Renormalization-group study of the superconducting-to-pseudogap transition

Springer, Daniel

2013

Springer, D. (2013). Renormalization-group study of the superconducting-to-pseudogap transition. Doctoral thesis, Nanyang Technological University, Singapore.

<https://hdl.handle.net/10356/59949>

<https://doi.org/10.32657/10356/59949>

Renormalization-Group Study of the Superconducting-to-Pseudogap Transition

NANYANG
TECHNOLOGICAL
UNIVERSITY

Daniel SPRINGER

School of Physical and Mathematical Science

A thesis submitted to the Nanyang Technological University
in fulfilment of the requirements for the degree of

Doctor of Philosophy

January 2013

Acknowledgements

I would like to express my sincere gratitude to my advisor Asst. Prof. CHEONG Siew Ann for his support of my research throughout the last four years.

*Contemporary physics is based on concepts somewhat analogous to
the smile of the absent cat.*

Albert Einstein

Contents

Contents	3
1 Introduction	8
2 High-Temperature Superconductivity (HTSC)	10
2.1 Theoretical models	13
2.2 The Pseudogap Phase	17
2.2.1 Magnetic Properties	18
2.2.2 Energy gap	20
2.2.3 Quasiparticle (QP) peak	22
2.2.4 Pseudogap in conventional superconductors	23
2.2.5 A two-gap scenario	24
2.2.6 Theoretical Background	26
3 The Renormalization Group	30
3.1 Fixed Points	31
3.1.1 Path Integral Formalism	31
3.1.2 Effective Action	34
3.1.3 Three RG steps to find Fixed Points	36
3.2 Obtaining the RG flow	38
3.2.1 Tree Level	39
3.2.2 Loop Corrections	40
4 The Origin of the PG	44
4.1 Details of the Model	44
4.2 Strong Correlation Effects	45
4.3 Implementing the RG approach	47
4.3.1 SC Effective Action	47
4.4 Superconducting Fixed Point at Tree Level	48
4.4.1 Invariance of S_0	51
4.4.2 Field Rescaling at the Superconducting Fixed Point	52

CONTENTS

4.5	Quantum Corrections of the Superconducting Fixed Point	53
4.5.1	Particle-Hole Channel	53
4.5.2	Particle-Particle Channel	56
4.6	Phase Coherence for Superconductors	58
4.6.1	The variational approach	58
4.7	Perturbations of the SC fixed point	62
4.7.1	Kinematically forbidden processes	63
4.7.2	Pair breaking processes	64
4.7.3	Dephasing processes	67
5	Conclusion	76
	References	79
	Appendix A: Stripe-like phase separation and electric fields	84
A.1	The Complex Ginzburg Landau Equation	84
A.1.1	Magnetic Fields	85
A.1.2	Electric Fields	87
	Appendix B: Grassmann Path Integration	89
B.1	Discretizing the Exponent	90
B.2	Limitations	91

Abbreviations

AF	Antiferromagnetic, Antiferromagnetism, antiferromagnetic
ARPES	Angle Resolved Photo Emission Spectroscopy
BCS	Bardeen-Cooper-Schrieffer
c	Fermion Annihilation Operator
$c^\dagger$	Fermion Creation Operator
Cu	Copper
E_F	Fermi Energy
HTSC	High-temperature superconductor(s), High-temperature superconductivity
K_F	Fermi Vector
λ	Momentum Cutoff
MI	Mott insulator, Mott insulating
O	Oxygen
PG	Pseudogap
Ψ_T	SC Trial wavefunction
ψ	Grassmann Field
QP	Quasi Particle
RG	Renormalization Group
S	Action
s	RG Scaling Factor
SC	Superconductivity, Superconductor(s), superconducting
STM	Scanning Tunneling Microscopy
T_c	SC Critical Temperature
T^*	PG Critical Temperature
θ	Quantum Phase
V	Coupling Potential
ω	Matsubara Frequency
Z	Quantum Partition Function

Abstract

The amount of hole- or electron-doping of a high-temperature superconductor determines the low-temperature long-range order. With increased doping the long-range order changes from a Mott insulating to a high-temperature superconducting phase. In between these two regimes a rather intriguing phase with a pre-formed energy gap but no superconductivity is observed.

Until recently no equivalent behaviour was observed for conventional superconductors. But scanning tunneling microscopy experiments on disordered thin film superconductors reveal that a pre-formed energy gap may as well exist in conventional superconductors. This supports the assumption that the pseudogap may not be a typical property of high-temperature superconducting materials but may be a phenomenon that is in general related to strongly correlated or disordered two-dimensional superconductors. According to this assumption a theoretical investigation of the pseudogap phase may not necessarily contain the full complexity of cuprate superconductors. Instead the phase transition from a superconducting state to the pseudogap phase may be studied based on a generalized description of superconductivity.

In this work we present a generalized description for a phase transition between a superconducting and a non-superconducting gapped state. To determine which microscopic mechanism induces this phase transition we use the perturbative momentum-space Renormalization Group (RG) method. After introducing a generalized effective action for a superconducting state, we determine the superconducting fixed point. We then analyze two types of perturbations that may be present in strongly correlated or disordered superconductors. The first breaks Cooper pairs and may induce a phase transition towards a gapless non-SC state. The second perturbation violates the quantum phase coherence condition found at the superconducting fixed point but conserves the paired state. Each of these two perturbations supports a different mechanism for the pseudogap. The former favors a scenario of pre-formed non-coherent Cooper pairs while the latter

indicates that the pseudogap is unrelated but in competition with superconductivity.

Our RG study shows that pair breaking perturbations due to strong correlations and disorder are irrelevant on macroscopic length scales. This means that Cooper pairs do not easily break up and the superconducting state is conserved in the presence of these perturbations. For pair conserving perturbations on the other hand we find a relevant RG flow. But this type of strong on-site correlation disrupts the global phase coherence of Cooper pairs. The superconducting state therefore vanishes while the energy gap persists. We conclude that the energy gap in the normal state of underdoped cuprates and disordered two-dimensional BCS-like superconductors may be understood as the result of dephasing correlations in an otherwise superconducting state.

Chapter 1

Introduction

With the discovery of superconductivity (SC) in 1911 [1] and its celebrated theoretical description by Bardeen-Cooper-Schrieffer (BCS) in 1957 [2] SC was believed to be understood. It therefore came as a surprise when in 1986 a potentially new flavour of SC that did not follow the conventional BCS theory was found in cuprates [3].

As physicists attempted to understand the unconventional SC mechanism, novel surprising effects were observed in high-temperature superconducting materials (HTSC). One of them is that an energy gap in the electronic spectrum, an integral part of any SC state, is also found in the non-SC doping regime. The possible connection between high- T_c SC and the pseudo-gap (PG) phase has made underdoped cuprates another frontier in the search for the SC mechanism. However, whether and how the SC and the PG phase are related remains as mysterious as the SC mechanism itself.

To uncover the relation between the SC and the PG phase we will investigate possible scenarios for the SC-PG transition. In particular we are interested whether and how a phase transition between a gapped SC phase and a gapped non-SC phase can be induced. An appropriate technique to analyze phase transitions is the perturbative momentum-space Renormalization-Group (RG) approach. With this method we analyze how perturbations that are typical for underdoped cuprates may change the long-range order of the system.

In chapter 2 of this thesis we will give a general survey of what is known about HTSC. As a part of this overview we discuss how strong on-site Coulomb repulsion influences the electron transport properties and eventually results in the formation of an antiferromagnetic (AF) Mott insulating (MI) phase. In addition we will give an introduction to theoretical models (section 2.1) that are generally used to describe the lattice dynamics of cuprates. In section 2.2 we will review experimental and theoretical results related to the PG phase.

In chapter 3 the perturbative momentum-space RG method is introduced. We

show how the effective action (see section 3.1.2) has to be chosen to identify a fixed point (see section 3.1.3). The field rescaling relation found at a fixed point can then be used to determine the importance of a perturbations and whether a phase transition towards a neighboring fixed point is induced.

In chapter 4 we use the RG technique to determine possible scenarios for a SC-PG transition. Before we can determine the SC fixed point and the corresponding field rescaling relation (section 4.4) we have to introduce a modified version of the effective action (section 4.3.1). In section 4.7 we introduce perturbations that may be expected to be present in the underdoped regime of HTSC or disordered two-dimensional BCS like SC. Using the RG transformation we will classify which perturbation is most capable to induce the SC-PG transition. Finally we discuss our findings in chapter 5.

Chapter 2

High-Temperature Superconductivity (HTSC)

With the discovery of superconductivity at unusual high temperatures in copper-oxides [3] condensed matter physics entered one of its richest and most complex fields. Today, more than 50 years after Bardeen-Cooper-Schrieffer presented their celebrated theory of conventional SC the field experiences a renaissance with the declared aim to realize superconductivity at room temperature. The possibility to design materials with a SC state at “living-room” conditions initiated immense theoretical and experimental efforts.

During 25 years of research in the HTSC field the number of reviews, highly cited papers and different perspectives has become enormous [4; 5; 6; 7; 8; 9]. Although this large variety of remarkable theories has led to a better understanding of HTSC materials a widely accepted theory for cuprate SC has yet to be found.

What is in general agreed upon [4; 5] is that the layered crystal structure (Figure 2.1) made up of copper-oxygen planes is an important piece in the HTSC puzzle. It is believed that most of the superconducting current flows along these layers only. The copper (Cu) atoms within these layers are doubly ionized in a d^9 configuration surrounded by six oxygen (O) atoms. In this octahedral environment the t_{2g} orbitals are completely filled. Due to a Jahn-Teller distortion of the octahedral shape along the z-axis, the e_g orbitals are split and the remaining electron occupies the $d_{x^2-y^2}$ orbital. In this configuration the band is half-filled and, according to band theory, a metallic state should emerge. The single $d_{x^2-y^2}$ -electron would then gain the kinetic energy $\bar{t}$ by hopping to a neighboring copper atom. But due to large on-site Coulomb repulsion $U_d \gg \bar{t}$ this process is strongly suppressed and the material is an insulator. This type of non-metals with an otherwise metallic band structure is known as Mott insulator (MI) [10].

In the phase diagram in Figure 2.2 (a) the MI phase (purple region) is located on the strongly underdoped side. The presence and location of the MI was

Figure 2.1: Schematic representation of the crystal structure of some Bi-based high-temperature superconductors: (a) Bi2201, (b) Bi2212 and (c) Bi2223. It is expected that the superconducting current mainly flows along the layered structure of the copper-oxygen plains. From [11]

found to be a common property among all HTSC materials. The lowest possible excitation of this configuration is the charge-transfer excitation. In this process the single hole of the d^9 configuration overcomes the energy barrier ($E_p - E_d$) between the Cu $3d$ and the nearest O $2p$ orbital to hop to the neighboring O atom (Figure 2.2 (b)). This process is energetically favourable if the gain in kinetic energy t_{pd} is larger than the energy barrier ($E_p - E_d$). To allow holes from two different Cu to hop to the same O the two holes must be antiferromagnetically (AF) aligned to maintain the Pauli principle. In this so called superexchange (Figure 2.3) two holes from neighboring Cu virtually hop to the oxygen's p orbital to gain the exchange energy J . The formation of AF order in undoped cuprates was confirmed experimentally [12; 13] and is a striking similarity of all HTSC materials.

However, the insulating AF state becomes unstable upon electron or hole doping. As can be seen from Figure 2.2 (a) the AF state rapidly vanishes when additional holes are doped into the system. The reason for this is the suppression of the superexchange mechanism by the doped hole. Due to the strong on-site repulsion U_d any additional hole resides on the O p orbital [14] (Figure 2.2 (b)). Such doped holes prevent superexchange between neighboring Cu atoms and the AF order is disturbed. The additional hole may also gain the kinetic energy t_{pd} by hopping to a neighboring Cu atom. From there, due to translational symmetry, it may hop to any of the neighboring O atoms where it again prevents

Figure 2.2: Left: Schematic phase diagram for hole doped HTSC materials. Without any hole doping an antiferromagnetic Mott insulating phase is realized. Upon low doping the magnetic order vanishes and the system enters the controversial pseudogap phase. Further increasing the hole concentration leads into the high-temperature superconducting phase. Here UD means underdoped, OD is overdoped and OPT denotes the optimally doped regime where the critical temperature T_c has its maximum. Right: Due to large Coulomb repulsion U_d doped holes (blue dashed arrow) will occupy the oxygen 2p orbital instead of the Cu $3d_{x^2-y^2}$ orbital.

Figure 2.3: Two possible scenarios of superexchange also known as the first Goodenough-Kanamori-Anderson rule. In this example the atoms to the left and right to the ligand atom have either none or one electron in their d_{z^2} orbitals. If electrons from both sides virtually hop to the ligand atom, their spins have to be antiparallel. Due to strong intraatomic Hund's coupling the remaining spins on each atom are parallel to the itinerant spins. This results in AF order.

superexchange. The hopping eventually activates the material's metallic character which is suppressed in the undoped state. This delocalization of doped holes and the suppression of the superexchange mechanism are the major reasons why

hole doping is very effective in disturbing the AF order. However, an explanation of unconventional SC in hole doped cuprates based on the instability of the AF phase remains elusive.

2.1 Theoretical models

After this overview of the microscopic properties of cuprates we next want to discuss theoretical models that are used to describe HTSC materials. In this section we will have a brief look at lattice models that are used to mimic those microscopic interaction discussed above. Although there is no consensus on the actual SC mechanism, there is little doubt that certain lattice models capture the most essential interactions of HTSC materials.

A first model to describe high- T_c materials was written down soon after their discovery. To account for all degrees of freedom of electrons moving along CuO planes the model Hamiltonian consists of three bands [15; 16; 17; 18]

$$\begin{aligned} \mathcal{H}_{3band} = & \epsilon_d \sum_{i,\sigma} n_{i,\sigma}^d + \epsilon_p \sum_{j,\sigma} n_{j,\sigma}^p + \sum_{\langle i,j \rangle, \sigma} t_{i,j}^{pd} (p_{j,\sigma}^\dagger d_{i,\sigma} + \text{H.c.}) \\ & + \sum_{\langle j,j' \rangle, \sigma} t_{j,j'}^{pp} (p_{j,\sigma}^\dagger p_{j',\sigma} + \text{H.c.}) \\ & + U_d \sum_i n_{i,\uparrow}^d n_{i,\downarrow}^d + U_p \sum_j n_{j,\uparrow}^p n_{j,\downarrow}^p + U_{pd} \sum_{\langle i,j \rangle} n_i^d n_j^p \end{aligned} \quad (2.1)$$

$$(2.2)$$

Here p_j (d_i) is the fermionic annihilation operator at the O (Cu) ions labeled j (i) and $p_j^\dagger$ ($d_i^\dagger$) is the corresponding creation operator. $\langle \rangle$ refers to summation over nearest neighbors. The first hopping term describes the hybridization between nearest neighbor Cu and O atoms while the second term corresponds to O-O hopping. U_d and U_p represent the repulsion of doubly occupied d or p orbitals with the occupation number operators $n_{j\uparrow}^d = d_{j\uparrow}^\dagger d_{j\uparrow}$ and $n_{j\uparrow}^p = p_{j\uparrow}^\dagger p_{j\uparrow}$ respectively. U_{pd} is the repulsion of holes on neighboring CuO atoms. The difference in on-site occupation energies of the O and Cu orbitals is accounted for by ϵ_d and ϵ_p . Due to the complexity of the three-band Hamiltonian simplified versions that only cover certain interactions were invented.

The $t - J$ model

One of the best known theories for unconventional SC assumes that the superconducting state emerges when the doped hole resonates on the four O atoms surrounding a single Cu site. The spin of the doped hole combines with the spin

on the Cu to form a singlet, also known as Zhang-Rice singlet [19]. This pair of holes gains energy by virtual hopping.

In a model that focuses to describe the Zhang-Rice singlet the three-bands can be simplified to a one-band tight-binding model on a square lattice. The nearest-neighbor hopping integral t and the on-site repulsion U form the exchange integral

$$J = \frac{4t^2}{U} \quad (2.3)$$

that describes magnetic exchange interaction between otherwise freely hopping electrons. Zhang and Rice concluded that that the $t - J$ model of the form

$$\mathcal{H}_{t-J} = -t \sum_{\langle ij \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + J \sum_{\langle ij \rangle} (\vec{S}_i \vec{S}_j - n_i n_j / 4) \quad (2.4)$$

is the effective Hamiltonian describing the physics of the three-band Hamiltonian (2.2). Here $c_{i,\sigma}^\dagger$ ($c_{i,\sigma}$) creates (annihilates) an electron at lattice site i with spin σ and $\langle ij \rangle$ restricts the sum to nearest neighbors. S_i is the spin and n_i the occupation number operator. The model describes an electron that gains kinetic energy t by hopping across the lattice or alternatively the exchange energy $J = 4t^2/U$ by aligning its spin with its nearest-neighbors.

The AF order found in high- T_c materials is obtained when $J > 0$. With this choice electrons that reside on neighboring lattice sites will have antiparallel spin orientation. But this AF order will be disturbed once a charge carrier changes its lattice position. For the case $t \gg J$ the gain in hopping energy dominates and the AF state will be completely destroyed in favour of freely moving electrons. If on the other hand the excess energy to destroy the AF state is too large $t \ll J$ the magnetic order is conserved and hopping will be suppressed.

A rather intriguing consequence of this competition between AF ordering and the free hopping of holes is the formation of stripes [20; 21; 22]. In [23] a variational ansatz is used to investigate the $t \ll J$ and the $t \gg J$ limit for the $t - J$ model. In both cases the separation into hole-rich and hole-free stripes is energetically favourable. The concentration of holes along striped patterns reduces the energy cost of hopping while the AF order is maintained in the hole-free regions. The supercurrent may then flow along these “rivers of charge” [24] without disturbing the AF order in a neighboring stripe. Experimental evidence for a striped phase in underdoped cuprate superconductors came from scanning tunneling microscopy (STM) [25] and neutron diffraction measurements [26].

However, it is still unclear whether these periodic modulations seen in experiment are of the same origin as phase separation in the $t - J$ model. One work contradicting the stripe picture [27] compares results from STM and angle resolved photoemission spectroscopy (ARPES) on the same cuprate sample. The

stripe patterns are identified to be the result of quasiparticle interference rather than the result of phase separation.

In a side project to the present work we investigated the response of stripe patterns to electric fields (Appendix A). In a phase-separated scenario it can be expected that hole-rich and hole-free regions react differently to the presence of an electric charge. Our analysis of a time-dependent Ginzburg-Landau equation showed that the width of stripes changes when an electric field is switched on.

Hubbard Model

Another microscopic model used to investigate transport dynamics in HTSC materials is the 2D single-band Hubbard model. It describes electron transport dynamics by focusing on the hybridization of the Cu $d_{x^2-y^2}$ orbitals with the O anions. The on-site repulsion is realized by adding a common Coulomb term. In fact the Hubbard Hamiltonian was already well known and applied in other fields long before the discovery of HTSC [28]. It became popular again due to its capability to describe the strong on-site repulsion that eventually causes the Mott insulating state in cuprates. The Hubbard model

$$\mathcal{H}_H = -t \sum_{\langle ij \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \quad (2.5)$$

is also one of the simplest lattice models with a superconducting phase. Here the first term describes free electron hopping while the second term accounts for on-site Coulomb repulsion. If the on-site repulsion is sufficiently large the free hopping of charge carriers will be suppressed in favour of a Mott insulating phase. Although the Hubbard model is a one-band model while cuprates are probably best described as three-band systems, equation (2.5) is believed to capture the essential physics seen in low energy HTSC.

To consider the layered structure of copper oxides extended versions of the Hubbard model (2.6) can be constructed. One possible scenario of a bilayer Hubbard model considers interlayer hopping. The charge carriers may then hop between two different but congruent layers labeled $p = 1, 2$ [29]. For interlayer hopping

$$\begin{aligned} \mathcal{H}_H = & -t \sum_p \sum_{\langle ij \rangle} \sum_{\sigma} (c_{p,i,\sigma}^\dagger c_{p,j,\sigma} + c_{p,j,\sigma}^\dagger c_{p,i,\sigma}) + U \sum_p \sum_i n_{p,i,\uparrow} n_{p,i,\downarrow} \\ & - t_{\perp} \sum_i \sum_{\sigma} (c_{1,i,\sigma}^\dagger c_{2,i,\sigma} + c_{2,i,\sigma}^\dagger c_{1,i,\sigma}) \end{aligned} \quad (2.6)$$

the intralattice coordinate of the charge carrier does not change. Here the term $t_{\perp}$ accounts for hopping between different layers. If instead of interlayer hopping interlayer Coulomb repulsion of the form $U \sum_i c_{1,i,\sigma}^\dagger c_{1,i,\sigma} c_{2,i,\sigma}^\dagger c_{2,i,\sigma}$ is added [30] to

the ordinary Hubbard model, the Hubbard phase diagram contains an insulating antiferromagnetic, a magnetic and non-magnetic d-wave superconducting as well as a spin liquid insulating region. The latter state is not seen in the single-band Hubbard model.

Resonating Valence Bond Model

Another model, initially developed to study AF coupled spins in low dimension [32; 33] assumes a liquid of singlet "valence bonds" between electrons. In this non-magnetic state some of the AF exchange energy can be regained when pairs resonate among many different pairing configurations. Theoretically the resonating valence bond (RVB) idea can be described as a Gutzwiller projection of BCS paired superconducting state. This projection limits each lattice site to single occupancy where two spins form a spin singlet. Such a non-magnetic liquid of pair bonds is visualized in Figure 2.4.

In the undoped half-filled state the RVB liquid state is comparable to a Mott insulator with AF order replaced by spin singlets. The mobility of carriers is strongly suppressed due to on-site Coulomb repulsion. Relieving this state by hole- or electron-doping breaks the translational symmetry of the repulsive interaction and carrier mobility is increased. Superconductivity is conjectured to emerge when a critical amount of doping facilitates the collective motion of the

8

Figure 2.4: Liquid of pair bonds envisioned in the RVB theory. Singlet valence bonds are localized due to strong Coulomb repulsion. Doping of holes (dashed circles) breaks the translational symmetry and increases carrier mobility to facilitate the formation of a supercurrent. From [31].

superfluid condensate.

Instead of phonons the pairing in the RVB theory is therefore mediated by the superexchange which usually causes AF order in Mott insulators. Due to the exchange pairing, the shape of the energy gap was predicted to be d-wave even before this was experimentally confirmed.

2.2 The Pseudogap Phase

Apart from the unconventional SC state the phase diagram in Figure 2.2 has at least one more intriguing region. When the Mott insulating state is perturbed by doping holes into the CuO layer the system does not immediately enter the SC regime. Instead, depending on temperature, an intermediate state with rather strange properties is realized. In this so called pseudogap (PG) phase [34] the energy spectrum for antinodal directions is gapped but no phase transition towards a SC order is observed. This came as a surprise since in conventional SC the emergence of SC and the formation of an energy gap go hand-in-hand. Located between the AF Mott insulating and the SC phase the PG phase is often understood as a pre-cursor state of unconventional SC. The pre-formed energy gap can then be attributed to pre-formed Cooper pairs which have, for some reason, not reached phase coherence. This view has raised hopes that understanding pair formation in the PG phase may reveal the cornerstones of the SC mechanism. Except from the pre-cursor scenario there are opinions that the PG may be in competition with SC. Then the energy gap in the PG phase should originate from a different microscopic interaction and thus be unrelated to Cooper pair formation.

However, to this point the origin of the PG phase is unclear. Given the controversy between the pre-formed pair scenario and the competing phase idea we want to theoretically investigate which neighboring phases can be accessed from a general SC state. We will use a Renormalization-Group approach that allows us to identify how a SC state can be perturbed to induce a transition towards a neighboring phase. We will then identify whether this neighboring phase is either (1) a non-coherent gapped state with the same gap as the SC state or (2) a gapped state with a gap of different origin.

In the sections to come we will discuss experimental studies related to the PG phase that will be the basis for our theoretical study. Since there are a number of excellent reviews about experiments conducted on underdoped cuprates [6] and high- T_c superconductors in general [4; 9; 35] we will only discuss a selection of works that are relevant to motivate the present work.

2.2.1 Magnetic Properties

In the undoped state high- T_c materials are Mott insulators where localized charge carriers on neighboring lattice sites have antiparallel spin orientation. By doping holes into the material this AF order is rapidly destroyed and the system enters the pseudogap phase. At a critical doping the system becomes superconducting and charge carriers are expected to form spin singlet ($S = 0$) Cooper pairs. Beyond the well understood spin-ordering in the AF and the SC phase, it is interesting to investigate the magnetic properties of the PG. If the PG phase is a precursor state of SC there should exist non-coherent pre-formed singlet pairs within the PG region.

A good measure to distinguish between the antiparallel AF order and antiparallel spin-singlet ordering is the spin susceptibility

$$\chi_s = \frac{1}{T} \sum_i \langle S_i^z S_0^z \rangle . \quad (1)$$

For AF ordering the spin susceptibility χ_s is usually larger than for systems with spin-singlet formation. Figure 2.5 shows the change of χ_s with temperature for underdoped $\text{YBa}_2\text{Cu}_4\text{O}_8$. For temperatures between 300 K and 700 K χ_s is constant as in an ordinary metal. However, below 300 K the spin susceptibility strongly decreases indicating increased magnetic order. This drop in χ_s could be expected to precede the transition to an AF state. Whether $\text{YBa}_2\text{Cu}_4\text{O}_8$ shows

Figure 2.5: Temperature dependence of the shift in the nuclear magnetic resonance frequency (Knight shift) observed in underdoped $\text{YBa}_2\text{Cu}_4\text{O}_8$ with a critical temperature $T_c = 79$ K. The decay indicates the formation of singlets well above the SC transition temperature. From [36].

Figure 2.6: Comparison of spin susceptibility for a Heisenberg antiferromagnet and differently doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$. Especially in underdoped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ χ_s drops below the value expected for an AF state. This suggests that AF long range order is replaced by spin-singlet formation. From [37].

AF ordering is best estimated by comparing χ_s from Knight shift measurements with idealized AF models. A theoretical description for the AF phase found in Mott insulators is given by the Heisenberg model

$$H_{\text{AF}} = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} . \quad (2.8)$$

Below the critical Neel temperature T_N the Heisenberg model describes a lattice where electrons on neighboring sites have antiparallel spin orientation. A comparison of χ_s in the Heisenberg model and differently doped $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ samples is shown in Figure 2.6. Especially for underdoped samples the Knight shift measurements reveal spin susceptibilities that are lower than theoretically predicted for Heisenberg-like AF. Therefore the reduction of spin susceptibility in underdoped high- T_c materials at low temperature is probably evidence for singlet formation rather than long range AF ordering. Thus the sharp drop of spin susceptibility is usually interpreted as the opening of a gap in the magnetic spectrum, a trend usually expected to precede the phase transition towards a SC state.

In [38] similar results were obtained from nuclear magnetic resonance (NMR) measurements on underdoped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. The observed reduction of magnetic susceptibility resembles that associated with pair formation below T_c in

optimally doped $\text{YBa}_2\text{Cu}_3\text{O}_{6+x}$. These results suggest that the pairing or more precisely spin singlet formation is not weakened in the underdoped regime. The magnetic properties of the PG are therefore more similar to a SC with $S = \text{Cooper pairs}$ than an AF.

2.2.2 Energy gap

While the steep drop in χ_s is interpreted as sign of a spin gap, evidence for charge gap was found in ARPES experiments [35]. In ARPES experiments the simultaneous measurement of momentum and energy of photo-emission electron allows us to map out the Fermi surface. During the SC phase transition the

Figure 2.7: (a)-(c) ARPES measurement on underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ with $T_c = 83$ K for three different points on the Fermi surface (d). The formation of gap corresponds to a shift of the leading edge of the spectrum (black line) to lower energies compared to a reference sample (red line). Along the directions (a) and (b) the gap is present at temperatures well above T_c . (e) shows the temperature dependence of the leading-edge midpoint for all three directions (a-c). From [39]

leading edge of the electronic spectrum is pushed back from the Fermi surface to lower energies. This energy gap Δ corresponds to the minimum energy required to excite electrons i.e. Δ is the binding energy between paired electrons. In conventional SC the gap is interpreted as the order parameter.

Figure 2.7 (a-c) shows ARPES data taken at three different points on the Fermi surface of underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$. For $T < T_c$ the leading edge of the spectral function is pushed to lower energies for all three directions. For comparison data obtained from a gapless reference sample is shown (red line). For $T > T_c$ the energy gap first closes in the nodal direction (Figure 2.7 (c)). But especially along the anti-nodal direction $(0, \pi)$ the gap is remarkably stable and persists up to the transition temperature $T^* = 120$ K and thus far into the normal state. This momentum dependent closing of the energy gap at different temperatures results in the formation of so called Fermi arcs (Figure 2.8). These arcs denote regions where the Fermi surface is present at a particular doping and temperature. The structure of the pseudo energy gap was found to have a $d_{x^2-y^2}$ shape similar to the SC gap [40; 41].

Figure 2.8: Illustration of the temperature evolution of the Fermi surface in underdoped copper oxides. For $T > T^*$ the gap first vanishes along the (π, π) direction. The ungapped point along the nodal directions starts to enlarge and the Fermi surface (dark line) becomes visible. With increasing temperature the destruction of the energy gap extends until the gapped state is reduced to the anti-nodal direction (π, π) . The pseudo energy gap has the same $d_{x^2-y^2}$ symmetry as the SC energy gap. From [39].

The temperature evolution of the energy gap is shown in Figure 2.9. Remarkably, T^* increases with decreasing hole doping and the spectrum remains gapped even in the immediate proximity of the AF Mott insulating phase (not shown). In the same doping regime the SC transition temperature T_c (dotted line) has a decreasing trend. Therefore, unlike for conventional SC high- T_c materials do not obey the relation $2\Delta = k_B T_c$ [42]. Therefore the energy gap is not the suitable

Figure 2.9: Doping trends of the superconducting gap $\Delta(T = 0)$ (circles), the pseudogap crossover temperature T^* (triangles and squares) and the critical temperature T_c (dashed line). The doping trends of $\Delta(0)$ and T^* both increase with underdoping. From [35].

order parameter for HTSC.

The presence of an energy gap without a superconducting phase cannot be explained by BCS theory. Intuitively, the emergence of an energy gap right before the transition to a SC phase motivates the idea of pre-formed Cooper pairs that have not achieved the necessary phase coherence to form a condensate. A possible way to determine whether the gap is caused by the formation of Cooper pairs is to probe for particle-hole symmetry with respect to the Fermi level. Evidence for particle-hole symmetry in the normal state in the anti-nodal region was found from ARPES measurements on $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$ [43].

2.2.3 Quasiparticle (QP) peak

Early theoretical approaches to explain high- T_c SC with the Bardeen-Cooper-Schrieffer (BCS) model were not successful. One reason is that phonon-mediated Cooper pair formation is unlikely to account for the high critical temperature of up to $T_c = 105$ K [44]. Therefore the energy gap Δ , identified to be the BCS order parameter, may not be the suitable order parameter to characterize HTS.

The advantage of ARPES to directly probe the momentum-resolved electron

structure allows us to resolve coherent QP line shapes near the Fermi energy E_F . The width of this lineshape carries information about the interaction within the material. The theory is that with a single photoexcited electron the remaining $N - 1$ electrons constitute a QP also called a photohole. Without interactions the lifetime of this QP is infinite. In a non-interacting Fermi system the ARPES lineshape would therefore be a δ -function. A distinct QP peak indicates well defined or long-lived electronic excitations. Switching on interactions causes a widening of the QP peak indicating a finite lifetime of the photohole. Effectively this means that the $N - 1$ electrons will rearrange to occupy an energetically more favourable configuration. The details of this rearrangement depend on the interactions within the material.

For high- T_c materials in the SC state a QP peak is found in ARPES measurements. In Figure 2.7 such excitation peaks are clearly visible below 70 K. However, at increased temperatures the QP peak abruptly disappears although the energy gap persists. Intuitively the opposite effect would be expected. When the energy gap closes the phase space available for scattering increases. This would lead to a broadened QP peak. Since experimental data report the opposite effect it can be concluded that the QP peak indicates the coherence of the SC state and is therefore unrelated to the energy gap [9].

2.2.4 Pseudogap in conventional superconductors

Although unrelated to high- T_c materials, a study on a BCS-like superconductor has revealed an interesting parallel related to pre-formed Cooper pairs. In [45] STM experiments are conducted on low and highly disordered InO films to study the superconductor-insulator transition. For $T < T_c$ the STM data of the less disordered sample reveal a peak of well defined electronic excitations accompanied by an energy gap. Heating the sample first removes the QP peak while the energy gap persists also at higher temperatures. In a highly disordered sample the energy gap shows similar temperature behavior as in the less disordered case. However, the QP peak is not present at all. In Figure 2.10 the black dotted line indicates the formation of the SC condensate which coincides with the formation of QP peaks. The missing coherence peak in the gapped highly disordered samples means that Cooper pairs do not split before the material becomes insulating. Instead, electron pairs are directly localized in the disordered state. This may be the BCS-like version of pre-formed Cooper pairs. In a different STM study on disordered titanium nitride (TiN) films the suppression of the single electron density of states is attributed to superconducting fluctuations [46].

Figure 2.10: Front and perspective view of the local tunneling current obtained from STM measurements on InO films. Figures (a,c) show results from low disordered samples while (b,d) are taken from highly disordered ones. In both cases an energy gap can be observed that closes for $T > T_c$. The spectra differ by the pronounced QP peak that can only be seen in the low disordered samples below the critical temperature T_c (black dashed line). If this peak is not present it indicates that there are no electronic excitations close to the Fermi surface and the InO film is insulating. From [45].

2.2.5 A two-gap scenario

When crossing through T_c experiments usually do not detect any changes of the gap. This indicates that the pseudo-gap as well as the SC energy gap have the same microscopic origin, hence a one-gap scenario. But in some recent works there are signs that the gap found in many experiments may consist of two gaps. Therefore, instead of closely related states the SC and PG phase may as well be in competition with each other.

In [47] STM measurements were conducted in ultra-high vacuum over a wide range of temperatures. The STM spectrum obtained shows the usual spatially homogeneous gap in the PG as well as in the SC phase (Figure 2.11 (a)). The inhomogeneity of the gap that does not depend on temperature is one of the cornerstones of a two-gap theory. Especially in the SC state one would expect a spatially homogeneous energy gap [48]. To distinguish between the low- and high-temperature part of the STM spectrum the normalized conductance is used in [47]. In this normalized spectrum a small, spatially homogeneous energy gap is

Figure 2.11: Figure (a) shows the energy gap $\Delta(r)$ for a particular region of a $(\text{Bi}_{1-y}\text{Pb}_y)_2\text{Sr}_2\text{CuO}_{6+x}$ sample. Red regions mean that no gap is detected ($\Delta = 0$ meV). The inhomogeneity of the gap across the shown region and its presence for $T > T_c$ is untypical for SC. Figure (b) shows the same region as (a) after removing the effective background of the high-temperature spectra. The gap amplitude is reduced, spatially homogeneous and vanishes when crossing through T_c . This indicates that the large energy gap found in ARPES and STM experiments may have to be separated into an inhomogeneous gap unrelated to SC and a smaller, homogeneous gap that indicates the formation of a SC state. From [47].

is identified that exists only below T_c (Figure 2.11 (b)). This suggests that there are two different energy scales: (1) a smaller one responsible for SC that is homogeneous across the sample and strongly temperature dependent and (2) a larger gap which is strongly inhomogeneous and almost temperature independent.

More evidence for a two-gap scenario comes from low-temperature ARPES measurements on strongly underdoped $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+x}$. In [49] the doping dependence of the energy gap in the anti-nodal direction and near the nodal direction are compared. It is shown that the gap along the anti-nodal direction decreases with increasing doping and therefore tracks T^* . Near the nodal directions where the gap is usually much smaller the gap increases with doping and a clear QP peak is visible (Figure 2.12). The nodal energy gap seems to follow the temperature dependence of the critical temperature T_c . Similar findings of a BCS-like gap near the node are reported in [50].

Figure 2.12: Doping dependence of ARPES spectrum along 8 different pairs (A) along the Fermi surface. A QP peak is only visible near the nodal direction. Along the anti-nodal direction the gap is larger but the QP peak is vanishing small. From [49].

2.2.6 Theoretical Background

Among the numerous theoretical attempts to capture the physics of the F regime there are two major paths. The PG is (1) an instability of the normal, non-Fermi liquid phase with two competing gaps or (2) an instability of the superconducting phase with a single gap.

A prominent example supporting (1) is the electron current-loop idea [51; 52]. According to this approach there are four different circulating current states each unit cell as depicted in figure 2.13. These current loops produce a pair of oppositely directed magnetic moments. A system taking on one of these four possible ground states may oscillate back and forth into the other three states. This kind of configuration breaks time-reversal and rotational symmetry. As a result an anisotropic gap emerges at the chemical potential of the single-particle spectrum [53] that may be attributed to the PG phase.

Another example supporting scenario (1) proposes that the PG originates from a $d_{x^2-y^2}$ density wave (DDW) state [54] that competes with superconductivity. The DDW order parameter is of the form

$$y = i \sum_{\mathbf{k}, s} f(\mathbf{k}) \langle c_{\mathbf{k}+\mathbf{Q}, s}^\dagger c_{\mathbf{k}, s} \rangle$$

with $f(\mathbf{k}) = \cos(k_x) - \cos(k_y)$. This state breaks parity and time-reversal symmetry.

Figure 2.13: The four possible ground-state configurations in the loop-current electronic order. Each configuration describes two loop-currents that generate oppositely directed magnetic momenta. If the material condenses into the top configuration it can oscillate back and forth between the top and the other three possible configurations. This results in three possible collective modes of oscillation. From [52].

metry as well as translational by one lattice spacing and rotation by $\pi/2$. The DDW picture successfully explains the d-wave-like PG as well as the properties of experimentally measured quantities such as the spin susceptibility, the superfluid density and the c -axis conductivity.

A different approach takes into account potentially large fluctuations of the classical and quantum phase [55]. A low zero-temperature phase stiffness

$$V_0 = \frac{\hbar n_s^2 a}{4m^*}$$

is characteristic for strong classical phase fluctuations. Since the superfluid density $n_s(0)$ is small in HTSC materials classical phase fluctuations should play an important role for the destruction of the SC state. The importance of quantum phase fluctuations is related to the number-phase uncertainty relation. In the superconducting state the phase coherence implies large relative number fluctuations which may cause strong Coulomb repulsion unless there is adequate screening. In unconventional SC the Coulomb screening is poor and hence quan-

tum phase fluctuations may destroy the SC state even at zero temperature. In general phase fluctuations are assumed to become important if the critical temperature T_c is close to the temperature T_θ^{max} at which phase order would disappear if all disordering effects were ignored. In metals T_θ^{max}/T_c is of the order of 10^5 while it approaches 1 in underdoped HTSC. The importance of phase fluctuations supports the idea that the PG is an instability of the superconducting phase.

A comparably simple explanation for the origin of the PG is given in terms of the RVB theory where it is assumed that spins form singlets. In such a liquid of singlets doped holes can hop in the background and the conductivity spectral weight in the ab plane remains unaffected by singlet formation. This is different for c -axis conductivity when an electron is transported between planes. For an electron to move between planes it is necessary to break a singlet. This requires a finite amount of energy. For photoemission experiments this finite energy required to break the singlet explains the pullback of the leading edge of the spectrum [4].

Pseudogap in the attractive Hubbard Model

Apart from the theoretical concepts discussed above numerical studies have been conducted to investigate the pseudogap in theoretical models. One work of particular importance for the present thesis investigates the formation of a pseudogap state in the Hubbard model. In [56] an attractive Hubbard model with on-site disorder was used to study the effects of disorder on superconductivity. In their Hamiltonian

$$H = -t \sum_{\langle ij \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}) - |U| \sum_i n_{i\uparrow} n_{i\downarrow} + \sum_{i, \sigma} (V_i - \mu) n_{i\sigma} \quad (2.9)$$

the first term describes the kinetic energy from electron hopping where c_i ($c_i^\dagger$) is the destruction (creation) operator for an electron with spin σ at site i of a square lattice. The second term accounts for attractive pairing interaction where $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ is the occupation number operator. In the third term μ is the chemical potential and $V_i \in [-V, V]$ is the random potential at lattice site i that controls the strength of the disorder. It is shown that the distribution $P(\Delta)$ of local pairing amplitudes Δ_i widens with increasing disorder (Figure 2.14 (a)). The authors interpret the inhomogeneous pairing amplitude as indication for the formation of SC islands with large Δ_i . To understand how the energy gap depends on disorder the density of states was plotted for different strengths of disorder (Figure 2.14 (b)). Surprisingly a finite spectral gap was observed even at high disorder where the SC order parameter sharply drops (Figure 2.15). This result suggests the existence of a non-superconducting paired state in highly disordered superconductors.

Figure 2.14: (a) The distribution $P(\Delta)$ of local pairing amplitudes widens with increasing disorder V . From [56]. (b)

Figure 2.15: (a) The distribution $P(\Delta)$ of local pairing amplitudes widens with increasing disorder V . Dependent on the local disorder strength V_i the formation of SC islands with large Δ_i is observed. From [56]. (b)

Chapter 3

The Renormalization Group

Instead of aiming for a complete theoretical description of high- T_c materials this work will be dedicated to investigating the SC-PG transition. To do that we will use experimental findings discussed in the previous chapter to define an appropriate phenomenological model. Based on what is known about underdoped cuprates we will then study how the SC-PG transition can be induced. From understanding the *how* of this transition we hope to elucidate the mechanism at work in the SC-PG transition. Among all available theoretical tools there is one method that is particularly suited to study phase transitions.

The renormalization group (RG) technique in condensed matter physics can be used to determine the long-range order of a given microscopic model. Effectively the RG idea can be compared to a photographer who snaps an anthill at different magnifications. At large magnification he is able to identify details of a single ant such as the length of their antennae or the number of legs. Reducing the zoom will show a number of ants, some of them communicating with each other, others carrying supplies for the colony. Another decrease of focal length will reveal that ants tend to move along tiny roads on and around the anthill. Only at the lowest magnification it becomes clear that the photographer is taking pictures of an anthill. Comparing the series of pictures taken at different magnifications allows the photographer to draw conclusions on how ant colonies are organised.

In condensed matter theory the RG approach acts as magnification glass for couplings. But while the photographer increases the spatial magnification, the momentum-space RG technique we use in our work changes the scale in Fourier space. The magnification in RG terms happens by integrating out modes far from the Fermi vector K_F . Comparison of couplings before and after this transformation allows us to define the RG flow. If the RG flow of a coupling increases with proximity to K_F , the coupling is important at large length scales. On the other hand if the RG flow decreases while approaching K_F , the coupling is irrelevant at the macroscopic level.

3.1 Fixed Points

To identify the coupling that determines the macroscopic appearance of a system an RG flow is defined for each coupling. The microscopic interaction with the strongest RG flow then determines the long range order of the system. But since the RG flow originates from a transformation of scale the flow is a relative measure with respect to some frame of reference. Such points of reference where the RG flow stops are called *fixed points*.

An important property at a fixed point is the scale invariance of the quantum partition function

$$\mathcal{Z} = \text{Tr}(e^{-\beta(H-\mu N)}) . \quad (3.1)$$

This property can be used to determine the fixed point of a system. If $\mathcal{Z}$ is the same before and after rescaling it means that the thermodynamic and transport properties are invariant. In (3.1) H is the Hamiltonian, μ is the chemical potential N is the particle number and $\beta = (k_b T)^{-1}$. The trace Tr can be written in terms of a summation over a complete set of Fock states $\{|n\rangle\}$

$$\mathcal{Z} = \sum_{\{n\}} \langle n | e^{-\beta(H-\mu N)} | n \rangle . \quad (3.2)$$

Fock states describe the configuration of a system in terms of the occupation of its quantum states. In its present form equation (3.2) is not suitable for momentum and energy rescaling. It would be desirable to work with quantum fields that are functions of momentum and energy. Before we obtain the SC fixed point we will transform $\mathcal{Z}$ into its path integral form to obtain a representation in terms of fermionic coherent states.

3.1.1 Path Integral Formalism

The Fock basis states used in (3.2) are not eigenstates of the fermionic creation ($c^\dagger$) and annihilation operator (c). When transforming $\mathcal{Z}$ into a Feynman path integral especially the exponent of the Boltzmann factor will be difficult to handle. As we will see later the calculation will be highly simplified if we introduce the coherent eigenstates $|\psi\rangle$.

Fermionic Coherent States

The eigenstates of the fermionic field operators can be defined as

$$|\psi\rangle = e^{-\sum_i \psi_i c_i^\dagger} |0\rangle \quad (3.3)$$

with the corresponding eigenvalue equations

$$\begin{aligned} c_i|\psi\rangle &= \psi_i|\psi\rangle \\ \langle\psi|c_i^\dagger &= \langle\psi|\bar{\psi}_i. \end{aligned} \quad (3.4)$$

The index i stands for all quantum numbers of the corresponding state e.g. (k, ω, σ) . Similar as the fermionic operators the corresponding eigenvalues have to obey anti-commutativity

$$[\psi_i, \psi_j]_+ = \psi_i\psi_j + \psi_j\psi_i = 0. \quad (3.5)$$

This implies that the eigenvalues ψ_i and $\bar{\psi}_i$ cannot be ordinary numbers. To account for the unconventional behaviour Grassmann numbers were introduced. Contrary to ordinary numbers they obey the integration rules

$$\begin{aligned} \int \psi d\psi &= 1 \\ \int d\psi &= 0. \end{aligned} \quad (3.6)$$

Since each state can only be occupied once the product of two identical eigenvalues has to vanish

$$\psi_i\psi_i = 0. \quad (3.7)$$

Now we want to replace the summation over Fock state in (3.2) by an integration over coherent states. To do that we insert the resolution of identity

$$id = \int \prod_i d\bar{\psi}_i d\psi_i e^{-\sum_i \bar{\psi}_i \psi_i} |\psi\rangle \langle\psi| \quad (3.8)$$

to obtain

$$\mathcal{Z} = \int d(\bar{\psi}, \psi) e^{-\sum_i \bar{\psi}_i \psi_i} \sum_n \langle n|\psi\rangle \langle\psi| e^{-\beta(H-\mu N)} |n\rangle \quad (3.9)$$

with $d(\bar{\psi}, \psi) = \prod_i d\bar{\psi}_i d\psi_i$. Since in the present work all terms within the Hamiltonian H as well as N consist of an even number of operators it is possible to rearrange equation (3.9) according to

$$\mathcal{Z} = \int d(\bar{\psi}, \psi) e^{-\sum_i \bar{\psi}_i \psi_i} \sum_n \langle\psi| e^{-\beta(H-\mu N)} |n\rangle \langle n|\psi\rangle. \quad (3.10)$$

Since the summation $\sum_n$ is over a complete set of Fock-states we finally obtain

$$\mathcal{Z} = \int d(\bar{\psi}, \psi) e^{-\sum_i \bar{\psi}_i \psi_i} \langle\psi| e^{-\beta(H-\mu N)} |\psi\rangle. \quad (3.11)$$

This defines the quantum partition function in terms of coherent states. However, the exponent $\beta(H-\mu N)$ still contains the Fock space operators c and $c^\dagger$. We want

to replace them by eigenvalues of the coherent states as well. To do that we split the matrix element in (3.11) into infinitesimal slices. At each intermediate step we sum over all possible configurations of the system and absorb this information into the Grassmann eigenvalues. We therefore write

$$\langle \psi | e^{-\beta(H-\mu N)} | \psi \rangle = \langle \psi | \wedge e^{-\frac{\beta}{N}(H-\mu N)} \wedge \dots \wedge e^{-\frac{\beta}{N}(H-\mu N)} \wedge | \psi \rangle \quad (3.12)$$

and at each position $\wedge$ we insert the resolution of identity (3.8) with an appropriate index n . Expression (3.11) then takes the form

$$\mathcal{Z} = \int \prod_{n=1}^{\tilde{N}} d(\bar{\psi}^n, \psi^n) e^{-\frac{\beta}{N} \sum_{n=0}^{\tilde{N}-1} [\frac{N}{\beta} (\bar{\psi}^n - \bar{\psi}^{n+1}) \psi^n + H(\bar{\psi}^{n+1}, \psi^n) - \mu N (\bar{\psi}^{n+1}, \psi^n)]} . \quad (3.13)$$

Here the creation ($c^\dagger$) and annihilation (c) operators were replaced by their corresponding eigenvalues according to

$$\begin{aligned} e^{c_k} e^{-\psi_k c_k^\dagger} |0\rangle &= (1 + c_k) (1 - \psi_k c_k^\dagger) |0\rangle \\ &= (1 - \psi_k c_k^\dagger - c_k \psi_k c_k^\dagger) |0\rangle \end{aligned} \quad (3.14)$$

$$= (1 - \psi_k c_k^\dagger + \psi_k - \psi_k^2 c_k^\dagger) |0\rangle \quad (3.15)$$

$$= e^{\psi_k} e^{-\psi_k c_k^\dagger} |0\rangle . \quad (3.16)$$

In (3.14) we have made use of the anticommutator relation for fermion operators and in expression (3.15) we have included the vanishing term $\psi_k^2 c_k^\dagger$ to complete the Taylor series expansion. Next we increase the number of 'time' slices by letting $\tilde{N} \rightarrow \infty$. Then the first term in the exponent in (3.13) can be written as

$$(\bar{\psi}^n - \bar{\psi}^{n+1}) \psi^n \rightarrow \bar{\psi} \partial_\tau \psi \quad (3.17)$$

and the summation over n can be interpreted as integral over the new variable τ . We then obtain the field representation which turns out to be equivalent to the action of the system

$$\begin{aligned} S[\bar{\psi}, \psi] &= \int_0^\beta d\tau \int_{-\lambda}^\lambda dk [\bar{\psi}(k) \partial_\tau \psi(k) + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi)] \\ &= \int_0^\beta d\tau \mathcal{L}(\bar{\psi}, \psi) . \end{aligned} \quad (3.18)$$

We see that the particular choice of coherent eigenstates allows to replace c and $c^\dagger$ by Grassmann numbers. For convenience the τ -integration in (3.18) can be replaced by a summation over Matsubara frequencies. This is done by Fourier transforming according to

$$\psi(\tau) = \frac{1}{\beta} \sum_{\omega_n} \psi_n e^{-i\omega_n \tau} \quad (3.19)$$

where

$$\omega_n = \begin{cases} 2n\pi k_B T, & \text{bosons} \\ (2n+1)\pi k_B T, & \text{fermions} \end{cases} \quad n \in \mathbb{Z} \quad (3.20)$$

are known as the Matsubara frequencies. Equation (3.18) then becomes

$$S[\bar{\psi}, \psi] = \int_{-\infty}^{\infty} d\omega \int_{-\lambda}^{\lambda} dk \left[-i\omega \bar{\psi}(k) \psi(k) + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi) \right] \quad (3.21)$$

where the summation over Matsubara frequencies was replaced by an integral. The quantum partition function in its path integral representation is of the form

$$\mathcal{Z} = \int \mathcal{D}[\psi] e^{-S[\psi]} . \quad (3.22)$$

Here $\mathcal{D}(\psi) = \prod_{n=1}^{\hat{N}} d(\bar{\psi}^n, \psi^n)$ denotes the integral over all possible configurations of the Grassman fields at all $\hat{N}$ time slices.

3.1.2 Effective Action

To obtain the fixed point of a theory we require the quantum partition function be invariant under RG transformations. From (3.22) we conclude that S must be invariant under RG transformations.

As discussed in the introduction the RG technique reduces the system to its long-range couplings by integrating out short-range fluctuations. To do that we will split the action into its long- and short-range components. In terms of momenta this means that we have to introduce an artificial cutoff between modes near and far from K_F . For this step it is helpful to shift the coordinates $k = K - K_F$ such that k determines the distance from K_F . We can then separate the fields into slow ($\psi_{<}$) and fast components ($\psi_{>}$)

$$\begin{aligned} \psi_{<} &= \psi(k) & |k| < \lambda/s \\ \psi_{>} &= \psi(k) & \lambda/s < |k| < \lambda . \end{aligned}$$

Here λ denotes the momentum cutoff imposed by the lattice constant and s is the artificial scaling parameter to distinguish between fast and slow modes.

For a lattice model such as the Hubbard or $t - J$ model the Hamiltonian usually consists of two parts. One term proportional to ψ^2 that describes the free hopping of charge carriers across the lattice ($\mathcal{H}_0$) and one interacting part, proportional to ψ^n with $n > 2$, that describes some sort of particle interaction ($\mathcal{H}_I$). It is important to note that due to momentum and energy conservation S_0 can only contain an integration over one momentum and one frequency variable. For terms with an order of fields $n > 2$ there are n momentum and energy integration variables while conservation is guaranteed by delta functions.

An example will illustrate the details more clearly. We imagine two action terms of the form

$$\begin{aligned} S_0 &\propto \int dk \bar{\psi}(k) \psi(k) \\ S_I &\propto \int \prod_i^4 dk_i \bar{\psi}(k_1) \bar{\psi}(k_2) \psi(k_3) \psi(k_4) \delta(k_1 + k_2 - k_3 - k_4) . \end{aligned}$$

If we split the momentum integration over slow and fast field components S_0 reads

$$S_0 \propto \int_{|k| < \lambda/s} dk \bar{\psi}_<(k) \psi_<(k) + \int_{\lambda/s < |k| < \lambda} dk \bar{\psi}_>(k) \psi_>(k) \quad (3.23)$$

where λ/s denotes the boundary of the small annulus around K_F that defines the location of slow modes. The two terms describe slow and fast field components and there is no mixing. On the other hand if we separate the integrations for S_I we see that a large number of mixed terms is possible

$$S_I \propto \int \prod_i^4 dk_i \bar{\psi}_<(k_1) \bar{\psi}_<(k_2) \psi_>(k_3) \psi_>(k_4) \delta(k_1 + k_2 - k_3 - k_4) \quad (3.24)$$

$$+ \int \prod_i^4 dk_i \bar{\psi}_>(k_1) \bar{\psi}_>(k_2) \psi_<(k_3) \psi_>(k_4) \delta(k_1 + k_2 - k_3 - k_4) \quad (3.25)$$

$$+ \dots \quad (3.26)$$

We can then write down the most general form for the action in terms of slow and fast fields

$$S[\psi_<, \psi_>] = S_0[\psi_<] + S_0[\psi_>] + S_I[\psi_<, \psi_>] . \quad (3.27)$$

Here $S_0[\psi_<]$ contains all terms that depend on slow modes only, $S_0[\psi_>]$ contains fast ones only and $S_I[\psi_<, \psi_>]$ keeps those terms where slow and fast fields are mixed.

With the RG procedure we will integrate out all contributions from fast field components. From (3.27) it is clear that especially the mixed terms will complicate this intention. However, we will now try to single out the slow modes from the partition function

$$\mathcal{Z} = \int \mathcal{D}[\psi_<] e^{S_0[\psi_<]} \int \mathcal{D}[\psi_>] e^{S_0[\psi_>]} e^{S_I[\psi_>, \psi_<]} \quad (3.28)$$

following the general approach described in [57]. We then define an effective action $S'[\psi_<]$ such that it depends on slow modes only

$$e^{S'[\psi_<]} = e^{S_0[\psi_<]} \int \mathcal{D}[\psi_>] e^{S_0[\psi_>]} e^{S_I[\psi_>, \psi_<]} . \quad (3.29)$$

Next we want to find a more useful form for the integration over fast fields. We can manipulate the integration in 3.29 to form a n-point or Greens function of the form

$$\langle \dots \rangle = \frac{\int \mathcal{D}[\psi](\dots)e^{S[\psi]}}{\int \mathcal{D}[\psi]e^{S[\psi]}} . \quad (3.30)$$

To do that we substitute the quantum partition function

$$\mathcal{Z}_{0>} = \int \mathcal{D}[\psi_{>}]e^{S_0[\psi_{>}]} \quad (3.31)$$

into S' . We note that the path integral in $\mathcal{Z}_0$ is taken with respect to fast modes with the action S_0 . We can then rearrange terms in (3.29) to find

$$\begin{aligned} e^{S'[\psi_{<}]} &= e^{S_0(\psi_{<})} \int \mathcal{D}[\psi_{>}]e^{S_0[\psi_{>}]}e^{S_I[\psi_{>},\psi_{<}]} \\ &= e^{S_0[\psi_{<}]} \frac{\int \mathcal{D}[\psi_{>}]e^{S_0[\psi_{>}]}e^{S_I[\psi_{>},\psi_{<}]}}{\int \mathcal{D}[\psi_{>}]e^{S_0[\psi_{>}]}} \int \mathcal{D}[\psi_{>}]e^{S_0[\psi_{>}]} \\ &= e^{S_0[\psi_{<}]} \left\langle e^{S_I[\psi_{>},\psi_{<}]} \right\rangle_{>0} \mathcal{Z}_{0>} . \end{aligned} \quad (3.32)$$

In the limit of large length scales $\mathcal{Z}_{0>}$ will be not important and merely add a constant to the effective action. The average $\langle \rangle_{>0}$ here is taken with respect to the fast modes with the action S_0 . This term integrates out or averages over short-range fluctuations. The RG theory assumes that once these fluctuations are averaged over the actual long range behaviour of the system is revealed. An exemplary introduction on how to calculate Grassmann path integrals such as $\langle \rangle_{>0}$ is given in Appendix B.

As discussed in the sections to come the perturbative treatment of the average $\langle \rangle_{>0}$ results in an infinite series of quantum corrections. Higher orders of this series can only be ignored if the coupling potential is small. The effective action given in (3.32) can therefore only be used for free electron systems subject to weak perturbations. To work with a superconducting system it will be necessary to define an appropriate effective action.

3.1.3 Three RG steps to find Fixed Points

After the introduction of the effective action S' the RG scale transformation can be performed easily. According to (3.32) we will split the fixed point calculation and first only work with those terms that contain slow modes. We will deal with the fast terms contained in the averages later. In physical terms this means that we will calculate the fixed point with respect to the non-interacting part of the action.

The first part of the procedure is the separation into slow and fast field components as discussed in the previous section. An illustration of this initial step is given in Figure 3.1 (a). The fast modes lie within the red region while the slow modes are confined to the small annulus (blue) around K_F . Contributions from fast modes are contained within the average $\langle \rangle_{>0}$ and will be integrated over. This reduces the momentum range to values from within $K_F \pm \lambda/s$.

But from a simple rescaling operation we do not expect a change in the domain of the rescaled variable i.e. the kinematic range before and after the scale transformation should be the same. Otherwise it is not possible to compare couplings before and after the RG transformation. In the second step the previous k - and ω -range is restored by rescaling the variables according to

$$k' = ks \quad \text{and} \quad \omega' = \omega s . \quad (3.33)$$

This rescaling of the kinematic range is shown in Figure 3.1 (b). By introducing the scaling factor s the rescaled momentum k' again takes on all values from the interval $[0, \lambda]$ and therefore covers the same kinematic range as before mode separation.

After mode separation and momentum and frequency rescaling the transformed free part of the effective action is of the form

$$S'_0[\bar{\psi}_<, \psi_<] = \int \prod_{ij} \frac{dk'_i d\omega'_j}{s^2} \times \left[-i \frac{\omega'_n}{s} \bar{\psi}_<(\frac{k'_m}{s}, \frac{\omega'_n}{s}) \psi_<(\frac{k'_m}{s}, \frac{\omega'_n}{s}) + H_0(\bar{\psi}_<, \psi_<) - \mu N(\bar{\psi}_<, \psi_<) \right] \quad (3.34)$$

where the respective arguments in H_0 and N as well as the factor $Z_{0>}$ have been dropped for convenience. As we can see the scaling factor s entered the equation and denotes that all variables and fields are rescaled versions of the original variables. The final step to obtain the fixed point with respect to S_0 is to make equation (3.34) independent of the scaling factor s . To do that it is necessary to rescale the fields according to

$$\psi'(k', \omega') = \eta \psi_<(\frac{k'}{s}, \frac{\omega'}{s}) . \quad (3.35)$$

Here the factor η will absorb all orders of s that appear as a result of the RG transformation. We then obtain for the RG transformed free part of the effective action

$$S'_0[\bar{\psi}', \psi'] = \int \prod_{ij} dk'_i d\omega'_j \times \left[-i \omega'_n \bar{\psi}'(k'_m, \omega'_n) \psi'(k'_m, \omega'_n) + H_0(\bar{\psi}', \psi') - \mu N(\bar{\psi}', \psi') \right] . \quad (3.36)$$

We note that the new fields ψ' are rescaled versions of the old fields ψ times the scaling factor $\eta = s^x$. Clearly the free part of the effective action has the same form as before the RG transformation. Therefore the quantum partition function and with it the physics remain scale invariant. We have therefore identified the non-interacting fixed point. Next we will use the scaling relation (3.35) to determine the RG flow caused by the remaining interacting part S_I with respect to S_0 .

Figure 3.1: (a) Shown is a segment of the Fermi surface (blue line) and the corresponding Fermi vector K_F . Within the cutoff region restricted by λ a thin annulus (blue) that contains the slow modes $\psi_<$ is defined. In the first step of the RG procedure momenta within the red region are integrated out i.e. contributions from this k -space region are averaged over and only contribute a constant factor. To compare couplings before and after integrating out fast components, it is necessary to rescale the momentum range back to its original kinematic scale. This is illustrated in (b) where the threshold of slow modes is expanded (red arrows indicate the rescaling $k' = ks$) to range up to the cutoff λ . The new variable k' covers the same kinematic range as before integrating out modes. Rescaling of fields $\psi' = \zeta \psi_<$ finally allows to determine the RG flow of a coupling.

3.2 Obtaining the RG flow

In the previous section we defined the fixed point of the non-interacting part of the action. Any RG flow obtained will be measured with respect to the defined fixed point.

We will now discuss the general treatment to determine the RG flow caused by the perturbation H_I . We recall that any coupling within H_I has to be small.

If the perturbation generates a relevant flow the previously found fixed point is unstable and the long range order of the system is determined by the interaction described by H_I . If we instead find an irrelevant flow, the system remains at the present fixed point and the phase of the system is then dominated by H_0 . If a marginal flow is found it is necessary to calculate higher orders of the yet to be discussed cumulant expansion (see section 3.2.2).

In general H_I contains more than two field operators. For example the Coulomb interaction between two spinless electrons can be written as

$$H_C = \frac{C}{N_d} \sum_{\langle ij \rangle} c_i^\dagger c_i c_j^\dagger c_j \quad (3.37)$$

where $\langle ij \rangle$ denotes summation over nearest neighbors and N_d accounts for double counting. As discussed in section 3.1.2 mode separation will in general mix slow and fast field components if the order of fields is $n > 2$. Mode separation for the interacting part will therefore create the following terms

$$S_I[\bar{\psi}, \psi] = S_I[\bar{\psi}_<, \psi_<] + S_I[\bar{\psi}_>, \psi_>] + S_I[\bar{\psi}_<, \bar{\psi}_>, \psi_<, \psi_>] . \quad (3.38)$$

All three terms in (3.38) have to be evaluated separately. The first term, also known as tree level and the second are the easiest to calculate. The first because it does not contain any mixed terms and the second because it can be ignored as it does not depend on slow modes at all i.e. it makes a constant contribution. For the mixed contribution we will have to calculate averages of the form found in (3.32).

3.2.1 Tree Level

Although in (3.32) we used the general expression $S[\psi_<, \psi_>]$ to account for all mixed terms we can see from (3.38) that there is one term that depends on slow modes only. We can deal with this term almost the same way as we did in the fixed point calculation. No averaging over fast fields is necessary. To obtain the contribution to the RG flow at tree level we use the usual three RG steps. After we separate modes and rescale momenta k and frequency ω according to (3.33) we obtain

$$\delta S_I[\bar{\psi}_<, \psi_<] = \int \prod_{ij} \frac{dk'_i d\omega'_j}{s^2} H_I(\bar{\psi}_<, \psi_<) . \quad (3.39)$$

Instead of choosing a field rescaling relation that makes the perturbation scale invariant we will insert the field rescaling relation obtained from the fixed point calculation (3.35). This will show whether δS_I becomes more or less important as we approach K_F . When we insert (3.35) into (3.39) we obtain

$$\delta S'_I[\bar{\psi}', \psi'] = \int \prod_{ij} dk'_i d\omega'_j \bar{\eta} H_I(\bar{\psi}', \psi') . \quad (3.40)$$

Here $\bar{\eta} = s^y$ contains the remaining orders of the scaling factor s i.e. y can be non-zero. The interaction term H_I contains a coupling potential V which is usually a function of k and ω . To analyze whether $V(k'/s, \omega'/s)$ increases or decreases with proximity to K_F the coupling potential is expanded in a power series

$$V\left(\frac{k'}{s}, \frac{\omega'}{s}\right) = V_{00} + V_{10} \frac{k'}{s} + V_{01} \frac{i\omega'}{s} + \dots \quad (3.41)$$

For the quantum partition function to remain invariant under the RG transformation we have to introduce a rescaled version of the coupling potential to absorb all remaining scaling factors within $\bar{\eta}$. We identify the rescaled interaction potential as

$$V'(k', \omega') = \bar{\eta} V\left(\frac{k'}{s}, \frac{\omega'}{s}\right) = s^y (V_{00} + V_{10} \frac{k'}{s} + V_{01} \frac{i\omega'}{s} + \dots) \quad (3.42)$$

A relevant flow is generated if $y > 0$. In that case the fixed point of the non-interacting part S_0 is unstable towards the perturbation S_I . The long-range order of the system will then be determined by the microscopic interaction within S_I . If on the other hand $y < 0$ the RG flow generated by the perturbation is irrelevant and the system remains at its current fixed point. If $y = 0$ higher orders of the cumulant expansion (section 3.2.2) are used to determine the relevance of the flow.

It is also possible to determine the differential form of the RG flow. This is done by setting $s = 1 + t$ where $t \ll 1$ which is equivalent to an infinitesimal rescaling step. Assuming that $y = n$ we rearrange the binomial series according to

$$\begin{aligned} V'(s_0 + t) &= (1 + t)^n V(s_0) \\ \frac{V'(s_0 + t) - V(s_0)}{t} &= \left(nV(s_0) + tV(s_0) \frac{n(n-1)}{2} + \dots \right) \end{aligned} \quad (3.43)$$

In the limit $\lim_{t \rightarrow 0}$ we find the differential RG flow for the coupling potential at the unperturbed fixed point

$$\frac{dV(s_0)}{dt} = nV(s_0) \quad (3.44)$$

Depending whether $n > 0$ or $n < 0$ the coupling potential grows or decays proportionally to V and will therefore become relevant or irrelevant for the macroscopic appearance of the system.

3.2.2 Loop Corrections

At tree level any term where slow and fast field components are mixed were ignored. These mixed terms may contribute quantum corrections to the expression

found at tree level. To evaluate these contributions path integrals emerging from

$$\left\langle e^{S_I[\psi_>, \psi_<]} \right\rangle_{>0} \quad (3.45)$$

have to be solved. Before we attempt to calculate such path integrals we perform a cumulant expansion. This will simplify the calculation.

Cumulant Expansion

Expression (3.45) can be rewritten in terms of its Taylor series expansion

$$\left\langle e^{S_I[\psi_>, \psi_<]} \right\rangle_{>0} = \sum_{n=0}^{\infty} \frac{1}{n!} \langle S_I^n \rangle_{>0} . \quad (3.46)$$

With the relation

$$\ln(1+x) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} x^n$$

it is possible to rearrange the right side of expression (3.46) according to

$$\begin{aligned} \ln \sum_{n=0}^{\infty} \frac{1}{n!} \langle S_I^n \rangle_{>0} &= \ln \left(1 + \langle S_I \rangle_{>0} + \frac{1}{2} \langle S_I^2 \rangle_{>0} + \dots \right) \\ &= \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} \left(\langle S_I \rangle_{>0} + \frac{1}{2} \langle S_I^2 \rangle_{>0} + \dots \right)^n . \end{aligned} \quad (3.47)$$

After exponentiating the average can then be written as

$$\left\langle e^{S_I[\psi_>, \psi_<]} \right\rangle_{>0} = e^{\langle S_I \rangle + \frac{1}{2} [\langle S_I^2 \rangle - \langle S_I \rangle^2] + \dots} . \quad (3.48)$$

Here the first term in the exponent ($\langle S_I \rangle$) is the tree level term. In this new expression the average over the exponential function was replaced by summations over averages of different orders of S_I . To further simplify expression (3.48) we can make use of the connected cluster theorem.

To use this theorem we have to distinguish between connected and disconnected vertices. Whenever the average is taken over two fields the two single lines are connected to become one internal line. If the average is taken over fields from two different vertices the internal line connects the two vertices to form a connected graph. A disconnected graph is formed if at least one vertex remains disconnected from all other vertices (Figure 3.2 (b)). We therefore call a graph connected if all vertices are connected directly or indirectly to each other (Figure 3.3).

We then note that $\langle S_I^2 \rangle$ produces all possible combinations of connected and disconnected graphs. The term $\langle S_I \rangle^2$ on the other hand only contains averages

over fields that belong to the same vertex i.e. only disconnected graphs are generated. It is then easy to see that in expression $\langle S_I^2 \rangle - \langle S_I \rangle^2$ only the connected graphs do not vanish. Therefore, instead of performing all possible averages we only have to consider the connected graphs at each order.

But there are even more graphs that can be ignored. By taking the average over fast modes a large number of loop diagrams is generated. However, not all of them are corrections for the vertex S_I . Only those loop diagrams that resemble the external structure of S_I , i.e. have the same number of external lines are valid quantum corrections. Those loop diagrams that use the S_I vertex as building blocks but do not resemble the external structure of S_I describe different physical processes and can be ignored.

To obtain the quantum correction emerging from a loop diagram it is necessary to calculate Grassmann path integrals of the form

$$\langle \dots \rangle = \frac{\int \mathcal{D}(\bar{\psi}, \psi) (\dots) e^{S[\bar{\psi}, \psi]}}{\int \mathcal{D}(\bar{\psi}, \psi) e^{S[\bar{\psi}, \psi]}}. \quad (3.49)$$

For a particular perturbation δS_I the first order loop correction is of the form

$$\langle \delta S_I^2 \rangle_{>0} = \frac{\int \mathcal{D}(\bar{\psi}_>, \psi_>) \delta S_I^2[\bar{\psi}_>, \psi_>, \bar{\psi}_<, \psi_<] e^{S_0[\bar{\psi}_>, \psi_>]}}{\int \mathcal{D}(\bar{\psi}_>, \psi_>) e^{S_0[\bar{\psi}_>, \psi_>]}}. \quad (3.50)$$

The slow and fast modes in $\delta S_I^2[\bar{\psi}_>, \psi_>, \bar{\psi}_<, \psi_<]$ have to be chosen such that the external lines resemble the original vertex δS_I . The path integral is then only calculated with respect to fast modes.

The action itself contains integrations over momentum k and Matsubara frequency ω . The numerator in equation (3.50) can then in general be written as

$$\left[\int_{|k| < \lambda/s} \int_{-\infty}^{\infty} dk d\omega \delta S_< \right] \left[\int_{\lambda/s}^{\lambda} \int_{-\infty}^{\infty} dk d\omega \int \mathcal{D}(\bar{\psi}_>, \psi_>) \delta S_> e^{S_0[\bar{\psi}_>, \psi_>]} \right]. \quad (3.51)$$

Here $\delta S_<$ denotes terms that contain slow modes only while $\delta S_>$ consists of fast modes. It is important that $\delta S_<$ resembles the same structure as the original vertex δS .

To truncate the infinite summation in (3.48) it is necessary that higher order loop diagrams vanish. In the weak coupling limit the perturbation is assumed to be small. Since loop diagrams of n -th order are proportional to the coupling potential at n -th order, the sum in (3.48) can be truncated.

Figure 3.2: (a) The initial vertex S_I . Corrections from the second order cumulant expansion must have the same number (4) of external legs. (b) A disconnected graph that originates from the expression $\langle S_I \rangle^2$ in the cumulant expansion. The average is taken over two identical vertices of the S_I type and loops are constructed by connecting two lines from the same vertex.

Figure 3.3: A connected graph. This diagram originates from the expression $\langle S_I^2 \rangle$ of the cumulant expansion. By integrating over two fields from different vertices the corresponding lines are connected. A loop is formed if two such connection exist between two vertices. The average $\langle S_I^2 \rangle$ also produces graphs of the form of Figure 3.2. Therefore all disconnected graphs vanish and only connected graphs account for corrections of S_I .

Chapter 4

The Origin of the PG

In this chapter we are going to investigate the origin of the PG phase found in underdoped cuprates and strongly disordered conventional SC. In particular we want to understand whether the pseudo energy gap is best explained with a single- or a two-gap scenario.

In section 4.1 we start our analysis and introduce the initial model. After we obtain the SC fixed point (section 4.4) we introduce perturbations (section 4.7) to induce the SC-PG phase transition. The choice of perturbations is based on our discussion of experimental findings from chapter 2. Using the RG scheme (see chapter 3) we identify the most relevant perturbation that induces the SC-PG transition. Finally we analyze whether the found perturbation supports a single- or a two-gap scenario.

4.1 Details of the Model

As shown in [45; 46] a PG phase may exist in strongly disordered thin film conventional superconductors. These experiments indicate the presence of localized Cooper pairs after the disorder induced superconductor-insulator phase transition. The disorder in thin film conventional SC has similar consequences like the reduction of hole doping in HTSC materials. While disorder induces a transition towards an insulator, reduced hole-doping in HTSC materials results in a Mott insulating state due to strong on-site Coulomb repulsion. In both cases the hopping of free charge carriers is strongly suppressed and charge carriers are localized.

The fact that a PG phase may exist in HTSC as well as in two-dimensional BCS-like SC gives rise to the hypothesis that the actual pairing mechanism behind SC may not be important to understand the PG phase. This implies that the PG phase in conventional and unconventional SC may originate from the same

microscopic mechanism. To study the transition from a SC to the PG phase we may then start from a generalized description of the SC state.

In a previous theoretical study of the PG phase the attractive Hubbard Hamiltonian was used [56]. This type of model has a SC state. The analysis in [56] shows that in the strongly disordered regime the SC state is destroyed while the SC energy gap persists; a behavior expected for a PG-like state.

In the present work we will use a reduced attractive Hubbard model

$$H = \sum_K E(K) c_K^\dagger c_K + \sum_{KL} V(KL) c_K^\dagger c_{-K}^\dagger c_L c_{-L} \quad (4.1)$$

where only fermions with pairwise antiparallel momenta interact. This restriction of the interaction term is reasonable and useful when we want to define the SC fixed point. Since in hole-doped cuprates it is assumed that charge transport is the result of mobile holes we will refer to holes rather than electrons from now on. We will use the same nomenclature as for fermion operators. Then the Hamiltonian (4.1) describes the kinetic energy of holes that move across a lattice subject to some attractive pairing potential $V > 0$. The operator $c_K^\dagger$ (c_K) creates (annihilates) a hole in a state with momentum $\hbar K$ and the dispersion relation of free holes

$$E(K) = -\cos(K_x) - \cos(K_y) . \quad (4.2)$$

The second term in 4.1 describes the scattering of paired holes with initial momenta $(K, -K)$ and final momenta $(L, -L)$. For simplicity we assume that the pairing potential is of s -wave form. This is reasonable if the SC-PG transition is a general feature found in conventional as well as unconventional SC as suggested by experiments. The discussion of a d -wave like gap mainly modifies the expansion of the pairing potential at the SC fixed point. The d -wave case will not be discussed in the present work.

4.2 Strong Correlation Effects

To induce the SC-PG phase transition we want to introduce an interaction that destroys the SC state. As discussed we assume that the underdoped region between the SC and the MI state suffers from a reduced number of free lattice sites. Cooper pairs may then find themselves in a strongly repulsive environment with a strongly-diminished hopping phase space. In such a scenario a paired hole will not only experience the pairing force that binds it into a Cooper pair, but also a repulsive force caused by occupied nearest neighbor sites. A similar scenario can be expected in strongly disordered conventional SC before the transition towards an insulator.

Figure 4.1: Illustration of Cooper pair (purple) hopping in strongly correlated environment. The pairwise hopping of holes (blue) is obstructed by a lack of free lattice sites (red). The pair experiences strong Coulomb repulsion (red region) that prevents the pair from hopping along the indicated path (arrows). Instead the paired holes hop to alternative free nearest neighbor lattice sites (white). This may disrupt the pairing and eventually may cause the Cooper pair to break up.

The strong correlation of paired charge carriers with their environment gives rise to two possible scenarios. In the first scenario the path of either one or both paired charge carriers can be obstructed by a lack of free lattice sites (Figure 4.1). Then the respective hole experiences an interaction with its local environment. In strongly correlated or strongly disordered materials this kind of interaction may cause the pair to break up.

In a second scenario where paired holes also interact with their local environment the pair may undergo recombination scattering. In this process both holes also experience individual scattering events but are scattered such that the pairwise motion of the pair is conserved (Figure 4.2).

Intuitively, our calculation can therefore have one of two possible conclusions. If our analysis shows that Cooper pairs tend to break due to strong on-site repulsion it means that another pairing mechanism unrelated to SC must be responsible for the observed energy gap of the PG phase. If on the other hand the SC pairing mechanism persists while the SC state is destroyed this would be consistent with the pre-formed pairs scenario.

Figure 4.2: As with Figure 4.1 a Cooper pair experiences strong Coulomb repulsion. But instead of disrupting the pairing, the pair remains intact but changes its direction of motion. In this scenario both holes experience an interaction with the respective environment but remain paired.

4.3 Implementing the RG approach

Before using the RG scheme for our problem it is necessary to adjust some parts of the general approach discussed in section 3. When we first studied the RG method we introduced an effective action to simplify the fixed point calculation. Due to mixing of slow and fast field components we separated the action into quadratic (S_0) and quartic (S_I) terms. We were then able to perform the fixed point calculation with respect to the non-interacting part S_0 . Later we treated the interaction term S_I perturbatively and identified the corresponding RG flow. This means that expression (3.32) can only be used to obtain the fixed point of the free term while interactions are treated perturbatively and generate a RG flow.

For our present problem this approach is not useful. To obtain the SC fixed point we want to include the interaction term into the fixed point calculation and not treat it as a perturbation. To do that we need to obtain an effective action that allows us to define a fixed point where pairing interactions are already present. Therefore we adjust the derivation in section 3.1.2.

4.3.1 SC Effective Action

In section 3.1.2 we separated the action into terms where slow and fast fields were mixed and those where the slow and fast fields do not mix. We will do the same

now but look a bit more carefully at the interaction part of the SC Hamiltonian (4.1). As usual the hopping term S_0 consists of quadratic terms i.e. mixing is impossible. For the interaction term on the other hand we can write after mode separation

$$S_I[\psi] = S_I[\psi_<] + S_I[\psi_>] + S_I[\psi_<, \psi_>] . \quad (4.3)$$

Here the first terms, $S_I[\psi_<]$ and $S_I[\psi_>]$ consist of slow and fast modes respectively and $S_I[\psi_<, \psi_>]$ contains fully mixed terms only. We will now use this refined expression to replace the generalized mixed term in (3.28). After rearranging terms we obtain

$$\mathcal{Z} = \int \mathcal{D}[\psi_<] e^{S_0[\psi_<] + S_I[\psi_<]} \int \mathcal{D}[\psi_>] e^{S_0[\psi_>] + S_I[\psi_>]} e^{S_I[\psi_>, \psi_<]} . \quad (4.4)$$

Again we substitute the partition function $\mathcal{Z}_>$ so that we can take the average over fast fields. With the same manipulations as in (3.32)

$$\begin{aligned} \mathcal{Z} &= \int \mathcal{D}[\psi_<] e^{S_0[\psi_<] + S_I[\psi_<]} \frac{\int \mathcal{D}[\psi_>] e^{S_0[\psi_>] + S_I[\psi_>]} e^{S_I[\psi_>, \psi_<]}}{\int \mathcal{D}[\psi_>] e^{S_0[\psi_>] + S_I[\psi_>]}} \mathcal{Z}_> \\ &= \int \mathcal{D}[\psi_<] e^{S_0[\psi_<] + S_I[\psi_<]} \langle e^{S_I[\psi_>, \psi_<]} \rangle_> \mathcal{Z}_> \end{aligned} \quad (4.5)$$

we finally obtain a slightly different expression for the effective action

$$e^{\tilde{S}'[\psi_<]} = e^{S_0[\psi_<] + S_I[\psi_<]} \langle e^{S_I[\psi_>, \psi_<]} \rangle_> \mathcal{Z}_> . \quad (4.6)$$

The average $\langle \rangle_>$ is now taken with respect to fast modes but with the action $S_0 + S_I$. The term $\mathcal{Z}_>$ will again contribute a constant that does not depend on $\psi_<$ and can therefore be ignored. The most important change comes from the exponential in front of the average. We manipulated the effective action in a way that the free as well as the interaction term depend on slow modes only. This allows us to perform the fixed point study with respect to the full action $S = S_0 + S_I$.

At the moment this neat manipulation appears to be advantageous over expression (3.32). But as we will see later, once we introduce perturbations for the SC fixed point the newly defined averages $\langle \rangle_>$ will emerge to be problematic to solve. A comprehensive discussion on this problem will be given in Appendix B.

4.4 Superconducting Fixed Point at Tree Level

To obtain the SC fixed point we will work with the Hamiltonian defined in equation (4.1). The first step is to replace field operators by their corresponding eigenvalues according to section 3.1.1. This gives the action of the system

$$S[\bar{\psi}, \psi] = \int_0^\beta d\tau \left[\bar{\psi} \partial_\tau \psi + H(\bar{\psi}, \psi) - \mu N(\bar{\psi}, \psi) \right] = S_0[\bar{\psi}, \psi] + S_{\text{SC}}[\bar{\psi}, \psi] . \quad (4.7)$$

The action contains a quadratic term (S_0) describing free hopping and a quartic term (S_{SC}) accounting for pairing hole-hole interaction. Combining the results from the previous sections we can write down the corresponding effective action after mode separation as

$$\begin{aligned}\bar{S}'[\psi_<] &= S_0[\psi_<] + S_{\text{SC}}[\psi_<] + \langle S_{\text{SC}}[\psi_<, \psi_>] \rangle_> \\ &+ \frac{1}{2} [\langle S_{\text{SC}}^2[\psi_<, \psi_>] \rangle_> - \langle S_{\text{SC}}[\psi_<, \psi_>] \rangle_>^2] + \dots\end{aligned}\quad (4.8)$$

To obtain the fixed point we look at those terms that depend on the slow modes only. Since there is no mixing and averaging involved these are easy to handle. We find for $S_0[\psi_<]$ and $S_{\text{SC}}[\psi_<]$

$$S_0[\psi_<] = \int_{\frac{1}{s}} \bar{\psi}_{(1,1)}^< (i\omega_1 - E(K_F + k_1) - \mu) \psi_{(1,1)}^< \quad (4.9)$$

$$S_{\text{SC}}[\psi_<] = \int_{\frac{1}{s}, \frac{1}{s}} V_{(12)} \bar{\psi}_{(1,1)}^< \bar{\psi}_{(-1,2)}^< \psi_{(2,3)}^< \psi_{(-2,4)}^< \quad (4.10)$$

with

$$\int_{\frac{1}{s}} = \frac{1}{(2\pi)^2} \int_{-\frac{\lambda}{s}}^{\frac{\lambda}{s}} K_F dk_1 \int_{-\infty}^{\infty} d\omega_1 \int_0^{2\pi} d\theta_1 \quad (4.11)$$

$$\int_{\frac{1}{s}, \frac{1}{s}} = \frac{1}{(2\pi)^6} \int_{-\frac{\lambda}{s}}^{\frac{\lambda}{s}} K_F^2 \prod_{i=1}^2 dk_i d\theta_i \int_{-\infty}^{\infty} \prod_{j=1}^4 d\omega_j \delta_\omega \quad (4.12)$$

Here and where it is obvious we replace the fields and the potential by short-hand notations of the form

$$\begin{aligned}\psi(k_i, \theta_i, \omega_j) &\rightarrow \psi_{(i,j)} \\ V(k_i, \omega_j) &\rightarrow V_{(i,j)}\end{aligned}$$

In equation (4.9) $E(K_F + k)$ denotes the dispersion relation of hopping holes, ω is the Matsubara frequency and μ is the chemical potential. For the small annulus around K_F we can always linearize the dispersion relation of hopping holes to obtain

$$E(K_F + k) - \mu \propto \mathcal{N}(K_F)k \quad (4.13)$$

where $\mathcal{N}(K_F)$ denotes a prefactor that depends on the density of holes and thus on the Fermi wavevector K_F . The δ_ω -functional maintains energy conservation and is of the form

$$\delta_\omega = \delta(\omega_1 + \omega_2 - \omega_3 - \omega_4) . \quad (4.14)$$

We note that momentum is always conserved.

From (4.11) and (4.12) we can see that expression (4.9) and (4.10) are defined on a reduced kinematic range compared to before mode separation. This prevents us from directly comparing the coupling function $V_{(i,j)}$ before and after mode separation. Following our discussion in chapter 3.1.3 we restore the previous kinematic range by rescaling momenta, frequency and the energy conserving delta-functional according to

$$\begin{aligned} k' &= sk \\ \omega' &= s\omega \\ \delta_{\omega'} &= \frac{\delta_{\omega}}{s} . \end{aligned} \quad (4.15)$$

In (4.11) and (4.12) we ignored the fact that the momentum integration after the shift of coordinates should be of the form

$$K dK = (K_F + k)dk . \quad (4.16)$$

This is because during momentum rescaling this expression changes to

$$(K_F + k)dk \rightarrow \left(K_F + \frac{k}{s}\right) \frac{dk}{s} . \quad (4.17)$$

By reducing the width of the annulus ($s \rightarrow \infty$) the term k/s can be neglected compared to K_F so that we can write

$$K dK \rightarrow K_F dk . \quad (4.18)$$

After mode separation and rescaling of momenta and frequency we obtain

$$S_0[\psi_<] = \int_{1'} \bar{\psi}_{(\frac{1'}{s}, \frac{1'}{s})}^< \left(i \frac{\omega'_1}{s} - \mathcal{N}(K_F) \frac{k'_1}{s} \right) \psi_{(\frac{1'}{s}, \frac{1'}{s})}^< \quad (4.19)$$

$$S_I[\psi_<] = \int_{i', j'} V_{(\frac{i'}{s}, \frac{j'}{s})} \bar{\psi}_{(\frac{1'}{s}, \frac{1'}{s})}^< \bar{\psi}_{(-\frac{1'}{s}, \frac{2'}{s})}^< \psi_{(\frac{2'}{s}, \frac{3'}{s})}^< \psi_{(-\frac{2'}{s}, \frac{4'}{s})}^< \quad (4.20)$$

with

$$\int_{1'} = \frac{1}{(2\pi)^2} \int_{-\lambda}^{\lambda} K_F \frac{dk'_1}{s} \int_{-\infty}^{\infty} \frac{d\omega'_1}{s} \int_0^{2\pi} d\theta_1 \quad (4.21)$$

$$\int_{i', j'} = \frac{1}{(2\pi)^6} \int_{-\lambda}^{\lambda} K_F^2 \prod_{i=1}^2 \frac{dk'_i}{s} d\theta_i \int_{-\infty}^{\infty} \prod_{j=1}^4 \frac{d\omega'_j}{s} s \delta_{\omega'} . \quad (4.22)$$

We can see that restoring the kinematic range to $[-\lambda, \lambda]$ introduces the factor s into our expressions. Since the RG transformation is only a scale transformation the physics must not change i.e. the quantum partition function and the action

of the system have to remain invariant. Therefore any additional factor s has to be absorbed by rescaling the fields according to

$$\psi'(k', \omega') = \zeta \psi\left(\frac{k'}{s}, \frac{\omega'}{s}\right). \quad (4.23)$$

If we want to choose ζ such that it absorbs all scaling factors within S_0 and S_I we notice that the orders of s in these two terms are different. Thus whatever field rescaling we choose, either S_0 or S_I will not be invariant during the RG transformation.

4.4.1 Invariance of S_0

Suppose we choose to keep S_0 invariant we obtain for the field rescaling

$$\psi'(k', \omega') = s^{-3/2} \psi\left(\frac{k'}{s}, \frac{\omega'}{s}\right) \quad (4.24)$$

which corresponds with earlier results [57]. Before we insert (4.24) into S_I we replace the pairing potential V by the power series

$$V\left(\frac{k'_1}{s}, \frac{k'_2}{s}, \frac{\omega'_1}{s}, \dots, \frac{\omega'_4}{s}\right) = V_{00} + V_{10} \frac{k'_1}{s} + V_{01} \frac{k'_2}{s} + \dots \quad (4.25)$$

We then insert the field rescaling as well as the power series of the coupling potential into (4.20) to obtain

$$S_I[\psi'] \propto \prod_{i=1}^2 \frac{dk'_i}{s} \prod_{j=1}^4 \frac{d\omega'_j}{s} s \delta_{\omega'} \zeta^{-4} \left(V_{00} + V_{10} \frac{k'_1}{s} + \dots \right). \quad (4.26)$$

We can see that the factor s^1 is not absorbed in S_I at zeroth order in V . This means that the interaction term grows when approaching K_F as $s \rightarrow \infty$ while S_0 remains invariant. Since S_{SC} describes the attracting force that eventually forms Cooper pairs, we conclude that the fixed point of the free part of our theory is unstable towards pair formation. This can be understood as the RG version of what was first described by Cooper in 1956 [58]. A Fermi liquid is unstable towards any infinitesimal pairing force between charge carriers. This result confirms findings in [57] where it is shown that electron-electron interactions can induce a relevant RG flow towards a SC state.

At this point it is important to discuss the difference between the present approach and previous works. In earlier works the RG formalism is used to obtain instabilities of the fixed point of a system of non-interacting electrons. The corresponding fixed point field scaling relation found in the literature [57] is

identical to equation (4.24). To obtain possible instabilities of the fixed point of free electrons, one usually introduces a very general perturbation that describes electron-electron interaction

$$H_{e-e} = \sum_{K_1 K_2 K_3 K_4} V c_{K_1}^\dagger c_{K_2}^\dagger c_{K_3} c_{K_4} .$$

For this general electron-electron interaction, the RG analysis in [57] reveals an RG flow that is marginal at tree level. Only at first order quantum correction it is possible to obtain a relevant flow. To be more specific, the RG flow becomes relevant only if the in- and outgoing momenta are antiparallel and if the interaction potential is attractive. This gives rise to the formation of a superconducting state.

The main difference of the present study compared to earlier works is that we use the restrictions found for the general electron-electron interaction at first order quantum correction and implement them directly into the initial Hamiltonian (4.1). Effectively we restrict the general electron-electron interaction to scattering of zero-momentum electron pairs with an attractive potential $V > 0$. When we analyse this interaction, we obtain a relevant flow at tree level. This result differs from the general electron-electron perturbation where the flow only becomes relevant at first order quantum correction. This difference in scaling emerges due to the restricted electron-electron interaction. By disallowing certain electron-electron interactions we assume that other types of interactions, except the attractive zero-momentum pairing are not important. This simplification should be reasonable for superconducting systems.

It is important to note that the field rescaling in (4.24) does not determine the fixed point of the Hamiltonian (4.1). Instead of making the system invariant, repeated RG transformations make S_I grow when approaching K_F .

4.4.2 Field Rescaling at the Superconducting Fixed Point

Next we aim for a field rescaling relation that makes S_I invariant and study how S_0 is affected by this choice. From (4.26) we can immediately see that the choice

$$\psi'(k', \omega') = s^{-5/4} \psi\left(\frac{k'}{s}, \frac{\omega'}{s}\right) \quad (4.27)$$

will absorb all factors of s within S_I . However, this is only valid at zeroth order of V . For higher orders of V we will obtain additional factors s^x with $x < 0$. But this is not a problem as these additional terms vanish in the limit $s \rightarrow \infty$. We also see that the invariance can only be achieved for the lowest order of V . If we chose to make higher order terms to become invariant factors, s^x with $x > 0$ would cause the lower order terms to diverge at K_F .

With the field rescaling (4.27) we note that the non-interacting part S_0 vanishes when we approach K_F . Therefore no relevant RG flow is induced by S_0 and we conclude that we have found the SC fixed point. The fact that S_0 vanishes in the limit $s \rightarrow \infty$ means that at the SC fixed point the free hopping of electrons becomes irrelevant for the long range order of the system.

4.5 Quantum Corrections of the Superconducting Fixed Point

Until now we have based the fixed point calculation only on the first two terms in equation (4.8). However, during the RG transformation higher order terms in the cumulant expansion (4.8) have to be considered as well. At this point we will not discuss the term $\langle \delta S_I[\psi_<, \psi_>] \rangle$ as it may only add a correction to the Fermi surface of freely moving fermions. This is not important in the present discussion. The quantum correction of second order is obtained by explicitly calculating the scaling of the term $\langle \delta S_I[\psi_<, \psi_>]^2 \rangle$. The cumulant expansion gives us an infinite number of corrections that may change the field rescaling relation (4.27) at the SC fixed point. To truncate the expansion at a certain order in V we assume that the pairing force between electrons is weak. It will then suffice to consider the first order loop diagrams and ignore all higher orders since $V^n \ll 1$ for $n > 2$.

4.5.1 Particle-Hole Channel

Before we start to determine the scaling of quantum corrections, we want to find out what kind of loop diagrams emerge. The first term of interest in the cumulant expansion is

$$\frac{1}{2} \left(\langle S_I^2 \rangle - \langle S_I \rangle^2 \right). \quad (4.28)$$

Since all non-connected diagrams cancel we will only be working with connected diagrams. The original vertex describing the scattering of Cooper pairs is shown in Figure 4.3. It consists of two incoming and two outgoing electrons with antiparallel momenta respectively. Now any quantum correction for this vertex has to have the same external structure as the original vertex. This means that only those diagrams with the same configuration of external legs will add a contribution.

One choice for the lowest order correction emerging from (4.28) is shown in Figure 4.4. It is constructed from two vertices of the form in figure 4.4 and is called the particle-hole channel. A connection (red line) between the vertices is established by taking the average over one in- and one outgoing leg each connected to one of the two vertices. To obtain a non-zero Grassmann integral, the momenta

Figure 4.3: For Cooper pair scattering the momenta are pairwise antiparallel before and after the scattering. Due to momentum and energy conservation the two momenta of the paired particles are effectively rotated by the same angle. Therefore they will always maintain the same distance to the Fermi surface.

of the in and outgoing lines have to be the same, hence the δ -functionals (for more details see Appendix B). Since both SC vertices within the loop diagram have pairwise antiparallel in- and out-going lines, the δ -functionals restrict the external momenta to be identical before and after the interaction. The corresponding scenario is shown in Figure 4.5.

If we compare the vertex in Figure 4.3 with its first-order loop correction shown in Figure 4.5, we see that the correction has a strongly diminished phase space. Instead of an infinite number of possible scattering events the final vectors have to be equal to the initial vector pair. The corresponding external lines resemble an interaction term of the form

$$H_I^{\text{LC}_1} = \sum_K V^{\text{LC}_1}(KK) c_K^\dagger c_{-K}^\dagger c_K c_{-K} \quad (4.29)$$

where the sum runs only over one momentum compared to the double sum of H_I in (4.1). Here $V^{\text{LC}_1}(KK)$ is proportional to V^2 and contains the contribution from the average over fast field components. Due to the strong reduction of possible scattering events compared to the initial vertex H_I , the first-order loop correction can be ignored. Therefore we do not need to evaluate the associated Grassmann path integrals.

However, before we proceed let us look at the second-order cumulant expansion. If the second and all higher orders can be ignored due to the same momentum restrictions we may not need to assume weak coupling in the first place. The diagram in Figure 4.6 is a straight forward extension of the first-order loop diagram with one additional vertex placed in between the first two vertices. As before connecting the vertices requires that the respective momenta are equal. We can see that with the additional vertex the in-going external lines become independent of the out-going ones. Therefore the second-order loop diagram allows the same number of scattering events as the original vertex and is not restricted

Figure 4.4: To construct a loop diagram we distinguish the internal and external part of the diagram. The external part has exactly the same number of legs as the vertex that is corrected by the loop diagram. Moreover for Cooper pair scattering the external legs have to be antiparallel pairwise. For the internal part we have to consider all possible connections (red line) between in- and out-going legs. The complete set of possible connections is obtained by taking the average over all internal lines and using Wick's theorem (see Appendix B).

to forward scattering. Therefore, to be able to truncate the cumulant expansion we have to remain in the weak coupling limit.

Figure 4.5: The one-loop correction at the SC fixed point. Both vertices describe Cooper pair scattering (Figure 4.3) i.e. in- and out-going momenta have to be pairwise antiparallel. Averaging over two legs connected to different vertices establishes an internal line only if the involved legs have the same momenta. Because of this restriction on the internal legs, the external legs cannot be chosen freely. Effectively the particle-hole one-loop diagram describes forward scattering of Cooper pairs. Compared to the original pair scattering process $(K_i, -K_i) \rightarrow (K_j, -K_j)$ in equation (4.1) the phase space of forward scattering $(K_i, -K_i) \rightarrow (K_i, -K_i)$ is strongly diminished.

Figure 4.6: The second-order quantum correction at the SC fixed point. While single-loop diagrams only add corrections to forwards scattered Cooper pairs, there is no such restriction for two-loop diagrams. Second order quantum corrections apply to all possible pair scattering events. However, in the weak coupling limit high-order loop diagrams can be ignored.

4.5.2 Particle-Particle Channel

Two vertices of the form shown in Figure 4.3 may as well be connected like in Figure 4.7. This diagram is known as the particle-particle channel or BCS loop diagram (here BCS does not refer to superconductivity but is of topological origin). For the case of free electrons which are subject to weak electron-electron interactions this particular quantum correction destabilizes the free electron fixed point in favor of a SC state [57] i.e. for a free electron system this diagram induces a relevant RG flow towards superconductivity.

Figure 4.7: Unlike for the particle-hole channel, the particle-particle channel does not restrict the external momenta. The internal lines can be evaluated without restricting the vertex to forward scattering. Therefore the vertex cannot be ignored and may add a quantum correction to the field rescaling at the superconducting fixed point 4.27.

An important difference between the particle-hole and the particle-particle

channel is that for the particle-particle channel the external lines are not restricted to forward scattering. The quantum correction in Figure 4.7 affects all possible scattering events of zero-momentum pairs. Therefore the BCS loop diagram cannot be ignored and may add a quantum correction to the field rescaling relation found for the superconducting fixed point at tree level (4.27). To actually evaluate this contribution we have to determine the contribution of internal lines in

$$\langle S_I^2 \rangle = \int_{\omega_i} \int_{0 < |k_i| < \lambda/s} V_0^2 \bar{\psi}_{<}^{ext} \bar{\psi}_{<}^{ext} \psi_{<}^{ext} \psi_{<}^{ext} \int_{\omega_i} \int_{\lambda/s < |k_i| < \lambda} \langle \bar{\psi}_{>}^{int} \bar{\psi}_{>}^{int} \psi_{>}^{int} \psi_{>}^{int} \rangle_{>}. \quad (4.30)$$

Here we have dropped the arguments (K_i, ω_i) . From the tree level analysis we know that the external part of the diagram with momenta in the thin annulus around K_F remains invariant under the choice (4.27). A change of the scaling behavior may be added by the term $\langle \bar{\psi}_{>}^{int} \bar{\psi}_{>}^{int} \psi_{>}^{int} \psi_{>}^{int} \rangle_{>}$. To evaluate this term we have to calculate the Grassmann path integrals in

$$\langle \bar{\psi}_{>} \bar{\psi}_{>} \psi_{>} \psi_{>} \rangle_{>} = \frac{\int \mathcal{D}(\bar{\psi}_{>}, \psi_{>}) \bar{\psi}_{>} \bar{\psi}_{>} \psi_{>} \psi_{>} e^{S_0 + S_I}}{\int \mathcal{D}(\bar{\psi}_{>}, \psi_{>}) e^{S_0 + S_I}} \quad (4.31)$$

where we again suppressed arguments for convenience. According to Figure 4.7 the momenta of the Grassmann fields that are averaged over are equal but antiparallel. Due to energy conservation the same holds for the Matsubara frequencies. In general integrals of Grassmann numbers follow very simple rules and can be evaluated easily. However, in the present case the exponent $S_0 + S_I$ makes an analytic calculation of the above integral impossible. An introduction to Grassmann numbers, Grassmann path integrals as well as a detailed discussion of the above integral can be found in Appendix B.

Instead of a lengthy numerical calculation we will discuss all possible outcomes of the above path integral. This is reasonable because we are not interested in the actual value of the integral, but just in its scaling behavior. Therefore we will distinguish between three cases. The path integral will add a scaling factor $s^{\delta\zeta}$ where $\delta\zeta$ may either be larger, smaller or equal to zero.

Certainly the simplest case would be that the averaging over fast fields $(\psi_{>})$ adds a factor s^0 i.e. a constant. In this case the field rescaling at tree level and at first order quantum correction are identical. Then the tree level field rescaling (4.27) does not have to be modified.

On the other hand, if we find a scaling behaviour where the exponent $\delta\zeta < 0$, the first order quantum correction vanishes when we approach the SC fixed point $s \rightarrow \infty$. This means that the classical diagram dominates the interaction at the SC fixed point.

Finally if $\delta\zeta > 0$ the BCS quantum correction grows under the field rescaling choice found at tree level. The growth of a diagram under rescaling operations

indicates that the diagram becomes more important when approaching K_F . In general this means that a relevant RG flow towards a *different* fixed point is induced. However, in the present case, the BCS loop diagram describes Cooper pair scattering. Therefore, this diagram is not a perturbation of the superconducting fixed point. Effectively a growing BCS loop-diagram means that quantum corrections of Cooper pair scattering become more important than the corresponding tree level term when approaching K_F . But this does not induce a flow towards a different fixed point i.e. the SC fixed point itself is not affected. We therefore conclude, that the BCS one-loop quantum correction in (4.8) can be ignored independent of the contribution by the integration over fast modes. The field rescaling found at tree level (4.27) therefore determines the SC fixed point and is not modified by quantum corrections.

4.6 Phase Coherence for Superconductors

In the SC state pairs of fermions behave like bosonic particles and therefore obey the Bose-Einstein instead of the Fermi-dirac statistics. This means that at $T = 0$ these effective bosons are able to form a Bose-Einstein condensate. Therefore, the SC phase can be interpreted as a state of condensed Cooper pairs.

In this section we will discuss the necessary condition for paired fermions to form a condensate. For this to happen we will show that all Cooper pairs have to share the same quantum phase [59].

4.6.1 The variational approach

Because the ground state is the state with the lowest possible energy, we can use a variational ansatz to obtain an approximate ground state wavefunction. In the Rayleigh-Ritz approximation, if the ground state energy E obeys the relation

$$H\psi_E = E\psi_E$$

where ψ_E is the real ground state, for any trial wavefunction ψ_T with

$$E' = \frac{\langle \psi_T^* | H | \psi_T \rangle}{\langle \psi_T^* | \psi_T \rangle} \quad (4.32)$$

it is always true that $E' > E$. To show that the ground state energy E is the minimum energy we will start with a trial wavefunction of the form

$$\psi_T = \psi_E + \alpha\phi. \quad (4.33)$$

We find that the variation of E' with respect to α vanishes in the proximity of an eigenfunction

$$\left. \frac{dE'}{d\alpha} \right|_{\alpha=0} = \frac{d}{d\alpha} \left[\frac{\langle \psi_E + \alpha\phi | H | \psi_E + \alpha\phi \rangle}{\langle \psi_E + \alpha\phi | \psi_E + \alpha\phi \rangle} \right]_{\alpha=0} \quad (4.34)$$

$$= E\langle \phi | \psi_E \rangle + E\langle \psi_E | \phi \rangle - E\langle \phi | \psi_E \rangle - E\langle \psi_E | \phi \rangle = 0 . \quad (4.35)$$

The Rayleigh-Ritz variational scheme can therefore be used to approximately determine the ground state wavefunction ψ_E from any trial wavefunction ψ_T . For our purposes we will vary an appropriate trial wavefunction with respect to the quantum phase to approximate the ground state.

The variational state

In a SC each paired momentum state $(K_i, -K_i)$ may either be occupied or empty. The corresponding trial wavefunction is of the form

$$|\psi_T\rangle = \prod_P \left(u_P u_{-P} + v_P v_{-P} c_P^\dagger c_{-P}^\dagger \right) |0\rangle . \quad (4.36)$$

Here $u_P u_{-P}$ and $v_P v_{-P}$ denote the probability amplitude that the pair state $(P, -P)$ is empty or occupied by two fermions. As usual for quantum mechanics these probability amplitudes are complex numbers that can be represented in terms of an amplitude and a phase factor. Since Cooper pairs are assumed to be composite particles we can assign a single probability amplitude to each pair state according to $u_P u_{-P} = \bar{u}_P$. The pair probability amplitudes are then of the form

$$\begin{aligned} \bar{u}_P &= |u_P| e^{i\alpha_P} \\ \bar{v}_P &= |v_P| e^{i\beta_P} \end{aligned}$$

The variational approach can now be used to minimize the energy expectation value with respect to amplitude and phase. The minimization with respect to amplitude was presented by Bardeen, Cooper and Schrieffer in one of their famous works [2]. For the rest of this thesis the variation with respect to amplitude will not be important. Instead we will analyze how the phase has to be chosen to obtain the variational ground-state wavefunction. To do that we first obtain the energy expectation value of the trial state (4.36)

$$\langle \psi_T | H_I | \psi_T \rangle = \langle \psi_T | \sum_{K,L} V(K,L) c_K^\dagger c_{-K}^\dagger c_L c_{-L} | \psi_T \rangle . \quad (4.37)$$

From the definition of the trial state we can see that ψ_T is not an eigenstate of the creation and annihilation operators. Instead the application of field operators results in the reduced state ψ_T^L where no particles occupy the L momentum state

$$\begin{aligned} c_L c_{-L} |\psi_T\rangle &= c_L c_{-L} \prod_P (\bar{u}_P + \bar{v}_P c_P^\dagger c_{-P}^\dagger) |0\rangle \\ &= c_L c_{-L} \bar{v}_L c_L^\dagger c_{-L}^\dagger \prod_{P \neq L} (\bar{u}_P + \bar{v}_P c_P^\dagger c_{-P}^\dagger) |0\rangle \\ &= -\bar{v}_L |\psi_T^L\rangle. \end{aligned} \quad (4.38)$$

When we insert expression (4.38) into (4.37) we get

$$\langle \psi_T | H_I | \psi_T \rangle = \sum_{K,L} V(K, L) \bar{v}_K^* \bar{v}_L \langle \psi_T^K | \psi_T^L \rangle \quad (4.39)$$

and see that the two trial states are not identical. While the product state ψ_T^L has no particles with momentum L the product state ψ_T^K has no particles with momentum K . Therefore in the scalar product $\langle \psi_T^K | \psi_T^L \rangle$ all terms with occupied L and K momenta vanish. When we rearrange the product states we can remove those terms that vanish in the scalar product. The product state $\psi_T^{K,L}$ where K and L momentum states are unoccupied are of the form

$$\begin{aligned} |\psi_T^L\rangle &= (\bar{u}_K + \bar{v}_K c_K^\dagger c_{-K}^\dagger) \prod_{P \neq L, K} (\bar{u}_P + \bar{v}_P c_P^\dagger c_{-P}^\dagger) |0\rangle \\ &= (\bar{u}_K + \bar{v}_K c_K^\dagger c_{-K}^\dagger) |\psi_T^{K,L}\rangle \end{aligned} \quad (4.40)$$

$$|\psi_T^K\rangle = (\bar{u}_L + \bar{v}_L c_L^\dagger c_{-L}^\dagger) |\psi_T^{K,L}\rangle. \quad (4.41)$$

The energy expectation value then reads

$$\begin{aligned} \langle \psi_T | H_I | \psi_T \rangle &= \sum_{K,L} V(K, L) \bar{u}_L^* \bar{v}_K^* \bar{u}_K \bar{v}_L \langle \psi_T^{K,L} | \psi_T^{K,L} \rangle \\ &= \sum_{K,L} V(K, L) |\bar{u}_L| |\bar{v}_K| |\bar{u}_K| |\bar{v}_L| e^{i(-\alpha_L - \beta_K + \alpha_K + \beta_L)}. \end{aligned} \quad (4.42)$$

Next we choose the origin of the phase by setting $\alpha_P = 0$ and define $\theta_P = \beta_P - \alpha_P$ to obtain

$$\langle \psi_T | H_I | \psi_T \rangle = \sum_{K,L} V(K, L) |\bar{u}_L| |\bar{v}_K| |\bar{u}_K| |\bar{v}_L| e^{i(\theta_L - \theta_K)}. \quad (4.43)$$

Phase independence of the hopping term

The careful reader may have noticed that the original BCS Hamiltonian also contains a term that describes free electron hopping (H_0). But since we have

shown that H_0 becomes irrelevant at the SC fixed point we have ignored it so far. However, for completeness we will show that the variational ground-state energy with respect to H_0 does not depend on our choice of the quantum phase. To do that it is sufficient to note that the creator ($c_K^\dagger$) and the annihilator (c_K) in H_0 both act on the same momentum state. Again we obtain the reduced trial states

$$\begin{aligned} c_K |\psi_T\rangle &= c_K \prod_P (\bar{u}_P + \bar{v}_P c_P^\dagger c_{-P}^\dagger) |0\rangle \\ &= c_K \bar{v}_K c_K^\dagger c_{-K}^\dagger \prod_{P \neq K} (\bar{u}_P + \bar{v}_P c_P^\dagger c_{-P}^\dagger) |0\rangle \\ &= \bar{v}_K c_{-K}^\dagger |\psi_T^K\rangle = \bar{v}_K |\bar{\psi}_T^K\rangle . \end{aligned} \quad (4.44)$$

For the corresponding energy expectation $\langle H_0 \rangle$ we then find that the phase factors cancel

$$\langle \bar{\psi}_T^K | H_0 | \bar{\psi}_T^K \rangle = \sum_K E(K) |v_K|^2 . \quad (4.45)$$

We can therefore ignore H_0 when we minimize the energy expectation with respect to the quantum phase.

The phase coherence condition

Finally we want to determine how θ has to be chosen to minimize $\langle H_I \rangle$. To do that we minimize with respect to the quantum phase θ_P

$$\begin{aligned} \frac{\partial \langle H_I \rangle}{\partial \theta_P} &= i \sum_{K,L} V(K,L) |\bar{u}_L| |\bar{v}_K| |\bar{u}_K| |\bar{v}_L| (\delta_{PL} - \delta_{PK}) e^{i(\theta_L - \theta_K)} \\ &= i \sum_K V(K,P) |\bar{u}_P| |\bar{v}_K| |\bar{u}_K| |\bar{v}_P| e^{i(\theta_P - \theta_K)} \\ &\quad - i \sum_L V(P,L) |\bar{u}_L| |\bar{v}_P| |\bar{u}_P| |\bar{v}_L| e^{i(\theta_L - \theta_P)} . \end{aligned} \quad (4.46)$$

In the simplest case we can assume that the coupling potential V is symmetric in its arguments so that we can rearrange the second sum to finally obtain

$$\frac{\partial \langle H_I \rangle}{\partial \theta_P} = \sum_K V(K,P) |\bar{u}_P| |\bar{v}_K| |\bar{u}_K| |\bar{v}_P| \sin(\theta_K - \theta_P) = 0 . \quad (4.47)$$

There are two cases when the above sum equals zero. In the first case each term in condition (4.47) is nonzero, but the sum vanishes. Why this is impossible is discussed in [59]. In the second scenario each single term of the sum vanishes. This implies that

$$\theta_K = \theta_P \quad (4.48)$$

which proves that Cooper pairs occupy a state with one common global phase θ_P . We should however note that far from K_F it is not necessarily true that $|u_K||v_K| \neq 0$. Strictly speaking the phase coherence condition is satisfied only in the region around K_F where the two distributions $|u_K|$ and $|v_K|$ are sufficiently smeared out. Deep inside the Fermi sphere where $|u_K| \rightarrow 0$ and $|v_K| \rightarrow 1$ the phase coherence condition is no necessary condition to minimize the energy expectation anymore. Since the RG scale transformation takes place in a small annulus around K_F it is safe to assume that the phase coherence condition is satisfied for all momenta $-\lambda < k < \lambda$. Therefore we conclude that the non-Fermi liquid fixed point we found in the previous section is the SC fixed point.

4.7 Perturbations of the SC fixed point

According to our discussion in section 4.1 we now want to introduce two types of perturbations. First we will investigate whether strong on-site Coulomb repulsion can cause a transition from a gapped to a gapless state. If we identify such a transition, this would indicate that the pseudo-gap originates from a coupling mechanism unrelated to SC pairing. Later we will look at a second type of perturbation that does not break Cooper pairs but disturbs the SC phase. Such a process would indicate that a one-gap scenario with pre-formed Cooper pairs is more plausible.

Before we start we have to clarify some technical details. Throughout the RG fixed point calculation as well as in the general introduction to RG in chapter 3 we have assumed that all involved interactions have to be in the weak coupling limit. Otherwise the cumulant expansion cannot be truncated. But HTSC materials are supposed to be strongly-correlated electron systems. Especially the MI phase is an exemplary case for strong electron-electron correlations. Thus, when we choose a perturbation that originates from strong correlations are we violating against the weak coupling restriction of the perturbative RG scheme? Not necessarily.

In a system with strong correlations between electrons we expect interactions that may not be present in weakly interacting systems. However, these additional strong correlation effects can also be described in the weak coupling limit. Then it is still possible to use the perturbative RG scheme to analyze these additional interactions. The important point to note is that without strong correlations the interactions discussed here are negligible or not present at all. We will now proceed to discuss strong correlation effects in the weak coupling regime.

4.7.1 Kinematically forbidden processes

The first class of perturbations we investigate describe Cooper pair breaking due to on-site repulsion. Such vertices consist of at least one Cooper pair that breaks when one of its constituents interacts with an occupied neighboring lattice site. The simplest version of this kind of interaction is shown in Figure 4.8. The vertex describes an incoming Cooper pair (incoming double arrow) that breaks up after interacting with a single hole (single arrow). After the interaction three unpaired fermions leave the vertex.

Before we obtain the RG flow for this vertex it will be interesting to discuss the condition for momentum conservation of this interaction. Since the incoming Cooper pair has zero momentum, the total momentum is conserved if the condition $K_1 = K_3 + K_4 + K_5$ (with $K_i = K_F + k_i$) is obeyed. This condition is shown graphically in Figure 4.9. The dashed green antiparallel arrows denote holes that are bound to form a Cooper pair. The black dashed line represents a single hole before the interaction while the three red solid arrows describe the outgoing unpaired particles after the interaction.

Physically any arrangement of momenta is allowed as long as total momentum is conserved. However, during the RG transformation the long range order of the system is determined by those momenta within the small annulus around K_F . Any momenta outside this region are considered to be short-range fluctuations that are not important on large length scales.

If we restrict all momenta such that the vertex in Figure 4.8 is relevant on a macroscopic scale we find that total momentum is only conserved if two outgoing lines are again antiparallel. Therefore we conclude that Cooper pairs cannot be split by interacting with a single neighboring hole. Effectively the vertex in Figure 4.8 describes short-range pair breaking which is irrelevant for the long range order of the system. We found that similar kinematic restrictions apply for square-like Fermi surfaces (not shown).

Since the paired state is conserved, it will be interesting to analyze whether the same is true for the SC phase. To do that we have to check whether the phase coherence condition (4.48) is valid for the present vertex. Effectively the vertex in Figure 4.8 describes the scattering of a Cooper pair in the presence of a third charge carrier. From Figure 4.9 it becomes clear that the momentum of the single charge carrier has to be the same before and after the interaction. The antiparallel momenta of the Cooper pair can be chosen freely. The corresponding Hamiltonian for this process is of the form

$$H_{1CP1e} = \sum_{K_i} \mathcal{V}_{1CP1e} c_{K_1}^\dagger c_{K_2}^\dagger c_{-K_2}^\dagger c_{K_1} c_{K_3} c_{-K_3} . \quad (4.49)$$

If we perform the same calculation as in section 4.6 we note that for the single hole the phase factors will cancel just as found for the free hopping term

Figure 4.8: The interaction vertex for hole-Cooper pair interaction. Here the double-arrow indicates paired holes while the single-arrows indicate unpaired charge carriers. After the interaction the pair splits and three unpaired holes leave the vertex. Momenta and frequencies have to be conserved for incoming and outgoing lines.

(compare section 4.6.1). Then we recover the same phase coherence condition as for conventional Cooper pair scattering. We conclude, that the interaction between one Cooper pair and a single hole not only conserves the pair but also the phase coherence condition. Therefore it is not important whether the vertex generates a relevant RG flow since in any case the SC state will be preserved and no SC-PG transition will be induced.

4.7.2 Pair breaking processes

Adding an additional hole or Cooper pair to the vertex in Figure 4.8 should make it easier to satisfy momentum conservation in a pair breaking process. These vertices are shown in Figure 4.10 and 4.11 respectively. In both vertices it is kinematically possible to have only holes in the outgoing state. The actions of the two vertices are of the form

$$\delta S_{1\text{CP}2\text{e}} = \int \prod_{i=1}^7 \frac{dk_i}{2\pi} \frac{d\omega_i}{2\pi} \frac{d\theta_i}{2\pi} \bar{\psi}_1 \bar{\psi}_{-1} \bar{\psi}_2 \bar{\psi}_3 \psi_4 \psi_5 \psi_6 \psi_7 \mathcal{V}_{1\text{CP}2\text{e}} \delta_k \delta_\omega, \quad (4.50)$$

$$\delta S_{2\text{CP}1\text{e}} = \int \prod_{i=1}^8 \frac{dk_i}{2\pi} \frac{d\omega_i}{2\pi} \frac{d\theta_i}{2\pi} \bar{\psi}_1 \bar{\psi}_{-1} \bar{\psi}_2 \bar{\psi}_{-2} \bar{\psi}_3 \psi_4 \psi_5 \psi_6 \psi_7 \psi_8 \mathcal{V}_{2\text{CP}1\text{e}} \delta_k \delta_\omega. \quad (4.51)$$

Here $\mathcal{V}_{1\text{CP}2\text{e}}$ and $\mathcal{V}_{2\text{CP}1\text{e}}$ denote interaction potentials which are functions of k and θ . The energy and momentum conserving functions are of the form

Figure 4.9: Graphical representation of the momentum conservation condition for a circular Fermi surface. The shaded grey area indicates the thin annulus of $K_F \pm \lambda$. All momenta have to lie within this narrow band. The dashed green (black) line indicates an incoming Cooper pair (a single hole). The red arrows are outgoing hole momenta. To satisfy momentum conservation two outgoing momenta have to be antiparallel again. This restriction prevents any momentum transfer.

$$\delta_\omega = \delta \left(\sum_{\text{in}} \omega_{\text{in}} - \sum_{\text{out}} \omega_{\text{out}} - \Delta \right) \quad (4.52)$$

$$\delta_k = \delta \left(\sum_{\text{in}} k_{\text{in}} - \sum_{\text{out}} k_{\text{out}} \right) . \quad (4.53)$$

To split a Cooper pair the unpaired scattering partners have to provide the excess energy Δ to overcome the pairing energy. Since we integrate over all frequencies $\omega = [-\infty, \infty]$ the energy gap Δ only causes a shift of the energy conservation condition.

More care, however, is needed when performing the momentum integration. If we choose the first $n-1$ momenta $K_1, K_2 \dots K_{n-1}$ freely from the shell $K_F \pm \lambda$, then the last momentum K_n can be as large as $(n-1)K_F$. This is of course not permitted. To prevent this we introduce the constraint

$$\theta(\lambda - |k_n(k_1, k_2, \dots, k_{n-1}, K_F)|) \quad (4.54)$$

for the remaining $(n-1)$ momenta with $K_i = K_F + k_i$. After rescaling this restriction changes to $\theta(\lambda - |k'_n(k'_1, k'_2, \dots, k'_{n-1}, sK_F)|)$. Since the θ -function is different before and after rescaling the allowed momenta that lie within the thin annulus $K_F \pm \lambda$ are reduced. Therefore, depending on the respective vertex only specific momentum configurations lie within $K_F \pm \lambda$. This restriction of momenta is not important for the remaining part of this work.

Figure 4.10: Interaction between two holes and a single Cooper pair (1CP2e) results in four unbound holes.

Figure 4.11: Two Cooper pairs can be split by a single hole (2CP1e) resulting in five unpaired outgoing lines.

To obtain the RG flow of the pair-breaking vertices we again perform the standard RG transformation. We start with mode separation and split δS_{1CP2e} and δS_{2CP1e} into slow ($\psi_{<}$), fast ($\psi_{>}$) and mixed field components. In the effective action

$$e^{\delta \tilde{S}'_{CPe}[\psi_{<}]} = e^{\delta S_{CPe}[\psi_{<}]} \left\langle e^{\delta S_{CPe}[\psi_{>}, \psi_{<}]} \right\rangle_{>} \quad (4.55)$$

we examine the contribution from the term consisting of slow field components only. Next we rescale momenta, frequency and fields according to

$$\begin{aligned} dk_i &\rightarrow \frac{dk'_i}{s} \\ d\omega_i &\rightarrow \frac{d\omega'_i}{s} \\ \psi_{<} \left(\frac{k'_i}{s}, \theta_i, \frac{\omega'_i}{s} \right) &= s^{5/4} \psi'(k'_i, \omega'_i, \theta) . \end{aligned} \quad (4.56)$$

Here equation (4.56) is the field rescaling relation we obtained at the SC fixed point. By rescaling the fields according to this relation we will obtain the RG flow

with respect to the SC fixed point. The momentum and frequency conserving functions δ_k and δ_ω scale inversely to their arguments. Finally any scaling factor s that emerges from our RG transformations needs to be absorbed by the rescaled interaction potentials $\mathcal{V}'$. To do that we expand the two coupling functions $\mathcal{V}_{1CP2e}$ and $\mathcal{V}_{2CP1e}$ into power series of the form

$$\mathcal{V} = \mathcal{V}^{00} + \sum_{ij} \left[\mathcal{V}^{ij} \frac{k'_i}{s} + \mathcal{V}^{ij} \frac{\omega'_j}{s} \right] + \dots \quad (4.57)$$

We then insert (4.57) into the action integrals (4.50) and (4.51) to obtain

$$\mathcal{V}'_{1CP2e} = s^{-2} \left(\mathcal{V}^{00}_{1CP2e} + \sum_{ij} \left[\mathcal{V}^{ij}_{1CP2e} \frac{k'_i}{s} + \mathcal{V}^{ij}_{1CP2e} \frac{\omega'_j}{s} \right] + \dots \right) \quad (4.58)$$

$$\mathcal{V}'_{2CP1e} = s^{-3/2} \left(\mathcal{V}^{00}_{2CP1e} + \sum_{ij} \left[\mathcal{V}^{ij}_{2CP1e} \frac{k'_i}{s} + \mathcal{V}^{ij}_{2CP1e} \frac{\omega'_j}{s} \right] + \dots \right) \quad (4.59)$$

Power counting reveals that only irrelevant terms with s^χ , $\chi < 0$ are generated. This means that at tree level the couplings $\mathcal{V}'_{1CP2e}$ and $\mathcal{V}'_{2CP1e}$ are irrelevant and do not induce a flow away from the SC fixed point. More precisely, Cooper pairs are preserved at large length scales.

Quantum corrections for the result obtained at tree level may come from higher-order terms of a cumulant expansion for the average in (4.55). To check these out path integrals of the form

$$\langle \dots \rangle = \frac{\int (\dots) e^{-S(\bar{\psi}, \psi)} \mathcal{D}(\bar{\psi}, \psi)}{\int e^{-S(\bar{\psi}, \psi)} \mathcal{D}(\bar{\psi}, \psi)} \quad (4.60)$$

have to be calculated. Evaluating Grassmann path integrals of this type is not trivial. In particular if the action contains two or more terms ($S = S_0 + S_I$) the Taylor expansion of the exponential function admits a large number of possible combinations. A comprehensive analysis of this problem is given in Appendix B.

Following the discussion in Appendix B we will ignore loop corrections of the tree level term and assume that any form of pair breaking induced by strong correlations is ineffective to destroy the SC state. This implies that Cooper pairs remain intact macroscopically even if strong correlation effects are introduced.

4.7.3 Dephasing processes

In the previous sections we showed that pair-breaking perturbations are either kinematically forbidden or irrelevant in RG terms. This implies that strong correlation induced pair breaking is not capable to destroy the SC order on large length scales.

To design a perturbation that may induce the SC-PG transition we want to understand from a technical point of view when a perturbation becomes relevant or irrelevant. We know that the SC fixed point is determined by the field rescaling relation

$$\psi'(k', \omega') = s^{-5/4} \psi\left(\frac{k'}{s}, \frac{\omega'}{s}\right). \quad (4.61)$$

If an action contains several fields ψ_i their scaling factors s^{n_i} are multiplied and the overall power is the sum of all exponents $\sum_i n_i$. But when more fields are introduced the number of integration variables dk and $d\omega$ that scale with s^{-1} increases as well. From a purely technical point of view we want a perturbation where the factors s emerging from rescaled fields outweigh the rescaling of integration variables. Then the rescaled coupling potential will absorb a factor s^n with $n > 0$ resulting in a relevant flow away from the original fixed point.

With this pragmatic point of view we note that any pair-breaking process *requires* more integration variables than a pair conserving process. The reason is simple. After a Cooper pair breaks the two formerly paired particles will have different momenta. In a pair conserving process on the other hand the particles will have antiparallel momenta before and after the interaction. This saves one momentum integration variable and therefore a factor s^{-1} .

After this technical discussion we now motivate an appropriate perturbation from a more physical point of view. In general a supercurrent forms when (1) a pairing force between electrons supports the formation of Cooper pairs and (2) when the temperature is low enough such that these bosons form a phase coherent condensate. For conventional SC the energy gap that indicates the formation of pairs was identified to be the SC order parameter. However, for HTSC materials the energy gap may not be the appropriate order parameter. Experimental data shows that the relation between the critical temperature T_c and the energy gap Δ

$$\frac{2\Delta}{k_B T_c} = \text{const.} \quad (4.62)$$

found for all BCS-like SC is not valid in cuprates. Instead it was shown [60] that T_c is proportional to the superfluid density or phase stiffness ρ_s according to

$$T_c \propto \text{const.} \times \rho_s(0) \quad \text{with} \quad \rho_s(T) = \mu_0 e^2 n_s / m^*. \quad (4.63)$$

Here μ_0 is the vacuum permeability, e is the electronic charge, n_s the density of superconducting charge carriers and m^* is their effective mass. This relation implies that it is not the strength of the pairing coupling that is important for the SC state, but the number of phase-coherent pairs. The breakdown of conventional and unconventional SC may therefore have rather different origins. For conventional SC Δ is much smaller than ρ_s and the breakdown of SC is therefore

related to the closing of the energy gap. For underdoped high- T_c materials the situation is reversed. The gap increases with underdoping [42; 61] while T_c scales with the superfluid density. The breakdown of unconventional SC should then be attributed to fluctuations of the coherent phase [22].

In this section we will therefore investigate whether non-phase coherent pair formation is possible. To do that we will again introduce perturbations caused by strong correlation effects. This time however we will enforce conservation of the paired state. This scenario is shown in Figure 4.2. Two paired charge carriers in an underdoped environment experience local on-site repulsion due to a lack of free nearest neighbor lattice sites. This results in individual interaction events of either both or one of the paired holes with their respective environment. We will now discuss two possible scenarios for this kind of interactions.

The 1CP1e Vertex

The simplest case when only one charge carrier within the Cooper pair interacts with its environment is described by the vertex in Figure 4.8. We have discussed this diagram earlier and already know that the phase coherence condition remains valid for this type of interaction. This means that even if this diagram generates a relevant RG flow the SC state will persist. We therefore ignore vertices of the 1CP1e type as they are ineffective to induce a phase transition.

The 1CP2e Vertex

The vertex that describes the interaction of both paired charge carriers with their respective environment is shown in Figure 4.12. A single incoming Cooper pair (double arrow) interacts with two unpaired holes (single arrows). Here the interaction with unpaired holes mimics strong on-site Coulomb repulsion that

Figure 4.12: In underdoped strongly correlated materials Cooper pairs may experience strong on-site repulsion due to a lack of free lattice sites. If the two paired charge carriers experience comparable momentum and energy transfer the paired state will be conserved.

disturbs the pairwise motion of the boson. To conserve the Cooper pair it is important that both paired holes experience individual but identical scattering events, which is probable only in strongly correlated systems. The respective interaction in k -space can then thus be written as

$$\begin{aligned} \delta \bar{S}_{1CP2e} = & \int_{k=-\lambda}^{\lambda} \int_{\omega} \prod_{i=1}^3 \prod_{j=1}^4 (K_i dK_i d\theta_i d\omega_j) dq dw \bar{V}_{1CP2e} \times \\ & \left[\bar{\psi}_{(1,1)} \bar{\psi}_{(-1,2)} \bar{\psi}_{(2,3)} \bar{\psi}_{(3,4)} \times \right. \\ & \left. \psi_{(1+q,1+w)} \psi_{(-1-q,2+w)} \psi_{(2-q,3-w)} \psi_{(3+q,4-w)} \right] . \end{aligned} \quad (4.64)$$

Again we replaced arguments by indices for convenience. Here we assume that each of the two paired fermions with initial momenta K_1 and $-K_1$ interacts with one of the two single holes (K_2 or K_3). To conserve the pair it is important that the momentum transfer q has to be equal in magnitude but opposite in direction i.e. $K_1 + q$ and $-K_1 - q$. Similarly the Matsubara frequency has to change by the same amount ω for both interactions.

Before we go ahead to perform the RG transformation we shift the momentum according to $k_i = K_i - K_F$ and obtain for the integration variables $dK_i = K_F dk_i$. With the same arguments as in section 4.4 we ignore the factor $k_i dk_i$ as it becomes irrelevant during the RG transformation. After mode separation and momentum rescaling we obtain at tree level

$$\begin{aligned} \delta \bar{S}_{1CP2e} = & \int_{k=-\lambda}^{\lambda} \int_{\omega} \prod_{i=1}^3 \prod_{j=1}^4 \left(K_F \frac{dk'_i}{s} d\theta_i \frac{d\omega'_j}{s} \right) \frac{dq'}{s} \frac{dw'}{s} \bar{V}_{1CP2e} \times \\ & \left[\bar{\psi}_{(1',1')}^< \bar{\psi}_{(-1',2')}^< \bar{\psi}_{(2',3')}^< \bar{\psi}_{(3',4')}^< \times \right. \\ & \left. \psi_{(1'+q',1'+w')}^< \psi_{(-1'-q',2'+w')}^< \psi_{(2'-q',3'-w')}^< \psi_{(3'+q',4'-w')}^< \right] . \end{aligned} \quad (4.65)$$

To obtain whether this perturbation generates a relevant RG flow with respect to the SC fixed point we have to insert the field rescaling relation (4.27)

$$\psi'(k', \omega') = s^{-5/4} \psi^<(k'/s, \omega'/s) \quad (4.66)$$

into (4.65) and expand the interaction potential $\bar{V}_{1CP2e}$ into a power series. When we absorb all remaining scaling factors from the integrand into the rescaled interaction potential we finally obtain the relation

$$\bar{V}'_{1CP2e} = s \left(\bar{V}_{00}^{00} + \bar{V}_{10}^{00} \frac{k_1}{s} + \bar{V}_{01}^{00} \frac{k_2}{s} + \bar{V}_{00}^{10} \frac{k_3}{s} + \dots \right) . \quad (4.67)$$

At zeroth order we find a relevant contribution and marginal contributions at first order. This means that the 1CP2e vertex generates a relevant flow away from the SC fixed point towards some neighboring phase.

However, at this stage it is unclear whether we have identified an RG flow towards another SC fixed point or whether the SC state is destroyed. To clarify this we have to check whether the phase coherence condition remains valid in the 1CP2e perturbation. To do that we repeat our calculation from section 4.6. Again we have to choose an appropriate trial state to calculate the matrix element $\langle H_{1\text{CP}2e} \rangle$. One possible choice may be the product state we used in section 4.6 to obtain the phase coherence condition for BCS-like SC. This trial state is of the form

$$|\Psi_{BCS}\rangle = \prod_K (\bar{u}_K + \bar{v}_K c_K^\dagger c_{-K}^\dagger) |0\rangle . \quad (4.68)$$

The essential difference between conventional Cooper pair scattering and the 1CP2e vertex are two additional single particle operators. We therefore have to check whether the wave function (4.68) is a suitable trial state. To do that we introduce the reduced product state

$$\begin{aligned} c_M |\Psi_{BCS}\rangle &= c_M \prod_K (\bar{u}_K + \bar{v}_K c_K^\dagger c_{-K}^\dagger) |0\rangle \\ &= c_M \bar{v}_M c_M^\dagger c_{-M}^\dagger \prod_{K \neq M} (\bar{u}_K + \bar{v}_K c_K^\dagger c_{-K}^\dagger) |0\rangle \\ &= \bar{v}_M c_{-M}^\dagger |\Psi_{BCS}^M\rangle . \end{aligned} \quad (4.69)$$

When a single fermion changes its momentum during the 1CP2e interaction we have to evaluate the expression

$$\langle \Psi_{BCS} | C(p) c_N^\dagger c_M | \Psi_{BCS} \rangle = \langle \Psi_{BCS}^N | C(p) \bar{v}_N^* c_{-N} \bar{v}_M c_{-M}^\dagger | \Psi_{BCS}^M \rangle \quad (4.70)$$

where $C(p)$ contains additional operators. In expression (4.70) the product-state Ψ_{BCS}^M does not contain any pairs with momenta $(M, -M)$ while the state Ψ_{BCS}^N does not contain $(N, -N)$ pairs. This means that all terms where N and M are occupied vanish in the scalar product. Thus we have

$$\begin{aligned} &\langle \Psi_{BCS}^N | C(p) \bar{v}_N^* \bar{v}_M c_{-N} c_{-M}^\dagger | \Psi_{BCS}^M \rangle \\ &= \langle \Psi_{BCS}^{MN} | C(p) \bar{u}_M \bar{v}_N^* \bar{u}_N \bar{v}_M c_{-N} c_{-M}^\dagger | \Psi_{BCS}^{MN} \rangle . \end{aligned} \quad (4.71)$$

However, in this expectation value the annihilation operator c_{-N} acts on Ψ_{BCS}^{MN} where the state N is not occupied. Therefore we find

$$\langle \Psi_{BCS} | c_N^\dagger c_M | \Psi_{BCS} \rangle \propto \delta_{MN} . \quad (4.72)$$

We see that the contribution to the energy expectation is nonzero only if the two unpaired fermions in the $\delta \bar{S}_{1\text{CP}2e}$ vertex have parallel momenta. Since this means a loss of generality the BCS trial state is not a good choice for our problem.

The 1CP2e trial state

The simplest alternative trial state is of the form

$$|\Phi_{1\text{CP}2\text{e}}\rangle = \tilde{\prod}_{KLM} (\bar{u}_K u_L u_M + \bar{v}_K v_L v_M c_K^\dagger c_{-K}^\dagger c_L^\dagger c_M^\dagger) |0\rangle. \quad (4.73)$$

Here the amplitudes u_K and v_K describe the occupation probability of fermionic states while $\bar{u}_K$ and $\bar{v}_K$ account for paired states. The notation $\tilde{\prod}$ indicates that configurations with multiple occurrence of the same index are not allowed i.e. $u_K^2 = 0$ or $\bar{v}_K u_K = 0$ and that each configuration appears only once. Then expression (4.73) describes product states of a single Cooper pair together with its local environment. This state neither allows isolated Cooper pairs nor isolated holes.

But before we replace the BCS trial state with expression (4.73) we have to verify that the new trial state reproduces the same phase coherence condition as found with the original BCS trial state. To do that we have to show that the application of c_{PC-P} on $\Phi_{1\text{CP}2\text{e}}$ reproduces relation (4.42). We write

$$c_{PC-P} \tilde{\prod}_{KLM} (\bar{u}_K u_L u_M + \bar{v}_K v_L v_M c_K^\dagger c_{-K}^\dagger c_L^\dagger c_M^\dagger) |0\rangle$$

and note that only those states where the paired state $(P, -P)$ is occupied give a non-zero contribution. Since double occupancy is not allowed and each configuration must appear only once we can write all terms with $(P, -P)$ occupied in front of the bracket according to

$$= \left[c_{PC-P} \bar{v}_P c_P^\dagger c_{-P}^\dagger \sum_{LM \neq \pm P} v_L v_M c_L^\dagger c_M^\dagger \right] \times \left[\tilde{\prod}_{KRS} (\bar{u}_K u_R u_S + \bar{v}_K v_R v_S c_K^\dagger c_{-K}^\dagger c_R^\dagger c_S^\dagger) \right] |0\rangle. \quad (4.74)$$

Here the product $\tilde{\prod}_{KRS}$ accounts for all linear combinations that do not appear in the first bracket.

Next we assume that the initial pair with $(P, -P)$ is scattered into the final state $(Q, -Q)$. When we apply the operator pair $c_Q^\dagger c_{-Q}^\dagger$ only terms with an empty $(Q, -Q)$ state do not vanish. Therefore we pull all terms where the pair $(Q, -Q)$

is not occupied in front of the bracket as well

$$\begin{aligned}
 &= - \left[\bar{v}_P \sum_{LM \neq \pm P, \pm Q} v_L v_M c_L^\dagger c_M^\dagger \right] \times \\
 &\quad \left[\bar{u}_Q \sum_{RS \neq \pm P, \pm Q, L, M} u_R u_S \right] \times \\
 &\quad \left[\tilde{\Pi}_{KXY} (\bar{u}_K u_X u_Y + \bar{v}_K v_X v_Y c_K^\dagger c_{-K}^\dagger c_X^\dagger c_Y^\dagger) \right] |0\rangle \\
 &= -\bar{v}_P \bar{u}_Q |\Phi_{1\text{CP}2e}^{PQ}\rangle. \tag{4.75}
 \end{aligned}$$

Here we already introduced the reduced product state $\Phi_{1\text{CP}2e}^{PQ}$. The product $\tilde{\Pi}_{KXY}$ runs over those indices that have not been determined in the first two brackets. Equation (4.75) is identical to the previously found relation (4.42). This means that the application of the operators $c_Q^\dagger c_{-Q}^\dagger c_P c_{-P}$ on the new trial state $\Phi_{1\text{CP}2e}$ will result in the same phase coherence condition as we found for the original BCS trial state [59]. This means that our new trial state $\Phi_{1\text{CP}2e}$ can also be used to describe a SC state.

Non-coherent paired states

Next we have to check whether the phase coherence condition remains valid when the 1CP2e interaction is introduced. To do that we have to minimize the energy expectation $\langle \Phi_{1\text{CP}2e} | 1\text{CP}2e | \Phi_{1\text{CP}2e} \rangle$ with respect to the quantum phase. If we find the same phase coherence condition as for ordinary Cooper pair scattering it means that the 1CP2e interaction causes a relevant RG flow towards another SC fixed point. A non-SC fixed point is found if the variational ground-state does not require phase coherence of paired charge carriers. The 1CP2e perturbation then describes Cooper pairs that lose their phase coherence due to interactions with their local environment.

Following the calculation in section 4.6 the matrix element can be simplified according to

$$\begin{aligned}
 &\langle \Phi_{1\text{CP}2e} | \delta \bar{S}_{1\text{CP}2e} | \Phi_{1\text{CP}2e} \rangle \\
 &= \sum_{\kappa} \langle \Phi_{1\text{CP}2e} | c_P^\dagger c_{-P}^\dagger c_Q^\dagger c_R^\dagger \mathcal{V}_{00}^{00} c_S c_{-S} c_T c_W | \Phi_{1\text{CP}2e} \rangle \\
 &= \sum_{\kappa} \mathcal{V}_{00}^{00} (u_P u_{-P} u_Q u_R v_P^* v_{-P}^* v_Q^* v_R^*) \langle \tilde{\Phi}_{1\text{CP}2e} | c_S c_{-S} c_T c_W | \tilde{\Phi}_{1\text{CP}2e} \rangle \\
 &= \sum_{\kappa} \mathcal{V}_{00}^{00} (u_P u_{-P} u_Q u_R v_P^* v_{-P}^* v_Q^* v_R^*) (u_S^* u_{-S}^* u_T^* u_W^* v_S v_{-S} v_T v_W). \tag{4.76}
 \end{aligned}$$

Here we write $\kappa = (P, Q, R, S, T, W)$ and replace the reduced wavefunctions by $\tilde{\Phi}_{1\text{CP}2e}$. For the complex probability amplitudes we use the polar representation

for single holes

$$\begin{aligned} u_K &= |u_K| e^{i\alpha_K} \\ v_K &= |v_K| e^{i\beta_K} \end{aligned}$$

and Cooper pairs

$$\begin{aligned} u_P u_{-P} &= |\bar{u}_P| e^{i\alpha_P} \\ v_P v_{-P} &= |\bar{v}_P| e^{i\beta_P} . \end{aligned}$$

Again we factor out the phase factor of all u_K and combine them to an overall constant phase. This is equivalent to choosing an origin for the quantum phase according to $\theta_K = \beta_K - \alpha_K$. In expression (4.76) we can then drop all amplitudes $|u_K|$ and $|v_K|$ and keep only the phase dependent factor

$$\sum_{\kappa} e^{i(\theta_S + \theta_T + \theta_W - \theta_P - \theta_Q - \theta_R)} . \quad (4.77)$$

Finally we have to minimize this expression with respect to the quantum phase according to the Rayleigh-Ritz approach. If we differentiate with respect to the quantum phase we obtain

$$\begin{aligned} \frac{\partial \langle \delta \bar{S}_{1\text{CP}2e} \rangle}{\partial \theta_K} &\propto \sum_{\kappa} \frac{\partial}{\partial \theta_K} \left[i e^{i(\theta_S + \theta_T + \theta_W - \theta_P - \theta_Q - \theta_R)} \right] \\ &\propto \sum_{\kappa} \left[i e^{i(\theta_S + \theta_T + \theta_W - \theta_P - \theta_Q - \theta_R)} \right] (\delta_{SK} + \delta_{TK} + \delta_{WK} - \delta_{PK} - \delta_{QK} - \delta_{RK}) . \end{aligned} \quad (4.78)$$

To simplify this expression we combine all δ -functions with the same sign according to

$$\begin{aligned} &\sum_{TWPQR} \left[i e^{i(\theta_K + \theta_T + \theta_W - \theta_P - \theta_Q - \theta_R)} \right] + \\ &\sum_{SWPQR} \left[i e^{i(\theta_S + \theta_K + \theta_W - \theta_P - \theta_Q - \theta_R)} \right] + \\ &\sum_{STPQR} \left[i e^{i(\theta_S + \theta_T + \theta_K - \theta_P - \theta_Q - \theta_R)} \right] + . \end{aligned} \quad (4.79)$$

Once we relabel the summation indices in expression (4.79) according to

$$\sum_{ABPQR} \left[i e^{i(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R)} \right] \quad (4.80)$$

it is easy to see that these sums are equivalent. We can do the same with the remaining three summations and after more relabeling we obtain

$$\begin{aligned}
 & 3 \sum_{ABPQR} \left[i e^{i(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R)} \right] - 3 \sum_{STWCD} \left[i e^{i(\theta_S + \theta_T + \theta_W - \theta_K - \theta_C - \theta_D)} \right] \\
 = & 3 \sum_{ABPQR} \left[i e^{i(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R)} \right] - 3 \sum_{STWCD} \left[i e^{-i(\theta_K + \theta_C + \theta_D - \theta_S - \theta_T - \theta_W)} \right] \\
 = & 3 \sum_{ABPQR} \left[i e^{i(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R)} - i e^{-i(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R)} \right] \\
 = & -6 \sum_{ABPQR} \sin(\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R) = 0 . \tag{4.81}
 \end{aligned}$$

As discussed in [59] each individual summand in this expression has to be zero. Then the condition to minimize the energy expectation value is

$$\theta_K + \theta_A + \theta_B - \theta_P - \theta_Q - \theta_R = 0 . \tag{4.82}$$

When we compare this result with the condition we found for conventional Cooper pair scattering $\theta_K - \theta_P = 0$ we see that in equation (4.82) the phases do not have to be constants. Instead for each summand to vanish there exists an infinite number of possible combinations. Certainly one possible choice is to make one or more phases constant and vary the remaining accordingly. However, it is clear that the condition does not restrict the phases to be constant and thus in general the constant phase condition found for conventional Cooper pair scattering does not apply for the 1CP2e process. This is an important finding. It shows that the relevant RG flow generated by the 1CP2e perturbation induces a phase transition towards a non-phase coherent state where charge carriers remain paired.

Chapter 5

Conclusion

In this thesis we investigated the origin of the energy gap found in the non-SC state of underdoped high- T_c materials. In particular we examined whether the pseudo-gap originates from (1) a mechanism unrelated to SC pair formation or (2) pre-formed non-coherent Cooper pairs.

To discriminate between the two above scenarios we used a perturbative momentum-space RG scheme (see chapter 3). To use this method we introduced a generalized effective action (see section 4.3.1) that allowed us to obtain the SC fixed point (see section 4.4). We then introduced two types of perturbations of the SC fixed point. The first breaks Cooper pairs and may induce a phase transition towards a gapless non-SC state (see section 4.7.2). The second perturbation violates the quantum phase coherence condition but conserves the paired state (see section 4.7.3).

At tree level we found that pair breaking induced by strong correlations does not generate a relevant RG flow away from the SC fixed point (see section 4.7.2). In addition our results showed that the RG flow becomes less relevant as more free charge carriers participate in the perturbation. Therefore pair breaking due to impurities is always irrelevant at tree level. We believe this result confirms what was first discussed by Cooper [58]. A Fermi liquid is unstable towards any infinitesimal attractive force between charge carriers. This tells us that Cooper pairs will form even in the presence of strong correlation effects as long as there is a pairing force. This pairing tendency was seen in Knight shift measurements on underdoped cuprates. The doping dependence of the spin susceptibility found (see section 2.2.1) suggests that spin singlet formation, instead of AF, is the dominant order in underdoped HTSC. Our theoretical results are therefore in qualitative agreement with experimental findings.

In contrast, we found that pair conserving processes generate a relevant RG flow away from the SC fixed point. Since these processes violate the quantum phase coherence condition (see section 4.7.3) the relevant RG flow suggests a

phase transition towards a gapped non-SC phase. This idea of non-coherent Cooper pairs is not new. In conventional SC the SC state vanishes once the energy gap closes. But due to the large energy gap of 50 meV compared to about 1 meV in conventional SC it was argued in [55; 62] that quantum phase fluctuations may be the weak link in unconventional SC. Additional support for this idea came from the fact that the quasiparticle peak seen in STM and ARPES experiments disappeared [9] when crossing through T_c (Figure 2.7 and ??). The QP peak in metals as well as in a SC is understood to be the signature of well defined electronic excitations. A vanishing QP peak in HTSC suggests that the existence of electronic excitations is related to the phase coherence of the superconducting state rather than to the energy gap.

Our results suggest that strong correlation effects, in particular strong on-site Coulomb repulsion does not cause pairs to break on a macroscopic scale. Instead strong correlations between paired charge carriers and their respective local environment causes a loss of phase coherence of Cooper pairs. Therefore, although the pairs persist, the global coherent phase condition is violated and the SC state is destroyed. Based on these findings we conclude that the pseudo-gap observed in underdoped cuprates originates from non-coherent Cooper pairs.

Our approach is also very general. In our generalized model we did not distinguish between conventional and unconventional SC. This may rise the question whether our calculation should be valid for any SC system. Clearly this is not the case. Although our initial Hamiltonian is very general and describes a SC state based on an arbitrary attractive interaction, we introduced perturbations that are untypical for BCS-like SC. By perturbing the system with strong correlation effects we exclude all materials which behave like Fermi liquids in the normal state.

We therefore conclude that our findings apply whenever a SC state is perturbed with local strong correlation effects. The actual origin or the mechanism of the SC state on the other hand is unimportant. We believe that experimental evidence for this generalization of the pre-formed Cooper pair scenario already exists. In [47] STM measurements on a highly disordered BCS like system revealed direct localization of Cooper pairs during the SC-insulator phase transition. This means that the attractive force between charge carriers persists even in the non-SC insulating state.

Apart from these findings we presented so far we also want to discuss some corollaries of the present work. For instance it is interesting that any paired state cannot be destroyed by local interactions such as on-site Coulomb repulsion. First of all this directly confirms the instability of Fermi liquids towards any form of pairing interaction between charge carriers. In addition it is reasonable to experimentally search for a PG like phase in BCS-like SC. This would support the idea that the presence of a PG phase is a common side-effect in SC systems

in the presence of strong correlation effects.

Another chapter of this work that may deserve more attention are kinematically forbidden processes. As discussed in section 4.7.1 the interaction of a Cooper pair with a single impurity does not disturb the SC state. Only the interaction of both paired charge carriers with impurities causes a dephasing of Cooper pairs and the break down of the SC state. This implies that materials with a large density of paired charge carriers should be more resilient towards a breakdown of the SC phase (see [60]). This relation between the critical temperature T_c and the density of superconducting pairs may be used to design new materials with even higher T_c .

In summary we believe that the work presented in this thesis gives a qualitative interpretation for the pseudo-gap problem in underdoped HTSC. A possible extension of the calculations presented here should include a treatment of loop corrections for the discussed perturbations. This will be part of a future publication.

References

- [1] Onnes, H. K. (1911) *Commun. Phys. Lab. Univ. Leiden* **12**, 120. 8
- [2] Bardeen, J., Cooper, L. N., and Schrieffer, J. R. (1957) *Phys. Rev.* **108**, 1175–1204. 8, 59
- [3] Bednorz, J. G. and Mueller, K. A. (1986) *Z. Physik B* **64**, 189–193. 8, 10
- [4] Lee, P. A., Nagaosa, N., and Wen, X.-G. (2006) *Rev. Mod. Phys.* **78**, 17–85. 10, 17, 28
- [5] Dagotto, E. (1994) *Rev. Mod. Phys.* **66**, 763–841. 10
- [6] Timusk, T. and Statt, B. (1998) *Rep. Prog. Phys.* **62**, 61–122. 10, 17
- [7] Damascelli, A., Hussain, Z., and Shen, Z.-X. (2003) *Rev. Mod. Phys.* **75**, 473–541. 10
- [8] Tsuei, C. C. and Kirtley, J. R. (2000) *Rev. Mod. Phys.* **72**, 969–1016. 10
- [9] Orenstein, J. and Millis, A. J. April 2011 *Science* **288**, 468–474. 10, 17, 23, 77
- [10] Mott, N. F. (1949) *Proc. Phys. Soc. A* **62**, 416–422. 10
- [11] Ott, H. R. (2008) *Superconductivity - Physics of Conventional and Unconventional Superconductors*, volume **2**, Springer-Verlag, Berlin Heidelberg. 11
- [12] Vaknin, D., Sinha, S. K., Moncton, D. E., Johnston, D. C., Newsam, J. M., Safinya, C. R., and King, H. E. (1987) *Phys. Rev. Lett.* **58**, 2802–2805. 11
- [13] Kastner, M. A., Birgeneau, R. J., Shirane, G., and Endoh, Y. (1998) *Rev. Mod. Phys.* **70**, 897–928. 11
- [14] Nuecker, N., Fink, J., Renker, B., Ewert, D., Politis, C., Weijs, P. J. W., and Fuggle, J. C. (1987) *Z. Phys. B* **67**, 9. 11

REFERENCES

- [15] Alloul, H., Bobroff, J., Gabay, M., and Hirschfeld, P. J. (2009) *Rev. Mod. Phys.* **81**, 45–108. 13
- [16] Emery, V. J. (1987) *Phys. Rev. Lett.* **58**, 2794. 13
- [17] Varma, C. M., Schmit-Rink, S., and Abrahams, E. (1987) *Solid State Commun.* **62**, 681. 13
- [18] Littlewood, P. B., Varma, C. M., and Abrahams, E. (1989) *Phys. Rev. Lett.* **63**, 2602. 13
- [19] Zhang, F. C. and Rice, T. (1988) *Phys. Rev. B* **37**, 3759–3761. 14
- [20] Kivelson, S. A., Bindloss, I. P., Fradkin, E., Oganessian, V., Tranquada, J. M., Kapitulnik, A., and Howavld, C. (2003) *Rev. Mod. Phys.* **75**, 1201–1241. 14
- [21] White, S. R. and Scalapino, D. J. (1998) *Phys. Rev. Lett* **80**, 1272–1275. 14
- [22] Emery, V. J. and Kivelson, S. A. (1994) *Physica C* **189**, 235–240. 14, 69
- [23] Emery, V. J., Kivelson, S. A., and Lin, H. Q. (1990) *Phys. Rev. Lett.* **64**, 475–478. 14
- [24] Emery, V. J., Kivelson, S. A., and Tranquada, J. M. (1999) *Proc. Natl. Acad. Sci. USA* **96**, 8814–8817. 14
- [25] Mesaros, A., Fujita, K., Eisaki, H., Uchida, S., Davis, J. C., Sachdev, S., Zaanen, J., Lawler, M. J., and Kim, E.-A. (2011) *Science* **333**, 426–430. 14
- [26] Tranquada, J. M., Sternlieb, B. J., Axe, J. D., Nakamura, Z., and Uchida, S. (1995) *Nature* **375**, 561–563. 14
- [27] Hoffman, J. A., McElroy, K., Lee, D.-H., Lang, K. M., Eisaki, H., Uchida, S., and Davis, J. C. (2002) *Science* **297**, 114. 14
- [28] Hubbard, J. (1963) *Proc. R. Soc. A* **276**, 238–257. 15
- [29] Lanata, N., Barone, P., and Fabrizio, M. (2009) *Phys. Rev. B* **80**, 224524–1–224524–8. 15
- [30] Han, J. H. and Jia, C. (2006) *Phys. Rev. B* **74**, 075105–1–075105–6. 15
- [31] Anderson, P. W., Lee, P. A., Randeria, M., Rice, T. M., Trivedi, N., and Zhang, F. C. (2004) *J. Phys.: Condens. Matter* **16**, R755–R769. 16

REFERENCES

- [32] Anderson, P. W. (1973) *Mater. Res. Bull.* **8**, 153. 16
- [33] Fazekas, P. and Anderson, P. W. (1974) *1974 Phil. Mag.* **30**, 432. 16
- [34] Alloul, H., Mendels, P., Casalta, H., Marucco, J. F., and Arabski, J. (1991) *Phys. Rev. Lett.* **67**, 3140–3143. 17
- [35] Campuzano, J. C., Norman, M. R., and Randeria, M. (2008) Superconductivity - Physics of Conventional and Unconventional Superconductors, volume **2**, Springer-Verlag, Berlin Heidelberg. 17, 20, 22
- [36] Curro, N. J., Imai, T., Slichter, C. P., and Dabrowski, B. (1997) *Phys. Rev. B* **56**, 877–885. 18
- [37] Nakano, T., Oda, M., Manabe, C., Momono, N., Miura, Y., and Ido, M. (1994) *Phys. Rev. B* **49**, 16000–16008. 19
- [38] Warren, W. W., Walstedt, R. E., Brennert, G. F., Cava, R. J., Tycko, R., Bell, R. F., and Dabbagh, G. (1989) *Phys. Rev. Lett.* **62**, 1193–1196. 19
- [39] Norman, M. R., Ding, H., Randeria, M., Campuzano, J. C., Yokoa, T., Takeuchi, T., Takahashi, T., Mochiku, T., Kadowaki, K., Guptasarma, P., and Hinks, D. G. (1998) *Nature* **392**, 157–160. 20, 21
- [40] Loeser, A. G., Shen, Z. X., Dessau, D. S., Marshall, D. S., Park, C. H., Fournier, P., and Kapitulnik, A. (1996) *Science* **273**, 325–329. 21
- [41] Williams, G. V. M., Tallon, J. L., Haines, E. M., Michalak, R., and Dupree, R. (1997) *Phys. Rev. Lett.* **78**, 721–724. 21
- [42] Harris, J. M., Shen, Z.-X., White, P. J., Marshall, D. S., and Schabel, M. C. (1996) *Phys. Rev. B* **54**, R15665–R15668. 21, 69
- [43] Yang, H.-B., Rameau, J. D., Johnson, P. D., Valla, T., Tsvelik, A., and Gu, G. D. (2008) *Nature* **456**, 77–80. 22
- [44] Gao, L., Xue, Y. Y., Chen, F., Xiong, Q., Meng, R. L., Ramirez, R., and Chu, C. W. (1994) *Phys. Rev. B* **50**, 4260–4263. 22
- [45] Sacepe, B., Dubouchet, T., Chapelier, C., Sanquer, M., Ovadia, M., Shahar, D., Feigel'man, M., and Ioffe, L. March 2011 *Nature Physics* **7**, 239–244. 23, 24, 44
- [46] Sacepe, B., Chapelier, C., Baturina, T. I., Vinokur, V. M., Baklanov, M. R., and Sanquer, M. (2010) *Nature Communications* **1**, 1–6. 23, 44

REFERENCES

- [47] Boyer, M. C., Wise, W. D., Chatterjee, K., Yi, M., Kondo, T., Takeuchi, T., Ikuta, H., and Hudson, E. W. September 2007 *Nature Physics* **3**, 802–806. 24, 25, 77
- [48] Fischer, O., Kugler, M., Maggio-Aprile, I., Berthod, C., and Renner, C. (2007) *Rev. Mod. Phys.* **79**, 353–419. 24
- [49] Tanaka, K., Lee, W. S., Lu, D. H., Fujimori, A., Fujii, T., Risdiana, Terasaki, I., Scalapino, D. J., Devereaux, T. P., Hussain, Z., and Shen, Z. X. (2006) *Science* **314**, 1910–1913. 25, 26
- [50] Lee, W. S., Vishik, I. M., Tanaka, K., Lu, D. H., Sasagawa, T., Nagaosa, N., Devereaux, T. P., Hussain, Z., and Shen, Z. X. (2007) *Nature* **450**, 81–84. 25
- [51] Varma, C. M. (1997) *Phys. Rev. B* **55**, 14554–14580. 26
- [52] Varma, C. M. (2006) *Phys. Rev. Lett.* **73**, 155113. 26, 27
- [53] Varma, C. M. (1999) *Phys. Rev. Lett.* **83**, 3538. 26
- [54] Chakravarty, S., Laughlin, R. B., Morr, D. K., and Nayak, C. (2001) *Phys. Rev. B* **63**, 094503. 26
- [55] Emery, V. J. and Kivelson, S. A. (1995) *Nature* **30**, 434–437. 27, 77
- [56] Ghosal, A., Mohit, R., and Nandini, T. (1998) *Phys. Rev. Lett.* **81**, 3940–3943. 28, 29, 45
- [57] Shankar, R. (1994) *Rev. Mod. Phys.* **66**, 129–192. 35, 51, 52, 56
- [58] Cooper, L. N. (1956) *Phys. Rev.* **104**, 1189–1190. 51, 76
- [59] Kouzoudis, D. (2009) *Eur. J. Phys.* **31**, 239–248. 58, 61, 73, 75
- [60] Uemura, Y. J. (1989) *Phys. Rev. Lett.* **62**, 2317–2320. 68, 78
- [61] Renner, C., Revaz, B., Genoud, J. Y., Kadowaki, K., and Fischer, O. (1998) *Phys. Rev. Lett.* **80**, 149–152. 69
- [62] Emery, V. J. and Kivelson, S. A. (1995) *Phys. Rev. Lett.* **74**, 3253–3256. 77
- [63] Springer, D. and Cheong, S. A. (2010) *arxiv.org* (cond-mat/1006.5775). 84
- [64] Winterbottom, D. (<http://codeinthehole.com/tutorials/cgl/index.html>). 84
- [65] Cox, S. M. and Matthews, P. C. (2002) *J. Comput. Phys.* **176**, 430–455. 84

REFERENCES

- [66] Morton, K. W. and Mayers, D. F. (2005) Numerical Solution of Partial Differential Equations, An Introduction, Cambridge University Press, . 85
- [67] Buscaglia, G. C., Bolech, C., and Lopez, A. (2001) Connectivity and Superconductivity, Springer, . 85

Appendix A: Stripe-like phase separation and electric fields

Stripe patterns seen in underdoped cuprates are often understood to originate from the competition between the SC and the AF phase. The supercurrent is then believed to flow along “rivers of charge” which are separated from each other by AF stripes. However, according to a different theory, stripes may be unrelated to the SC and AF phase but originate from quasiparticle interference.

In a side project [63] to this thesis we investigated theoretically whether and how stripes that originate from phase separation behave in the presence of an external electric field. In a phase separated state the charge carrier rich and charge carrier poor regions should react differently to the application of external fields. According to our results experiments may be designed to either confirm or disprove our results. This would help to classify the origin of stripe patterns seen in underdoped high- T_c materials.

A.1 The Complex Ginzburg Landau Equation

The basic assumption of our work is that the SC order parameter of high- T_c materials can be described by the complex Ginzburg-Landau equation (CGL) which is of the form

$$\partial_t \Psi = \Psi + (1 + i\alpha)\nabla^2 \Psi - (1 + i\beta)|\Psi|^2 \Psi . \quad (\text{A.1})$$

Then the strength of the SC state is proportional to the absolute value of the complex SC order parameter Ψ . Here α and β are phenomenological parameters.

To obtain Ψ along a square grid we use a numerical pseudo-spectral method [64]. After a Fourier transformation the CGL simplifies to an ordinary non-linear first-order differential equation. Such problems can be solved using the exponential time differentiation scheme [65]. Based on random initial conditions stripe pattern formation can be observed after a certain number of time iterations. In Figure A.1 red regions ($|\Psi| \approx 1$) indicate strong SC tendencies while blue areas

Figure A.1: When we start from random initial conditions we observe the formation of stripe patterns. Red color indicates SC regions while blue regions indicate AF ordering.

signal AF order ($\Psi \approx 0$).

A.1.1 Magnetic Fields

Before we introduce an electric field into the CGL we verify that the order parameter Ψ is suitable to describe the SC state. For any SC material it is well known that a critical magnetic field strength will destroy the SC state. Using the minimal coupling approach we introduce a vector potential A into the CGL equation and see whether a suppression of SC regions can be observed. To solve the modified CGL we have to use a different numerical scheme.

We integrate the CGL using a finite-difference approach [66] with Adam-Bashforth time-stepping. In the so called ψU method [67] the phase factors

$$\mathcal{U}^x = \exp \left\{ -i \int_{x_0}^x \mathbf{A}_x(\epsilon, y) d\epsilon \right\} \quad (\text{A.2})$$

$$\mathcal{U}^y = \exp \left\{ -i \int_{y_0}^y \mathbf{A}_y(x, \mu) d\mu \right\} \quad (\text{A.3})$$

contain the local change of the vector potential. The Laplacian in our gauge-

Figure A.2: Starting from well developed stripes, we see that a magnetic field destroys the stripe phase. Within times that are short compared to the typical time scale of stripe dynamics, we observe the formation of uniformly-spaced vortex-like structures across the surface. Both figures show the absolute values of the numerical solutions.

invariant finite difference approximation then reads

$$\begin{aligned}
 & (\nabla - i\mathbf{A})^2 \psi \big|_{(x_i, y_i)} \\
 = & \frac{U_{i,j}^x \psi_{i+1,j} - 2\psi_{i,j} + \bar{U}_{i-1,j}^x \psi_{i-1,j}}{a_x^2} + \\
 & \frac{U_{i,j}^y \psi_{i,j+1} - 2\psi_{i,j} + \bar{U}_{i,j-1}^y \psi_{i,j-1}}{a_y^2}
 \end{aligned} \tag{A.4}$$

where U are the link variables

$$U_{i,j}^x = \bar{U}_{i,j}^x U_{i+1,j}^x, \quad U_{i,j}^y = \bar{U}_{i,j}^y U_{i,j+1}^y. \tag{A.5}$$

For the simulation in the presence of a magnetic field we start from an initial condition where stripes have already formed. When we switch on the magnetic field we observe that the stripe patterns vanish and the SC state reduces to small equidistantly spaced islands (see Figure A.2). From this we conclude that the variable Ψ in the CGL equation may indeed be interpreted as the SC order parameter.

A.1.2 Electric Fields

Similar as for the magnetic field we use the minimal coupling approach to introduce a scalar potential ϕ to mimic an electric field

$$\left(\partial_t + \frac{iq}{\hbar}\phi\right)\Psi = \Psi + (1 + i\alpha)\nabla^2\Psi - (1 + i\beta)|\Psi|^2\Psi. \quad (\text{A.6})$$

We can again use the pseudo-spectral approach to obtain the SC order parameter Ψ . The simulation starts from random initial conditions. For the case $\phi = 0$ we obtain the pattern shown in Figure A.3 (a). In the same figure we also plot the Fourier coefficients (b) which are indicative for the width of the stripes. When we repeat the simulation with the same initial conditions but with a negative bias voltage the observed stripe patterns appear to be widened. The corresponding Fourier coefficients of the pattern shown in Figure A.4 (a) are shifted towards lower k -values i.e. larger wavelengths.

According to our findings for a phase separated system where SC and AF are in competition with each other, it can be expected that external electric fields will change the width of stripe patterns. Based on this result it may be possible to design an experiment that allows to investigate the influence of electric fields on underdoped high- T_c materials. If experiments confirm that stripe patterns change their width in the presence of an electric field this would be indicative that stripes are the result of competing phases. If on the other hand stripes remain unchanged in the presence of electric fields the quasiparticle interference scenario is the more plausible description.

Figure A.3: (a) Ginzburg-Landau order parameter Ψ of the stripe solution in the absence of fields and (b) the amplitudes of Fourier coefficients. There are no preferred orientations for the stripes in the isotropic CGLE, Eq. A.6.

Figure A.4: (a) The Ginzburg-Landau order parameter Ψ under the influence of a negative bias voltage forms wider stripes. (b) The Fourier amplitudes then become shifted to smaller values compared to the field-free case.

Appendix B: Grassmann Path Integration

To obtain the contribution that emerges from loop diagrams it is necessary to solve integrals of the form

$$\langle \dots \rangle = \frac{\int \mathcal{D}(\bar{\psi}, \psi) (\dots) e^{\mathcal{S}[\bar{\psi}, \psi]}}{\int \mathcal{D}(\bar{\psi}, \psi) e^{\mathcal{S}[\bar{\psi}, \psi]}} . \quad (\text{B.1})$$

If $\bar{\psi}$ and ψ were ordinary numbers these type of integrals are known as Gaussian integrals. However, since $\bar{\psi}$ and ψ are Grassmann numbers they obey very simple integration rules. Here we list those relations that will be sufficient to solve any Grassmann path integral

$$\int d\psi \, \psi = 1 \quad (\text{B.2})$$

$$\int d\psi \, 1 = 0 \quad (\text{B.3})$$

$$\int d\psi_i \, [\psi_i \psi_i] = 0 \quad (\text{B.4})$$

$$\int d(\psi_1, \psi_2) \, [\psi_1 \psi_2] = 1 . \quad (\text{B.5})$$

With these simple rules we can immediately solve integrals of the form

$$\int d\psi e^{\psi} = \int d\psi (1 + \psi) = 1 \quad (\text{B.6})$$

where it is important to note that the Taylor expansion of the exponential has only two non-zero terms. All higher orders vanish due to the anti-commutation rules. For integrals of the form

$$\int d\bar{\psi} d\psi \, e^{\bar{\psi}\psi} = \int d\bar{\psi} d\psi \, (1 + \bar{\psi}\psi) = - \int d\bar{\psi} \, \bar{\psi} \int d\psi \, \psi = -1 \quad (\text{B.7})$$

an additional minus sign emerges when we re-order the integrand. In path integrals that emerge during the evaluation of loop diagrams the exponent S usually contains an integration over momentum and Matsubara frequency.

B.1 Discretizing the Exponent

Before we deal with integrals in the exponent we look at simple summations. This is equivalent to discretizing e.g. the momentum integration. If the action S would only contain a momentum integration that can be discretized to a sum over two values we would obtain an expression of the form

$$\begin{aligned} & \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 e^{a_1 \bar{\psi}_1 \psi_1 + a_2 \bar{\psi}_2 \psi_2} \bar{\psi}_1 \psi_1 \\ &= \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 \left(1 + a_1 \bar{\psi}_1 \psi_1 + a_2 \bar{\psi}_2 \psi_2\right) \bar{\psi}_1 \psi_1 \\ &= a_2 . \end{aligned} \tag{B.8}$$

To completely evaluate expression (B.1) we calculate for the denominator

$$\begin{aligned} & \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 e^{a_1 \bar{\psi}_1 \psi_1 + a_2 \bar{\psi}_2 \psi_2} \\ &= \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 \left[1 + \frac{1}{2} \left(a_1 \bar{\psi}_1 \psi_1 + a_2 \bar{\psi}_2 \psi_2\right)^2\right] \\ &= \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_2 d\psi_2 \left[a_1 \bar{\psi}_1 \psi_1 a_2 \bar{\psi}_2 \psi_2\right] \\ &= a_1 a_2 . \end{aligned} \tag{B.9}$$

Then for the simplified version of expression (B.1) with only two possible configurations of ψ we find

$$\langle \bar{\psi}_1 \psi_1 \rangle = \frac{1}{a_1} . \tag{B.10}$$

It is straight forward to extend this result to cases with more than two field configurations. In the numerator the Taylor expansion of the exponential function will contribute a single term where all configurations of ψ_i appear once except the configuration of the integrand. According to the integratin rules for Grassmann

numbers we obtain

$$\int \prod_m d\bar{\psi}_m d\psi_m e^{\sum_m a_m \bar{\psi}_m \psi_m} (\bar{\psi}_i \psi_i) \quad (\text{B.12})$$

$$= \int \prod_m d\bar{\psi}_m d\psi_m \sum_n \left[\frac{(a_1 \bar{\psi}_1 \psi_1 + a_2 \bar{\psi}_2 \psi_2 + \dots)^n}{n!} \right] (\bar{\psi}_i \psi_i) \quad (\text{B.13})$$

$$= \prod_{m \neq i} a_m . \quad (\text{B.14})$$

For the denominator on the other hand we find all possible configurations. Therefore, we can write a generalized form of (B.11)

$$\langle \bar{\psi}_i \psi_i \rangle = \frac{\prod_{m \neq i} a_m}{\prod_m a_m} = \frac{1}{a_i} . \quad (\text{B.15})$$

We note that due to the integration rules (B.5) only terms where all field configurations appear exactly once are non-zero. Therefore if the action consists of a single summation of the form $\sum_m \bar{\psi}_m \psi_m$ only a single term can obey this requirement. Here it is important to note that for terms where each ψ_m is linear the factor $\frac{1}{n!}$ from the Taylor expansion will always cancel with a factor $n!$ from the multinomial theorem. Therefore the number of possible field configurations does not matter. We can now replace the summation over discrete indices m by an integral over a continuous variable k . For convenience we write from now on $\prod_m d\bar{\psi}_m d\psi_m = d(\bar{\psi}, \psi)$ and obtain

$$\langle \bar{\psi}(p) \psi(p) \rangle = \frac{\int d(\bar{\psi}(k), \psi(k)) (\bar{\psi}(p) \psi(p)) e^{\int a(k) \bar{\psi}(k) \psi(k) dk}}{\int d(\bar{\psi}(k), \psi(k)) e^{\int a(k) \bar{\psi}(k) \psi(k) dk}} = \frac{1}{a(p)} . \quad (\text{B.16})$$

B.2 Limitations

We now want to extend the calculation from the previous section such that the exponent contains two or more expressions e.g. $S = S_0 + S_I$. To obtain the nonzero terms we need to find those terms where each field configuration appears exactly once. Again we start with a simple example with only two allowed field configurations. We assume that S_I describes some arbitrary interaction

$$\begin{aligned} & \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_{-1} d\psi_{-1} e^{[a_1 \bar{\psi}_1 \psi_1 + a_{-1} \bar{\psi}_{-1} \psi_{-1}] + [b_{11} \bar{\psi}_1 \bar{\psi}_{-1} \psi_1 \psi_{-1}]} \bar{\psi}_1 \psi_1 \\ &= \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_{-1} d\psi_{-1} [a_{-1} \bar{\psi}_{-1} \psi_{-1}] \bar{\psi}_1 \psi_1 \\ &= a_{-1} . \end{aligned} \quad (\text{B.17})$$

For the denominator we then find

$$\begin{aligned} & \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_{-1} d\psi_{-1} e^{[a_1 \bar{\psi}_1 \psi_1 + a_{-1} \bar{\psi}_{-1} \psi_{-1}] + [b_{11} \bar{\psi}_1 \bar{\psi}_{-1} \psi_1 \psi_{-1}]} \\ &= \int d\bar{\psi}_1 d\psi_1 d\bar{\psi}_{-1} d\psi_{-1} [a_1 a_{-1} \bar{\psi}_1 \psi_1 \bar{\psi}_{-1} \psi_{-1} + b_{11} \bar{\psi}_1 \bar{\psi}_{-1} \psi_1 \psi_{-1}] \\ &= a_1 a_{-1} - b_{11} \end{aligned} \quad (\text{B.18})$$

and the average becomes

$$\langle \bar{\psi}_1 \psi_1 \rangle = \frac{a_{-1}}{a_1 a_{-1} - b_{11}} . \quad (\text{B.19})$$

We will now look at the same example but allow four different field configurations. In addition we assume that the quartic term S_I describes antiparallel field configurations only i.e. $\bar{\psi}_1 \bar{\psi}_{-2} \psi_2 \psi_{-1} = 0$. We then find

$$\int d(\bar{\psi}, \psi) e^{\left[\sum_{n=-2}^2 a_n \bar{\psi}_n \psi_n + \sum_{i,j=1}^2 b_{ij} \bar{\psi}_i \bar{\psi}_{-i} \psi_j \psi_{-j} \right]} \bar{\psi}_1 \psi_1 . \quad (\text{B.20})$$

We then extract all terms where each field configuration appears once and obtain

$$\begin{aligned} &= \int d(\bar{\psi}, \psi) \left[a_2 a_{-1} a_{-2} (\bar{\psi}_2 \psi_2 \bar{\psi}_{-1} \psi_{-1} \bar{\psi}_{-2} \psi_{-2}) (\bar{\psi}_1 \psi_1) \right. \\ &+ \left. b_{22} a_{-1} (\bar{\psi}_2 \bar{\psi}_{-2} \psi_2 \psi_{-2} \bar{\psi}_{-1} \psi_{-1}) (\bar{\psi}_1 \psi_1) \right] \\ &= a_2 a_{-1} a_{-2} - b_{22} a_{-1} . \end{aligned} \quad (\text{B.21})$$

Due to the special form of S_I the quartic term contributes only one term. All others vanish due to $\psi_1 \psi_1 = 0$. We also note that the presence of a single $b_{i,j}$ will flip the sign. If we do the same for the denominator we find

$$a_1 a_2 a_{-1} a_{-2} - a_1 a_{-1} b_{22} - a_2 a_{-2} b_{11} + b_{11} b_{22} + b_{12} b_{21} . \quad (\text{B.22})$$

If we group terms together we can write for the average

$$\langle \bar{\psi}_1 \psi_1 \rangle = \frac{a_{-1} (a_2 a_{-2} - b_{22})}{a_1 a_{-1} (a_2 a_{-2} - b_{22}) - b_{11} (a_2 a_{-2} - b_{22}) + b_{12} b_{21}} \quad (\text{B.23})$$

$$= \frac{a_{-1} (a_2 a_{-2} - b_{22})}{(a_1 a_{-1} - b_{11}) (a_2 a_{-2} - b_{22}) + b_{12} b_{21}} . \quad (\text{B.24})$$

Unfortunately the obtained averages for 2 and 4 field configurations are not the same. We see that the first part of expression (B.24) resembles the result found in (B.19). However, the additional term $b_{12} b_{21}$ in the denominator does

not cancel. When we allow 6 possible field configurations we obtain the result

$$\langle \bar{\psi}_1 \psi_1 \rangle = \frac{a_{-1} [(a_2 a_{-2} - b_{22})(a_3 a_{-3} - b_{33}) + b_{23} b_{32}]}{(a_1 a_{-1} - b_{11}) [(a_2 a_{-2} - b_{22})(a_3 a_{-3} - b_{33}) + b_{23} b_{32}] + A} \quad (\text{B.25})$$

with

$$A = b_{12} b_{21} a_3 a_{-3} + b_{13} b_{31} a_2 a_{-2} - b_{12} b_{21} b_{33} - b_{13} b_{31} b_{22} - b_{12} b_{23} b_{31} - b_{21} b_{13} b_{32} . \quad (\text{B.26})$$

Compared to the previous cases we note that the additional factor that does not cancel is growing with the number of allowed field configurations. If we would replace the discrete summation in (B.20) by an integral over a large number of field configurations, the factor A in the denominator would consist of an even larger number of terms.

It is therefore not possible to analytically solve path integrals that emerge in loop corrections discussed in section 4.7.2. We note that the complications originate in our definition of the effective action in section 4.3.1. This means that the ability to determine the fixed point of a system with interactions comes with the restriction that the RG flow analysis is limited to tree level. Whether this limitation can be circumvented will be subject of further studies.