Phase structure and critical properties of an abelian gauge theory

by

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Abstract

The main new results are presented in the form of three papers at the end of this thesis. The main topic is Monte-Carlo studies of the phase structure and critical properties of the phenomenological Ginzburg-Landau model, i.e. an abelian gauge theory. However, the first paper is totally different and deals with microscopic theory for lattice-fermions in a magnetic field.

Paper I is about "Fermion-pairing on a square lattice in extreme magnetic fields". We consider the Cooper-problem on a two-dimensional, square lattice with a uniform, perpendicular magnetic field. Only rational flux fractions are considered. An extended (real-space) Hubbard model including nearest and next nearest neighbor interactions is transformed to "k-space", or more precisely, to the space of eigenfunctions of Harper's equation, which constitute basis functions of the magnetic translation group for the lattice. A BCS-like truncation of the interaction term is performed. Expanding the interactions in the basis functions of the irreducible representations of the point group $C_{4\nu}$ of the square lattice simplify calculations. The numerical results indicate enhanced binding compared to zero magnetic field, and thus re-entrant superconducting pairing at extreme magnetic fields, well beyond the point where the usual semi-classical treatment of the magnetic field breaks down.

Paper II is about the "Hausdorff dimension of critical fluctuations in abelian gauge theories". Here we analyze the geometric properties of the line-like critical fluctuations (vortex loops) in the Ginzburg-Landau model in zero magnetic background field. By using a dual description, we obtain scaling relations between exponents of geometric and thermodynamic nature. In particular we connect the anomalous scaling dimension η of the dual matter field to the Hausdorff- or fractal dimension D_H of the critical fluctuations, in the original model. We also discuss the connection between the values of η and D_H, and the possibility of having a thermodynamic transition in finite background field.

Paper III is about "The order of the metal to superconductor transition". Here we present results from large-scale Monte Carlo simulations on the full Ginzburg-Landau model, including fluctuations in the amplitude and the phase of the matter-field, as well as fluctuations of the non-compact gauge-field of the theory. From this we obtain a precise critical value of the Ginzburg-Landau parameter $\kappa_{\rm tri}$ separating a first order metal to superconductor transition from a second order one, $\kappa_{\rm tri} = (0.76 \pm 0.04)/\sqrt{2}$. This agrees remarkably well with earlier analytical results based on a disorder theory of the superconductor to metal transition, where the value $\kappa_{\rm tri} = 0.798/\sqrt{2}$ was obtained. To achieve this, we have done careful infinite volume and continuum limit extrapolations. We argue that $\kappa_{\rm tri}$ is also the value that separates type-I from type-II behavior.

Preface

This thesis is submitted to the Norwegian University of Science and Technology (NTNU) in partial fulfillment of the requirements for the Norwegian academic degree *Doktor ingeniør*. The work has been carried out at the Department of Physics at NTNU where I was fully employed from February 1998 to December 2001. During this period I have spent one year taking courses and nearly one year assisting in the teaching of undergraduate students.

The thesis is organized in two parts.

Part I Introduction

In Chapter 1, 2, 3, and 4 I give a rather short introduction to superconductivity, microscopic theory, phase transitions, and Monte Carlo simulations. This is mostly meant for non-specialists and new students in the field, and I also give some references to relevant literature for further reading. Chapter 2 is about microscopic theory and the main topic is Cooper pairing in different settings, but I also give a short introduction to the Hofstadter problem of lattice fermions on a square lattice in a perpendicular magnetic field. This chapter is intended to help the understanding of Paper I and is thus a bit aside of the main topic in the thesis which is phase transitions and critical phenomena. Chapter 3 is about phase transitions, and here I give a short introduction to the important concepts of spontaneous symmetry breaking, scaling, and renormalization. In the last section I stress some of the main differences between first order and second order phase transitions. Chapter 4 is about Monte-Carlo simulations and is meant to give a short elementary introduction to this field. I also introduce the important, but somewhat more advanced, topic of reweighting.

Chapter 5, 6, and 7, are more closely related to the specific projects I have worked on, are meant to illuminate and clarify some aspects in Paper II and Paper III. Chapter 5 deals with the Ginzburg-Landau model. Here I introduce the model and some of the various parametrizations of it, present some perturbative (mean-field) results, and introduce the concept of topological defects (vortices) and duality. Chapter 6 is closely related to Paper II and introduce the concept of fractal dimension and the relation between the vortex excitations of the original theory and the dual field theory. Chapter 7 is closely related to Paper III where we studied the order of the metal to superconductor phase transition. To do this we had to do careful infinite volume and continuum limit extrapolations. We also had to consider ultraviolet renormalization since the Ginzburg-Landau theory is a continuum field theory with no inherent short scale cut-off. To reduce auto-correlation times we added several improvements to the standard Metropolis algorithm in the Monte-Carlo simulations, the most important improvement being an overrelaxation algorithm for the scalar field and a global update of the scalar amplitude.

Part II Papers

See the list at page vii.

Acknowledgments

First of all I want to thank my supervisor Professor Asle Sudbø for giving me a number of very challenging and interesting problems during these years. His enthusiasm for the field and ability to explain the physics behind the formulas have been highly appreciated.

I will also thank my colleagues in the Superconductivity Group at NTNU for many interesting discussions and a pleasant environment: Professor Kristian Fossheim, Dr. Sai-Kong Chin, Dr. Anh Kiet Nguyen, Dr. John Ove Fjærestad, Dr. Jørgen Nyhus, Joakim Hove, Ulrik Thisted, Jo Smiseth, and Eivind Smørgrav. Here I will specially thank Jo for proofreading the manuscript and in particular Joakim which I have worked closely together with on the simulation problems. The cooperation has been very fruitful, and also the help with different computer problems has been highly appreciated.

There have also been many project and diploma students connected to our group during these years contributing to the good environment. Here I will specially thank Håvard Alnes for asking many interesting questions during his diploma work.

In May 2001 Joakim and I visited Dr. Kari Rummukainen at the Nordic Institute for Theoretical Physics (NORDITA) in Copenhagen. This visit was very inspiring and instructive for us, since Kari is an expert on lattice gauge simulations and knows all the technical details of the art of performing such simulations. The help we got greatly improved our ability to extract data from our simulations and the software we got for Ferrenberg-Swendsen reweighting in fact made it possible to finish our last project, at least in a reasonable amount of time.

I also thank the Norwegian Research Council via Grant No. 124106/410 and the High Performance Computing Program, and Department of Physics at NTNU for financial support.

List of papers

I *Fermion-pairing on a square lattice in extreme magnetic fields*,
Sjur Mo and Asle Sudbø,
Submitted to Phys. Rev. B,
e-print: cond-mat/0111279.
(See page 67)

II *Hausdorff dimension of critical fluctuations in abelian gauge theories*,
Joakim Hove, Sjur Mo and Asle Sudbø,
Phys. Rev. Lett. **85**, 2368 (2000),
e-print: cond-mat/0008112.
(See page 77)

III *The order of the metal to superconductor transition*,
Sjur Mo, Joakim Hove, and Asle Sudbø,
Submitted to Phys. Rev. B,
e-print: cond-mat/0109260.
(See page 83)

Contents

Part I

Introduction

Chapter 1

Introduction to superconductivity

Superconductivity and superfluidity are among the most fascinating phenomena in Nature. The reason is that quantum coherence effects are observable on a truly macroscopic scale. This quantum behavior causes spectacular and strange effects such as zero resistivity, perfect diamagnetism (Meissner-effect), flux quantization, and Josephson tunneling in superconductors and zero viscosity in superfluids, i.e. ^{3}He and ^{4}He. Superconductivity was discovered already in 1911 by Kammerlingh Onnes [118], but it took almost fifty years before a satisfactory theoretical explanation was achieved. In 1957 Bardeen, Cooper and Schrieffer proposed a complete microscopic theory of superconductivity, the famous BCS-theory [11]. This is without doubt one of the most successful, if not *the* most successful, theories of condensed matter physics. They showed that superconductivity in conventional metallic superconductors was caused by pairs of fermions ("Copper pairs") with an effective *attractive* interaction. The pairs condense, with some analogies to Bose-Einstein condensation, into the superconducting phase. New materials with higher critical temperature T_c were found during the years, reaching an apparent barrier of $T_c \simeq 23$ K in the alloy Nb_3Ge. This barrier was broken in 1986 when Bednorz and Müller discovered superconductivity with an onset of $T_c \simeq 30$ K in the cuprate oxide $La_{2-x}Ba_xCuO_4$ [13]. The critical temperature was later increased to $T_c \simeq 38$ K. Soon after, superconductivity in other cuprates was also found and the "high-T_c revolution" was started. Already in 1987 a T_c of ~ 92 K, which is above that of liquid nitrogen, was discovered in $YBa_2Cu_3O_{7-\delta}$. These discoveries opened a whole new field of research and the "world-record" today is $T_c \simeq 133$ K in some mercury based cuprate. See e.g. [38, 143] for more details.

The high-T_c-materials all have in common a structure with planes of copper oxide which are assumed to dominate the superconducting properties. Between the planes are ions like La, Y, Ba, and Th serving as charge reservoirs. The materials are typically hole-doped antiferromagnetic insulators that become metallic upon doping. A typical phase diagram in the doping-temperature plane is shown schematically in Fig. 1.1 on the following page.

There is still, 15 years after the discovery, no accepted *microscopic* theory explaining the high-T_c superconductivity. Spin-singlet Cooper pairs seem to be essential, but the order parameter/gap seems to have d-wave symmetry in contrast to the s-wave symmetry found in conventional superconductors. This was experimentally shown by van Harlingen [61] and Tsuei *et al.* [144]. In addition the "normal" state is very different from the metallic state in the conventional superconductors. This indicates that a description in terms of a normal Fermi liquid may be inadequate due to strong fermion-fermion correlations as realized by P. W. Anderson already in 1987 [8]. For more references see e.g. [51]. It is claimed that the most difficult problem may be to understand the unusual "normal" phase of these materials, when this is achieved the understanding of the superconducting phase may be comparable simpler. Despite these fundamental and difficult problems it must be said that even if no microscopic theory has become accepted many interesting properties of the materials can be studied theoretically. At a phenomenological level different variants of the Ginzburg-Landau model [55] work well and have been extensively studied in the latest years.

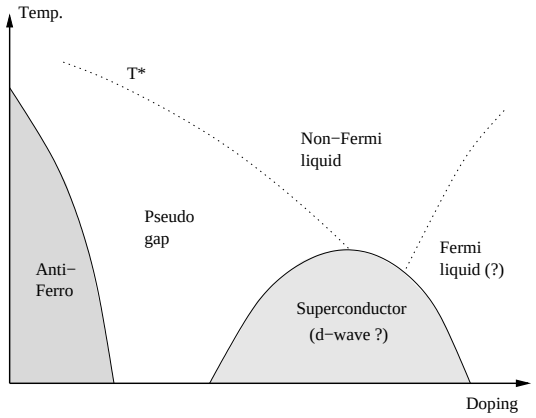

Figure 1.1: Schematic phase diagram for a high-T_c superconductor in the doping-temperature plane. Here *Anti-ferro* is an abbreviation for the anti-ferromagnetic phase (see [32]) and T^* is the temperature where Cooper-pairs start to *form*. This temperature must not be confused with the superconducting transition temperature T_c which is the temperature where the pairs start to *condense*.

The high-T_c cuprates are extreme type-II superconductors and have very large fluctuation effects compared to conventional superconductors and also compared to most other condensed matter systems. This makes them perfect systems for the study of phase transitions and critical phenomena. The strong fluctuation effects are related to the fact that the high-T_c cuprates are strong coupling superconductors arising out of doped Mott-Hubbard insulators. The latter fact gives rise to a low superfluid density ρ_s and thus a low phase stiffness since

$$\rho_s \sim \frac{\partial^2 f}{\partial(\Delta\theta)^2}, \tag{1.1}$$

where $\Delta\theta$ is a twist in the superconducting order parameter over the size of the system, and f is the free energy density. The strong coupling effects give rise to a large T_c and thus increased thermal fluctuations. In Paper II [71] and Paper III [108] we have done Monte Carlo simulation on the Ginzburg-Landau model to study the fluctuation effects in a non-perturbative manner and this is the topic of the main part of this thesis. However the next chapter is devoted to microscopic theory and gives an introduction to the Cooper problem in zero magnetic field. The same problem in non-zero field is studied in Paper I [109].

Chapter 2

Microscopic theory

The BCS theory of superconductivity [11] is a striking success of quantum theory of solids. It accounts for the essential effects associated with superconductivity in an ingenious and higly nontrivial manner. The essential mechanism is an effective *attractive* interaction between electrons. In conventional superconductors the attraction is caused by indirect interactions between electrons mediated by phonons. One electron polarizes the medium and leaves a net positive charge in a region, a second electron is attracted to this region. This is possible since the ions relax relatively slowly compared to the fast moving electrons, thereby allowing the first electron to disappear before the second electron enters the region. By waiting just long enough, i.e. not so long that the ions have relaxed, this attraction can be larger than the (screened) Coulomb repulsion. The phonon mediated interaction is however not essential for the BCS-theory as such. The important thing is the possibility of effective attractive interactions, not the microscopic mechanism causing them.

The first suggestion that unusual properties would result from such an attraction was made by Cooper [34]. In the next section I will give a short review of this, for more details see e.g. the textbooks [38, 43, 83, 135, 143]. To prepare for Paper I [109], I also give a short introduction to the Cooper problem on a two-dimensional square lattice for zero magnetic field ($B = 0$), and to the problem of non-interacting electrons on the same lattice with a perpendicular field ($B \neq 0$), the so called Harper [62] or Hofstadter [70] problem.

2.1 Cooper pairs

Suppose that we have an inert Fermi sea at zero temperature ($T = 0$) and zero external magnetic field ($B = 0$). Add two electrons of opposite momenta and opposite spins just above the Fermi surface as shown in Fig. 2.1. These two electrons interact with each other, but not with the

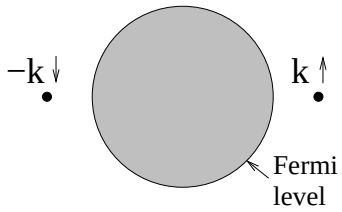

Figure 2.1: A Cooper pair is made up of two electrons with opposite momenta and opposite spins ($\boldsymbol{k}\uparrow$, $-\boldsymbol{k}\downarrow$) on top of an inert Fermi sea.

electrons in the sea, except via the exclusion principle. The two-particle wave function can be

expanded in a sum of non-interacting two-particle states, i.e. simply plane waves, as

$$\psi(\boldsymbol{r}_1, \boldsymbol{r}_2) = \sum_{\boldsymbol{k}} a_{\boldsymbol{k}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}_1} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_2}. \tag{2.1}$$

Assuming a spin-singlet pair gives an anti-symmetric spin wave function and thereby a symmetric spatial wave function

$$\psi(\boldsymbol{r}_1 - \boldsymbol{r}_2) = \sum_{k>k_F} a_{\boldsymbol{k}} \cos[\boldsymbol{k}\cdot(\boldsymbol{r}_1 - \boldsymbol{r}_2)]. \tag{2.2}$$

By inserting this into the Schrödinger equation of the problem, $(H_0 + V)\psi = E\psi$, where $H_0 = \frac{\boldsymbol{p}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$, one can show that the coefficients $a_{\boldsymbol{k}}$ and the energy eigenvalue E are to be determined by solving

$$(E - 2\epsilon_{\boldsymbol{k}})a_{\boldsymbol{k}} = \sum_{|\boldsymbol{k}'|>k_F} V_{\boldsymbol{k},\boldsymbol{k}'} a_{\boldsymbol{k}'}. \tag{2.3}$$

Here $\epsilon_{\boldsymbol{k}} = \frac{\hbar^2 k^2}{2m}$ is the energy of a free electron,

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \frac{1}{\Omega}\int d\boldsymbol{r}\; V(\boldsymbol{r}) e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \tag{2.4}$$

is a matrix element of the interaction potential (see Fig. 2.2), Ω is the normalization volume, and $\boldsymbol{r}$ is the distance between the two electrons. For conventional superconductors the interaction can

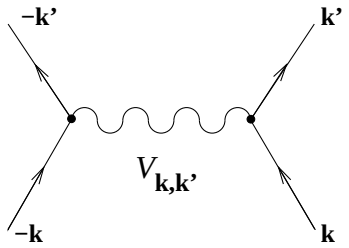

Figure 2.2: Diagram representing the interaction $V_{\boldsymbol{k},\boldsymbol{k}'}$ spreading a pair from the state labeled by $(-\boldsymbol{k}, \boldsymbol{k})$ to $(-\boldsymbol{k}', \boldsymbol{k}')$. The interaction term is a function of the difference $\boldsymbol{k} - \boldsymbol{k}'$, i.e. $V_{\boldsymbol{k},\boldsymbol{k}'} = V(\boldsymbol{k} - \boldsymbol{k}')$.

be treated as approximately wave-vector independent, i.e. $V_{\boldsymbol{k},\boldsymbol{k}'} = -V$, for $\boldsymbol{k}$-states in the interval $|\epsilon_{\boldsymbol{k}} - E_F| \leq \hbar\omega_D$, where $\hbar\omega_D$ is the Debye-energy and $E_F = \frac{\hbar^2 k_F^2}{2m}$ is the Fermi energy. Then

$$a_{\boldsymbol{k}} = V\frac{\sum_{|\boldsymbol{k}'|>k_F} a_{\boldsymbol{k}'}}{2\epsilon_{\boldsymbol{k}} - E}, \tag{2.5}$$

which gives

$$\frac{1}{V} = \sum_{|\boldsymbol{k}|>k_F} \frac{1}{2\epsilon_{\boldsymbol{k}} - E} \tag{2.6}$$

by summing over $\boldsymbol{k}, (|\boldsymbol{k}| > k_F)$. By replacing the summation over $\boldsymbol{k}$ by an energy integration and measuring the energy relative to the Fermi level, i.e. $E - 2E_F \to E$, we get

$$\frac{1}{V} = N(0)\int_0^{\hbar\omega_D} \frac{d\epsilon}{2\epsilon - E} = \frac{1}{2}N(0)\ln\frac{E - 2\hbar\omega_D}{E}, \tag{2.7}$$

where $N(0)$ is the density of states at the Fermi level. For $N(0)V \ll 1$ thus

$$E \approx -2\hbar\omega_D e^{-2/N(0)V}, \tag{2.8}$$

and the electrons are bound since the energy is negative. What is unusual is that the pairs bind *independent* of the strength of the attraction. Normally two particles which attract will not bind unless the attraction is stronger than some lower limit.

For high-T_c superconductors the interaction $V_{\boldsymbol{k},\boldsymbol{k}'}$ may depend on the direction of $\boldsymbol{k}$ and $\boldsymbol{k}'$ since the pairing is assumed to have d-wave symmetry rather than s-wave symmetry. A transformation to energy-integration will then normally be impossible, and the equation must be solved numerically in a self-consistent manner. However if the interaction represented by the diagram in Fig. 2.2 on the preceding page is separable in "before" and "after" variables, as in Eq. 2.12c, the problem is easier to solve.

In the above treatment we have assumed that we can distinguish one pair of electrons from the rest of the electrons. This is of course not possible in a real many-particle system, since the electrons are identical particles, and the complicated many-particle problem must be solved in a self-consistent way. Still, the forming of Cooper pairs is essential for the understanding of this problem. In the full BCS-theory [11] pairs are formed until the Fermi sea is so much altered that the energy gain by making another pair becomes zero. Thus the problem of calculating the expectation value $\langle c_{\boldsymbol{k}\uparrow} c_{-\boldsymbol{k}\downarrow}\rangle$, which is order parameter like, must be solved in a self-consistent manner. I have neither time nor space to go into more details here, for more details see e.g. the textbooks [83, 135, 143]. In the next section I will consider the Cooper problem on a lattice. The treatment is limited to a square lattice in two dimensions.

2.2 Hubbard model

Since most of the physics in the high-T_c cuprates is assumed to take place in the copper-oxide planes a two-dimensional description should be adequate for most purposes. An often used model is the Hubbard-model

$$H = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma} \right) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} \tag{2.9}$$

where $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$ are creation and annihilation operators for fermions (electrons or holes) in Wannier orbitals with spin σ at lattice site i, $n_{i,\sigma} = c^\dagger_{i,\sigma} c_{i,\sigma}$ is the number operator, and $\langle i,j\rangle$ denotes all pairs of nearest neighbor sites i and j. The first term describes hopping between neighbors while the second describes on-site Coulomb interactions. The model can be extended with more distant neighbor hopping and interactions.

2.2.1 Cooper pairing on a square lattice

To prepare for the treatment of Cooper pairing in a plane with a perpendicular magnetic field (Paper I [109]), I here give a short review of the problem in zero field. For more details see [121,122]. The extended Hubbard model is defined by

$$\begin{aligned} H = & -t \sum_{\langle i,j\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - t' \sum_{\langle\langle i,j\rangle\rangle,\sigma} c^\dagger_{i,\sigma} c_{j,\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} \\ & + \frac{1}{2} \left[U \sum_i n_{i,\uparrow} n_{i,\downarrow} + V \sum_{\langle i,j\rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} + W \sum_{\langle\langle i,j\rangle\rangle,\sigma,\sigma'} n_{i,\sigma} n_{j,\sigma'} \right] \end{aligned} \tag{2.10}$$

where $\langle i,j\rangle$ and $\langle\langle i,j\rangle\rangle$ denote nearest and next nearest neighbor pairs respectively. No particular microscopic mechanism is considered, but it is assumed that the different interactions U, V, and W can be either repulsive or attractive. By transforming to a plane-wave basis given by

$$c_{\boldsymbol{k},\sigma} = \frac{1}{\sqrt{N}} \sum_j e^{-i\boldsymbol{k}\cdot\boldsymbol{r}_j} c_{j,\sigma}, \tag{2.11}$$

where N is the number of lattice sites, and doing a standard BCS truncation, where only states with opposite spins and wave vectors interact as in Fig. 2.2 on page 6, the Hamiltonian can be written as

$$H = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} c^\dagger_{\boldsymbol{k},\sigma} c_{\boldsymbol{k},\sigma} + \sum_{\boldsymbol{k},\boldsymbol{k}'} V_{\boldsymbol{k},\boldsymbol{k}'} c^\dagger_{\boldsymbol{k},\uparrow} c^\dagger_{-\boldsymbol{k},\downarrow} c_{-\boldsymbol{k}',\downarrow} c_{\boldsymbol{k}',\uparrow}. \tag{2.12a}$$

Here (after rescaling of t' and μ)

$$\epsilon_{\boldsymbol{k}} = -2t[\cos(k_x) + \cos(k_y) - 2t' \cos(k_x)\cos(k_y) - (2 - 2t' - \mu)] \tag{2.12b}$$

is the spectrum for non-interacting electrons, and

$$V_{\boldsymbol{k},\boldsymbol{k}'} = \sum_{\eta=1}^{5} \lambda_\eta B_\eta(\boldsymbol{k}) B_\eta(\boldsymbol{k}') \tag{2.12c}$$

is the interaction term where $\boldsymbol{\lambda} = (\frac{U}{2}, V, W, V, W)$ and the set $\{B_\eta(\boldsymbol{k})\}$ forms a basis[1] for the irreducible representations of the symmetry group C_{4v} of the square lattice. The set is finite due to the short range of the interactions.

For the non-interacting case we define a two-particle state $|\boldsymbol{k},\sigma;-\boldsymbol{k},-\sigma\rangle_0$ obeying the Schrödinger equation

$$H_0|\boldsymbol{k},\sigma;-\boldsymbol{k},-\sigma\rangle_0 = 2\epsilon_{\boldsymbol{k}}|\boldsymbol{k},\sigma;-\boldsymbol{k},-\sigma\rangle_0. \tag{2.13}$$

By using $|\boldsymbol{k},\sigma;-\boldsymbol{k},-\sigma\rangle_0$ as a basis for the general case, a two-particle state can be written as

$$|1,2\rangle = \sum_{k>k_F,\sigma} a_{\boldsymbol{k},\sigma} |\boldsymbol{k},\sigma;-\boldsymbol{k},-\sigma\rangle_0, \tag{2.14}$$

where the exact two-particle state obeys the Schrödinger equation

$$(H_0 + H_{\rm int})|1,2\rangle = E|1,2\rangle. \tag{2.15}$$

By inserting Eq. 2.14 in Eq. 2.15 and using Eq. 2.12c we get

$$\sum_\eta B_\eta(\boldsymbol{k}') \underbrace{\sum_{k>k_F} \lambda_\eta a_{\boldsymbol{k}} B_\eta(\boldsymbol{k})}_{\equiv A_\eta} = (E - 2\epsilon_{\boldsymbol{k}'}) a_{\boldsymbol{k}'}, \tag{2.16}$$

where now the spin index is neglected since the energy is spin independent. The expansion coefficients $a_{\boldsymbol{k}}$ are then given by

$$a_{\boldsymbol{k}} = \frac{\sum_\eta A_\eta B_\eta(\boldsymbol{k})}{E - 2\epsilon_{\boldsymbol{k}}}, \quad \epsilon_{\boldsymbol{k}} > \epsilon_{k_F}. \tag{2.17}$$

[1] The basis $\{B_\eta(\boldsymbol{k})\}$ is given by

$$\begin{aligned}
B_1(\boldsymbol{k}) &= \frac{1}{\sqrt{N}} \\
B_2(\boldsymbol{k}) &= \frac{1}{\sqrt{N}}(\cos(k_x) + \cos(k_y)) \\
B_3(\boldsymbol{k}) &= \frac{2}{\sqrt{N}}(\cos(k_x)\cos(k_y)) \\
B_4(\boldsymbol{k}) &= \frac{1}{\sqrt{N}}(\cos(k_x) - \cos(k_y)) \\
B_5(\boldsymbol{k}) &= \frac{2}{\sqrt{N}}(\sin(k_x)\sin(k_y)).
\end{aligned}$$

The reason for the number $\eta \leq 5$ is that the gap must be symmetric for $\vec{k} \to -\vec{k}$. Without this symmetry one may have to include both even and odd symmetries, then $\eta \leq 9$.

This can then be inserted back in the Schrödinger equation 2.16 and we get the equation

$$\sum_{\eta'} \lambda_{\eta'} B_{\eta'}(\boldsymbol{k}') \sum_{\eta} A_{\eta} \underbrace{\sum_{k>k_F} \frac{B_{\eta}(\boldsymbol{k}) B_{\eta'}(\boldsymbol{k}')}{E - 2\epsilon_{\boldsymbol{k}}}}_{\equiv D_{\eta\eta'}(E)} = \sum_{\eta'} A_{\eta'} B_{\eta'}(\boldsymbol{k}'). \tag{2.18}$$

By using the linear independence of the functions $\{B_{\eta}(\boldsymbol{k})\}$ we get

$$\sum_{\eta} A_{\eta} \underbrace{\lambda_{\eta'} D_{\eta\eta'}(E)}_{\equiv T_{\eta\eta'}(E)} = A_{\eta'}, \tag{2.19}$$

which can be written in terms of vectors as

$$[\mathsf{T}(E) - \mathbb{1}]\boldsymbol{A} = 0. \tag{2.20}$$

This equation has a solution only for such values of the energy E that the determinant vanishes, i.e. $\det(\mathsf{T}(E) - \mathbb{1}) = 0$. By defining $\chi_{\boldsymbol{k}} = 1/(E - 2\epsilon_{\boldsymbol{k}})$ and using that $\chi_{\boldsymbol{k}}$ transforms as an s-wave and in addition using the orthogonality properties of the set $\{B_{\eta}(\boldsymbol{k})\}$ we can conclude that the wave function must have *either* s-wave or d-wave symmetry, i.e.

$$a_{\boldsymbol{k}}^{\text{s-wave}} = \sum_{\eta=1}^{3} A_{\eta} B_{\eta}(\boldsymbol{k}), \quad a_{\boldsymbol{k}}^{\text{d-wave}} = \sum_{\eta=4}^{5} A_{\eta} B_{\eta}(\boldsymbol{k}); \quad \epsilon_{\boldsymbol{k}} > \epsilon_{k_F}. \tag{2.21}$$

The real space Cooper wave function (in the center of mass system) can be found by an inverse lattice Fourier transform

$$\psi(\boldsymbol{r}) = \frac{1}{N} \sum_{k_x=0}^{n_k-1} \sum_{k_y=0}^{n_k-1} a_{\boldsymbol{k}} \exp\left(i \frac{2\pi}{n_k} \boldsymbol{k} \cdot \boldsymbol{r}\right) \tag{2.22}$$

where $\boldsymbol{r}$ is the vector between the two electrons comprising the Cooper pair and $\boldsymbol{k} = (k_x, k_y)$.

For low magnetic fields the behavior of the system can be estimated by treating the field in a perturbative manner. By using the zero field correlation length one can find a value for the upper critical field H_{c2}. The limitations of this approach is that it neglects the change in the wave-functions of the Cooper pairs due to the magnetic field. For very large magnetic fields, a more appropriate approach to the problem is to solve the single-particle spectrum first in the presence of the magnetic field, and then introduce the pairing interaction as a singular perturbation on this problem as done in Paper I [109]. That problem is more involved since a plane-wave basis no longer is a suitable starting point. In the next section I give a short introduction to the single-electron spectrum and wave-functions in this setting.

2.3 Hofstadter's butterfly

The spectral properties of electrons in a spatially periodic potential have been studied since the early days of quantum mechanics. The well known Bloch form of the eigenfunctions

$$\psi_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r}) e^{i\boldsymbol{k}\cdot\boldsymbol{r}}, \quad u_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{R}) = u_{\boldsymbol{k}}(\boldsymbol{r}), \tag{2.23}$$

where $\boldsymbol{R}$ is a lattice vector, is a consequence of invariance under lattice translations. Using group theory this can be formally proven, see e.g. [74, 83]. Likewise the eigenstates of electrons living in a continuumin a constant magnetic field ($B \neq 0$) give the well known Landau levels. These eigenstates are the quantum mechanical analogues of classical electrons with circular motion. The electrons only propagate in the direction parallel to the field. The problem is much more peculiar for electrons living in both a periodic potential and a magnetic field. This problem can also be

treated by group theory, but now one has to consider *magnetic translations* on a lattice. The eigenfunctions of the Schrödinger equation for this problem constitute a basis for the irreducible representations of the magnetic translation group. This formal treatment was introduced by Brown [27,28] and Zak [154,155]. It turns out that this is one of the few places in physics where the difference between rational and irrational numbers is important. In this problem we have two competing length scales: (1) the period of the potential, which is equal to the lattice spacing a, and (2) the magnetic length $\ell_{\rm magn} = \sqrt{\hbar/eB}$. We will consider this problem for a two-dimensional lattice in the xy-plane with a magnetic field in the z-direction, $\boldsymbol{B} = B_z\hat{e}_z$. The competing length scales in general give frustration in the system, the only exceptions are when the flux piercing a plaquette in the lattice is a *rational* multiple of the elementary flux quantum $\phi_0 = h/e$, i.e.

$$\frac{\phi}{\phi_0} = \frac{Ba^2}{h/e} = \frac{a^2}{2\pi\ell_{\rm magn}^2} \equiv \frac{p}{q}. \tag{2.24}$$

It is only for rational $\frac{p}{q}$ the concept of a magnetic translation group is well defined, however here I will continue in a less formal way as in Paper I [109]. The Hamiltonian for non-interacting electrons living on a lattice is given by

$$H_0 = \sum_{i,\sigma}[\epsilon(\sigma) - \mu]c^\dagger_{i,\sigma}c_{i,\sigma} - t\sum_{\langle i,j\rangle,\sigma} e^{\theta_{ij}}c^\dagger_{i,\sigma}c_{j,\sigma} - t'\sum_{\langle\langle i,j\rangle\rangle,\sigma} e^{\theta_{ij}}c^\dagger_{i,\sigma}c_{j,\sigma}, \tag{2.25}$$

where μ is the chemical potential and t, t' are hopping amplitudes to the nearest and next nearest neighbors respectively. The Peierl's phase factor [124] for hopping from lattice site j to i is

$$\theta_{ij} \equiv -\frac{2\pi}{\phi_0}\int_j^i \boldsymbol{A}\cdot d\boldsymbol{\ell}. \tag{2.26}$$

By using the Landau-gauge $\boldsymbol{A} = Bx\hat{\boldsymbol{e}}_y$, introducing $g = 2\pi p/q = 2\pi Ba^2/\phi_0$ and setting $a = 1$ the phase factor can be written as

$$\theta_{ij} = \begin{cases} 0 & \text{if} \quad \boldsymbol{r}_i - \boldsymbol{r}_j = m\hat{\boldsymbol{e}}_x \\ g\frac{x_i+x_j}{2}n & \text{if} \quad \boldsymbol{r}_i - \boldsymbol{r}_j = m\hat{\boldsymbol{e}}_x + n\hat{\boldsymbol{e}}_y \end{cases} \tag{2.27}$$

where m, n are integers. Using this and writing the wave function as[2]

$$\psi_{\mu,\nu,\ell}(x_m, y_n) = \langle \boldsymbol{r}_m|\boldsymbol{\kappa}, l\rangle = e^{i(\mu x_m + \nu y_n)}u_{\mu,\nu,\ell}(x_m), \tag{2.28}$$

where we have introduced $\boldsymbol{\kappa} = (\mu, \nu)$, the Schrödinger equation can be written as

$$\begin{aligned} &- e^{i\mu}\left\{t + 2t'\cos[g(m+1/2)+\nu]\right\}u_{\mu,\nu,\ell}(x_{m+1}) \\ &- e^{-i\mu}\left\{t + 2t'\cos[g(m-1/2)+\nu]\right\}u_{\mu,\nu,\ell}(x_{m-1}) \\ &- \left\{2t\cos[gm+\nu]\right\}u_{\mu,\nu,\ell}(x_m) = \epsilon_{\mu,\nu,\ell}u_{\mu,\nu,\ell}(x_m). \end{aligned} \tag{2.29}$$

Here x is taken modulo q due to the periodicity for $m \to m+q$, i.e. $u(x)$ is the periodic part of the Bloch functions on the *magnetic lattice*. The equation can be written as a $q\times q$ matrix. It is easy to see that the equation is periodic for $\nu \to \nu+2\pi$. By introducing $\hat{u}_{\mu,\nu,\ell}(x_m) = e^{i\mu x_{(m \bmod q)}}u_{\mu,\nu,\ell}(x_m)$ it is easily shown that the equation for $\hat{u}_{\mu,\nu,\ell}(x_m)$ is periodic for $\mu \to \mu + 2\pi/q$. Since $x_m - x_{(m \bmod q)} = nq$ it is clear that $\psi_{\mu,\nu,\ell}(x_m, y_n)$ must have the same periodicity. The different eigenvalues are numbered with ℓ and each value corresponds to different Harper- or Hofstadter-bands. Eq. 2.29 is the well known Harper's equation which has been extensively studied especially for $t' = 0$, see e.g. [62,63,70,115,116,134,142] and [54, chapter 9]. The spectrum is the so called Hofstadters butterfly as shown (for t'=0) in the upper part of Fig. 2.3 on the next page. Here only rational fluxes with $q \le 40$ are shown and we observe that the energy bands split into q

[2] We have chosen the normalization $\sum_{i=1}^{N}|u_{\mu,\nu,\ell}(x_i)|^2 = 1$ where N is the number of lattice sites.

sub-bands. The lower part of this figure also shows the butterfly for a non-zero value of the next nearest neighbor hopping, i.e. $t' \neq 0$. It is clear that the additional possibility of next nearest neighbor hopping distorts the butterfly, but the number of sub-bands is still given by q, for more details see e.g. [60]. For irrational flux ratios the spectrum is a Cantor set [70].[3] In Paper I [109] pairs are made of electrons living in Hofstadter-bands. Thus the wave-functions in Eq. 2.28 replace the plane wave basis used in the zero field case, Eq. 2.11.

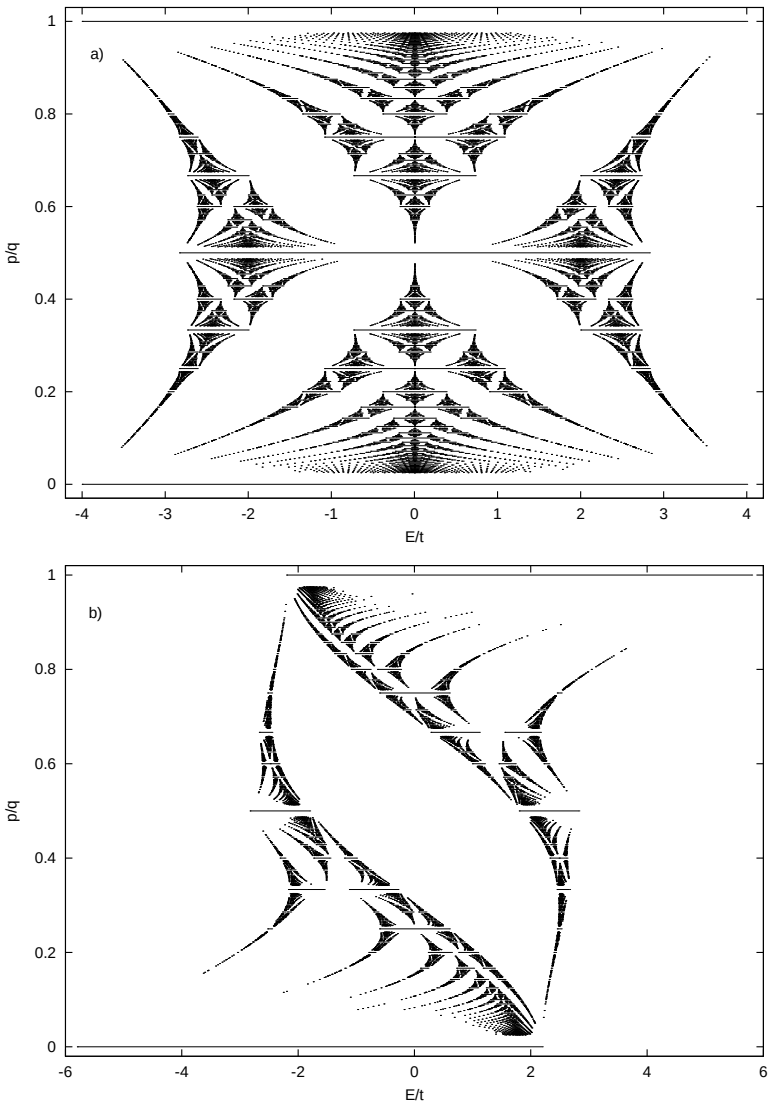

Figure 2.3: Hofstadter's butterfly for rational flux ratios $\phi/\phi_0 = p/q$ where $q \leq 40$. The next nearest to nearest neighbor hopping ratios are given by: a) $t'/t = 0$ and b) $t'/t = 0.45$.

[3]The Cantor set appears when one starts with the interval $[0, 1]$ and in the first step removes the interval $[\frac{1}{3}, \frac{2}{3}]$ from the middle. In the next step one removes one third from the middle of the remaining two intervals, and so on. The measure of the remaining set, after an infinite number of steps, is zero, and the fractal dimension is ≈ 0.63. The term Cantor set is often used more generally to describe every set with measure zero and fractal dimension less than unity.

Chapter 3

Phase transitions

When a large number ($N_A \sim 10^{23}$) of interacting particles are put together, many new and interesting phenomena emerge. This was stated as "More is different" in a famous paper by P. W. Anderson [7]. Phase transitions may be the most familiar such phenomena from our daily life, with the transitions in water as prime examples. In this chapter I will give a very short introduction to this field, for more details see e.g. some chapters in the general texts on statistical mechanics [31, 73, 123, 129] and the more specialized literature about critical phenomena, e.g. [5, 24, 30, 56, 75, 76, 104, 156]. In addition there are many review articles worth reading [19, 37, 50, 125, 136, 139, 150, 151].

We know that ice melts into water when we increase the temperature above $T_m = 0°\mathrm{C}$ and that water becomes vapor upon heating above $T_b = 100°\mathrm{C}$. At both of these phase transitions two phases coexist, respectively ice/water and water/steam. These phase transitions are associated with discontinuities in the internal energy, and a latent heat must be supplied. They are named first order or discontinuous phase transitions. Let us study the liquid–gas transition slightly more in detail, the phase diagram in the (T, p)-plane is shown in Fig. 3.1. If we increase the pressure and the temperature the density difference between the liquid and gaseous phases becomes smaller and the latent heat diminishes. Finally we reach a *critical point* ($T_c \simeq 374°\mathrm{C}$, $p_c \simeq 222$ atm) where the difference disappears. At this point the transition is classified as second order or continuous. At the critical point the behavior is strongly influenced by thermal fluctuations leading to a highly

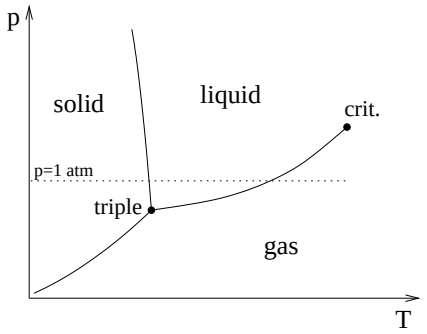

Figure 3.1: Schematic phase diagram for water. Here the point marked with *crit.* is the critical point and the point marked with *triple* is the triple point ($T_t = 0.01°\mathrm{C}$, $p_t \simeq 0.06$ atm).

correlated state with many unusual and interesting properties. The understanding of critical phenomena is among the most difficult problems in theoretical physics. The reason is that many-particle effects are essential and no clear separation of length scales is inherent in the problem. This differs from the normal situation one encounters in most physical problems where one or a few length scales dominate and dimensional analysis gives useful results. This normally means that one can integrate out fluctuations on shorter length scales and define effective theories for slowly

varying, low energy phenomena. A well known example is hydrodynamics where fluctuations at an atomic level can be neglected and only be incorporated in the values of the viscosity and other relevant parameters. Near phase transitions no such clear separation of length scales is possible since there are fluctuations on every length scale, from the microscopic scale to the correlation length, and the fluctuations on short scales influence the ones at larger scales. At critical points the correlation length goes to infinity and thus fluctuations spanning the whole system must be accounted for. Since fluctuations on *all* length scales have almost identical properties, the system becomes *self-similar* or *scale invariant*. This means that it looks similar at many length scales, a fact that is very important in the understanding of critical phenomena. The fluctuations give rise to singular behavior in many observables of the systems, such as diverging heat capacity and compressibility. The diverging correlation length is accompanied by a phenomena called critical slowing down. This is caused by a slowing down in the dynamics of a system related to the large number of local updates necessary to update portions of the system determined by the correlation length.

Even if the development of methods to analyze such systems with fluctuations on many length scales have been a major challenge to physicists, the diverging correlation length also leads to some important simplifications. The point is that most of the microscopic details of a particular system will not influence the large scale properties at the critical point. This is called universality, and a coarse-grained description in terms of an effective theory with an order parameter field is often possible. This order parameter can be the magnetization for spin systems or the density difference between liquid and gas. Models with totally different microscopic description may belong to the same universality class if they have the same dimensionality and the order parameter has the same symmetry. Spontaneous symmetry breaking occurs when an invariance of the Hamiltonian of a physical system is not an invariance of its ground state. This extremely important concept in modern physics will be introduced in the next section.

3.1 Spontaneous symmetry breaking

The first part of this section is based on the very clear expositions of these matters in [128]. In statistical mechanics and quantum field theory, the (macroscopic) state of the system is specified by the *observables* which are expectation values of different functions $\langle f[\psi] \rangle$ of the possible configurations ψ of the system. In thermal equilibrium the state is given by

$$\langle f[\psi] \rangle = Z^{-1} \sum_{\{\psi\}} f[\psi] e^{-\beta H[\psi]}, \tag{3.1}$$

where $\beta = 1/k_B T$ and Z is defined by demanding that $\langle 1 \rangle = 1$. Z is the partition function and is obviously a function of temperature, but it is also a function of the energy levels in the system, i.e. the boundary conditions such as the size of the system. The definition in Eq. 3.1 can be extended to the infinite volume case by defining the system in a d-dimensional box of size L^d, and taking $L \to \infty$. In this so called *thermodynamic limit* the observables may be non-analytic, and the possible non-analyticities are called *phase transitions*.

Let the Hamiltonian $H_{L,h}[\psi]$ describe a model defined on a lattice of size L^d, where $H_{L,h}$ is a linear function of the real variable h (typically an external field coupling to ψ). For $h = 0$ the Hamiltonian is assumed to be invariant under some transformation Λ of the fields, i.e.

$$H_{L,h=0}[\Lambda\psi] = H_{L,h=0}[\psi]. \tag{3.2}$$

We denote the expectation value of some local function $f[\psi]$ of the fields by

$$\langle f[\psi] \rangle_{L,h} = Z_{L,h}^{-1} \sum_{\{\psi\}} f[\psi] e^{-\beta H_{L,h}[\psi]}, \tag{3.3}$$

where h and L can take any value. If the average

$$\langle f[\psi] \rangle \equiv \lim_{h \to 0} \lim_{L \to \infty} \langle f[\psi] \rangle_{L,h} \tag{3.4}$$

is non-invariant for any $f[\psi]$, i.e.

$$\langle f[\Lambda\psi]\rangle \neq \langle f[\psi]\rangle \tag{3.5}$$

the symmetry is said to be *spontaneously broken* in the thermodynamic limit. Then the equilibrium state is non-unique, because it is related by a symmetry transformation to another state, which can be obtained by using $H_{L,h}(\Lambda\psi)$ instead of $H_{L,h}(\psi)$ in Eq. 3.3. This means that $\langle f[\Lambda\psi]\rangle$ is discontinuous at $h = 0$ and the system is at a first order transition line. Often the symmetry is broken only for low temperatures and the first order line will end at some point corresponding to a critical temperature T_c. Here the system undergoes a first order or a second order transition to the symmetric phase.

Note that strictly speaking spontaneously symmetry breaking only can occur in the thermodynamic limit. For finite system sizes there is a finite probability to go anywhere in configuration-space if one waits for a sufficiently long time, i.e. the system is ergodic. At short time scales one will observe meta-stable states since the system can be trapped in local minima for rather long times.

It is also possible to have phase transitions without breaking of local symmetries. The prime example is the 2DXY-model with its Kosterlitz-Thouless phase transition [14,91,92]. The Mermin-Wagner theorem [106] states that no long-range order is possible for two-dimensional systems with continuous symmetry. No local order parameter can thus be associated with this phase transition and in fact the transition was found to be driven by an unbinding of topological defects (vortices), see Chapter 5 for more details. In the 3DXY-model a local order parameter can be defined, the broken symmetry being a global $U(1)$-symmetry. However, also here the phase transition is driven by unbinding of topological defects, here in the form of vortex-loops, see e.g. [113] and references therein. For models with a *local gauge symmetry*, as the Ginzburg-Landau model,[1] things are more complicated. Elitzur's theorem [45] states that a gauge symmetry can never be spontaneously broken since the mean value of any local order-parameter on the orbit of the gauge group is zero. This does not mean that there cannot be phase transitions as such, but the possible phase transitions must have a more subtle origin than simply breaking of the gauge symmetry. The transitions are typically driven by a proliferation of topological defects, e.g. a vortex-loop blowout. The transitions must be found either by jumps in local order-parameter like quantities, as we have done in Paper III [108], or by using non-local order-parameters, as the vortex tension or the mass of the fields, see e.g. [77,79], or the more abstract Wilson loop or Polyakov loop [90].

3.2 Scaling and renormalization

This is a short introduction to scaling and renormalization meant only to give a glimpse of this broad and interesting field. The account is based on [30,100]. The partition function of a system can be written as

$$Z = \sum e^{-\mathcal{H}}, \quad \mathcal{H} = \beta H \tag{3.6}$$

where $\beta = 1/k_B T$ and the sum is over all configurations of the system. The idea behind the renormalization group (RG) is to do this summation in a successive manner by integrating out degrees of freedom on longer and longer length scales. This gives an effective Hamiltonian $\mathcal{H}'$ describing the physics on longer length scales. Since this physics should be left unaffected we must have

$$e^{-\mathcal{H}'} = \sum{}' e^{-\mathcal{H}}. \tag{3.7}$$

where the mark on the sum means that only short wavelength fluctuations should be summed over. Note that this coarse-graining procedure may be carried out in different ways such as e.g. block spin transformations (real-space) or by integrating over short-wavelength modes (k-space). This coarse-graining will increase the microscopic length scale a by a factor ℓ and we must do

[1] Another important example is the Ising lattice gauge model introduced by F. Wegner [147]. The simplest gauge-invariant order parameter for this model is the Wilson loop [149]. The Wilson loop and the Polyakov loop are the best known non-local order parameters for lattice gauge theories, see e.g. the review article by J. Kogut [90] for more details.

the rescaling $a' = a\ell$ to be able to compare the effective Hamiltonian with the original one. The correlation length will then transform as $\xi' = \xi/\ell$ and the system will move away from the critical point unless we start precisely at the critical point. The coarse-graining combined with the rescaling can be formally written as

$$\mathcal{H}' = \mathcal{R}_\ell(\mathcal{H}). \tag{3.8}$$

This transformation is of course very difficult to do in practice and can only be done approximately. The conceptual picture that emerges is still very useful. By iterating this transform one gets a (RG-)flow in the space of possible Hamiltonians. In this space of RG-trajectories there are a few special points named fixed points where

$$\mathcal{H}^* = \mathcal{R}_\ell(\mathcal{H}^*). \tag{3.9}$$

Normally only points associated with diverging correlation lengths, corresponding to phase transitions, are interesting. The other points correspond either to infinite or zero temperature, see Fig. 3.2.

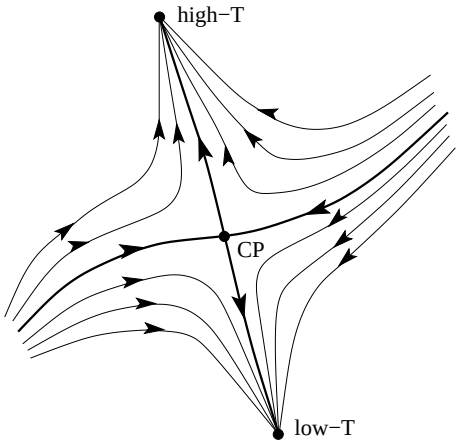

Figure 3.2: Schematic RG-flow in a two-dimensional parameter space. The critical point (CP) is unstable in the temperature direction.

The fact that many different microscopic models flow to the same fixed point is the underlying reason for the *universality* observed at critical points. The Hamiltonian can normally be written on the form

$$\mathcal{H} = \sum_i K_i \theta_i(\{S\}) \tag{3.10}$$

where K_i are elements in a vector $\boldsymbol{K}$ of coupling constants[2] and θ_i are local operators of the degrees of freedom $\{S\}$. The RG-transform may then formally be written as

$$\boldsymbol{K}' = \mathcal{R}_\ell \boldsymbol{K}, \tag{3.11}$$

and gives a flow in the space of coupling constants. Even if one starts with only a finite number of short range interactions, each step in the coarse graining procedure gives more couplings. Thus in general the number of components in the coupling vector $\boldsymbol{K}$ have to be infinite, and one normally have to do some kind of approximations. By linearizing around a fixed point we can write

$$\boldsymbol{K}^* + \delta\boldsymbol{K}' = \mathcal{R}(\boldsymbol{K}^* + \delta\boldsymbol{K}) = \underbrace{\mathcal{R}(\boldsymbol{K}^*)}_{=\boldsymbol{K}^*} + \mathsf{M}\delta\boldsymbol{K} + \mathcal{O}(\delta\boldsymbol{K}^2), \tag{3.12}$$

[2]Normally the (inverse) temperature is proportional to one of the components of this coupling constant vector.

where the matrix M has the elements

$$M_{ij} = \left.\frac{\partial \mathcal{R}(K_i)}{\partial K_j}\right|_{\boldsymbol{K}=\boldsymbol{K}^*}. \tag{3.12'}$$

Thus

$$K_i' - K_i^* = \sum_j M_{ij}(K_j - K_j^*). \tag{3.13}$$

By changing to a basis $g_n = \sum_i c_i K_i$ where the matrix M is diagonal it becomes clear that the eigenvalues can be related to critical exponents. The scaling fields g_n transform as

$$g_n' = \ell^{y_n} g_n, \tag{3.14}$$

and the relevance of these fields are determined by the sign of the eigenvalues y_n, i.e.

- $y_n > 0$: g_n is relevant, increases under RG.
- $y_n < 0$: g_n is irrelevant, decreases under RG.
- $y_n = 0$: g_n is marginal and nonlinear terms have to be included to determine the behavior.

The irrelevant couplings normally flow to zero and can be neglected, except for some special situations where they are dangerously irrelevant, see e.g. [31].

3.2.1 Critical exponents

Since the partition function is invariant under RG-flow the free energy density $f = F/L^d = -L^{-d} \ln Z$ transforms as

$$f(\boldsymbol{K}) = \ell^{-d} f_s(\boldsymbol{K'}) + h(\boldsymbol{K}), \tag{3.15}$$

where h is non-singular. The singular part has the scaling form

$$f_s(g_1, g_2, \ldots) = \ell^{-d} f_s(\ell^{y_1} g_1, \ell^{y_2} g_2, \ldots), \tag{3.16}$$

and critical exponents are derived by taking appropriate derivatives. For a system with one relevant coupling $t = T/T_c - 1$ the specific heat is given by

$$c_v \propto \frac{\partial^2 f(t)}{\partial t^2} = \ell^{2y_t - d} f''(t\ell^{y_t}), \tag{3.17}$$

and by setting $t\ell^{y_t} \approx 1$ one easily finds $\alpha = 2 - d/y_t$ by using the definition of the exponent α, $c_v \propto t^{-\alpha}$. For a finite system L^{-1} is a relevant scaling field and we can write

$$f_s(g_1, g_2, \ldots, L^{-1}) = L^{-d} \tilde{f}_s(L^{y_1} g_1, L^{y_2} g_2, \ldots). \tag{3.18}$$

Then

$$c_v = L^{2y_t - d} \widetilde{F}(tL^{y_t}) \tag{3.19}$$

and we see that the singular behavior is rounded and the divergence is replaced with a finite peak at a shifted temperature. Such finite size scalings are very useful in Monte Carlo simulations where the systems, for obvious reasons, necessarily have to be finite.

3.3 First order transitions

Here I will give a short review of some of the main differences between first order and second order transitions, for more details see e.g. the review by Binder [20], as well as some sections in [95].

First order phase transitions are much more common than second order ones. Typically, lines of first order transitions end in a single critical point where second order behavior is observed. Despite this, first order transitions are much less understood than critical phenomena. The reason is that critical phenomena are associated with a diverging correlation length. Close to the critical point this length tends to infinity, and only the structure of the system on very long length scales is important. The behavior on length scales comparable to the direct interactions, which typically are a few lattice constants, becomes irrelevant. This is the reason why universal behavior is observed and is also the basis for the renormalization group approach. At first order transitions there are no diverging correlation lengths and one cannot restrict attention to long-wavelength phenomena, thus no such universality as for critical phenomena is to be expected. This means that details on microscopic scales in the models are important. *For continuum models which are artificially discretized to make simulations possible, this means that one has to carefully take the continuum limit, where the lattice spacing tends to zero, to remove lattice artifacts.* This will be a central point in Chapter 7 and Paper III [108].

At first order transitions, the ordered and disordered phase have the same free energy and coexistence may be observed. This is in contrast to second order transitions where the difference between the two phases disappears. Here, the diverging correlation length means that the whole system will be correlated and thus in the same phase. At a first order transition this is not so and parts of the system may be ordered while others are disordered. If we start with a disordered system and decrease the temperature, small droplets of the ordered phase will start forming. For high temperatures, these droplets will be small and have short life-times. By reducing the temperature the droplets will increase in size and finally, when the temperature is decreased below the transition temperature, droplets of a critical size will appear. The surface free energy will be lower than the gain in bulk free energy and they will start to increase in size thereby ordering the system. Normally droplets start forming at some defects, such as dust in the air. For very clean samples there are very few defects and formation of droplets may be suppressed until temperatures considerable below the normal transition point. The system will then be in a meta-stable state, which means that the free energy is not minimized since the system is in a local but not a global minimum in the energy landscape. Doing simulations or experiments on first order transitions one must be very careful not to be stuck in such local minima. For strong first order transitions this can be a severe problem since tunneling between the ordered and disordered state is very rare. Concerning Monte Carlo simulations the solution is either to use standard sampling methods such as Metropolis with a very high number of sweeps, or to use more advanced techniques such as "Multicanonical Monte-Carlo simulations", see e.g. [16]. We have studied weak first order transitions where this problem is less important, but in compensation we got other problems since weakly first order transitions are difficult to classify.

3.3.1 Lee-Kosterlitz method

The identification of the order of a weakly first order transition is problematic. In a finite system the discontinuities are rounded and thus difficult to separate from second order behavior. Lee and Kosterlitz [97, 98] proposed an ingenious and clear-cut scheme to distinguish first and second order transitions. This scheme has turned out to be remarkable effective, even for rather small systems. By using this method they were able to determine *numerically*[3] that the transition in the 2D q-state Potts model is first order for $q > 4$. As mentioned, first order transitions may have coexisting ordered and disordered phases, while second order transitions cannot. Thus, for first order transitions histograms of some order parameter like quantity should show a clear double-peak structure as shown in Fig. 3.3 on the facing page. The recipe is then to do a long simulation

[3]The same result had been found analytically much earlier, see the review [153], but simulations had given contradictory results for the limiting value of q.

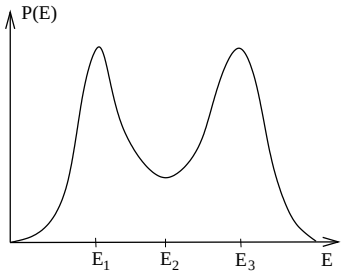

Figure 3.3: The difference in free energy between the pure phases with energy E_1, E_3 and the coexisting phase with energy E_2 is given by $\Delta F(L) = \ln P_{\max}(E) - \ln P_{\min}(E)$. Here $P(E)$ is a histogram of E where $P_{\max}(E) = P(E_1) = P(E_3)$ and $P_{\min}(E) = P(E_2)$

.

at a temperature quite near the phase transition, i.e. one has to be so near that both peaks, if they are present, are visible in the histograms. The peaks are then made equal high by the use of reweighting techniques as explained in Section 4.4. The difference in free energy between the pure phases and a mixture of the two phases is then given by

$$\Delta F(L) = \ln P_{\max}(E) - \ln P_{\min}(E), \tag{3.20}$$

where $P_{\max}(E)$ and $P_{\min}(E)$ are respectively the maximum and minimum probabilities for a given state to occur, see Fig. 3.3. This procedure is repeated for different lattice sizes L and if $\Delta F(L)$ diverges when $L \to \infty$ the transition is first order, if not it is second order. More precisely, in a d-dimensional system, one should observe the scaling

$$\Delta F(L) \propto L^{d-1} \tag{3.21}$$

for L above some lower limit. Thus, the difference in free energy between the pure phases and the coexisting ordered and disordered phase scales as a surface in a d-dimensional space, i.e. it represents the surface energy between the two phases.

Chapter 4

Monte Carlo simulations

This is a very short introduction to some of the aspects of Monte Carlo simulations. There are several excellent books available that should be consulted for a more thorough introduction, see especially the book by Landau and Binder [95], but also e.g. the books [22, 141], [23](≈ [21]) and [24, chapter 4]. In a Monte Carlo simulation we try to follow the evolution in time for a model that evolves in a stochastic manner which depends on a sequence of random numbers which is generated during the simulation. This is in contrast to a model which evolves in time according to e.g. Newton's laws of motion. *A stochastic time evolution is typical for effective models on long length and time scales where the microscopic fluctuations enter only as random noise* (e.g. a thermal reservoir).

4.1 Statistical mechanics

For an effective model with a Hamiltonian $H[\psi]$ that is a functional of the (microscopic) "state"[1] or configuration ψ of the system the thermal average of a physical quantity $A[\psi]$ is defined as

$$\langle A \rangle = \frac{1}{Z} \sum_{\{\psi\}} A[\psi] e^{-\beta H[\psi]} \tag{4.1a}$$

where

$$Z = \sum_{\{\psi\}} e^{-\beta H[\psi]} \tag{4.1b}$$

is the partition function and $\beta = 1/k_B T$. From the partition function one can find the free energy

$$F = -\frac{1}{\beta} \ln Z = -k_B T \ln Z, \tag{4.2}$$

the internal energy

$$U = \langle H \rangle = \frac{\partial(\beta F)}{\partial \beta} = -T^2 \frac{\partial (F/T)}{\partial T}, \tag{4.3}$$

and the specific heat

$$C_V = \left(\frac{\partial U}{\partial T} \right)_V = \frac{1}{k_B T^2} \left(\langle H^2 \rangle - \langle H \rangle^2 \right). \tag{4.4}$$

More generally if the Hamiltonian has a term of the form $\delta H = -XY$, where e.g. X is the magnetization and Y is the magnetic field, the mean value of X is defined by

$$\langle X \rangle = \frac{1}{\beta} \frac{\partial \ln Z}{\partial Y} \bigg|_{Y=0} = -\frac{\partial F}{\partial Y} \bigg|_{Y=0}, \tag{4.5}$$

[1] Note the different use of the word "state" here compared to e.g. Section 3.1. Unfortunately both are common.

and the susceptibility of X by

$$\chi_x = \frac{1}{\beta}\frac{\partial\langle X\rangle}{\partial Y}\bigg|_{Y=0} = \frac{1}{k_B T}\left(\langle X^2\rangle - \langle X\rangle^2\right). \tag{4.6}$$

The entropy is given by

$$S = -k_B \ln P = \left(\frac{\partial F}{\partial T}\right)_V \tag{4.7}$$

where the probability for the system being in state ψ_i is

$$P_i = \frac{e^{-\beta H[\psi_i]}}{Z}. \tag{4.8}$$

If the entropy at $T = 0$ is known one can find the entropy at other temperatures by integrating the specific heat C_V. Since constant volume gives $dU = TdS = C_V dT$ then

$$S(T) = S(0) + \int_0^T \frac{C_V(T')}{T'}dT'. \tag{4.9}$$

Note that this formula only makes sense for Ising-type systems where $C(T \to 0) \to 0$. For classical systems where $C(T \to 0) \to$ const. the entropy will diverge, $S(T \to 0) \to -\infty$. The free energy can be found by integrating the internal energy $\beta F = \int U d\beta$, i.e.

$$\frac{F(T)}{k_B T} = -\frac{S(\infty)}{k_B} + \int_0^{1/k_B T} U(T')d(1/k_B T'). \tag{4.10}$$

The essential task in statistical mechanics is to do multi-dimensional sums or integrals such as in Eq. 4.1a. The Monte Carlo simulation method is a very effective method to do this and relies on the *ergodic hypothesis*

$$\langle A\rangle = \frac{1}{Z}\sum_{\{\psi\}} A[\psi]e^{-\beta H[\psi]} = \lim_{t\to\infty}\frac{\int_0^t dt' A[\psi(t')]e^{-\beta H[\psi(t')]}}{\int_0^t dt' e^{-\beta H[\psi(t')]}}, \tag{4.11}$$

where t is the Monte Carlo time and $\psi(t)$ is now a dynamical variable in a Markov chain. For the Monte Carlo method to be efficient one has to use importance sampling.

4.2 Importance sampling

Due to the enormous number of available states it is not efficient to use simple sampling where each configuration has the same probability. Instead the new states should be chosen according to their probability of appearance. If the probability for a given state in the Markov chain is given by the Boltzmann weight

$$p_{\rm eq}(\psi) = \frac{e^{-\beta H[\psi]}}{Z}, \tag{4.12}$$

the average is simply the sum

$$\langle A\rangle = \lim_{N\to\infty}\sum_{n=0}^{N} A[\psi(t_n)]. \tag{4.13}$$

This is called *importance sampling*. The question is then how one should generate new configurations such that the probabilities are according to Eq. 4.12. The most general method is given by a Markov chain with transition probability $\mathcal{P}(\psi'|\psi) = \mathcal{P}(\psi \to \psi')$ satisfying the following set of three conditions

Sum rule At each step the system must go somewhere, i.e.

$$\sum_{\psi'} \mathcal{P}(\psi \to \psi') = 1 \tag{4.14}$$

.

Accessibility From a given starting configuration it must be possible to evolve the system to any of its other configurations in a finite number of Monte-Carlo steps.

Microreversibility To make the probabilities $p_n(\psi)$ converge to $p_{eq}(\psi)$ the following must be true,

$$p_{\rm eq}(\psi)\mathcal{P}(\psi \to \psi') = p_{\rm eq}(\psi')\mathcal{P}(\psi' \to \psi). \tag{4.15}$$

This is also called *detailed balance.*

Suppose that we have chosen $\mathcal{P}$ such that this is fulfilled, and that each configuration ψ appears with probability $p_n(\psi) = p_{\rm eq}(\psi)$ at step n in a Markov chain. Then

$$p_{n+1}(\psi) = \sum_{\psi'} p_{\rm eq}(\psi')\mathcal{P}(\psi' \to \psi) = p_{\rm eq}(\psi) \underbrace{\sum_{\psi'} \mathcal{P}(\psi \to \psi')}_{=1} = p_{\rm eq}(\psi), \tag{4.16}$$

and the distribution is unchanged. If $p_n(\psi)$ differs from the wanted probability distribution, i.e. $p_n(\psi) \neq p_{\rm eq}(\psi)$, we can define

$$D_n = \sum_{\psi} \Big| p_n(\psi) - p_{\rm eq}(\psi) \Big|, \tag{4.17}$$

and thereby

$$\begin{aligned} D_{n+1} &= \sum_{\psi} \Big| p_{n+1}(\psi) - p_{\rm eq}(\psi) \Big| \\ &= \sum_{\psi} \Big| \sum_{\psi'} p_n(\psi')\mathcal{P}(\psi' \to \psi) - p_{\rm eq}(\psi) \Big| \\ &= \sum_{\psi} \Big| \sum_{\psi'} \left[p_n(\psi') - p_{\rm eq}(\psi) \right] \mathcal{P}(\psi' \to \psi) \Big|. \end{aligned}$$

Since $\mathcal{P}$ is a probability we have $\mathcal{P} \geq 0$, which implies

$$\begin{aligned} D_{n+1} &\leq \sum_{\psi,\psi'} \Big| p_n(\psi') - p_{\rm eq}(\psi') \Big| \mathcal{P}(\psi' \to \psi) \\ &= \sum_{\psi'} \Big| p_n(\psi') - p_{\rm eq}(\psi') \Big| \\ &= D_n, \end{aligned}$$

and we see that the difference gets smaller. Thus the difference from the Boltzmann distribution, given in Eq. 4.12, decreases steadily along the Markov chain.

4.2.1 Metropolis algorithm

The most frequently used algorithm for the Markov process was invented by Metropolis *et al.* [107]. If the system is in state ψ, a new state ψ' should be chosen with probability

$$\mathcal{P}(\psi \to \psi') = \min\left(1, \frac{p(\psi')}{p(\psi)}\right), \tag{4.18}$$

Metropolis algorithm
For each variable s_i:

- Generate new configuration ($\psi \to \psi'$ by letting $s_i \to s_i'$).
- Calculate energy change ($\Delta E = E_{\psi'} - E_\psi \equiv E' - E$).
- Calculate $\mathcal{P} = \min\left(1, e^{-\beta \Delta E}\right)$.
- Find random variable r uniform on $[0, 1]$.
- Accept move if $r \leq \mathcal{P}$.

Figure 4.1: Metropolis algorithm

which gives the algorithm shown in Fig. 4.1. Another often used algorithm is the heat-bath method [35] where the new configuration is accepted with probability[2]

$$\mathcal{P}(\psi \to \psi') = \frac{e^{-\beta E'}}{e^{-\beta E'} + e^{-\beta E}} = \frac{1}{1 + e^{\beta \Delta E}}. \tag{4.21}$$

This method may be particular useful if the acceptance ratios for the Metropolis method are low.

4.2.2 Parallelization

For very large systems the turnaround time for each simulation may become a severe problem. By doing such simulations in a parallel manner, i.e. using several processors on a single job, the turnaround time may be drastically reduced. For our largest systems we have used 32 processors which reduces the waiting time from months to days. Monte-Carlo simulations for lattice systems with short range interactions are ideally suited for parallelization since the system can be divided into a number of subsystems equal to the number of processors. The subsystem on each processor is further divided into a black and a white part which are run in an alternating manner, i.e. when one processor runs its black part the neighbors are running their white parts and vice versa. The purpose of this division in black and white subsystems is to avoid that the neighboring processors change the boundary conditions before all processors are finished. Each processor perform simulation on its part of the system, and when all processors are finished with one sweep new boundary conditions are exchanged with the neighbors. Since this exchange of data takes time there is an upper limit of processors that can be used in an efficient manner, i.e. the system

[2] Strictly speaking, this is only an approximation to the original definition of the heat-bath method where new states are chosen with probability $\propto e^{-\beta E'}$, i.e. *independent* of the old configurations. Thus, for the Ising model, the probabilities for finding spin up or spin down are given by $p(\uparrow') = Z_i^{-1} e^{-\beta E_i(\uparrow')}$, $p(\downarrow') = Z_i^{-1} e^{-\beta E_i(\downarrow')}$ respectively, where $Z_i = p(\uparrow') + p(\downarrow')$. Here, E_i is the local energy, i.e. the part of the energy that depends on the spin at site i. More generally the probability for a state α_i' is given by

$$p(\alpha_i') = Z_i^{-1} e^{-\beta E_i(\alpha_i')}, \quad Z_i = \sum_{\{\alpha_i''\}} e^{-\beta E_i(\alpha_i'')} \tag{4.19}$$

where $\{\alpha_i\}$ is the set of possible values of the local variable α_i and E_i is defined as above. For continuous variables new states should be drawn from a distribution

$$p(\psi_i') = Z_i^{-1} e^{-\beta E_i(\psi_i')}, \quad Z_i = \int d\psi_i'' e^{-\beta E_i(\psi_i'')}. \tag{4.20}$$

Hence, it is necessary that it should be possible to find random numbers with this distribution in a simple manner if the method is to be useful. This is only possible for rather simple models, typically quadratic in ψ_i, where the inverse $\psi(p)$ can be found. For more complicated theories involving coupled scalar fields, e.g. ψ^4 terms, and gauge fields this is generally impossible. The compromise is then to draw a new state randomly and accept this state by comparing its energy to the old state and accept it with probability according to Eq. 4.21. Thus, we in some sense assume that the new trial state and the old state are the only states present in the system and weigh these relative to each other as for the Ising model.

should not be divided in too small pieces. The parallel algorithm is then given schematically as shown in Fig. 4.2. If disk place not allows saving of the whole time-series of measurements, one

Parallel algorithm:

1. Initialize by specifying the start configuration and boundary conditions for each subsystem, i.e. each processor.
2. Parallel simulation. Each processor updates either the black or white part of its subsystem by using standard Metropolis algorithm. If desired this algorithm can be enhanced as shown in Chapter 7.
3. Update the boundary conditions for each subsystem by exchanging updated values with the neighboring subsystems.
4. Repeat step 2 and 3 with the opposite color.
5. Do measurements at each processor and collect the results on a "master" processor. Store the data temporarily in a matrix.
6. When the matrix is filled up: write to file.
7. If more sweeps left: repeat from 2.
8. Use the time series to calculate averages, error-estimates, histograms and so fort.

Figure 4.2: Parallel algorithm

has to calculate averages, variances and often also one- or multi-dimensional histograms during the simulations. The main problem with this method is that one has to think about "everything" before the simulations start. Here "everything" means things such as the number of bins in the histograms and the highest momenta of the measured data that may become necessary for future calculations.

4.3 Error analysis

Since Monte Carlo simulations are statistical by nature, error analysis is an important part of every simulation project. For *uncorrelated* measurements the standard formula for the error in the mean value of N uncorrelated measurements of a quantity A is

$$\sigma^2_{\langle A\rangle} = \frac{\sigma^2_A}{N} \tag{4.22a}$$

where the variance is given in the standard way by

$$\sigma^2_A = \frac{1}{N-1}\sum_{i=1}^{N}\left(A_i - \langle A\rangle\right)^2 . \tag{4.22b}$$

In Monte Carlo simulations successive measurements are normally strongly correlated due to the local nature of the update. This is especially problematic near a critical point where correlated domains of sizes comparable to the system size appear since the correlation length ξ diverges. It is intuitively clear that changing the fields considerably in such large domains by only using local updates will take much time. This phenomena is called critical slowing down, and is measured by a correlation time given by $\tau = \xi^z$, where z is an critical exponent. This slowing down can

be drastically reduced by using cluster updating algorithms such as Swendsen-Wang [137, 138] and Wolff [152]. The problem is that such algorithms are difficult to use efficiently on parallel computers and they are not yet developed for use in more complicated theories with typically coupled scalar and gauge fields. Normally therefore, successive states in Monte Carlo simulations are strongly correlated and the error estimates must incorporate this. For *correlated* measurements the formula corresponding to Eq. 4.22, is[3]

$$\sigma^2_{\langle A\rangle} = \frac{\sigma_A^2}{N}\left(1+\frac{2\tau_A}{\delta t}\right) \equiv \frac{\sigma_A^2}{n_{\rm eff}}, \tag{4.23}$$

where τ_A is the integrated correlation time defined by

$$\tau_A \equiv \int_0^\infty \psi_A(t)dt, \tag{4.24}$$

δt is the time interval between two successive measurements, and $n_{\rm eff}$ is defined as an *effective* number of measurements where the effect of the correlation time is incorporated. For $\tau_A \gg \delta t$ we then have the error

$$\sigma^2_{\langle A\rangle} \approx \sigma_A^2\frac{2\tau_A}{N\delta t} = \sigma_A^2\frac{2\tau_A}{t}, \tag{4.25}$$

and we see that it only depends on the ratio t/τ_A and not the time interval δt. The calculation of the correlation times normally gives large errors, and other methods to estimate the error are more common. An alternative method is to group the measured data N into N_B bins of size $n = N/N_B$. If the size of each bin is larger than the correlation time the mean value of the data in each bin

$$\theta_i = \frac{1}{n}\sum_{j=n(i-1)+1}^{ni} A_j, \quad i = 1,\ldots,N_B \tag{4.26}$$

should be approximately uncorrelated. Then the formula in Eq. 4.22 can be used to calculate the error. Normally one starts with relatively small bins and increases the size until the results seem to converge towards a limiting value.

If one tries to calculate the mean value and the error in some nonlinear function $f(A)$ one should use Jackknife analysis to reduce the bias in the results, see e.g. [15]. Let $\theta_1,\ldots,\theta_{N_B}$ represent a sample of N_B independent and identically distributed random variables and let $\langle\theta\rangle$ be the estimator of the average calculated using all members of the sample. Deleting the i$^{\rm th}$ member one then calculates the estimator $\langle\theta_{-i}\rangle$ based on the remaining groups. The estimator

$$\overline{\theta} = \frac{1}{N_B}\sum_{i=1}^{N_B}\widetilde{\theta}_i, \quad \widetilde{\theta}_i = N_B\langle\theta\rangle - (N_B-1)\langle\theta_{-i}\rangle \tag{4.27}$$

eliminates the order $1/N_B$ bias. The mean value $\overline{f^J}$ and the corresponding error in the mean $\sigma^2_{\overline{f^J}}$ can then be found from the formulas

$$\begin{aligned}
\theta_i^J &= \frac{1}{N_B-1}\sum_{j\neq i}\theta_j = \frac{1}{N_B-1}(N_B\overline{\theta}-\theta_i)\\
f_i^J &= f(\theta_i^J)\\
\overline{f^J} &= \frac{1}{N_B}\sum_{i=1}^{N_B} f_i^J\\
\sigma^2_{\overline{f^J}} &= \frac{N_B-1}{N_B}\sum_{i=1}^{N_B}\left(f_i^J-\overline{f^J}\right)^2.
\end{aligned} \tag{4.28}$$

[3]Note that for each new temperature a number of measurements N_0 in the beginning must be rejected to ensure that the system has reached thermal equilibrium before averages are calculated. The length of this thermalization period will depend on the initial configuration of the system and the autocorrelation time for the given temperature. If the whole time series is stored the value of N_0 can be found by increasing the number of rejected measurements until the averages seem to settle at a constant value.

To compare this result with the standard error formula in Eq. 4.22 we can set $f = \theta$ and $N_B = N$ which gives

$$\begin{aligned} \overline{\theta} \equiv \overline{\theta^J} &= \frac{1}{N}\sum_{i=1}^{N}\theta_i^J \\ \sigma_{\overline{\theta}}^2 &= \frac{N-1}{N}\sum_{i=1}^{N}\left(\theta_i^J - \overline{\theta}\right)^2, \end{aligned} \tag{4.29}$$

which is similar to Eq. 4.22, except that the prefactor $1/(N-1)$ is replaced by $(N-1)$.

4.4 Reweighting

Near phase transitions, physical quantities may show divergent behavior, e.g. the peak in the specific heat for a second order transition. To study such a peak in detail one needs very high temperature resolution. The most naive solution is of course to do many runs at slightly different temperatures.[4] This is however not the most efficient use of simulation time and the concept of reweighting comes into play. The idea, put forward in its modern form by Ferrenberg and Swendsen [48], is that the results from a (long) simulation at one temperature can be used to extract information about near-lying temperatures by reweighting. Thus one can calculate physical quantities as *continuous* functions of temperature, which of course is very useful in dealing with narrow peaks. This procedure can be improved further by combining several temperatures in the reweighting procedure [49]. During the simulations one can either store histograms of the outcome of some quantity or the whole time series. If disk place allows it, storing the whole time series is clearly recommended. Doing so will ease further data analysis and one avoids saving multi-dimensional histograms with its obvious limitations on precision since the number of bins in each direction must be rather small. Here I will use, as an illustrative example the Ising model with partition function

$$Z(K) = \sum_E e^{-KE}, \quad E = \sum_{\langle i,j\rangle}\sigma_i\sigma_j \tag{4.30}$$

where $K = J/k_BT$. Here $\langle i,j\rangle$ is a nearest neighbor pair. This is clearly a very simple example, but the formulas are easily adopted to other, more complicated, models. The probability of observing the system with internal energy E and magnetization M is then

$$P_K(E,M) = \frac{W(E,M)e^{-KE}}{Z(K)}, \tag{4.31}$$

where $W(E,M)$ is the number of configurations with energy E and magnetization M. Note that reweighting only gives reliable results when reweighting to near-lying temperatures where the probability distribution for the reweighted temperature have considerable overlap with the distributions sampled during simulations. If this is not fulfilled statistical errors will be severe due to the low number of measurements at the tails of the distributions, see e.g. [95, chapter 7] for more details. It is also possible to let the reweighting become an integrated part of the simulations where the new configuration are chosen from distributions that do not have Boltzmann weights. This technique is named *multicanonical sampling*, see [16, 17, 95] for more details. Here I will give the essential formulas for reweighting from one or several runs based on histograms or not.

[4] I use temperature here, but more generally the term coupling constant should be used, e.g. one can do a simulation at one magnetic field and reweight to another.

4.4.1 Histogram methods

By doing a simulation at K_0 and making a histogram $H_{K_0}(E,M)$ one gets an estimate of the probability distribution at this coupling by

$$\widetilde{P}_{K_0}(E,M) \approx \frac{H_{K_0}(E,M)}{N} = \frac{\widetilde{W}(E,M)e^{-K_0 E}}{Z(K_0)} \tag{4.32}$$

where N is the number of measurements. This gives an estimate of $W(E,M)$,

$$\widetilde{W}(E,M) = \frac{Z(K_0)H(E,M)e^{K_0 E}}{N}, \tag{4.33}$$

and we can easily find an estimate of $P_K(E,M)$,

$$P_K(E,M) = \frac{H(E,M)e^{-(K-K_0)E}}{\sum_{E,M} H(E,M)e^{-(K-K_0)E}}. \tag{4.34}$$

With this averages can be computed simply as

$$\langle f(E,M)\rangle_K = \sum_{E,M} f(E,M)P_K(E,M). \tag{4.35}$$

It is also possible to combine several runs at different couplings by weighting each run according to the autocorrelation times τ_j with a weight factor $g_j = 1 + 2\tau_j$. This method is often called Ferrenberg-Swendsen multi-histogram reweighting [49]. The probability distribution at coupling K obtained from R independent simulations, each with n_j configurations is then given by

$$P_K(E,M) = \frac{\sum_{i=1}^{R} g_i^{-1} H_i(E,M)e^{-KE}}{\sum_{j=1}^{R} n_j g_j^{-1} e^{-K_j E + f_j}} \tag{4.36a}$$

where

$$e^{-f_j} = \sum_{E,M} P_{K_j}(E,M). \tag{4.36b}$$

This determines the set $\{f_j\}$ up to an additive constant, which corresponds to different normalizations. The set of equations 4.36 must be solved self consistently by using e.g. multi-dimensional Newton-Raphson methods. This calculation is rather tricky, due to the size of the numbers involved, typically numbers are $\exp(\pm V)$, where V is the volume of the system. To avoid overflow and underflow one has to use the logarithm of most quantities during the calculations. Averages can be calculated as

$$\langle f(E,M)\rangle_K = \frac{\sum_{E,M} f(E,M)P_K(E,M)}{\sum_{E,M} P_K(E,M)}. \tag{4.37}$$

The main problem with this method is that the simulation results must be saved in histograms. If one only is interested in functions of E this is no problem, but as soon as one has to consider functions of both E and M (or even more variables for more complicated models), this becomes problematic. To store multi-dimensional histograms one normally has to use rather few bins in each direction to be able to store the data in the memory, and much information is lost. An other problem is unevenly distributed data with e.g. rapid variations for small E and a long tail for higher E. To handle this one needs either a high number of bins in this direction or bins with different sizes, but bins of varying sizes are complicated to implement technically. If one has stored the whole time-series during the simulation this problem is easily resolved.

4.4.2 Reweighting without histograms

Assume that we have done a simulation at coupling K_0 and stored the time-series of measurements $E(t)$ and $M(t)$ where $t = 1, 2, \ldots, n_0$. An average at K_0 is then simply

$$\langle f(E,M)\rangle_{K_0} = \frac{\sum_{t=1}^{n_0} f[E(t),M(t)]}{\sum_{t=1}^{n_0} 1}, \tag{4.38}$$

and the reweighted result at K is

$$\langle f(E,M)\rangle_{K} = \frac{\sum_{t=1}^{n_0} f[E(t),M(t)]e^{-(K-K_0)E}}{\sum_{t=1}^{n_0} e^{-(K-K_0)E}}. \tag{4.39}$$

It is also possible to combine several runs as in the previous section without using histograms. For some reason this method seems to be very rarely mentioned in the literature [110]. Assume that we have done R independent runs with different lengths n_j. The time series will then have an index indicating the run. Then the essential reweighting formulas are given by

$$P_\ell(t,K) = \frac{g_\ell^{-1} e^{-K E_\ell(t)}}{\sum_{j=1}^{R} n_j g_j^{-1} e^{-K_j E_j(t)+f_j}}, \tag{4.40a}$$

where

$$e^{-f_j} = \sum_{\ell=1}^{R}\sum_{t=1}^{n_\ell} P_\ell(t,K_j). \tag{4.40b}$$

This set is solved self-consistently as for Eq. 4.36. One can then calculate averages as

$$\langle f(E,M)\rangle_{K} = \frac{\sum_{\ell=1}^{R}\sum_{t=1}^{n_\ell} f[E(t),M(t)]P_\ell(t,K)}{\sum_{\ell=1}^{R}\sum_{t=1}^{n_\ell} P_\ell(t,K)}. \tag{4.41}$$

This completely non-binning method for multi-run reweighting is extensively used in Paper III [108].

Chapter 5

Ginzburg-Landau theory

This is a short introduction to the Ginzburg-Landau (GL) model, for more details see e.g. the textbooks [38, 43, 85, 143]. The first understanding of superconductors on a phenomenological level was obtained by the two-fluid model proposed by Fritz and Heinz London in 1935 [102]. This model could explain the Meissner effect by assuming that a fraction n_s of the total electron density n could flow without resistivity, thereby modifying Ohm's law. The next step forward came in 1950 when Ginzburg and Landau [55] proposed their famous phenomenological model for superconductors which could account for spatial varying densities of superconducting electrons and link this density to magnetic fields and electric currents. This is a description in terms of a kind of macroscopic wave functions $\psi(\boldsymbol{r})$, where the local density of superconducting electrons is proportional to $|\psi(\boldsymbol{r})|^2$, and a vector potential $\boldsymbol{A}$ corresponding to a magnetic field $\boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}$. Note that this magnetic field is due *both* to external fields and super-currents in the sample. If $\psi(\boldsymbol{r})$ is small, which is the case near a critical point, and varies slowly in space, the free energy density can be expanded in a series of the form

$$f = f_{\text{normal}} + \alpha(T)|\psi|^2 + \frac{u}{2}|\psi|^4 + \frac{\hbar^2}{2m^*}\left|(\boldsymbol{\nabla} - ie^*\boldsymbol{A})\,\psi\right|^2 + \frac{1}{2\mu_0}\left(\boldsymbol{\nabla}\times\boldsymbol{A}\right)^2 . \tag{5.1}$$

Here f_{normal} is the contribution from the normal electrons, e^* and m^* are effective charge and mass parameters, and u is a self coupling for the scalar field ψ. We have also introduced the temperature dependent coefficient $\alpha(T)$ given by

$$\alpha(T) = \alpha_0 \frac{T - T_c^{\text{MF}}}{T_c^{\text{MF}}} \equiv \alpha_0 \tau \tag{5.1'}$$

where $T = T_c^{\text{MF}}$ is the mean-field critical temperature. In 1957 Bardeen Cooper and Schrieffer proposed their famous BCS-theory [11] and it was realized that superconductivity was caused by forming pairs of fermions, so called "Cooper pairs" [34], condensing for sufficiently low temperatures.[1] This made a more microscopic interpretation of Eq. 5.1 possible, and it became clear that the effective charge should be interpreted as $e^* = 2e/\hbar$, where $2e$ is the total charge of the two fermions constituting a Cooper pair. A microscopic derivation of the Ginzburg-Landau free energy from the BCS-theory was given in 1959 by Gorkov using Green function techniques [2, 57]. He showed that the Ginzburg-Landau free energy was a limiting case for the BCS theory near the critical temperature. The Ginzburg-Landau model has been very successful in dealing with spatial inhomogeneities, such as the mixed state in type-II superconductors, and even high-T_c superconductors where no microscopic mechanism so far has been found, at least not to everybody's satisfaction. Therefore investigations of the GL-theory has the advantage of yielding

[1] In fact for conventional superconductors the pairs are created and condense at approximately the same temperature T_c which is to a very good approximation equal to the mean-field transition temperature $T = T_c^{\text{MF}}$. For high-T_c superconductors the pairs are created at a rather high temperature T^* and condense at a considerably lower temperature T_c, see Fig. 1.1 on page 4. To incorporate this in the GL-model, the fields must be allowed to fluctuate. Then one can identify $T^* = T_c^{\text{MF}}$.

model-independent results. For high-T_c superconductors thermal fluctuations become important due to the high temperature and short correlation length, as mentioned in Chapter 1. The free energy density in Eq. 5.1 then has to be replaced with the functional integral

$$\begin{aligned} Z &= \int D[\psi]D[\boldsymbol{A}]e^{-H[\psi,\boldsymbol{A}]/k_BT}, \\ H[\psi,\boldsymbol{A}] &= \int d^3r \left[\alpha(T)\left|\psi\right|^2+\frac{u}{2}\left|\psi\right|^4+\frac{\hbar^2}{2m^*}\left|(\boldsymbol{\nabla}-ie^*\boldsymbol{A})\,\psi\right|^2+\frac{1}{2\mu_0}\left(\boldsymbol{\nabla}\times\boldsymbol{A}\right)^2\right]. \end{aligned} \tag{5.2}$$

This theory has a local $U(1)$ symmetry (gauge-symmetry) and is invariant under the transformation

$$\psi(\boldsymbol{r}) \to e^{i\theta(\boldsymbol{r})}\psi(\boldsymbol{r}), \quad \boldsymbol{A}(\boldsymbol{r}) \to \boldsymbol{A}(\boldsymbol{r}) + \boldsymbol{\nabla}\theta(\boldsymbol{r})/e^* \tag{5.3}$$

where $\theta(\boldsymbol{r})$ is an arbitrary real-valued function.[2] When T is far enough from the critical temperature, fluctuations are assumed to be negligible, and one can derive the Ginzburg-Landau equations by minimizing $H[\psi,\boldsymbol{A}]$ with respect to $\boldsymbol{A}$ and ψ. From these equations one can find the amplitude of the scalar field for different temperatures,

$$|\psi(T)| = \begin{cases} |\psi_0||\tau|^{1/2} & \tau \leq 0 \\ 0 & \tau > 0 \end{cases}, \quad |\psi_0| = \sqrt{\alpha_0/u}. \tag{5.4}$$

This field is often given the name order field since it, at the mean-field level, develops a finite value in the superconducting phase. In zero external magnetic field the minimum for the vector potential is for $\boldsymbol{A}=0$. Thus the solution for $T > T_c^{\mathrm{MF}}$ is trivial and both fields ψ and $\boldsymbol{A}$ vanish. For $T < T_c^{\mathrm{MF}}$ things are more interesting and the system appears to be in a broken phase since $\psi \neq 0$. The finite value of ψ is a basic ingredient in the Higgs mechanism [6,46,68,69] which gives the photon a non-zero mass and thereby explains the Meissner effect. This can be seen as a finite value of the magnetic penetration length λ, given in mean-field theory as [143]

$$\lambda(T) = \lambda_0|\tau|^{-1/2}, \quad \lambda_0 = \sqrt{\frac{m^*u}{4e^2\mu_0\alpha_0}}. \tag{5.5}$$

In addition we can define a correlation length ξ which gives the length scale for variations in $\psi(\boldsymbol{r})$ due to a point-perturbation. At the mean-field level we find [143]

$$\xi(T) = \xi_0|\tau|^{-1/2}, \quad \xi_0 = \sqrt{\frac{\hbar^2}{2m^*\alpha_0}}. \tag{5.6}$$

We can thus conclude that we have a second order phase transition at the mean-field level because the order parameter goes continuously to zero and both $\lambda(T)$ and $\xi(T)$ diverge at the critical temperature $T = T_c^{\mathrm{MF}}$. The Ginzburg-Landau parameter κ is defined by the ratio

$$\kappa = \frac{\lambda}{\xi} \tag{5.7}$$

and divides the superconductors in type-I and type-II according to their response to an external magnetic field. In type-I superconducting materials the magnetic field is completely expelled until a critical field H_c is reached, above this field the materials become completely normal. For type-II superconducting materials the flux is completely expelled only up to a lower critical field H_{c1}. Above this field, but below an upper critical field H_{c2}, magnetic flux can penetrate the sample

[2] This model is also used to describe a great number of other phenomena in Nature, including such widely separated phenomena as the Higgs mechanism in particle physics, [33] phase transitions in liquid crystals, [42,103] crystal melting, [86] the quantum Hall effect, [127,148] and it is also used as an effective field theory describing phase transitions in the early Universe. [145] In quantum field theory this model is often referred to as 3d $U(1)$+Higgs, Abelian Higgs (3d) or scalar QED (3d).

as lines of quantized flux [1]. Above H_{c2} the materials become completely normal. At the mean-field level the point of separation between type-I and type-II superconductors is given by the well known textbook value $\kappa_{\mathrm{I/II}} = 1/\sqrt{2}$,[3] but fluctuations may alter this result, and in fact they do, as we have demonstrated in Paper III [108]. Before saying more about fluctuations, I will mention some of the different parametrizations of the Ginzburg-Landau model which sometimes may be a bit confusing.

5.1 Parametrization of the model

The standard textbook version of the Ginzburg-Landau model in connection with superconductors is given in Eq. 5.2. Since this model has so many fields and couplings it can be written in many different forms by different rescalings. This is of course trivial in principle, but in practice the different ways to write the model, and the connection between them may be rather confusing. Here I will give some details about the transformation from the form Eq. 5.2 to the form in Eq. 5.12, which we have used in our simulations on the full GL-model with fluctuating amplitude, phase, and gauge fields. For other parametrizations see e.g. [85, part II, chapter 3].

Starting with Eq. 5.2 it is convenient to define $\gamma = \hbar^2/m^*$ and $\widetilde{m}^2 = \alpha_0 \tau$. We absorb μ_0, γ, and the temperature $\widetilde{T} = k_B T$ by defining new fields and couplings:

$$\boldsymbol{A}'^2 = \frac{\boldsymbol{A}^2}{\mu_0 \widetilde{T}},\ q^2 = e^{*2}\mu_0 \widetilde{T},\ |\psi'|^2 = \frac{\gamma|\psi|^2}{\widetilde{T}},\ m^2 = \frac{\widetilde{m}^2}{\gamma},\ u' = \frac{u\widetilde{T}}{\gamma^2}, \tag{5.8}$$

which gives the action ($S = H/\widetilde{T}$)

$$S[\psi', \boldsymbol{A}'] = \int d^3r' \left[m^2 |\psi'|^2 + \frac{u'}{2}|\psi'|^4 + \frac{1}{2}|(\boldsymbol{\nabla} - iq\boldsymbol{A}')\psi'|^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A}')^2 \right]. \tag{5.9}$$

Now the charge q is dimensionful and can be used to define dimensionless quantities

$$\psi = \psi'/q, \quad \boldsymbol{A} = \boldsymbol{A}'/q, \quad \boldsymbol{r} = \boldsymbol{r}'q^2, \quad y = m^2/q^4, \quad x = u'/q^2. \tag{5.10}$$

This gives the action

$$S[\psi, \boldsymbol{A}] = \int d^3r \left[y|\psi|^2 + \frac{x}{2}|\psi|^4 + \frac{1}{2}|(\boldsymbol{\nabla} - i\boldsymbol{A})\psi|^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2 \right] \tag{5.11}$$

or

$$S[\psi, \boldsymbol{A}] = \int d^3r \left[y|\psi|^2 + x|\psi|^4 + |(\boldsymbol{\nabla} - i\boldsymbol{A})\psi|^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2 \right] \tag{5.12}$$

by letting $\psi \to \sqrt{2}\psi$, $x \to x/2$, and $y \to y/2$. Then one can relate the parameters x, y in Eq. 5.12 to the parameters α, u in the original theory Eq. 5.2 on page 32 by going backwards

$$x \to \frac{2u'}{q^2} \to \frac{2u\widetilde{T}}{\mu_0\gamma^2 e^{*2}\widetilde{T}} \to \frac{m^{*2}\hbar^2 u}{2\mu_0\hbar^4 e^2} \to \frac{1}{8\pi\alpha_s\hbar c}\left(\frac{m^* c}{\hbar}\right)^2 u \tag{5.13a}$$

$$y \to \frac{2m^2}{q^4} \to \frac{2\widetilde{m}^2}{\mu_0^2\gamma e^{*4}\widetilde{T}^2} \to \frac{2m^2 m^*\hbar^4}{\hbar^2\mu_0^2(k_BT)^2 16e^4} \to \frac{m^* c^2}{128\pi^2\alpha_s^2(k_BT)^2}\alpha(T) \tag{5.13b}$$

where $\alpha_s = \frac{\mu_0 e^2 c}{4\pi\hbar}$ is the fine-structure constant. Note the *huge* numerical ratios entering here. This means that one should be aware that clear effects seen in the effective action Eq. 5.12 may be unobservably small in real superconductors. This is e.g. so for the fluctuation induced first order jump predicted for strongly type-I superconductors [59], [78, appendix A].

[3] Note that $\kappa_{\mathrm{I/II}}$ is also the value where the sign of the electromagnetic part of the interaction between two vortices changes, as first discussed by Bogomolnyi [26].

5.2 Fluctuations

In a seminal paper by Halperin, Lubensky, and Ma [59] a "fluctuation induced" or "Coleman-Weinberg" type [33] first order phase transition was predicted. It was shown that for a constant scalar field, fluctuations in the gauge-field induce a first order transition. Here I will give a short review of this, partly following [85, 89]. The Lagrange density of the Ginzburg-Landau model in Eq. 5.9 can be written as

$$\mathcal{L} = \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2 + \frac{1}{2}|(\boldsymbol{\nabla} - iq\boldsymbol{A})|^2 + m_\psi^2|\psi|^2 + \frac{u}{2}|\psi|^4, \tag{5.14}$$

where

$$m_\psi^2 = \xi_0^{-2}\tau = \xi_0^{-2}\frac{T - T_c^{\rm MF}}{T_c^{\rm MF}}, \tag{5.14'}$$

and ξ_0 is the zero temperature correlation length. In the London limit[4] we can write

$$\psi(\boldsymbol{r}) = \psi_0 e^{i\theta(\boldsymbol{r})}, \tag{5.15}$$

and the Lagrange density becomes

$$\mathcal{L} = \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2 + \frac{1}{2}(\boldsymbol{\nabla}\theta - q\boldsymbol{A})^2 + \underbrace{m_\psi^2\psi_0^2 + \frac{u}{2}\psi_0^4}_{\equiv \mathcal{V}_0(\psi_0)}. \tag{5.16}$$

The integrating of the $\theta(\boldsymbol{r})$ field (in the gauge $\boldsymbol{\nabla}\cdot\boldsymbol{A} = 0$) results in a massive gauge field, $m_A = q\psi_0$, since a term $\frac{1}{2}m_A^2\boldsymbol{A}^2$ appears in the the action. By integrating out the gauge field we obtain a one-loop effective potential

$$\begin{aligned}
\mathcal{V}_{\rm eff}(\psi_0) &= \int_{k<\Lambda} \frac{d^3k}{(2\pi)^3} \ln\left(k^2 + m_A^2\right) \\
&= \frac{1}{2\pi^2}\int_{k=0}^{\Lambda} dk k^2 \ln\left(k^2 + m_A^2\right) \\
&= \frac{1}{2\pi^2}\left[\frac{1}{3}\Lambda^3 \ln\left(\Lambda^2 + m_A^2\right) - \frac{2}{9}\Lambda^3 + \frac{2}{3}m_A^2\Lambda - \frac{2}{3}m_A^3 \arctan\frac{\Lambda}{m_A}\right] \\
&\approx \frac{1}{3\pi^2}\Lambda^3 \ln\Lambda - \frac{1}{9\pi^2}\Lambda^3 + \frac{1}{2\pi^2}q^2\psi_0^2\Lambda - \frac{1}{6\pi}q^3\psi_0^3, \quad m_A/\Lambda \ll 1.
\end{aligned} \tag{5.17}$$

Here we note that the two first terms are independent of ψ_0 and can be absorbed in the total energy, the third term can be absorbed in the mass by defining

$$\widetilde{m}^2 = m_\psi^2 + \frac{q^2}{2\pi^2}\Lambda = \widetilde{\xi}_0^{-2}\left(\frac{T}{\widetilde{T}_c} - 1\right) \tag{5.18}$$

where $\widetilde{\xi}_0^2 = \xi_0^2[\Upsilon(\Lambda) - 1]^{-1}$, $\widetilde{T}_c = T_c^{\rm MF}[\Upsilon(\Lambda) - 1]$, and $\Upsilon(\Lambda) = (q^2\xi_0^2/2\pi^2)\Lambda$. Hereafter we remove the tilde for notational simplicity. We then have the effective potential

$$\mathcal{V}(\psi_0) = \mathcal{V}_0(\psi_0) + \mathcal{V}_{\rm eff}(\psi_0) = m_\psi^2\psi_0^2 - \frac{1}{6\pi}q^3\psi_0^3 + \frac{u}{2}\psi_0^4, \tag{5.19}$$

and a simple mean-field calculation shows that the term $\propto \psi_0^3$ gives a first order transition. The phase transition will be for a temperature T_1 given by

$$\begin{aligned}
m_\psi^2 \equiv \xi_0^{-2}\left(\frac{T_1}{T_c} - 1\right) &= \frac{1}{18}\left(\frac{q^3}{2\pi}\right)^2\frac{1}{u} \\
\Rightarrow T_1 &= T_c\left(1 + \frac{q^6\xi_0^2}{72\pi^2 u}\right)
\end{aligned} \tag{5.20}$$

[4] In the London limit the scalar amplitude is assumed to be spatially constant. It can be shown that for *second order* transitions this approximation is justified since the amplitude-fluctuations are negligible compared to the phase-fluctuations, see e.g. [87, 113]. Note however that amplitude fluctuations must be incorporated to allow first order transitions, as in Paper III [108].

which is *above* T_c, and the corresponding jump in the order parameter ψ_0 is given by

$$\Delta\psi_0 = \frac{q^3}{6\pi u}. \tag{5.21}$$

In the above calculations we have assumed that the amplitude is approximately constant, an assumption that is not always valid. The Ginzburg criterion tells us that fluctuations will become important for

$$|\tau_G| \lesssim u^2\xi_0^2 \tag{5.22a}$$

which corresponds to

$$\frac{\tau_G}{\tau_1} \sim \frac{u^3}{\xi_0^2} \sim \kappa^6 \tag{5.22b}$$

where we have set $\tau_1 = T_1/T_c - 1$. This means that the predicted first order jump will take place *inside* the Ginzburg region for a type-II superconductor. In this region the London limit of a spatial constant amplitude may not be valid and we must be suspicious to the above result. By using a perturbative approach one neglects topological defects, such as vortex loops, since they can only be included by going to infinite order in the perturbation series, an impossible task. For type-II superconductors the neglect of vortices is clearly problematic since there is strong evidence that topological effects in form of vortex loops drive the phase transition. In fact the phase transition is associated with a vortex loop blowout as clearly demonstrated by Monte Carlo simulations in e.g. [71, 113]. We have studied the order of the metal to superconductor phase transition in a non-perturbative manner by doing Monte Carlo simulations on the full Ginzburg-Landau model in Paper III [108]. See also Chapter 7 for more details.

5.3 Topological defects

A topological defect is in general characterized by some core region (e.g. a point or a line) where the order is destroyed and a far away region where the fields are slowly varying and the order is almost restored. Since topological excitations are collective excitations they are largely independent of microscopic details of the underlying theory, and their nature are instead determined by broad characteristics of the underlying model like its symmetries and dimensionality. Thus they give a convenient mesoscopic description of the system. Qualitatively their importance are related to their ability to destroy order at long distances at a low cost in energy. Macroscopical fluctuations in form of topological excitations allow large deviations from the perturbative ground state and are triggering phase transitions. Whenever their configurational entropy exceed their energy, they proliferate, thereby inducing singularities in thermodynamic quantities.

Topological defects are important in the understanding of many phase transitions and have different names depending on the broken symmetry. In superfluid ^{4}He and XY-models they are called *vortices* (2D) or *vortex loops* (3D), in periodic crystals, *dislocations*, and in liquid crystals, *disclinations*. The prime example is the phase transition in the 2DXY-model which can be used as a model for the superfluid-to-normal phase transition in a ^{4}He-film. In two dimensions the Mermin-Wagner theorem [106] states that a continuous symmetry cannot be broken. Therefore the phase transition must be related to something more complicated than simply breaking of the rotational invariance for the spin direction, or the $U(1)$-symmetry for the two-dimensional ϕ^4-model. This means that no *local* order parameter can be defined. The solution was found independently by Berezinskii [14] and by Kosterlitz and Thouless [91, 92]. In the low temperature phase the dominant excitations are spin waves, where the directions of spins vary slowly in space, and the correlation length is infinite. By increasing the temperature the spins fluctuate more wildly and the periodicity of their direction angle must be accounted for. Thus small vortex-antivortex pairs, as shown in the lower part of Fig. 5.1 on the next page, can be created. Such pairs only disturb the spin alignment in their nearest neighborhood and are therefore not important for the large-scale properties of the system near a critical point. This is seen by realizing that pairs of finite size always will be coarse grained away upon renormalization. However, at high enough temperatures

the pairs will unbind thereby creating vortices and antivortices arbitrarily far apart as shown in the upper part of Fig. 5.1. Such isolated vortices become the dominating excitations rendering the correlation length finite, and we have a phase transition at the point where the vortex-antivortex pairs unbind. An isolated vortex is topological stable since it can only be removed by rotating a macroscopically large number of spins. In contrast a vortex-antivortex pair, as shown at the bottom in Fig. 5.1, only disturb the overall alignment in a finite region, and the pair can be made to disappear by a continuous transformation which brings the pair together thereby annihilating. For more details see e.g. the book by Chaikin and Lubensky [31, chapter 9].

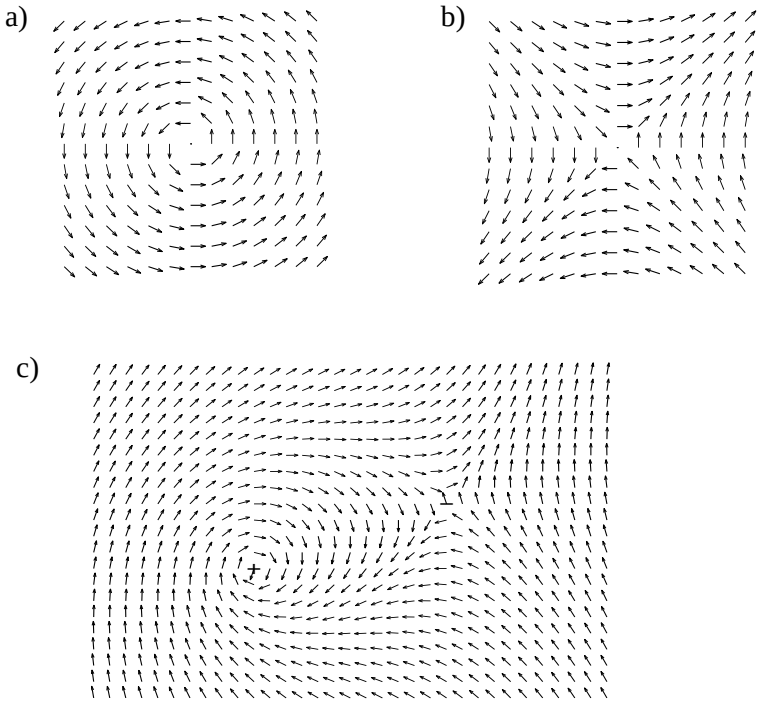

Figure 5.1: Vortex excitations in a 2DXY-model: a) vortex with *topological* charge $q = +1$, b) vortex with *topological* charge $q = -1$, and c) vortex-antivortex pair ($q = \pm 1$).

In three dimensions the Mermin-Wagner theorem does not forbid breaking of continuous symmetries, and phase transitions in theories exhibiting *global symmetries* can be associated with a local order parameter acquiring a finite value in the broken phase. In the broken phase the ground state of 3DXY-model has perfect spin alignment, which corresponds to a broken $U(1)$-symmetry in the ϕ^4 model. For low temperatures the dominating excitations are spin waves as in two dimensions. Lars Onsager [119, 120] realized that the phase transition from superfluid to normal ^{4}He could be driven by a proliferation of vortex loops. Such loops are closed lines with fractal dimension, in contrast to the point vortices present in two dimensions, and the configurational entropy is therefore much higher. This picture of a vortex loop driven phase transition has later been verified by extensive numerical simulations on the 3DXY-model, see e.g. [112, 113] and references therein. This model is assumed to belong to the same universality class as the ϕ^4-model.

In a classic and brilliant paper, Alexei A. Abrikosov [1] showed, by using the Ginzburg-Landau equations, that the ground state for a type-II superconductor in an external magnetic field is a lattice of vortex lines, each line carrying a magnetic flux $\Phi_0 = \frac{h}{2e}$. In the interior of a vortex line the order field disappears and the magnetic flux can penetrate. In a type-II superconductor the magnetic penetration depth λ is larger than the correlation length ξ and the structure of a vortex line is as shown schematically in Fig. 5.2 on the facing page. In the high-T_c cuprates there are strong fluctuation effects near the phase transition, and in addition to the field induced vortex lines also thermally induced vortex loops must be included, see e.g. [25, 113]. These materials

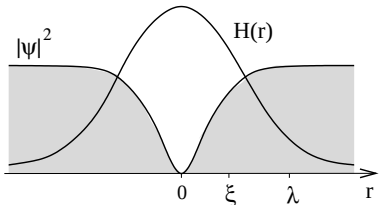

Figure 5.2: Structure of isolated vortex line for type-II superconductor where $\kappa = \lambda/\xi \gtrsim 1$.

are strongly type-II which means that the magnetic penetration length is much larger than the correlation length. The fluctuations in the gauge field can therefore to a good approximation be neglected. This means that the phase transition in zero field may be described by the 3DXY-model and the phase transition is driven by a proliferation of thermally induced vortex loops. The behavior in a finite field is more complicated and I refer to the extensive review of these matters in Anh Kiet Nguyen's PhD-thesis [111]. The finite field-transition is also mentioned in Paper II [71] where the behavior is related to the fractal dimension of the vortex loops. If the thermally induced vortices fill space more effectively than the field induced ones, the zero-field phase transition in terms of a vortex loop blowout is assumed to persist.

To illustrate the importance of the vortices in the phase-field a simple example will be given in the next section. An effective Hamiltonian for phase-fluctuations is constructed and the vortices are seen to clearly modify the behavior of the model.

5.3.1 Effective Hamiltonian for transverse phase fluctuations

Naively the effective Hamiltonian for phase fluctuations in the London model, see e.g. Eq. 5.16, is $\mathcal{H} = 0$ since the phase degree of freedom can be removed by a suitable gauge-transformation. This is however too naive since the London model is known to sustain delta-function vortices leading to a multiply connected geometry which complicates matters. The calculations below were done to understand, in a simple setting, the effect of gauge fluctuations on the lower limit on the anomalous dimension of the scalar field in the Ginzburg-Landau model. In Paper II [71] we gave the resulting formulas, but the details had to be skipped due to lack of space. The same problem has later also been considered in [101] where the influence of vortices on the Higgs mechanism [6, 46, 68, 69] is studied.

The equation that defines the delta-function vortices is

$$\boldsymbol{\nabla} \times (\boldsymbol{\nabla}\theta)_T = \sum_{\boldsymbol{r}_i} n(\boldsymbol{r}_i)\delta(\boldsymbol{r} - \boldsymbol{r}_i)\hat{\boldsymbol{e}}_i, \tag{5.23}$$

where $n(\boldsymbol{r}_i)$ is a local vortex density, $\hat{\boldsymbol{e}}_i$ is a unit vector giving the local direction of the vorticity, and $(\boldsymbol{\nabla}\theta)_T$ denotes a transverse phase fluctuation. Operating from the left with $\boldsymbol{\nabla}\times$ and using that $\boldsymbol{\nabla} \times \boldsymbol{\nabla} \times \boldsymbol{A} = \boldsymbol{\nabla}(\boldsymbol{\nabla} \cdot \boldsymbol{A}) - \boldsymbol{\nabla}^2\boldsymbol{A}$, and $\boldsymbol{\nabla} \cdot (\boldsymbol{\nabla}\theta)_T = 0$, we get

$$-\boldsymbol{\nabla}^2(\boldsymbol{\nabla}\theta)_T = \sum_{\boldsymbol{r}_i} n(\boldsymbol{r}_i)\boldsymbol{\nabla} \times \delta(\boldsymbol{r} - \boldsymbol{r}_i)\hat{\boldsymbol{e}}_i. \tag{5.24}$$

By using the the Fourier transforms

$$\boldsymbol{S}_{\boldsymbol{k}} = \int d^3r (\boldsymbol{\nabla}\theta)_T e^{i\boldsymbol{k}\cdot\boldsymbol{r}} \quad \Leftrightarrow \quad (\boldsymbol{\nabla}\theta)_T = \int \frac{d^3k}{(2\pi)^3} \boldsymbol{S}_{\boldsymbol{k}} e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{5.25}$$

and the definition of the delta-function

$$\delta(\boldsymbol{r} - \boldsymbol{r}_i) = \int \frac{d^3k}{(2\pi)^3} e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}_i)}, \tag{5.26}$$

we can solve for the Fourier transform of $(\boldsymbol{\nabla}\theta)_T$,

$$k^2 \boldsymbol{S}_{\boldsymbol{k}} = \sum_{\boldsymbol{r}_i} n(\boldsymbol{r}_i) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} (-i\boldsymbol{k}) \times \hat{\boldsymbol{e}}_i. \tag{5.27}$$

By defining

$$\boldsymbol{n}_{\boldsymbol{k}} \equiv \frac{1}{2\pi} \sum_{\boldsymbol{r}_i} n(\boldsymbol{r}_i) e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} \hat{\boldsymbol{e}}_i, \tag{5.28}$$

this can be written as

$$\boldsymbol{S}_{\boldsymbol{k}} = -2\pi i \frac{\boldsymbol{k} \times \boldsymbol{n}_{\boldsymbol{k}}}{k^2}. \tag{5.29}$$

After these introductory calculations we are ready to study the vortex influence on the effective theory for phase fluctuations. Let the Hamiltonian density be given by

$$\mathcal{H}_{\psi,\boldsymbol{A}} = m_\psi^2 |\psi|^2 + \frac{u_\psi}{2} |\psi|^4 + |(\boldsymbol{\nabla} - iq\boldsymbol{A})\psi|^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2. \tag{5.30}$$

By defining $\psi = |\psi| e^{i\theta}$, neglecting amplitude fluctuations by setting $|\psi| = 1$, and neglecting constant terms, we get the Hamiltonian density in the London limit,

$$\mathcal{H}_{\theta,\boldsymbol{A}} = (\boldsymbol{\nabla}\theta - q\boldsymbol{A})^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2. \tag{5.31}$$

This can be split in contributions from longitudinal and transverse phase-field fluctuations in the following way

$$\mathcal{H}_{\theta,\boldsymbol{A}} = [(\boldsymbol{\nabla}\theta)_L - q\boldsymbol{A}_L]^2 + [(\boldsymbol{\nabla}\theta)_T - q\boldsymbol{A}_T]^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A}_T)^2. \tag{5.32}$$

Here the longitudinal part can be removed by a suitable gauge transform and we will not consider them further. By writing the Hamiltonian density for the remaining transverse terms in terms of Fourier modes we find

$$\mathcal{H}_{\theta,\boldsymbol{A}} = \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} - q(\boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{A}^T_{-\boldsymbol{k}} + \boldsymbol{S}_{-\boldsymbol{k}} \cdot \boldsymbol{A}^T_{\boldsymbol{k}}) + \left(\frac{k^2}{2} - q^2\right) \boldsymbol{A}^T_{\boldsymbol{k}} \cdot \boldsymbol{A}^T_{-\boldsymbol{k}}, \tag{5.33}$$

where $\boldsymbol{A}^T_{\boldsymbol{k}}$ is the Fourier-transform of the transverse part gauge-field. Note that in the presence of vortices the phase $\theta(\boldsymbol{r})$ itself does not have a well-defined Fourier-transform because of its singularities. However the gradient of the phase has a well defined longitudinal and transverse part since this is a velocity. By completing squares in $\boldsymbol{A}^T_{\boldsymbol{k}}, \boldsymbol{A}^T_{-\boldsymbol{k}}$ we obtain

$$\mathcal{H}_{\theta,\boldsymbol{A}} = \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} + \Xi^2 \left[\boldsymbol{A}^T_{\boldsymbol{k}} - \frac{q\boldsymbol{S}_{\boldsymbol{k}}}{\Xi^2}\right] \cdot \left[\boldsymbol{A}^T_{-\boldsymbol{k}} - \frac{q\boldsymbol{S}_{-\boldsymbol{k}}}{\Xi^2}\right] - \frac{q^2 \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}}}{\Xi^2}, \tag{5.34}$$

where $\Xi^2 = \frac{k^2}{2} + q^2$. Here we can integrate out the shifted gauge-field defined by $\widetilde{\boldsymbol{A}}^T_{\boldsymbol{k}} = \boldsymbol{A}^T_{\boldsymbol{k}} - q\boldsymbol{S}_{\boldsymbol{k}}/\Xi^2$, thereby giving us the effective Hamiltonian density for the transverse phase fluctuations describing fluctuating vortices

$$\mathcal{H}_\theta = \left(1 - \frac{q^2}{\Xi^2}\right) \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}} = \frac{k^2}{2q^2 + k^2} \boldsymbol{S}_{\boldsymbol{k}} \cdot \boldsymbol{S}_{-\boldsymbol{k}}. \tag{5.35}$$

Here it is interesting to study some special cases. By setting $q = 0$ we see that the gauge-field fluctuations soften the fluctuations by introducing a factor $1/[2(q/k)^2 + 1] \leq 1$ multiplying the effective Hamiltonian density. In a charged model, i.e. $q \neq 0$, *without vortices* we have $\boldsymbol{S}_{\boldsymbol{k}} = 0$, and thus $\mathcal{H} = 0$ as claimed in the beginning of this section. This is of course a rather boring theory! However the presence of vortices gives $\mathcal{H} \neq 0$ and results in a model with many interesting properties.

This simple example illustrated the importance of *transverse phase fluctuations* in the form of vortices. A field theoretic description of these vortices in terms of a dual, or disorder, field theory is the topic of the next section.

5.4 Duality

It is well known that the Schrödinger theory of an arbitrary number of particles N can be formulated as a second quantized field theory, see e.g. [58]. In the field description the single field $\psi(\boldsymbol{r}, t)$ replaces the N particle orbits and their canonical momenta. We also know that all quantum mechanical properties have a statistical analogue by simply continuing time to imaginary values $t \to i\tau$. It is easy to show that the thermal analogue of a free quantum particle is a random walk. The thermal partition function is thus equivalent to a grand canonical ensemble of particles performing random walks in a thermal environment. Defect lines can be handled in a similar way by replacing the time by a length parameter. For an extensive account of these matters see the book by Kleinert [85, particularly chapter 6].

By doing a duality transformation it is possible to find a field theory describing the defects in the original theory, a so called *disorder field theory*. In the disorder theory one can define a (dis)order parameter which acquires a finite expectation value in the disordered phase of the original theory. It thus plays a role that is opposite to the usual order parameter in the sense of Landau. The duality transform maps a strong coupling regime to a weak coupling regime. This is useful when doing perturbative calculations. For a thorough introduction to this subject see [85, 130].

Here I will first start with the London model, which is the GL-model with frozen amplitude, on a lattice. The reason is that in this model the duality transformations can be done rather straightforwardly. To achieve this we have to introduce the so called Villain approximation. In the continuum limit no such formal mathematical connection between the original and dual theory has been developed, but relying on some unproven assumptions a dual theory can be found. Then a very clear and intuitive picture emerges.

5.4.1 Duality in the lattice London model

Here I will only give a short review of some of the techniques involved in the duality transformations on a lattice. For a more thorough introduction to these matters see e.g. [65, 82, 131, 132] and in particular the book by Kleinert [85].

The action for the lattice London model can be written as a sum over lattice sites i

$$\begin{aligned} \mathcal{S}_L &= \widetilde{\beta} J_0 \sum_i \left[-\cos\left(\boldsymbol{\Delta}\theta_i - \widetilde{\boldsymbol{A}}_i\right) + \frac{\lambda^2}{2} (\boldsymbol{\Delta} \times \widetilde{\boldsymbol{A}}_i)^2 \right] \\ &= \sum_i \left[-\beta \cos\left(\boldsymbol{\Delta}\theta_i - q\boldsymbol{A}_i\right) + \frac{1}{2} (\boldsymbol{\Delta} \times \boldsymbol{A}_i)^2 \right], \end{aligned} \tag{5.36}$$

where $\beta = \widetilde{\beta} J_0$, $q^2 = 1/\widetilde{\beta} J_0 \lambda^2$, $\boldsymbol{A}_i = \widetilde{\boldsymbol{A}}_i / q$, and λ is the magnetic penetration length. In addition we have introduced a lattice derivative given by $\Delta_\mu = \theta_{i+\hat{\mu}} - \theta_i$. The partition function can be written as

$$\begin{aligned} Z(\beta, q) = \int_{-\pi}^{\pi} \left[\prod_i \frac{d\theta_i}{2\pi} \right] \int_{-\infty}^{\infty} \left[\prod_{i\mu} dA_{i\mu} \right] \\ \times \exp\left[\beta \sum_{i\mu} \cos(\Delta_\mu \theta_i - q A_{i\mu}) - \frac{1}{2} \sum_i (\boldsymbol{\Delta} \times \boldsymbol{A}_i)^2 \right], \end{aligned} \tag{5.37}$$

where the gauge-field is non-compact, $A_{i\mu} \in \mathbb{R}$. In the Villain approximation [146] Eq. 5.37 can

be rewritten as

$$Z(\beta,q)=\int_{-\pi}^{\pi}\left[\prod_i\frac{d\theta_i}{2\pi}\right]\int_{-\infty}^{\infty}\left[\prod_{i\mu}dA_{i\mu}\right]\sum_{n_{i\mu}=-\infty}^{\infty}\times\exp\left[-\frac{\beta}{2}\sum_{i\mu}(\Delta_\mu\theta_i-qA_{i\mu}-2\pi n_{i\mu})^2-\frac{1}{2}\sum_i(\boldsymbol{\Delta}\times\boldsymbol{A}_i)^2\right].\tag{5.38}$$

The kinetic term can be linearized by introducing an auxiliary field $\boldsymbol{v}_i=v_{i\mu}\hat{\boldsymbol{e}}_\mu$ such that

$$e^{-\frac{\beta}{2}(\Delta_\mu\theta_i-qA_{i\mu}-2\pi n_{i\mu})^2}\propto\int_{-\infty}^{\infty}dv_{i\mu}e^{-\frac{1}{2\beta}v_{i\mu}^2+i(\Delta_\mu\theta_i-qA_{i\mu}-2\pi n_{i\mu})v_{i\mu}}.\tag{5.39}$$

The sums over $n_{i\mu}$ restrict $v_{i\mu}$ to integers $\ell_{i\mu}$. The θ_i integrals give that $\boldsymbol{\Delta}\cdot\boldsymbol{v}_i=0$, which can be achieved by introducing an integer valued gauge field $\boldsymbol{h}_i$

$$\boldsymbol{\ell}_i=\boldsymbol{\Delta}\times\boldsymbol{h}_i.\tag{5.40}$$

In order to be able to treat $\boldsymbol{h}_i$ as a continuous variable we introduce a new integer-valued field $\boldsymbol{m}_i$ by the Poisson summation formula

$$\sum_{\ell_{i\mu}=-\infty}^{\infty}\delta(\ell_{i\mu}-h_{i\mu})=\sum_{m_{i\mu}=-\infty}^{\infty}e^{-2\pi i m_{i\mu}h_{i\mu}}.\tag{5.41}$$

Then the partition function can be written as

$$Z(\beta,q)=\int_{-\infty}^{\infty}\left[\prod_{i\mu}{}'dh_{i\mu}\right]\int_{-\infty}^{\infty}\left[\prod_{i\mu}{}'dA_{i\mu}\right]\sum_{m_{i\mu}=-\infty}^{\infty}{}'e^{-\sum_i\mathcal{S}_i}\tag{5.42}$$

where

$$\mathcal{S}_i=2\pi i\boldsymbol{m_i}\cdot\boldsymbol{h}_i+\frac{1}{2\beta}(\boldsymbol{\Delta}\times\boldsymbol{h}_i)^2-iq(\boldsymbol{\Delta}\times\boldsymbol{h}_i)\cdot\boldsymbol{A}_i+\frac{1}{2}(\boldsymbol{\Delta}\times\boldsymbol{A}_i)^2.\tag{5.43}$$

The marks on the products and sums mean

$$\boldsymbol{\Delta}\cdot\boldsymbol{A}_i=\boldsymbol{\Delta}\cdot\boldsymbol{h}_i=\boldsymbol{\Delta}\cdot\boldsymbol{m}_i=0.\tag{5.44}$$

Integrating out the gauge field $\boldsymbol{A}_i$ gives

$$Z(\beta,q)=\int_{-\infty}^{\infty}\left[\prod_{i\mu}{}'dh_{i\mu}\right]\sum_{m_{i\mu}=-\infty}^{\infty}{}'\times\exp\left[-\sum_i\left\{2\pi i\boldsymbol{m_i}\cdot\boldsymbol{h}_i+\frac{1}{2\beta}(\boldsymbol{\Delta}\times\boldsymbol{h}_i)^2+\frac{q^2}{2}\boldsymbol{h}_i^2\right\}\right].\tag{5.45}$$

This is a theory where vortex segments $m_{i\mu}$ have a Biot-Savart type interaction mediated by a massive dual gauge field $\boldsymbol{h}_i$. By integrating out $\boldsymbol{h}_i$ we obtain the London model in a vortex representation and it is easily seen that the mass of $\boldsymbol{h}$ gives a finite range of the interactions. Note that the massiveness of the gauge-field reduces the symmetry from a local gauge symmetry to a global $U(1)$ symmetry.

5.4.2 Continuum dual model

In the continuum London model the duality transformation cannot be performed without introducing additional assumptions regarding the continuum limit of the lattice transform. Several attempts have been made using slightly different attacks, see e.g. [65,82,131,132]. Here I will only give the resulting dual theory without any mathematical justification. Note that what follows is *only* valid in three dimensions.

Although the formal relation between the original and dual theory relies on some unproven assumptions the picture that emerges is however very clear and intuitive. It is useful to start by defining a "super-theory"

$$\mathcal{H}_{\mathrm{s}}^{q,m_\Lambda}[\Phi,\mathbf{\Lambda}] = |(\boldsymbol{\nabla} - iq\mathbf{\Lambda})\Phi|^2 + m_\Phi^2|\Phi|^2 + \frac{u_\Phi}{2}|\Phi|^4 + \frac{m_\Lambda^2}{2}\mathbf{\Lambda}^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\mathbf{\Lambda})^2, \tag{5.46}$$

where $\mathbf{\Lambda}$ is a gauge field coupling to the scalar field Φ. Here the charge q and the mass of the gauge field m_Λ are allowed to take any value *including* zero. This theory is similar to the Ginzburg-Landau model if the mass of the gauge field m_Λ vanishes, i.e.

$$\begin{aligned}\mathcal{H}_{\mathrm{GL}}[\psi,\boldsymbol{A}] &= \mathcal{H}_{\mathrm{s}}^{q_{\mathrm{GL}},0}[\psi,\boldsymbol{A}] \\ &= |(\boldsymbol{\nabla} - iq_{\mathrm{GL}}\boldsymbol{A})\psi|^2 + m_\psi^2|\psi|^2 + \frac{u_\psi}{2}|\psi|^4 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{A})^2.\end{aligned} \tag{5.47}$$

This theory has a *local* $U(1)$ symmetry (gauge-symmetry). Here $|\psi|^2$ gives the Cooper pair density and the magnetic field is given by $\boldsymbol{B} = \boldsymbol{\nabla}\times\boldsymbol{A}$. The dual Hamiltonian density can be written in several ways, e.g.

$$\begin{aligned}\mathcal{H}_{\mathrm{dual}}[\phi,\boldsymbol{h}] &= \mathcal{H}_{\mathrm{s}}^{q_{\mathrm{dual}},m_h}[\phi,\boldsymbol{h}] \\ &= |(\boldsymbol{\nabla} - iq_{\mathrm{dual}}\boldsymbol{h})\phi|^2 + m_\phi^2|\phi|^2 + \frac{u_\phi}{2}|\phi|^4 + \frac{m_h^2}{2}\boldsymbol{h}^2 + \frac{1}{2}(\boldsymbol{\nabla}\times\boldsymbol{h})^2.\end{aligned} \tag{5.48}$$

Here $q_{\mathrm{dual}} = 2\pi m_h/q_{\mathrm{GL}}$ and $m_h = q_{\mathrm{GL}}\rho$, where ρ is the amplitude of the *order field* ψ. The *disorder* field ϕ describes a grand canonical ensemble of fluctuating magnetic vortex loops. It is minimally coupled to the massive vector field $\boldsymbol{h}$, representing the local magnetic induction. Since the gauge field $\boldsymbol{h}$ is massive the symmetry is lowered to a *global* $U(1)$ symmetry. The critical dual theory can be further simplified by observing that the exact RG-transformation for the mass of the dual gauge field is given by [40]

$$\frac{\partial m_h^2}{\partial \ln \ell} = m_h^2, \tag{5.49}$$

where ℓ is a length scale.[5] For $m_h \neq 0$ this gives $\lim_{\ell\to\infty} m_h^2 = \infty$. Thus $\boldsymbol{h} \to 0$ and we are left with the *effective* dual theory

$$\mathcal{H}_{\mathrm{dual}}^{\mathrm{eff}}[\phi] = |(\boldsymbol{\nabla}\phi|^2 + m_\phi^2|\phi|^2 + \frac{u_\phi}{2}|\phi|^4. \tag{5.50}$$

This is the theory for an uncharged superfluid. The dual of *this* theory can be found by setting $q_{\mathrm{GL}} = 0$ in Eq. 5.47. Then the gauge field and the scalar field decouple. Now $m_h = 0$ in Eq. 5.48 and we immediately observe that the dual of the noncharged theory Eq. 5.50 is isomorphic to the charged theory in Eq. 5.47.

If we define a duality operator $\mathbb{D}$ we can formally write

$$\mathbb{D}\mathcal{H}_{\mathrm{s}}^{q\neq 0,0}[\psi,\boldsymbol{A}] = \mathcal{H}_{\mathrm{s}}^{q=0,0}[\psi,0] \tag{5.51a}$$

and

$$\mathbb{D}\mathcal{H}_{\mathrm{s}}^{q=0,0}[\psi,0] = \mathcal{H}_{\mathrm{s}}^{q\neq 0,0}[\psi,\boldsymbol{A}]. \tag{5.51b}$$

[5] See Section 3.2 for a short introduction to the renormalization group (RG).

Thus

$$\mathbb{D}^2\,\mathcal{H}_{\rm s}^{q\neq 0,0}[\psi,\boldsymbol{A}] = \mathbb{D}\mathcal{H}_{\rm s}^{q=0,0}[\psi,0] = \mathcal{H}_{\rm s}^{q\neq 0,0}[\psi,\boldsymbol{A}] \tag{5.51c}$$

and $\mathbb{D}^2 = 1$.

The picture that emerges can then be summarized as follows. The vortex lines in a neutral superfluid are closed loops with long-rang Biot-Savart type interactions due to their long-range phase distortions. The disorder field theory has a complex scalar field coupled to a gauge field and is thus of the Ginzburg-Landau type which normally is used to describe superconductivity, i.e. a charged superfluid. We also know that the Ginzburg-Landau model has its own vortex lines. These only have short-range interactions since the long range phase fluctuations of the scalar field are nonphysical gauge modes which are unobservable. The magnetic field is screened by the Meissner effect. The disorder theory then have only short range interactions which, in renormalization group sense, can be replaced with steric interactions since this does not change the universality class. The disorder theory of the Ginzburg-Landau model is thus in the same universality class as the ϕ^4-model, which has only a complex scalar field and no gauge field. This disorder theory thus describes a neutral superfluid. These theories are thus not self-dual since the original and the dual theory belong to different universality classes.

A strong indication of the validity of the dual approach is the fact that properties of the dual field can be calculated from the geometrical properties of the vortices in the original model. This is the topic of Chapter 6 and Paper II [71].

5.5 Charged fixed point

In Fig. 5.3 the RG-flow[6] in the space of (renormalized) couplings $(\hat{u},\hat{q}^2)$ for the Ginzburg-Landau model (see e.g. Eq. 5.47) is shown in a schematic way. The fixed point structure in this plane contains four fixed points [18, 39, 53, 66]. A noncharged model lives on the $\hat{u}$-axis. Since the

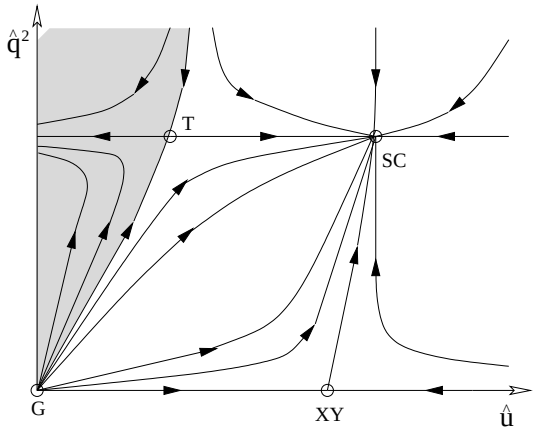

Figure 5.3: Schematic RG-flow diagram at the critical surface $T = T_c$ for the Ginzburg-Landau model. Here $\hat{u}$ is the steric coupling and $\hat{q}^2$ is the charge coupling. The four fixed points are the Gaussian (G), the uncharged (XY), the tricritical (T), and the charged fix point corresponding to a superconductor (SC). The shaded region to the left corresponds to first order transitions.

Gaussian fixed point is unstable the model will flow to the XY critical point upon renormalization. The critical exponents are thus determined by this fixed point.

For non-zero charge the picture is more interesting. In the shaded region to the left we observe runaway trajectories which are assumed to correspond to first order behavior, in agreement with

[6]The concept of a renormalization group flow (RG-flow) in the space of couplings is presented very shortly in section 3.2.

the conclusion in the seminal paper of Halperin, Lubensky, and Ma [59]. To the right of this region all trajectories flow to the charged fixed point (SC). The separatrix between these regions is given by the (line of) couplings which flow to the tricritical point (T). The tricritical point was predicted by Kleinert in 1982 [84] using duality arguments. He gave an estimate of the value of the Ginzburg-Landau parameter $\kappa = \sqrt{u/q^2}$ at this point, $\kappa_{\rm tri} \simeq 0.8/\sqrt{2}$. An early Monte-Carlo result was given by Bartholomew [12]: $\kappa_{\rm tri} \simeq 0.4/\sqrt{2}$. To our knowledge, this old simulation has *not* been revisited in a serious manner, and given the enormous development in computing power, we felt it would be worthwhile to do the simulations over again. We have studied the order of the normal metal to superconductor phase transition in Paper III [108] and found $\kappa_{\rm tri} = (0.76 \pm 0.04)/\sqrt{2}$. *Here we also claim that the line separating first and second order transitions coincides with the line separating type-I and type-II superconductors.* The charged fixed point has many interesting properties and has been intensively studied in recent years, both analytically [18,39–41,53,65–67,81,82,88,96,114], and by Monte Carlo simulations [71, 72, 113, 117]. Near this point fluctuations in the gauge-field become important and the anomalous dimension of the gauge field changes from $\eta_A = 0$ to $\eta_A = 1$. This is an exact result due to gauge symmetry [66]. Using this it is possible to show that $\lambda \sim \xi$, in contrast to the result $\lambda \sim \xi^{1/2}$ found in the XY-regime where gauge-field fluctuations are negligible.

The phase transition can also be studied by using the dual theory. From the last section we know that the dual of a charged theory, i.e. a theory with gauge field, is a pure scalar field theory corresponding to zero charge. The critical properties of this theory are thus determined by the XY fixed point. The values of observable exponents, such as ν, have to be the same since the original and dual formulations are two descriptions of the same physics. Note however that the temperature axis is reversed in the dual model, giving rise to the often used description "inverted XY". However the anomalous dimension η of the original and the dual scalar field do not have to be equal, and in fact they are not. In the charged model η is gauge-dependent and is not directly observable, the value is negative in contrast to the (slightly) positive value found in the uncharged model. Thus the term "inverted XY" should not be understood in the sense that the charged fixed point belongs to the same universality class as the uncharged XY fixed point, only with the temperature axis reversed.

Chapter 6

Geometrical description of phase transitions

The search for a geometrical description of phase transitions has a long history going back to the ideas put forward by Onsager [64, 119, 120] to describe the λ-transition in ^{4}He. In this transition the relevant geometrical objects are topological line defects in the form of vortex loops which are the stable topological defects of $U(1)$ matter fields. These loops may have a very complicated self-similar or fractal geometry allowing a very high configurational entropy. The phase transition in this picture is characterized by a fundamental change in the loop size, or equivalently the *connectivity* of the vortex-loop tangle at the critical point. In the superfluid phase only finite loops exist due to the finite line tension, at the critical point an effective line tension vanishes and infinite loops appear. This picture has many analogies to the sudden appearance of a percolating cluster in percolation phenomena at criticality, a fact that is exploited in [133].

The *Hamiltonian density* in the Ginzburg-Landau model can be written as

$$\mathcal{H}(q, u_\phi) = m_\phi^2 |\phi|^2 + \frac{u_\phi}{2} |\phi|^4 + |(\boldsymbol{\nabla} - iq\boldsymbol{A})\phi|^2 + \frac{1}{2}(\boldsymbol{\nabla} \times \boldsymbol{A})^2. \tag{6.1}$$

The *anomalous dimension* η_ϕ for the scalar field ϕ is defined by

$$G(\boldsymbol{x}, \boldsymbol{y}) = \langle \phi(\boldsymbol{x}) \phi^\dagger(\boldsymbol{y}) \rangle = \frac{\mathcal{G}(|\boldsymbol{x} - \boldsymbol{y}|/\xi)}{|\boldsymbol{x} - \boldsymbol{y}|^{d-2+\eta_\phi}}, \tag{6.2}$$

where $\mathcal{G}$ is some scaling function, ξ is the correlation length, and d is the dimension of the system. This anomalous dimension will turn out to be related to geometric properties of the vortex loops, not in the original theory, but in the *dual theory*. In fact the anomalous dimension η_ϕ is related to the fractal dimension D_H of the vortex loops in the dual theory by the remarkable simple formula

$$D_H + \eta_\phi = 2. \tag{6.3}$$

Equivalently, the fractal dimension of the vortex-loop tangle of the original theory is connected to the anomalous scaling dimension of the dual theory. Eq. 6.3 is one of the main results of Paper II [71]. It shows directly a deep connection between geometry and criticality in this particular problem. In the following I will introduce some concepts used in the paper and do some calculations in more detail.

6.1 Fractal dimension

A fractal dimension can be defined in several ways. The *capacity dimension*, which is essentially the same as the *Hausdorff* dimension, of a set of points embedded in a d-dimensional space is given by

$$D_H = \lim_{\epsilon \to 0} \frac{\ln N(\epsilon)}{\ln \epsilon^{-1}}, \tag{6.4}$$

where $N(\epsilon)$ is the number of cubes of size $V = \epsilon^d$ necessary to cover all points in the set. The fractal dimension of a vortex loop could therefore, in principle, be found by measuring its length $L(\ell)$ using finer and finer scales, i.e. increase the resolution. By reducing the length scale ℓ we can find the limit

$$D_H = \lim_{\ell \to 0} \frac{\ln L(\ell)}{\ln \ell^{-1}}. \tag{6.5}$$

Since the shortest length scale on a lattice is $\ell = a$ this method is not well defined. An alternative is to study vortex loops with increasing diameter[1] D using the lattice constant as a length scale. If one *defines* $D \equiv 1$, the lattice spacing a will be given by $a = 1/N_D$ where N_D is the diameter measured in units of a. Then

$$D_H = \lim_{N_D \to \infty} \frac{\ln L(N_D)}{\ln N_D}, \tag{6.6}$$

and the concept of fractal dimension is well defined when the size of the vortex loops tends to infinity.

6.2 Random walks and Gaussian field theories

To relate the fractal dimension of the vortex loops with the anomalous dimension we have to find the length distribution of loops. To do this it is convenient to start with the fairly simple problem of relating random walks and a Gaussian field theory.

Let us assume that we have non-interacting *closed* strings with a finite line tension or energy ε per length a. This length is the lattice constant in a d-dimensional cubic lattice where the number of nearest neighbors is $z = 2d$. The following results are a short recapitulation of some of the results in the extensive account of these matters in [85, part II, chapter 6], but also [10].

For an open string the number of configurations of length N is $(2d)^N$, and the entropy is $S = -N \ln 2d$ where the Boltzmann constant $k_B = 1$. Note that backtracking is allowed in these formulas, resulting in some over-counting. For a closed string the number of configurations is $\Omega(N) = (2d)^N D(N)$ where $D(N)$ is the probability that a string of length N will close (summed over lattice sites). The partition function for a single string can then be written as

$$Z^1 = \sum_N D(N)(2d)^N e^{-\beta N \varepsilon} = \sum_N D(N) e^{-\beta \varepsilon_{\text{eff}}(T) N} \tag{6.7a}$$

where we have defined an effective string tension by

$$\varepsilon_{\text{eff}}(T) = \frac{E - TS}{N} = \left(1 - \frac{T}{T_H}\right)\varepsilon \tag{6.7b}$$

where $T_H = \varepsilon / \ln 2d$ is the Hagedorn temperature. The effective line tension becomes negative for $T > T_H$ and strings of infinite size appear. An ensemble of strings is described by the partition function $Z = \exp(Z^1)$. To proceed we have to find $D(N)$ and it is useful to introduce $P(\boldsymbol{x}, \boldsymbol{y}; N)$ denoting the probability density that a string of length N begins at $\boldsymbol{x}$ and ends at $\boldsymbol{y}$. In the continuum limit $a \to 0$, which implies $N \to \infty$ for constant $L = Na$, it can be shown that $P(\boldsymbol{x}, \boldsymbol{y}; N)$ satisfies the diffusion equation [85]

$$\frac{\partial P}{\partial N} = \frac{1}{2d} \nabla^2 P \tag{6.8a}$$

with solution

$$P(\boldsymbol{x}, \boldsymbol{y}; N) \equiv P(|\boldsymbol{x} - \boldsymbol{y}|; N) = \left(\frac{d}{2\pi N}\right)^{d/2} \exp\left[-\frac{d}{2}\left(\frac{|\boldsymbol{x} - \boldsymbol{y}|}{N^{1/2}}\right)^2\right]. \tag{6.8b}$$

[1] Since the vortex loops are not circular we define the diameter of a vortex loop by the size of the smallest box that can contain the whole loop.

This expression should include a coefficient $\theta(N-|\boldsymbol{x}-\boldsymbol{y}|)$ to ensure that the extension of a string is less than its length, but the Gaussian damping factor has approximately the same effect. The normalized distribution of loops of perimeter N is then given by

$$D(N) \propto \frac{1}{N}\sum_{\boldsymbol{x}} P(\mathbf{0};N) \propto N^{-\alpha}, \tag{6.9}$$

where the extra factor N^{-1} comes from the arbitrariness in defining the starting position along the loop. For a pure random walker then $\alpha = \frac{d}{2}+1$. Note that this result is only valid where $\varepsilon_{\text{eff}}(T)=0$, more generally $D(N)$ contains an exponential factor suppressing large loops

$$D(N) \propto N^{-\alpha} e^{-\beta\varepsilon_{\text{eff}}(T)N}, \tag{6.10}$$

where $\varepsilon_{\text{eff}}(T)$ is the effective line tension defined in Eq. 6.7b.

For a random walk of length N in d dimensions, the probability of going from $\boldsymbol{x}$ to $\boldsymbol{y}$ is given by Eq. 6.8b. The correlation function $G(\boldsymbol{r}) \equiv G(\boldsymbol{x},\boldsymbol{y})$ of the corresponding Gaussian field theory is found by summing up $P(\boldsymbol{r};N) \equiv P(\boldsymbol{x}-\boldsymbol{y};N)$ for all N

$$\begin{aligned} G(\boldsymbol{r}) &\sim \int dN P(\boldsymbol{r};N) \\ &\propto \int dN N^{-d/2} \exp\left[-\frac{\boldsymbol{r}^2 d}{2N}\right] \\ &= \frac{1}{|\boldsymbol{r}|^{d-2}} \int dN' N'^{-d/2} \exp\left[-\frac{1}{2N'}\right] \quad (N' = \frac{N}{r^2 d}) \\ &\propto \frac{1}{|\boldsymbol{r}|^{d-2}}, \end{aligned} \tag{6.11}$$

and we immediately conclude that $\eta_\phi = 0$ by comparing with Eq. 6.2. The distance between two points $\boldsymbol{x}$ and $\boldsymbol{y}$ N walks apart is given by

$$\langle |\boldsymbol{x}-\boldsymbol{y}|^2 \rangle \propto N^{2\Delta}, \tag{6.12}$$

where in the Gaussian case the *wandering exponent* $\Delta = 1/2$, and the Hausdorff dimension is seen to be given by

$$D_H = \frac{1}{\Delta} = 2. \tag{6.13}$$

After this we are prepared to attack the more complicated problem with interacting loops corresponding to more general walks. That is the main theoretical development in Paper II [71].

6.3 General case

By assuming that the functional form in Eq. 6.8b survives in the interacting case, the probability of going from $\boldsymbol{x}$ to $\boldsymbol{y}$ by a general walk of length N in d dimensions can be defined by [71]

$$P(\boldsymbol{x}-\boldsymbol{y};N) \propto \frac{1}{N^\rho} F\left(\frac{|\boldsymbol{x}-\boldsymbol{y}|}{N^\Delta}\right). \tag{6.14}$$

For the random walk $\rho = d/2$ and $\Delta = 1/2$. The probability distribution must be normalizable which implies $\rho = d\Delta$ since

$$\int d^d r P(\boldsymbol{r};N) \overset{(r=N^\Delta r')}{=} \underbrace{N^{d\Delta-\rho}}_{\Rightarrow \rho = d\Delta} \int d^d r' P(\boldsymbol{r}';1), \tag{6.15}$$

where $\boldsymbol{r} = \boldsymbol{x}-\boldsymbol{y}$. By using Eq. 6.9 we easily relate ρ and α

$$D(N) \propto \frac{1}{N^{\rho+1}} \propto \frac{1}{N^\alpha} \Rightarrow \rho = \alpha - 1. \tag{6.16}$$

The correlation function can be found in the same way as for the random walk by summing over all N in Eq. 6.14

$$\begin{aligned} G(\boldsymbol{r}) &\sim \int dN P(\boldsymbol{r}; N) \\ &\propto \int dN N^{-\rho} F\left(\frac{|\boldsymbol{r}|}{N^{\Delta}}\right) \\ &= \frac{1}{|\boldsymbol{r}|^{(\rho-1)/\Delta}} \int dN' N'^{-\rho} F\left(\frac{1}{N'^{\Delta}}\right) \quad \left(N'^{\Delta} = \frac{N^{\Delta}}{|\boldsymbol{r}|}\right) \\ &\propto \frac{1}{|\boldsymbol{r}|^{(\rho-1)/\Delta}}. \end{aligned} \tag{6.17}$$

This immediately gives the scaling relation [71]

$$\eta_{\phi} = \frac{\rho - 1}{\Delta} + 2 - d, \tag{6.18}$$

which implies

$$\eta_{\phi} + D_H = 2, \qquad D_H = \frac{d}{\alpha - 1}. \tag{6.19}$$

This is clearly satisfied by the Gaussian theory where $\alpha = d/2 + 1$, $\eta_{\phi} = 0$, and $D_H = 2$. This simple relation is the connection between the Hausdorff dimension of the vortex loops and the anomalous dimension of the dual theory, i.e. a relation between geometric properties of the vortex loops and a thermodynamic exponent η_{ϕ} [71]. This relation was also found independently in [133] by relating the problem to percolation. In the simulations we have measured the loop distribution $D(N)$ and found $\alpha = -\ln D(N)/\ln N$. A more direct measurement of D_H by using Eq. 6.6 was also tried and this gave consistent results, but with larger error-bars.

Chapter 7

Simulations on the full Ginzburg-Landau model

In this chapter I will give some details about the simulations we have done on the full Ginzburg-Landau model to find a precise numerical value of the Ginzburg-Landau parameter κ separating the first and second order phase transitions. The focus will be on technical details and the reader is advised to read Paper III [108] for a broader introduction to the problem. To achieve our goal we had to carry out infinite volume and continuum limit extrapolations. Normally only the former limit has to be considered when studying critical phenomena if only universal quantities, such as exponents or amplitude ratios, are studied. The microscopic details are not important since only length scales comparable to the (diverging) correlation length matter. *This is not so if one wants to find precise numerical values of critical coupling constants or is studying first-order transitions without a diverging length scale.* One solution is to do perturbation theory on the continuum theory, but proceeding in a naive manner will give ultraviolet divergences and the theory must be renormalized. Another problem is that vortices are nonperturbative by nature. The other solution is to discretize the theory, i.e. putting it on an auxiliary mathematical lattice, thereby introducing a lower length scale which eliminates ultraviolet divergences. Since the lattice is artificial the continuum limit has to be approached by letting the lattice constant go to zero.

7.1 Renormalization

The action for the ϕ^4-theory, which corresponds to the Ginzburg-Landau model with $q = 0$, can be written as

$$S_u[\phi] = \int d^3r \left[|\nabla\phi|^2 + m^2|\phi|^2 + u|\phi|^4 \right]. \tag{7.1}$$

The free theory, i.e. $S_{u=0}[\phi]$, can be solved analytically, and all correlation functions can be given a closed form. This is no longer the case when we are dealing with interacting fields, i.e. $u \neq 0$. The only way to proceed analytically is to perform a perturbative analysis in the coupling constant u by expanding $\exp(u|\phi|^4)$ in a series. It turns out that this is problematic since the perturbation series involves divergent momentum integrals. This is clearly nonphysical and is related to ultraviolet divergences. To avoid this one has to introduce some sort of arbitrary upper cut-off Λ on allowed momenta thereby *regularizing* the theory. Then one can *renormalize* the theory by defining scale dependent parameters $m^2(\Lambda), u(\Lambda)$ in such a way that one can remove the arbitrary cut-off by letting $\Lambda \to \infty$. In addition the field ϕ must normally be scaled by a Λ-dependent number. If defining a finite number of scale dependent parameters, such as m^2, u, ϕ above, renders every possible correlation function finite, the theory is said to be renormalizable. The renormalization procedure removes the divergences, but the exact values of the parameters must be decided by demanding that the value of physical observables coincide with experimental ones. For a thorough introduction to these matters see e.g. the textbooks [5, 24, 156].

The Ginzburg-Landau theory has similar ultraviolet divergences and must also be renormalized. As we have seen in Chapter 5 the continuum action for the Ginzburg-Landau theory can be written in several different ways. Here we choose the form [78]

$$S[\phi, \boldsymbol{A}] \equiv \int d^3r \mathcal{L}[\phi, \boldsymbol{A}] = \int d^3r \left[\frac{1}{4} F_{ij}^2 + |D_i \phi|^2 + m^2 |\phi|^2 + u |\phi|^4 \right], \tag{7.2}$$

where $F_{ij} = \partial_i A_j - \partial_j A_i$, and $D_i = \partial_i - iqA_i$. To get rid of ultraviolet divergences the theory has to be renormalized. It can be shown that in three dimensions the couplings q^2 and u in Eq. 7.2 are not renormalized in the ultraviolet, but that there is a linear 1-loop and a logarithmic 2-loop divergence for the mass parameter m^2. In the $\overline{\text{MS}}$ (minimal subtraction) dimensional regularization scheme[1] in $3 - 2\epsilon$ dimensions, the renormalized mass parameter at a scale μ becomes [47]

$$m^2(\mu) = \frac{-4q^4 + 8uq^2 - 8u^2}{16\pi^2} \log \frac{\Lambda_m}{\mu}, \tag{7.3}$$

where Λ_m is a scale independent physical mass parameter of the theory. It is however more convenient to use $m^2(q^2)$ by choosing q^2 to set the scale. The physics of the theory will then depend on the two dimensionless ratios

$$y = \frac{m^2(q^2)}{q^4}, \quad x = \frac{u}{q^2}. \tag{7.4}$$

A problem with this approach is that vortices only can be included by going to infinite order in the perturbation series, a hopeless task for the Ginzburg-Landau model. To incorporate vortices one has to consider lattice regularization, which of course has much in common with the momentum cut-off since a lattice constant is related to the momentum cut-off by $a \sim 1/\Lambda$.

7.1.1 Lattice regularization

To be able to do numerical simulations on the Ginzburg-Landau model it must be discretized by introducing an auxiliary mathematical lattice. The lattice constant a can then be used to define dimensionless quantities. By defining a lattice field by

$$|\phi|^2_{\text{cont}} = \frac{\beta_H}{2a} |\psi|^2_{\text{latt}} \tag{7.5}$$

where β_H is a so far undetermined constant, and also defining $\vec{x} = \vec{r}/a$, $\alpha_i = aqA_i$, $F_{ij} = \alpha_i(\vec{x}) + \alpha_j(\vec{x} + \hat{\imath}) - \alpha_i(\vec{x} + \hat{\jmath}) - \alpha_j(\vec{x})$, and $U_i(\vec{x}) = e^{i\alpha_i(\vec{x})}$, we can write the discrete version of Eq. 7.2 as

$$\begin{aligned} S = \sum_{\vec{x}} \Bigg[& \frac{\beta_G}{4} F_{ij}^2 + \frac{\beta_H}{2} \left(6 |\psi|^2 - 2 \sum_i \mathsf{Re}[\psi^*(\vec{x}) U_i(\vec{x}) \psi(\vec{x} + \hat{\imath})] \right) \\ & + \frac{\beta_H y}{2\beta_G{}^2} |\psi|^2 + \frac{x\beta_H{}^2}{4\beta_G} |\psi|^4 \Bigg]. \end{aligned} \tag{7.6}$$

[1] Dimensional regularization is an alternative to the momentum cut-off regularization. The idea is to analytically continue the diverging integrals to a dimension where they can be evaluated. Here the dimension is allowed to take any value, not only positive integers. The answer is typically in terms of Gamma-functions of relations involving the dimension d. The divergences are removed by so called minimal subtraction. If divergences appearing in three dimensions are to be removed this normally gives a small parameter $\varepsilon = 3 - d$, where d is the dimension of the system. For more information see the article by 't Hooft and Veltman [140] who introduce the dimensional regularization scheme, the early review article [99], and e.g. the books [24, 105, 156]. One of the advantages of this scheme is that symmetries are conserved. This is generally not so for the momentum cut-off method and to conserve the symmetries upon renormalization complicated methods such as Pauli-Villars, see e.g. [156], have to be introduced.

Here $\beta_G = 1/aq^2$ and x, y are defined in Eq. 7.4. The first term can be rewritten using that $\sum_{ij} \frac{1}{4} F_{ij}^2 = \sum_{i<j} \frac{1}{2} F_{ij}^2$, while the hopping term can be rewritten by defining $\psi = \rho e^{i\theta}$ as

$$\mathsf{Re}[\psi^*(\vec{x}) U_i(\vec{x}) \psi(\vec{x}+\hat{\imath})] = \rho(\vec{x})\rho(\vec{x}+\hat{\imath}) \cos\left[\theta(\vec{x}+\hat{\imath}) - \theta(\vec{x}) + \alpha_i(\vec{x})\right]. \tag{7.7}$$

For historical reasons, it is customary to exploit a freedom in choosing β_H such that the theory can be written as

$$S = \beta_G \sum_{\vec{x}, i<j} \frac{1}{2} F_{ij}^2 - \beta_H \sum_{\vec{x}, i} \mathsf{Re}[\psi^*(\vec{x}) U_i(\vec{x}) \psi(\vec{x}+\hat{\imath})] + \sum_{\vec{x}} |\psi|^2 + \beta_R \sum_{\vec{x}} \left[|\psi|^2 - 1\right]^2 \tag{7.8}$$

where $\beta_R = \frac{x {\beta_H}^2}{4\beta_G}$. This is achieved provided β_H satisfies the relation

$$\frac{\beta_H}{2}\left[6 + \frac{y}{{\beta_G}^2}\right] + 2\beta_R = 1 \quad \Leftrightarrow \quad 2{\beta_G}^2 \left(\frac{1}{\beta_H} - 3 - \frac{x\beta_H}{2\beta_G}\right) = y, \tag{7.9a}$$

which, when solved for β_H, gives

$$\beta_H = \varrho\left[-1 + \sqrt{1 + \frac{2\beta_G}{x\varrho^2}}\right], \text{ where } \varrho = \left(3 + \frac{y}{2{\beta_G}^2}\right)\frac{\beta_G}{x}. \tag{7.9b}$$

7.1.2 The relation between lattice- and $\overline{\text{MS}}$-regularization

Due to different ultraviolet behavior of the lattice and continuum theory one must be very careful when comparing results from perturbation theory and simulations. To study the continuum theory in Eq. 7.2 it is crucial to keep the continuum variables x and y fixed when discretizing the theory. The linear and logarithmic mass divergences are renormalized in the continuum theory in the $\overline{\text{MS}}$ scheme, see Eq. 7.3. Discretization in itself is another scheme. The two schemes have to be related so that correlators measured in the lattice scheme go to the correct continuum ones at given x, y in the limit that the lattice spacing a goes to zero. From [93,94] the three-dimensional $U(1)$+Higgs theory, which corresponds to the Ginzburg-Landau theory, on a lattice is defined by the Lagrangian

$$\begin{aligned}\mathcal{L}_{\text{lat}}(\vec{x}) = {} & \frac{\gamma^2}{a^4 q^2} \sum_{i<j} \left[1 - \cos\left(\frac{\arg\left[P_{ij}(\vec{x})\right]}{\gamma}\right)\right] \\ & + \frac{2}{a^2} \sum_i \left[|\phi(\vec{x})|^2 - \mathsf{Re}[\phi^*(\vec{x}) U_i(\vec{x}) \phi(\vec{x}+\hat{\imath})]\right] \\ & + m^2 |\phi(\vec{x})|^2 + u |\phi(\vec{x})|^4,\end{aligned} \tag{7.10a}$$

where

$$P_{i,j}(\vec{x}) = U_i(\vec{x}) U_j(\vec{x}+\hat{\imath}) U_i^*(\vec{x}+\hat{\jmath}) U_j^*(\vec{x}), \quad U_i(\vec{x}) = e^{iaqA_i(\vec{x})}. \tag{7.10b}$$

Here $\gamma = 1$ corresponds to a compact gauge field, $A_i(\vec{x}) \in [-\pi, \pi)$, while the non-compact case, $A_i(\vec{x}) \in \mathbb{R}$, follows from the limit

$$\lim_{\gamma\to\infty} \gamma^2 \left[1 - \cos\left(\frac{\alpha}{\gamma}\right)\right] = \frac{1}{2}\alpha^2. \tag{7.11}$$

The continuum Lagrangian is defined in Eq. 7.2. It can be shown that the perturbative renormalization of the continuum theory by $\overline{\text{MS}}$ regularization and the lattice regularization are made equal to two-loop order by defining the bare mass parameter as

$$\begin{aligned} m^2 = {} & m^2(\mu) - (2q^2 + 4u)\frac{\Sigma}{4\pi a} \\ & - \frac{1}{16\pi^2}\left[\left(-4q^2 + 8uq^2 - 8u^2\right)\left(\ln\frac{6}{a\mu} + \zeta\right)\right. \\ & \left. + q^4\left(\frac{1}{4}\Sigma^2 - 1 - 2\delta - 4\rho + \frac{8\pi}{3}\frac{\Sigma}{\gamma^2}\right) + 8uq^2\left(\frac{1}{4}\Sigma^2 - \delta\right)\right],\end{aligned} \tag{7.12a}$$

where the numerical constants are $\Sigma = 3.175911535625$, $\delta = 1.942130(1)$, $\rho = -0.313964(1)$, $\zeta = 0.08849(1)$. Thus the numerical value of the last term in (7.12a) is

$$-\frac{1}{16\pi^2}\left[\left(-1.1068+\frac{26.6065}{\gamma^2}\right)q^4+4.6358uq^2\right]. \tag{7.12b}$$

Similarly the lattice and continuum condensates are related by

$$\langle\phi^*\phi\rangle_{\rm cont} = \langle\phi^*\phi\rangle_{\rm latt} - \frac{\Sigma}{4\pi a} - \frac{q^2}{8\pi^2}\left(\ln\frac{6}{a\mu}+\zeta+\frac{1}{4}\Sigma^2-\delta\right) \tag{7.13}$$

where $\zeta + \frac{1}{4}\Sigma^2 - \delta = 0.66796(1)$.

For our model with a non-compact gauge field this means that to relate the lattice (7.8) and continuum theory (7.2) we have to substitute ($y = m^2/q^4$)

$$y \to y - \frac{3.1759115(1+2x)\beta_G}{2\pi} - \frac{(-4+8x-8x^2)(\log 6\beta_G + 0.09) - 1.1 + 4.6x}{16\pi^2} \tag{7.14}$$

in the lattice formulas, see [93, 94] for more details.[2] Note that the complicated counter-terms only affect the value of y_c for a given x, not the qualitative structure of the phase diagram. The counter-terms guarantee that $\lim_{a\to 0} y_c$ exist and must be used if we want to find this limit. The relation between the continuum (at the scale $\mu = q^2$) and lattice condensates is [94]

$$\frac{\langle\phi^*\phi(q^2)\rangle_{\rm cont}}{q^2} = \frac{1}{2}\beta_H\beta_G\langle\psi^*\psi\rangle_{\rm latt} - \frac{3.1759115\beta_G}{4\pi} - \frac{\log 6\beta_G + 0.668}{8\pi^2}, \tag{7.15}$$

where the first term is the rescaling from Eq. 7.5. Note that the complicated counter-terms are not needed for calculating the discontinuity $\Delta\langle\phi^*\phi\rangle_{\rm cont}$ in a first order transitions since they are independent of y.

7.2 Monte-Carlo simulation

We have performed standard Metropolis update, see section 4.2.1 on page 23, for the gauge field, and the amplitude as well as phase of the scalar field. The acceptance ratios are, as far as possible, adjusted to lie between 60% and 70% by adaptively adjusting the maximum allowed changes in the above mentioned fields. Note that the change in variables from ψ, ψ^* to ρ, θ, where $\psi = \rho e^{i\theta}$, must be accounted for in the Metropolis update scheme for the amplitude. The measure transforms as $d\psi^* d\psi \to \rho d\rho d\theta$, thus the probability for amplitude updates must be changed to

$$P(\rho \to \rho') = \min\left(1, \frac{\rho'}{\rho}e^{-[S(\rho')-S(\rho)]}\right), \tag{7.16}$$

where ρ' is drawn from a flat distribution. We find the trial state by multiplying by e^ξ, where $\xi \in [-\epsilon, \epsilon]$ is drawn from a flat distribution, i.e. $\rho' = e^\xi\rho$. Thus $d\rho \propto e^\xi d\xi$ and

$$P(\rho \to \rho') = \min\left(1, e^{2\xi - \Delta S(\rho\to\rho')}\right), \tag{7.17}$$

where ΔS is the change in the action and 2ξ comes from the change in the measure. For the amplitude we have also used a *global* update, where ρ is multiplied by the same factor over the whole lattice, to reduces autocorrelation times [44, 80]. The probability for updating is then given by $P(\xi) = \min\left(1, e^{2V\xi - \Delta S(\xi)}\right)$, where V is the volume of the system. Due to the factor V the multiplication factor e^ξ has to be very close to unity for the global update to have non-negligible $P(\xi)$. Finally we have added an *overrelaxation* step for the updating of the scalar field. Normally the scalar field will have longer correlation times than the gauge field and we have therefore chosen not to implement overrelaxation for the gauge field. One sweep with these improvements then consists of

[2] In [9] similar relations for the ϕ^4-model was found and used in simulations on this model. However due to the simplicity of the ϕ^4-model compared to the GL-model they were also able to calculate higher order corrections, $\mathcal{O}(a), \mathcal{O}(a^2)$.

- Standard Metropolis update for the amplitude, phase, and gauge-field. The acceptance ratio is kept between 60% and 70% by adaptive adjustment of maximum allowed changes.
- Metropolis update for a global change in the amplitude, where the amplitude is multiplied by the same factor over the whole lattice. The acceptance ratio is also here kept between 60% and 70% as above.
- Overrelaxation update for the amplitude and phase of the scalar field. This is normally several "sweeps" through the whole lattice.

The overrelaxation method is explained in the next section.

7.2.1 Overrelaxation

The overrelaxation method, as invented by Adler [3, 4], is a generalization of the heat-bath algorithm where the field evolution is deterministic and microcanonical (conserves energy). To restore ergodicity one has to use a combination of standard ergodic updates (e.g. Metropolis or heat-bath) and nonergodic overrelaxation updates in an alternating manner [29, 36, 52]. The purpose of incorporating overrelaxation is to reduce autocorrelation times. The principle is based on choosing new states rather far away from the initial state without having to pay a high energy penalty. This is possible by going to the "opposite side" of a minimum in the effective potential. Since the successive states are quite different one should expect a rather rapid flow through phase space. The method also has direct relations to the successive overrelaxation methods used in minimization schemes for e.g. solving linear equations [126, 141]. Here the minimum for a given variable is indirectly influenced by the variable itself since the neighbors were updated based on the value of the variable. This means that the variable will be correlated to its old value. The problem can to some extent be overcome by realizing that the most efficient update is not to go to the minimum, but past the minimum to the other side, thereby anticipating future corrections.

The Higgs/scalar potential at $\vec{x}$ can be written in the form [44, 80]

$$\overline{V}(\psi(\vec{x})) = -\boldsymbol{a}\cdot\boldsymbol{F} + \rho^2(\vec{x}) + \beta_R\left[\rho^2(\vec{x})-1\right]^2, \tag{7.18a}$$

where $\psi(\vec{x}) = \rho(\vec{x})e^{i\theta(\vec{x})}$, and

$$\boldsymbol{a} = \begin{bmatrix}\rho(\vec{x})\cos\theta(\vec{x})\\ \rho(\vec{x})\sin\theta(\vec{x})\end{bmatrix}, \quad \boldsymbol{F} = \begin{bmatrix}\beta_H\sum_i \rho(\vec{x}+\hat{\imath})\cos\left[\theta(\vec{x}+\hat{\imath})+\alpha_i(\vec{x})\right]\\ \beta_H\sum_i \rho(\vec{x}+\hat{\imath})\sin\left[\theta(\vec{x}+\hat{\imath})+\alpha_i(\vec{x})\right]\end{bmatrix}, \tag{7.18b}$$

by using that $\cos(a-b) = \cos a\cos b + \sin a\sin b$. We then define new variables by

$$X = \boldsymbol{a}\cdot\boldsymbol{f}, \quad \boldsymbol{Y} = \boldsymbol{a} - X\boldsymbol{f}, \tag{7.19}$$

where $\boldsymbol{f} = \boldsymbol{F}/|F|$. Note that $\boldsymbol{Y}\cdot\boldsymbol{f} = 0$ and $\rho^2 = X^2 + Y^2$. The potential may then be rewritten as

$$V\left(X,F,Y^2\right) = -XF + \underbrace{\left[1+2\beta_R\left(Y^2-1\right)\right]}_{\equiv B(Y^2)}X^2 + Y^2\left(1-2\beta_R\right) + \beta_R\left(X^4+Y^4\right). \tag{7.20}$$

The $\boldsymbol{Y}$ updating is the reflection $\boldsymbol{Y}\to\boldsymbol{Y}' = -\boldsymbol{Y}$ or

$$\boldsymbol{a}' = -\boldsymbol{a} + 2X\boldsymbol{f} \quad\Rightarrow\quad \theta' = \arctan\frac{2Xf_2 - a_2}{2Xf_1 - a_1}. \tag{7.21}$$

The X updating is done by solving the equation

$$\left[\frac{\partial V(X')}{\partial X'}\right]^{-1} e^{V(X')} = \left[\frac{\partial V(X)}{\partial X}\right]^{-1} e^{V(X)} \tag{7.22}$$

for X', where the derivatives had to be included to account for the change in measure. This is necessary since X is a nonlinear function of X' [52].

Instead of solving Eq. 7.22, we solve the auxiliary equation

$$V(X') = V(X), \tag{7.23a}$$

and accept the solution with probability

$$p(X') = \min(1, p_0), \quad p_0 = \left| \frac{\partial V(X)/\partial X}{\partial V(X')/\partial X'} \right|. \tag{7.23b}$$

Since $X' = X$ is a solution, we may factor out $(X' - X)$ and reduce the equation to a cubic one

$$X'^3 + XX'^2 + \frac{B(Y^2) + \beta_R X^2}{\beta_R} X' + \frac{\beta_R X^3 + B(Y^2)X - F}{\beta_R} = 0, \tag{7.24a}$$

where

$$B(Y^2) = 1 + 2\beta_R(Y^2 - 1). \tag{7.24b}$$

In realistic cases the parameters of $V(X)$ are such that there always is only one real root and it is straightforward to write a closed expression for X'. The new amplitude and phase are given by

$$\rho'(\vec{x}) = \sqrt{X'^2 + Y'^2}, \quad \theta'(\vec{x}) = \arctan \frac{Y_2' + X' f_2}{Y_1' + X' f_1}. \tag{7.25}$$

7.3 Reweighting

The action Eq. 7.8 can be written as

$$S = \beta_G S_G + \beta_{\phi^2} S_{\phi^2} + \beta_H S_{\text{hopping}} + \beta_R S_{(\phi^2-1)^2} = \beta_i S_i, \tag{7.26}$$

where $\beta_{\phi^2} \equiv 1$. Note that both couplings β_H and β_R depend on the temperature-like variable y. This will make reweighting more complicated compared to the normal situation where one e.g. reweights with respect to β in $S = \beta H$. There is however an easy way to solve this problem. If we remember the action Eq. 7.6 *before* the special choice of β_H in Eq. 7.9, we note that there y only appeared once. Thus by defining the field $\Phi = \sqrt{\frac{\beta_H}{2\beta_G}}\psi$ the action can be written as

$$\begin{aligned} S = \beta_G \sum_{\vec{x}, i<j} \frac{1}{2} F_{ij}^2 - 2\beta_G^2 \sum_{\vec{x}, i} \mathsf{Re}[\Phi^*(\vec{x}) U_i(\vec{x}) \Phi(\vec{x} + \hat{\imath})] \\ + (6\beta_G^2 + y) \sum_{\vec{x}} |\Phi|^2 + x\beta_G^3 \sum_{\vec{x}} |\Phi|^4, \end{aligned} \tag{7.27}$$

where $\beta_G = 1/aq^2$. By sampling

$$S_y = \sum_{\vec{x}} |\Phi|^2 = \frac{\beta_H}{2\beta_G^2} \sum_{\vec{x}} |\psi|^2 \tag{7.28}$$

during the simulations, reweighting with respect to y is easily performed. The essential reweighting formulas for completely non-binning reweighting with respect to y are then given by a modified version of Eq. 4.40:

$$P_\ell(t, y) = \frac{g_\ell^{-1} e^{-y S_y^\ell(t)}}{\sum_{j=1}^R n_j g_j^{-1} e^{-y_j S_y^j(t) + f_j}}, \tag{7.29a}$$

where

$$e^{-f_j} = \sum_{\ell=1}^R \sum_{t=1}^{n_\ell} P_\ell(t, y_j). \tag{7.29b}$$

Here R is the number of y-values used and n_ℓ is the length of the time-series $S_y^\ell(t)$ for y_ℓ. One can then calculate the average for a quantity W at y by using the time-series $W_\ell(t)$ for this quantity

$$\langle W \rangle(y) = \frac{\sum_{\ell=1}^{R} \sum_{t=1}^{n_\ell} W_\ell(t) P_\ell(t,y)}{\sum_{\ell=1}^{R} \sum_{t=1}^{n_\ell} P_\ell(t,y)}. \tag{7.30}$$

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Part II

Papers

Paper I

Fermion-pairing on a square lattice in extreme magnetic fields [109]

Paper II

Hausdorff dimension of critical fluctuations in abelian gauge theories [71]

Paper III

The order of the metal to superconductor transition [108]