi}_j \mathcal{J}_j}, \tag{B.2.1}$$

where $\mathcal{J}$ and $\xi$ are Grassmann-variables, and $A_{ij}$ need to fulfill the same criteria as for the complex-variable case. For Grassmann variable we define $\mathcal{D}\bar{\xi}\mathcal{D}\xi = \prod_k d\bar{\xi}_k d\xi_k$. Completing the square in the integration variable, and introducing the new variable $\tilde{\xi} = \xi + \mathcal{J}_j A_{ji}^{-1}$ gives

$$\int \mathcal{D}\bar{\tilde{\xi}}\mathcal{D}\tilde{\xi} e^{-\bar{\tilde{\xi}}_i A_{ij}\tilde{\xi}_j + \bar{\mathcal{J}}_i A_{ij}^{-1}\mathcal{J}_j} \tag{B.2.2}$$

$$= e^{\bar{\mathcal{J}}_i A_{ij}^{-1}\mathcal{J}_j} \int \mathcal{D}\bar{\tilde{\xi}}\mathcal{D}\tilde{\xi} e^{-\bar{\tilde{\xi}}_i A_{ij}\tilde{\xi}_j} \tag{B.2.3}$$

For Grassmann variables, we have that

$$\int d\bar{\xi} d\xi e^{-\bar{\xi} a \xi} = \int d\bar{\xi} d\xi (1 - \bar{\xi} a \xi) = a, \tag{B.2.4}$$

where we have used that $\int d\xi \bar{\xi}\xi = -\bar{\xi}$. This allows us to write

$$\int \mathcal{D}\bar{\tilde{\xi}}\mathcal{D}\tilde{\xi} e^{-\bar{\tilde{\xi}}_i A_{ij}\tilde{\xi}_j} \tag{B.2.5}$$

$$= \int \mathcal{D}\bar{\eta}\mathcal{D}\eta e^{-\sum_n \lambda_n \bar{\eta}_n \eta_n} \tag{B.2.6}$$

$$= \int \mathcal{D}\bar{\eta}\mathcal{D}\eta (1 - \sum_n \lambda_n \bar{\eta}_n \eta_n) \tag{B.2.7}$$

$$= \prod_n \lambda_n = \det(A) \tag{B.2.8}$$

which gives us that

$$I_{\text{fermion}} = \int \mathcal{D}\bar{\xi}\mathcal{D}\xi e^{-\bar{\xi}_i A_{ij}\xi_j + \xi_i \bar{\mathcal{J}}_i + \bar{\xi}_j \mathcal{J}_j} \tag{B.2.9}$$

$$= \det(A) e^{\bar{\mathcal{J}}_i A_{ij}^{-1}\mathcal{J}_j}. \tag{B.2.10}$$

where we can observe that the determinant is now in the numerator and not in the denominator as for the bosonic case.

# Appendix C

# Fourier Transforms

First we define the Fourier transform for the fermion operator as

$$c_{i,\sigma} = \frac{1}{\sqrt{N\beta}} \sum_k c_{\mathbf{k},\sigma} e^{ik\cdot r_i}. \tag{C.0.1}$$

The volume of the four-momentum space is $N\beta$, hence, the factor $(\sqrt{N\beta})^{-1}$. The electron-electron-interaction we want to Fourier transform

$$H_{\text{int}} = \sum_{\sigma,\sigma'} \sum_{i,j} V_{\sigma,\sigma'}(r_i - r_j) c^\dagger_{i\sigma} c_{i,\sigma} c^\dagger_{j,\sigma'} c_{j,\sigma'}. \tag{C.0.2}$$

Inserting the Fourier transforms for the fermionic operators gives

$$H_{\text{int}} = \frac{1}{(N\beta)^2} \sum_{\substack{i,j \\ \sigma,\sigma'}} \sum_{\substack{k_1,k_2 \\ k_3,k_4}} V_{\sigma,\sigma'}(r_i - r_j) c^\dagger_{k_1,\sigma} e^{-ik_1\cdot r_i} c_{k_2,\sigma} e^{ik_2\cdot r_i} c^\dagger_{k_3,\sigma'} e^{-ik_3\cdot r_j} c_{k_4,\sigma'} e^{ik_4\cdot r_j} \tag{C.0.3}$$

Next, we redefine the position $r_i$ an $r_j$ to be relative position $r$ and center of mass position $R$

$$R = \frac{r_i + r_j}{2}, \quad r = r_i - r_j. \tag{C.0.4}$$

When performing the sum over the center of mass position, we get

$$H_{\text{int}} = \frac{1}{N\beta} \sum_{r,\sigma,\sigma'} \sum_{\substack{k_1,k_2 \\ k_3,k_4}} V_{\sigma,\sigma'}(r) c^\dagger_{k_1,\sigma} c_{k_2,\sigma} c^\dagger_{k_3,\sigma'} c_{k_4,\sigma'} e^{-i(k_1-k_2-k_3+k_4)\cdot r/2} \delta(-k_1 + k_2 - k_3 + k_4). \tag{C.0.5}$$

where we used that $\frac{1}{N\beta} \sum_R e^{i(-k_1+k_2-k_3+k_4)\cdot R} = \delta(-k_1 + k_2 - k_3 + k_4)$, which gives that

$$k_1 - k_2 = -(k_3 - k_4). \tag{C.0.6}$$

We will now look at two different ways to index the creation and annihilation operators. The first one corresponds to the term we use for the CDW interaction and the second one for the SC interaction.

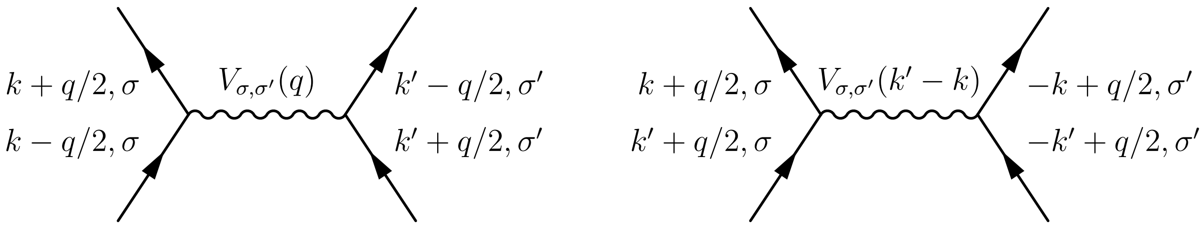


Figure C.1: Two representations of a Feynmann diagram for an electron-electron interaction, with a potential $V$.

**First alternative** We define the center of mass momentum, $k$ and $k'$, and the relative momentum, $q$ as

$$k = \frac{k_1 + k_2}{2}, \quad k' = \frac{k_3 + k_4}{2}, \quad q = k_1 - k_2. \tag{C.0.7}$$

Inserting the new definitions into the Hamiltonian gives us

$$H_{\text{int}} = \frac{1}{N\beta} \sum_{q,k,k'} \sum_{r} V_{\sigma,\sigma'}(r) e^{-ir\cdot q} c^\dagger_{k+q/2,\sigma} c_{k-q/2,\sigma} c^\dagger_{k'-q/2,\sigma'} c_{k'+q/2,\sigma'}. \tag{C.0.8}$$

Next, we define

$$V_{\sigma,\sigma'}(q) \equiv \frac{1}{N\beta} \sum_{r} V_{\sigma,\sigma'}(r) e^{-ir\cdot q}, \tag{C.0.9}$$

which leaves us with the final expression for the Fourier-transformed interaction-term

$$H_{\text{int}} = \sum_{q,k,k'} \sum_{\sigma,\sigma'} V_{\sigma,\sigma'}(q) c^\dagger_{k+q/2,\sigma} c_{k-q/2,\sigma} c^\dagger_{k'-q/2,\sigma'} c_{k'+q/2,\sigma'}, \tag{C.0.10}$$

where $q$ is the exchanged momentum in the interaction, $k + q/2$ is the initial momentum of the left fermion in figure C.1 and $k - q/2$ the outgoing momentum of the left fermion.

**Second alternative** An alternative way of renaming the momenta is

$$k = \frac{k_1 - k_3}{2}, \quad k' = \frac{k_2 - k_4}{2}, \tag{C.0.11a}$$

$$q = k_1 + k_3 = k_2 + k_4. \tag{C.0.11b}$$

This gives us a Hamiltonian on the form

$$H_{\text{int}} = \sum_{q,k,k'} V_{\sigma,\sigma'}(k'-k) c^\dagger_{k+q/2,\sigma} c_{k'+q/2,\sigma} c^\dagger_{-k+q/2,\sigma'} c_{-k'+q/2,\sigma'}, \tag{C.0.12}$$

where

$$V_{\sigma,\sigma'}(k'-k) \equiv \frac{1}{N\beta} \sum_{r} V_{\sigma,\sigma'}(r) e^{i\mathbf{r}\cdot(k'-k)}. \tag{C.0.13}$$

This interaction is shown as a Feynmann diagram on the right in figure C.1.

# Appendix D

# General Formula for Matsubara Summation

This appendix will follow the lecture notes from Lecture Notes in Functional Integral Methods in Condensed Matter Physics by Asle Sudbø [46]. First, we want to perform the following sums

$$\sum_{\omega_n} \frac{1}{i\omega_n - \xi_{\mathbf{k}}} = \frac{\beta}{1 + e^{\beta\xi_{\mathbf{k}}}}. \tag{D.0.1}$$

To do this we will use Cauchy's residue theorem. We will use the Fermi distribution is given by

$$f(z) = \frac{1}{1 + e^{\beta z}}, \tag{D.0.2}$$

We can see that it has poles in $i\omega_n$. The Cauchy´s residue theorem tells us that

$$\oint dz g(z) = 2\pi i \sum_i \operatorname*{Res}_{z \to z_0} [g(z_i)]. \tag{D.0.3}$$

By integrating over the Fermi distribution and using the theorem, we have

$$\oint dz f(z) = 2\pi i \lim_{z \to i\omega_n} [(z - i\omega_n) f(z)] = 2\pi i \lim_{z \to i\omega_n} \frac{z - i\omega_n}{1 + e^{\beta z}} \tag{D.0.4}$$

$$= 2\pi i \lim_{z \to i\omega_n} \frac{z - i\omega_n}{1 + e^{\beta(z - i\omega_n + i\omega_n)}} = 2\pi i \lim_{z \to i\omega_n} \frac{z - i\omega_n}{1 - e^{\beta(z - i\omega_n)}} \tag{D.0.5}$$

$$= 2\pi i \lim_{z \to i\omega_n} \frac{z - i\omega_n}{1 - (1 + \beta(z - i\omega_n) + ...)} \approx 2\pi i \lim_{z \to i\omega_n} \frac{z - i\omega_n}{-\beta(z - i\omega_n)} = -\frac{2\pi i}{\beta} \tag{D.0.6}$$

where we have used that $\omega_n = \frac{(2n+1)\pi}{\beta}$. Integrating over a curve $C$ that encloses all the poles of $f(z)$, but non of the poles in $g(z) = \frac{1}{z - \xi_{\mathbf{k}}}$, we have that

$$\sum_{i\omega_n} g(i\omega_n) = -\frac{\beta}{2\pi i} \oint_C dz g(z) f(z). \tag{D.0.7}$$

The deformation of the curve must be such that it is covering the poles of $f(z)$ and not

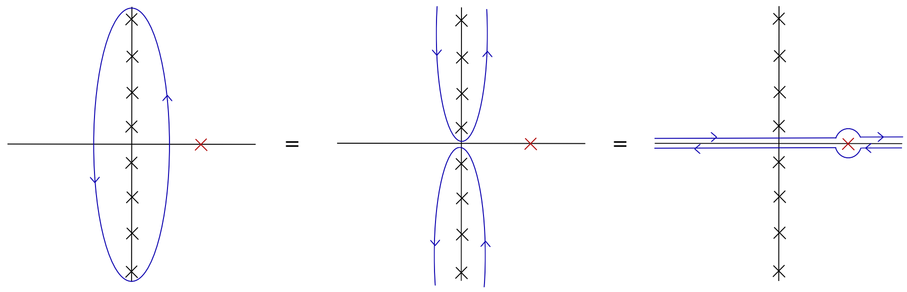


Figure D.1: Deformation of the curve C

the poles of $g(z)$. We will use the deformation in D.1. The integral is

$$\frac{\beta}{2\pi i}\oint_C dz g(z) f(z) = \frac{\beta}{2\pi i}\int_{-\infty}^{\infty} d\epsilon \left[\frac{f(\epsilon+i\delta)}{\epsilon+i\delta-\xi_{\mathbf{k}}} - \frac{f(\epsilon-i\delta)}{\epsilon-i\delta-\xi_{\mathbf{k}}}\right]. \tag{D.0.8}$$

Since $f(x)$ is continuous we can write this as

$$\frac{\beta}{2\pi i}\int_{-\infty}^{\infty} d\epsilon f(\epsilon) \left[\frac{1}{\epsilon+i\delta-\xi_{\mathbf{k}}} - \frac{1}{\epsilon-i\delta-\xi_{\mathbf{k}}}\right]. \tag{D.0.9}$$

Next, we want to divide the integral into tree parts, namely for $\epsilon > \xi_{\mathbf{k}} + i\delta$, $\xi_{\mathbf{k}} - i\delta < \epsilon < \xi_{\mathbf{k}} + i\delta$ and $\epsilon < \xi_{\mathbf{k}} + i\delta$

$$\int_{-\infty}^{\infty} = \int_{-\infty}^{R} + \int_{\gamma\pm} + \int_{R}^{\infty}, \tag{D.0.10}$$

where $\gamma_\pm$ is the upper/lower circle around the pole of $g(x)$. The integral will now be

$$\frac{\beta}{2\pi i}\left[\int_{-\infty}^{R} d\epsilon \frac{f(\epsilon)}{\epsilon+i\delta-\xi_{\mathbf{k}}} + \int_{\gamma+} d\epsilon \frac{f(\epsilon)}{\epsilon+i\delta-\xi_{\mathbf{k}}} + \int_{R}^{\infty} d\epsilon \frac{f(\epsilon)}{\epsilon+i\delta-\xi_{\mathbf{k}}}\right. \tag{D.0.11}$$

$$\left.- \int_{-\infty}^{R} d\epsilon \frac{f(\epsilon)}{\epsilon-i\delta-\xi_{\mathbf{k}}} - \int_{\gamma-} d\epsilon \frac{f(\epsilon)}{\epsilon-i\delta-\xi_{\mathbf{k}}} - \int_{R}^{\infty} d\epsilon \frac{f(\epsilon)}{\epsilon-i\delta-\xi_{\mathbf{k}}}\right] \tag{D.0.12}$$

$$= \frac{\beta}{2\pi i}\left[\int_{\gamma+} d\epsilon \frac{f(\epsilon)}{\epsilon+i\delta-\xi_{\mathbf{k}}} - \int_{\gamma-} d\epsilon \frac{f(\epsilon)}{\epsilon-i\delta-\xi_{\mathbf{k}}}\right]. \tag{D.0.13}$$

For the integrals where the curve is not over the pole, we can remove $\pm i\delta$. Using Cauchy principal value we get

$$\oint_C dz g(z) f(z) = -\frac{\beta}{2\pi i} 2\pi i f(\xi_{\mathbf{k}}). \tag{D.0.14}$$

Going back to equation (D.0.7), we see that

$$\sum_{\omega_n} g(i\omega_n) = \frac{\beta}{1+e^{\xi_{\mathbf{k}}\beta}}, \tag{D.0.15}$$

which is what we wanted to prove.

**Higher-powers** Next, we want to give a general formula for higher powers of the denominator in the sum. We want to prove that

$$\sum_n \frac{1}{(i\omega_n - \xi)^m} = \frac{\beta}{(m-1)!}\partial_\xi^{m-1} f(\xi). \tag{D.0.16}$$

We will make use of the following expression for the derivative

$$\partial_\xi^m \frac{1}{i\omega_n - \xi} = \frac{m!}{(i\omega_n - \xi)^{m+1}}. \tag{D.0.17}$$

By inserting this into (D.0.16), we get

$$\sum_n \frac{1}{(i\omega_n - \xi)^m} = \sum_n \frac{1}{(m-1)!}\partial_\xi^{m-1} \frac{1}{i\omega_n - \xi} \tag{D.0.18}$$

$$= \frac{1}{(m-1)!}\partial_\xi^{m-1} \sum_n \frac{1}{i\omega_n - \xi} = \frac{1}{(m-1)!}\partial_\xi^{m-1} \beta f(\xi), \tag{D.0.19}$$

which gives us the desired result.

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