Vortex Fluctuations in Superconductors

Peter Olsson

The thesis is based on the following papers:

I Extension of a set of renormalization equations for the Kosterlitz-Thouless transition

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III On the helicity modulus, the critical temperature and Monte Carlo simulations for the two-dimensional $XY$-model

IV Effective vortex interaction in the two-dimensional $XY$ model
   Peter Olsson, submitted to Phys. Rev. B.

V Interplay between one- and two-dimensional fluctuations for a class of $XY$ models

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Vortex fluctuations in superconductors

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Abstract

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This thesis may be considered to consist of two parts. The first is concerned with two models that have often been used as models for 2D superconductors, the 2D Coulomb gas and the 2D $XY$ model. The second part contains analyses related to high-temperature superconductivity.

Through analysis of some renormalization equations for the Kosterlitz-Thouless (KT) transition, it is shown that the region governed by the KT critical behavior is very small and only applies at very low values for the flux-flow resistance. It is concluded that this critical behavior not is observable in superconductors, and, furthermore, that the only available method to test for 2D fluctuations at the onset of resistance, is through comparison with the 2D resistance scaling function.

The critical temperature for the 2D $XY$ model is determined by means of a finite-size scaling relation for the helicity modulus. The linearly screened potential in the $XY$ model is written in terms of a correlation function. The analogy to the 2D Coulomb gas is found to be exact with a temperature-dependent bare interaction and a new expression for vorticity. It is also demonstrated that the Coulomb gas scaling concept may be applied to $XY$-type models.

An analysis of resistance data for YBCO/PBCO superlattices in terms of the 2D resistance scaling function gives evidence for 2D behavior in the cases with large separation of the superconducting layers. In the superlattices with stronger interlayer coupling, the crossover to three-dimensional behavior is seen as a deviation from the scaling function as $T_c$ is approached from above.

The anisotropic three-dimensional (3D) $XY$ model is examined as a model for high-temperature superconductors. It is shown that the density of vortices above $T_c$ are closely equal in the anisotropic 3D model and the 2D model. This is taken as evidence that the 3D to 2D crossover found in the superlattices also is present in the anisotropic 3D $XY$ model.

Keywords: Superconductor, Two dimensions, Vortex, Coulomb gas, $XY$ model, Kosterlitz-Thouless transition, high-$T_c$. 

ISBN 91-7174-708-7
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iii
Publications

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Related, but not included in the present thesis are:

IX Quasi two-dimensional vortex fluctuations in high-$T_c$ superconductors

X Reply to Comment on Paper VIII.
# Contents

**Preface** vii

1 **Introduction** 1
  1.1 Statistical mechanics ................................................. 1
    1.1.1 The Ising model ................................................. 1
    1.1.2 Temperature ...................................................... 2
    1.1.3 Computer simulations – Monte Carlo ......................... 3
    1.1.4 Phase transitions .............................................. 4
  1.2 The 2D $XY$ model .................................................. 5
  1.3 Metropolis Monte Carlo ............................................. 7
    1.3.1 Speeding up with integers .................................... 7

2 **Two dimensions** 8
  2.1 Superconductivity ................................................... 8
    2.1.1 Ginzburg-Landau theory of superconductivity ................. 9
    2.1.2 Dissipation in thin superconducting films ................. 11
    2.1.3 Ginzburg-Landau Coulomb gas ................................ 13
    2.1.4 Coulomb gas scaling .......................................... 15
    2.1.5 The $XY$ model and superconductivity ................... 15
  2.2 The two-dimensional Coulomb gas ................................. 17
    2.2.1 The Kosterlitz-Thouless transition .......................... 18
    2.2.2 Kosterlitz’ renormalization group equations ............... 19
    2.2.3 Minnhagen’s self-consistent renormalization equations (I) . 20
    2.2.4 Size of the critical region (II) ............................ 23
  2.3 The two-dimensional $XY$ model .................................. 24
    2.3.1 General ......................................................... 26
    2.3.2 Spin-spin correlation ........................................ 27
    2.3.3 The helicity modulus ........................................ 28
    2.3.4 Determination of $T_c$ (III) ................................. 29
    2.3.5 Effective vortex interaction in the 2D $XY$ model (IV) .... 31
    2.3.6 Formal separation of the current (IV) ....................... 31
    2.3.7 The bare superfluid density in the $XY$ model ............ 33
    2.3.8 Coulomb gas scaling in the 2D $XY$ model (V) ........... 35

3 **Layered systems – three dimensions** 37
  3.1 High-$T_c$ superconductors ....................................... 37
    3.1.1 Two-dimensional behavior ................................... 38
    3.1.2 YBCO/PBCO superlattices (VI) .............................. 38
3.2 The layered XY model ................................................. 40
  3.2.1 The isotropic model ............................................. 40
  3.2.2 Analysis in terms of coupled layers (VII) ............... 42
  3.2.3 Vortex density (VIII) .......................................... 43

4 Conclusion 46

References 48

Acknowledgement 51

Papers I–VIII
Preface

Theoretical physics is a comprehensive and fascinating subject. It is, however, not easy to convey this feeling to innocent friends who ask what the research is all about. The obvious reason is that many of the central concepts in physics are abstract and foreign to ordinary human experience.

As an attempt to bridge this gap, this thesis begins with a short introduction in a popular style, Secs. 1.1–1.2. The purpose is to introduce some basic concepts and methods which are fundamental for this field of physics – statistical physics.

Some words about a confusing simplification: An important constant in statistical mechanics is the Boltzmann’s constant $k_B$, which acts as a conversion constant from temperature to energy. This constant almost never appears in this thesis. The reason is that the temperature, in accordance with a convention in much of the literature, is chosen to have the same dimension as energy. One may think of this as being due to the substitution $k_B T \rightarrow T$. The conversion factor is, however, necessary in order to make comparisons with experiments where the temperature is measured in ordinary units.

For the sake of clarity, it should also be pointed out that the roman numerals refer to the Publications listed on page iv. Papers I through VIII are included as the second part of the thesis.
1 Introduction

The first part of this section is a popular introduction to some concepts and methods used throughout this thesis. The second part, Sec. 1.3, is a short introduction to Monte Carlo calculations.

1.1 Statistical mechanics

The major part of the papers in this thesis concern the study of some simple models. This preoccupation with such 'toy models' may at first seem strange and stupid. But there are actually several good reasons for the study of simple models:

- The first reason is that real systems are very complex, which means that it is impossible to do the calculations one would like to do for a realistic physical model. To obtain something manageable it is therefore necessary to neglect several complicating factors.

- It is also often an advantage to analyze simple models since it is a means to improve the understanding. In the simple models we are able to isolate certain characteristics of the system and learn how they affect its behavior.

- The third reason for the study of simple models is related to the occurrence of universality. This means that certain characteristics of a system are independent of details and only depend on some general properties, as the number of dimensions and the symmetry properties. From this follows that these quantities may be the same for a simple model as for the complete system and they may therefore be calculated from the properties of the simple model.

1.1.1 The Ising model

A good example of a simple model is the Ising model in two dimensions. Imagine a large piece of paper with a large number of dots in a regular square pattern so that each dot has four nearest neighbors. This is now a ‘lattice’. Let the points be numbered, 1, 2, 3, ... and put arrows (spins), $s_1, s_2, s_3, ...$, which may point in two directions, say up and down, at these points. This is illustrated in Fig. 1a. The model is defined when we have specified the rules for calculating the energy:

- The energy may be thought of as being located between neighboring arrows. For each link between two adjacent arrows the energy is $-1$ if the arrows point in the same direction and $+1$ otherwise.
The total energy in the system is obtained by summing the energies for all such links between adjacent arrows.

The expression for the total energy is often called the Hamiltonian, and the energy is therefore denoted by $H$.

The main interest in statistical physics is the behavior of very large systems, actually systems of infinite size. One reason for this is that the real systems, which we ultimately would like to compare our results with, consist of a huge number of atoms, molecules, or other relevant entities. A complicating factor, from the computational point of view, is that the behavior of a model often is highly dependent on the system size, and that it is impossible to do Monte Carlo calculations on very large systems. It is, however, possible to eliminate the boundary which is the most problematic feature of a finite system. This is done by means of 'periodic boundary conditions', which means that the leftmost column is used as the neighboring column to the rightmost one and the uppermost row is thought of as also being below the lowest row.

An important concept in statistical mechanics is a 'configuration'. To specify a configuration we have to give directions for all the arrows, e.g. $s_1 = \uparrow$, $s_2 = \downarrow$, $s_3 = \uparrow$, $s_4 = \uparrow$, ..., The number of different configurations for a system increases rapidly with the size of the lattice. Already the $5 \times 5$ lattice with 25 arrows in Fig. 1a has more than 30 million different configurations; and this figure is doubled for each arrow that is added to the system.

### 1.1.2 Temperature

A main question in statistical mechanics is how the behavior of a system depends on temperature. A crucial issue is therefore how to introduce the temperature in a theoretical analysis of a model system. The simple case is the behavior at the lowest
possible temperature – zero temperature (-273.15 °C). Since the temperature, e.g. of a bottle of water, increases if we supply energy and thereby increase its internal energy, one might conclude that the converse is true too – the lowest possible temperature corresponds to the minimum value of the energy. Since the energy associated with a link is −1 if the two arrows are parallel and +1 if they point in opposite directions, it follows that the lowest possible energy for the whole system is obtained if all the arrows point in the same direction, i.e. all ↑ or all ↓.

To consider the case of non-zero temperatures we may think of our model system in thermal contact with a large ‘reservoir’ at a certain temperature. The thermal contact means that energy can flow in and out, and the energy is therefore not a constant. The basic assumption of statistical mechanics is now that the probability for a certain configuration to show up only depends on its energy $H$.

From this assumption one may deduce that with a system at temperature $T$ the probability depends on the ratio $H/T$ in a certain way: If $H/k_B T$ for two configurations only differ by a small amount $\delta$, the probability for the configuration with the lower energy to show up is $(1 + \delta)$ times larger. Here $k_B$ is Boltzmann’s constant $= 1.38 \times 10^{-23}$ J/K that relates temperature (Kelvin) to energy (Joule).

Mathematically this may be expressed in terms of the ‘Boltzmann factor’. The probability for a certain configuration is proportional to $\exp(-H/k_B T)$, where $H$ is its energy.

### 1.1.3 Computer simulations – Monte Carlo

As mentioned above, the total energy in a small system is not a constant. It is, however, possible to calculate the average value – the expectation value – for the energy. In this calculation it seems fair to give a larger weight to the configurations that should appear more often, and to let this weight for each configuration be proportional to the probability – the Boltzmann factor.

The calculation of this kind of expectation values seems to be an ideal problem for a computer. The task is just to generate all possible configurations, measure the energy, and sum the relevant quantity weighted by the Boltzmann factor.

There is, however, one problem with this approach which is linked to our desire to study fairly large systems. The problem with these large systems is that the number of configurations becomes enormous. For a 64 × 64 system – a rather large system – the number of configurations in the Ising model is about $10^{1233}$, and it is clear that even with a good computer with, say, $10^9$ operations per second, this direct approach is useless.

The solution to this dilemma is, not to make use of all possible configurations in the calculation. The next idea is therefore to make configurations by letting the computer ‘toss the coin’ – up or down – for each lattice point. But it turns
out that this is no good idea, either. The problem is now that practically all the configurations that are generated in this way happen to be very disordered and therefore have large energy. This means that their probability is small; most of them would never occur.

The situation is like making an opinion poll among the students in Umeå about the election to the “students’ union”. Since the participation in the election is below 10%, one would waste a lot of time on people who don’t influence the outcome.

The solution to this problem is called importance sampling. This means that one generates configurations with different probability which depends on their energy. There are various ways to do this, but the common idea is to generate configurations in a sequence where each configuration is generated from the previous one through the flipping of arrows. The decision of flipping or not is made by means of some clever rules involving the temperature and the change in energy caused by the flip.

The problem with this kind of approach is that the configurations are generated from each other. The succeeding configurations may therefore look very much the same, and this has important bearings on the simulations since we would like to have a large number of independent configurations and measurements. Nobody with a serious wish to make a good opinion poll restricts himself to questioning a single family.

1.1.4 Phase transitions

The 2D Ising model may be characterized by means of the magnetization, i.e. the net arrow which is obtained upon summing all the arrows. At zero temperature, where all the spins point in the same direction, the magnetization per arrow is equal to one. Since misalignments become more common with increasing temperature, the net arrow, the magnetization, decreases as the temperature is increased.

One could well imagine that the magnetization in an infinite system should decrease smoothly to lower and lower values as the temperature is increased. However, the more exciting possibility - a phase transition - happened to be true for the 2D Ising model. The magnetization decreases rapidly as the transition temperature is approached and becomes equal to zero at \( T_c \approx 2.269 \). The demonstration of this\[49\] has been described as ‘one of the major achievements of 20th century science’.

The abrupt approach to zero for the magnetization is, however, only found in very large systems. The solid symbols in Fig. 2 show how the magnetization approaches zero for two different system sizes: \( 32 \times 32 \) (circles) and \( 64 \times 64 \) (squares). The concept magnetization is obviously derived from the similarity with a fer-
romagnet. Each atom in a piece of iron has a property – spin – which gives rise to a small magnetic field in a certain direction. In a normal piece of iron these small magnets are randomly oriented which implies that they cancel each other out. In a permanent magnet, on the other hand, the spins tend to point in a common direction and this may be detected as a certain magnetization. Just as in the Ising model the magnetization in a ferromagnet decreases upon heating, and approaches zero at a certain temperature – the Curie point. Despite this similarity the 2D Ising model is not a very good model of a ferromagnet.

The phase transition is more clearly seen in the heat capacity, which measures how fast the average energy changes with increasing temperature. The open symbols in Fig. 2 show the heat capacity per spin.

1.2 The 2D XY model

With a small modification of the two-dimensional Ising model one obtains the two-dimensional XY model. The change is simply to let the arrows point in arbitrary directions in a plane instead of only up or down. A possible configuration for the 2D XY model is shown in Fig. 1b. The direction of an arrow is now conveniently described by an angle. As in the Ising model the energy depends on the difference in direction between neighboring arrows. For the cases parallel and anti-parallel
**1 INTRODUCTION**

- **a)** No current
- **b)** Current ⇒
- **c)** Circulating current

Figure 3: Currents in the $XY$ model.

$(0^\circ, 180^\circ)$ the energy for a nearest-neighbor pair is the same as in the Ising model, $-1$ and $+1$, respectively. For intermediate angles the energy varies smoothly with the angle.

The fact that makes the 2D $XY$ model a model of a thin superconductor, is that a superconductor, in each point, may be characterized by an arrow with a certain direction or angle. At lowest conceivable temperature and in the absence of currents, this angle is the same throughout the whole superconductor. Putting a current through the superconductor makes the angle increase gradually in the direction of the current. Figure 3 shows this arrow at certain points in a part of a superconductor at zero temperature. Panel a) is in the absence of currents and panel b) is a configuration with a certain current to the right.

As is often the case, things are simple at zero temperature. With a twist of, say, 0.01 in some units, the current per link would also be 0.01. At temperatures above zero, things become much more complicated since we are then interested in the behavior averaged over a huge number of configurations. It is, however, possible to analyze how the average current per link in the $XY$ model varies with temperature (keeping the twist the same) by means of MC calculations described above. The result, which turns out to be highly dependent on the system size, is shown in Fig. 12. The curves show the fraction

$$\frac{\text{average current}}{\text{twist}},$$

which illustrates how the superconducting ability is lost as the temperature is increased.

This loss of superconducting ability turns out to be intimately related to the existence of whirls – vortices – in the current distribution. Figure 3c shows a configuration with such a vortex – a circulating current. These vortices normally occur in pairs with opposite sense of rotation, cf. Fig. 10.
1.3 Metropolis Monte Carlo

It is possible to use different algorithms in Monte Carlo (MC) calculations. The one used in the work for the present thesis, which is also the most commonly used, is the Metropolis algorithm[36].

In the Metropolis algorithm a configuration is generated from the previous one by iteration of the following steps:

- Select one site at the lattice.
- Get a suggested new direction for the spin.
- Calculate $\Delta E$, the change in energy caused by this change in spin direction.
- If $\Delta E < 0$, accept the change.
- If $\Delta E > 0$, accept the change with probability $e^{-\Delta E/T}$.

In the calculations for the present work the sites were chosen sequentially. In an ordinary run it was four sweeps through the lattice between consecutive measurements, and the results were stored in the data file as sums over 1024 measurements. The distribution of these group values around their corresponding means, was used to get measures of the statistical errors.

1.3.1 Speeding up with integers

Since some of the computers used are considerably faster with integer than floating point arithmetics, some effort were taken to convert the update routine to integer arithmetics as much as possible. Besides discretizing the angles and putting cosinus and sinus for the relevant angles in a table, the exponentiation for the Boltzmann factor was also made unnecessary.

To this end, firstly, a table with integers proportional to $\cos(\phi)/T$ (where $\phi$ is an angular difference) was used to calculate LNP, the logarithm of the Boltzmann factor. Secondly, a random number generator with integers as output was used. The twelve most significant bits were used as an index IX in a vector LNR with the logarithm of the random number stored. In the case LNP < LNR(IX) the change is accepted, if LNR > LNR(IX+1) the change is rejected, and if LNR(IX) < LNP < LNR(IX+1) the floating point arithmetics with an ordinary exponentiation is used to arrive at a decision.
2 Two dimensions

This section contains a short introduction to superconductivity and the two models used in this thesis for the theoretical analysis of thin superconducting films. The first model, the two-dimensional Coulomb gas, is suitable for an analytical approach. Papers I and II are concerned with the derivation and numerical analysis of a set of equations for this model. The second model, the two-dimensional $XY$ model, is more suitable for MC calculations. Papers III and IV are devoted to the study of this model and Paper V contains an analysis of some closely related models.

There are often more or less direct relations between different physical models. Such relations are very important and are therefore the subject of several of the following subsections. The relation between the superconductor and the 2D CG is given in Sec. 2.1.3, and the corresponding relation to the 2D $XY$ model is given in Sec. 2.1.5. One of the issues discussed in Paper IV is the precise relation between the two latter models. This is also discussed in Sec. 2.3.6.

2.1 Superconductivity

The phenomenon superconductivity was discovered in 1911 by H. Kammerlingh Onnes\cite{26} through measurements on mercury at very low temperatures. He found that the electrical resistivity appeared to vanish below 4.2 K.

Superconductivity has, since then, been found in many different materials, both elements and alloys, and it has been shown that the resistivity in a superconductor actually is identically zero. This has been done in experiments with a current in a superconducting ring; the current has been observed to flow without measurable decrease for more than a year. We may therefore say that a hallmark of a superconductor is perfect conductivity.

The microscopic mechanism for superconductivity was not found until 1957 – nearly fifty years after the discovery of the phenomenon – by Bardeen, Cooper, and Schrieffer (BCS). The essential of the BCS theory is that the electrons are bound together in pairs – Cooper pairs – by a weak force caused by phonons, and that these paired electrons are the superconducting charge carriers.

Before the advent of the microscopic theory there were some phenomenological theories of superconductivity. One successful approach is due to F. and H. London (1935). They introduced the ‘number density’ of superconducting electrons $n_s$, and suggested two equations which contain the basic electrodynamic properties. These equations give at hand that an external magnetic field induces currents that makes the magnetic field vanish in the interior of the superconductor – the Meissner effect. This is the second important characteristics of the superconducting state.
2.1 Superconductivity

The magnetic field will, however, penetrate a thin layer of the superconductor. The equations show that the thickness of this layer, the penetration depth, obeys

\[ \lambda_L = \sqrt{\frac{mc^2}{4\pi n_s e^2}}. \]

### 2.1.1 Ginzburg-Landau theory of superconductivity

The present work is based on the Ginzburg-Landau (GL) theory of superconductivity which was formulated in 1950, seven years before the presentation of the microscopic theory. The reason for using the phenomenological GL theory instead of the BSC theory is mainly that the GL theory is simpler, but still includes the most important features of the superconducting state on a macroscopic scale. Furthermore, it is possible to derive the GL theory from the BCS theory. On the other hand, one can imagine situations where the GL theory is valid even if the BSC theory is not.

The first assumption in the GL theory is that a superconductor at each point is characterized by a complex 'order parameter' \( \psi(\mathbf{r}) \)

\[ \psi(\mathbf{r}) = |\psi(\mathbf{r})|e^{i\theta(\mathbf{r})}, \]

where both the magnitude and the phase are important. The magnitude of the order parameter is directly related to the density of superconducting electrons

\[ |\psi(\mathbf{r})|^2 = \frac{1}{2} n_s. \]

The factor of one half gives the density of Cooper pairs.

The second assumption in the GL theory is that the free energy may be written in powers of \( \psi \) and \( \nabla \psi \) [31]:

\[ F = \int d\mathbf{r} \left[ \frac{B^2}{8\pi} + \frac{\hbar^2}{2m^*} \left( \nabla - \frac{ie^*}{\hbar c} \mathbf{A} \right) \psi \right]^2 + \alpha(T)|\psi|^2 + \frac{\beta}{2} |\psi|^4, \]

where \( m^* = 2m \) and \( e^* = 2e \) are the mass and charge, respectively, of a Cooper pair, and \( \mathbf{B} = \nabla \times \mathbf{A} \) is the magnetic induction. The first term in the free energy is the magnetic energy. The second term is equal to the expression for the kinetic energy in quantum mechanics; the vector potential \( \mathbf{A} \) is included to get a gauge invariant expression. The function \( \alpha(T) \) in the third term is equal to zero at \( T_{c0} \), the mean-field temperature, and negative at lower temperatures. It is assumed that this function, to a good approximation, is given by the first term in an expansion around \( T_{c0} \),

\[ \alpha = \alpha'(T - T_{c0}). \]
Finally, \( \beta \) in the last term is a positive constant.

The equilibrium value of \( |\psi| \) is determined by the condition that the free energy is a minimum. In the absence of external fields this means that the total mass density of superconducting electrons is given by

\[
\rho_0 = m^*|\psi|^2 = -m^* \frac{\alpha(T)}{\beta} = m^* \frac{\alpha'}{\beta} (T_{c0} - T).
\]

(2)

The subscript '0' at both the transition temperature and the mass density signifies that they are mean-field quantities.

The requirement that the free energy is a minimum with respect to small variations of the vector potential \( \delta A \), gives an expression for \( \nabla \times B \) which may be identified with Maxwell's equation \( \nabla \times \mathbf{B} = (4\pi/c)\mathbf{j} \). The expression for the current density then becomes

\[
\mathbf{j} = -\frac{i e^* h}{2m^*} (\psi^* \nabla \psi - \psi \nabla \psi^*) - \frac{e^2}{m^* c} |\psi|^2 \mathbf{A} = \frac{e^*}{m^*} |\psi|^2 \left( h\nabla \theta - \frac{e^*}{c} \mathbf{A} \right),
\]

(3)

where \( \psi^* \) denotes the complex conjugate of \( \psi \). We see that, neglecting the magnetic contribution, it is \( \nabla \theta \) – the gradient of the phase – that determines the current.

Another important parameter in the GL theory is the Ginzburg-Landau coherence length which is a measure of the size of the region with correlated \( \psi \). It is given by

\[
\xi_{GL} = \frac{\hbar}{\sqrt{2m^*|\alpha(T)|}},
\]

and diverges due to the temperature dependence of \( \alpha \), as the mean-field temperature \( T_{c0} \) is approached from below.

The ratio of the two characteristic lengths defines the Ginzburg-Landau parameter, \( \kappa = \lambda_L / \xi_{GL} \). It was shown by Abrikosov\cite{1} that a superconductor with large GL parameter behaves differently in the presence of a magnetic field. With \( \kappa > 1/\sqrt{2} \) the flux can penetrate the superconductor without destroying the superconducting state. This different kind of materials is called type-II superconductors.

We will in the following restrict ourselves to the extreme type-II limit, \( \xi_{GL} \ll \lambda_L \). In this limit the magnetic effects due to the charge transport associated with the current is negligible. This turns out to be a good approximation in the case of thin, 'dirty' type-II superconducting films\cite{3}.

The GL theory of superconductivity has much in common with superfluidity – the remarkable property of \(^4\text{He}\) to flow without resistance\cite{40,19}. This is the reason that \( \rho_0 \) and \( \rho_s \) often are called the 'bare superfluid density' and the (macroscopic) 'superfluid density', respectively.
2.1 Superconductivity

Figure 4 is a sketch of the resistivity as a function of temperature for both a bulk superconducting material and a thin superconducting film. As shown in the figure, there is an abrupt onset of the resistivity in the bulk material, whereas the resistivity in the thin film comes smoothly as the temperature is increased.

One notes that the appearance of resistivity in a bulk superconductor nearly coincides with the vanishing of $\rho_0$, the density of superconducting electrons. This seems very reasonable. But in the thin films things are different. It turns out that the resistivity shows up while we still have a large density of superconducting electrons in the film. This calls for a mechanism that produces resistivity in spite of the fact that the sample is superconducting on a microscopic level. For the region close to the onset of dissipation, the vortex unbinding transition is the well established mechanism behind this effect.

We first note that if a film is thin enough, the order parameter does not change very much as one goes through the film. It is therefore justified to describe it as a two-dimensional system. In this context $\rho_0$ is a two-dimensional density.

Consider now a superconducting ring of a thin film with an uniform circulating current, as in Fig. 5a. That the current is uniform means that the gradient of the phase is the same everywhere. The phase rotates as one goes around the ring, and the number of revolutions – the winding number – has to be an integer. An
important point is that the winding number not is easily changed. The winding number for the ring may only change if an object with winding number ±1 – a vortex – forms at one of the boundaries (Fig. 5b), moves across the film, and crosses the opposite boundary – or through an equivalent process involving several vortices. A reduction of the winding number is equivalent to a degradation of the current and this will be perceived as a non-zero resistivity in the sample.

In this scenario the vortices – the objects with winding number ±1 – are the main actors, and the major part of this thesis concerns the effects of vortices, in one way or the other. A property of vortices which is directly related to the appearance of resistivity, is that they, at low temperatures, are bound together into neutral pairs. This is important since the movement of a vortex pair across the ring not changes the winding number and therefore not gives rise to any dissipation. To have dissipation it is necessary to have free vortices.

It is this ‘vortex unbinding’ – the change as the temperature is increased above a certain threshold value from a system with only bound vortex pairs to a system with some free vortices – which is the hallmark of the Kosterlitz-Thouless (KT) transition[28]. This transition is central to several of the papers in the present thesis.

From the above reasoning one may conclude that the resistance is proportional to the number of free vortices. A further step was taken by Bardeen and Stephen[2] who showed that the ‘flux-flow resistance’ $R$, is given by

$$\frac{R}{R_N} = 2\pi \xi_{GL}^2 n_F,$$

where $R_N$ is the normal-state resistance and $n_F$ is the density of free charges.
2.1.3 Ginzburg-Landau Coulomb gas

In order to analyze the system of vortices in a superconductor we first separate the mass current density into two parts[40], one with vortex excitations and one with spin waves, cf. Fig. 10. We write

\[ g(r) = g_\perp(r) + g_\parallel(r), \]

where the two parts obey

\[ \nabla \times g_\parallel(r) = 0, \quad g_\parallel(r) = \nabla \Phi(r), \]
\[ \nabla \cdot g_\perp(r) = 0, \quad g_\perp(r) = \nabla \times \hat{z} W(r), \]

and \( \hat{z} \) is the unit vector perpendicular to the plane. In the expressions for \( g_\perp(r) \) the contribution from the vector potential is omitted, which, as pointed out above, is justified in the extreme type-II limit.

In the simplest description of a vortex one might keep the magnitude of the complex order parameter fixed \( \rho_0 = m^*|\psi|^2 \), and only consider the variation in the phase \( \theta \). In this way the vorticity is concentrated to a single point. This is, however, unphysical since the current density becomes infinite at the vortex core, cf. Eq. (3). To avoid singularities in \( \nabla \psi \) one has to require \( \rho_0 = 0 \) at the center of the vortex and smoothly varying around.

A more realistic description of a vortex has been obtained through a minimization of the GL free energy, Eq. (1), under the constraint that the phase rotates by \( 2\pi \) around the origin[42]. This kind of analysis gives rise to a certain mass current density field \( g_v(r) \), from which one may extract a vorticity distribution \( f_{r_0}(r) \)

\[ \nabla \times g_v(r) = 2\pi f_{r_0}(r) \frac{\rho_0 \hbar}{m^*}, \]

where \( r_0 \) is the extension of a vortex. A further information from this kind of vortex description is the energy \( E_c \) associated with the reduction of \( |\psi| \) in the vortex core[42].

With Eq. (5) the above expression leads to

\[ \nabla^2 W(r) = -2\pi f_{r_0}(r) \frac{\rho_0 \hbar}{m^*} \]
\[ = \frac{\rho_0 \hbar}{m^*} \int dr' f_{r_0}(r') \nabla^2 V(r - r'), \]

where \( \nabla^2 V(r) = -2\pi \delta(r) \). We also get an explicit expression for \( W \):

\[ W(r) = \frac{\rho_0 \hbar}{m^*} \int dr' f_{r_0}(r') V(r - r'). \]
To describe the system with several vortices we define the vorticity density

\[ n(r) = \sum_i q_i f_{\tau_0}(r - r_i), \]  

(8)

where the summation runs over all the vortices; \( r_i \) is the position and \( q_i \) the vorticity of the vortex with index \( i \). It is also convenient to generalize \( W \) to a system with several vortices, \( W_{\text{tot}}(r) = \sum_i q_i W(r - r_i) \).

The vortex contribution to the energy consists of two parts. The first is related to the currents in the system, and the second is associated with the reduction of \( |\psi| \) in the vortex core[40]. We may write

\[ H_{\text{vortex}} = \frac{1}{2\rho_0} \int dr \, g_\perp^2(r) + NE_c, \]

where the integrand may be written \( g_\perp^2(r) = (\nabla \times \hat{z} W_{\text{tot}})^2 = (\nabla W_{\text{tot}})^2 \), and after a partial integration the integral becomes

\[ \int dr \, g_\perp^2(r) = - \int dr \, W_{\text{tot}}(r) \nabla^2 W_{\text{tot}}(r). \]

Through Eqs. (6) and (7), which holds for \( W_{\text{tot}} \) after the substitution \( f_{\tau_0}(r) \rightarrow n(r) \), cf. Eq. (8), the vortex contribution to the energy may be written

\[ H_{\text{vortex}} = 2\pi \rho_0 \left( \frac{\hbar}{m^*} \right)^2 \frac{1}{2} \int dr \, dr' n(r) V(r - r') n(r') + NE_c. \]

(9)

It is now possible to transform this result to a 2D Coulomb gas. With an effective interaction \( U(r) \) between the vortices with vorticity distribution \( f_{\tau_0}(r) \), the energy may be written as a sum over all vortex pairs

\[ H_{\text{CG}} = \frac{1}{2} \sum_{i,j} q_i q_j U(r_{ij}) + NE_c, \]

\[ = \frac{1}{2} \sum_{i \neq j} q_i q_j [U(r_{ij}) - U(r_0)] + NE_c, \]

where the neutrality condition \( \sum_i q_i = 0 \), has been used to get the second line.

The prefactor in Eq. (9) is now included in the new temperature variable – the Coulomb gas temperature \( T_{\text{CG}} \). This is obtained from the requirement that the statistical weight for a certain vortex configuration should be equal to the same quantity for the corresponding Coulomb gas configuration, i.e.,

\[ \frac{H_{\text{vortex}}}{T} = \frac{H_{\text{CG}}}{T_{\text{CG}}}. \]
This gives
\[ T^{CG} = T / \left[ 2\pi \rho_0 \left( \frac{\hbar}{m^*} \right)^2 \right], \tag{10} \]
for the Coulomb gas temperature, and the important observation that the bare superfluid density \( \rho_0 \), and its temperature dependence is central for a comparison between the superconductor and the 2D CG.

### 2.1.4 Coulomb gas scaling

The main idea behind Coulomb gas scaling\[37,40\] is that the superconducting films are described by a Coulomb gas with the properties of the charges (size, charge distribution, and creation energy), governed by the Ginzburg-Landau description. A consequence of this is that the quantities characterizing a superconducting film which may be expressed in terms of Coulomb gas quantities should be identical for different superconducting samples.

A link between experiments on 2D superconductors and the CG is given by the Bardeen-Stephen formula for the flux-flow resistance, Eq. (4). Since \( R/R_N \) may be expressed in terms of Coulomb gas quantities it is a possible candidate for CG scaling, and, noting that it is a dimensionless quantity, it may be concluded that it can only be a function of the dimensionless Coulomb gas temperature \( T^{CG} \). The scaling variable is then, in order to get rid of the unknown parameters \( a' \) and \( \beta \), chosen to be
\[ X(T) = \frac{T^{CG}(T)}{T^{CG}(T_c)} = \frac{T}{T_c} \left( \frac{T_{c0} - T_c}{T_{c0}} \right), \]
where the second step is from Eqs. (2) and (10).

The 2D resistance scaling function is shown in Fig. 6. In the interval \( 1.1 < X < 4 \) it is to a very good approximation parametrized by (Paper IX)
\[ |\ln(R/R_N)| = \left[ (4.824 + \frac{1.143}{X - 0.98})^{-a} + \theta(X - 1.2) \left( 0.2744 + \frac{2.977}{X - 1.2} \right)^{-a} \right]^{-1/a}, \tag{11} \]
where \( \theta \) is the step function and \( a = 2.566 \).

This scaling function will be used in Sec. 3.1.2 to test for two-dimensional behavior in the resistance data from YBCO/PBCO superlattices.

### 2.1.5 The XY model and superconductivity

The starting point in our description of superconductors, so far, has been the GL free energy Eq. (1). The purpose with this section is to show that the XY model
Figure 6: The 2D resistance scaling function. The open circles have been determined from experimental data and the solid curve is the parametrization given by Eq. 11.

may be motivated directly from the GL free energy, and therefore is a model of a superconductor. The arguments are valid in three as well as two dimensions.

The motivation involves several simplifications:

- Neglect the magnetic energies.

- Assume that the spatial variation in the magnitude of the order parameter is unimportant. The magnitude of the order parameter is put to a constant which only depends on temperature, \( m^*|\psi|^2 = \rho_0(T) \), the mass density of superconducting electrons. This means that the phase \( \theta(r) \) is the only remaining degree of freedom.

- Discretize the space so that the phase \( \theta \), only is defined at certain lattice points, \( r_i \). In this discretization the lattice constant \( a \) is identified with the Ginzburg-Landau coherence length \( \xi_{GL} \), since they are both of the same order of magnitude as a vortex in the respective systems.

- Change the interaction potential:

\[
\frac{1}{2} \rho_0 \left( \frac{\hbar}{m^*} \right)^2 |\nabla \theta(r)|^2 \rightarrow -J \cos(\theta_i - \theta_j),
\]

(12)

where \( i \) and \( j \) are nearest neighbors.
2.2 The two-dimensional Coulomb gas

The resulting Hamiltonian is

\[ H_{XY} = -J \sum_{(ij)} \cos(\theta_i - \theta_j), \]

where \((ij)\) denotes a summation over all nearest-neighbor links.

2.2 The two-dimensional Coulomb gas

The two-dimensional Coulomb gas (2D CG) describes the behavior of charged particles, with positive and negative charge, interacting through the Coulomb interaction \(V(r)\). This is defined by the Poisson's equation \(\nabla^2 V(r) = -2\pi \delta_r\), which is logarithmic in two dimensions.

In order to get a well-defined model it is necessary to include a short-distance cutoff in the interaction. This may be done in several ways. One way is to specify a charge distribution \(f_{r_0}\), since this will stop the interaction from diverging at \(r \to 0\). This happened to be the case for the GL CG in Sec. 2.1.3. Another way is to include the prescription that two charges never can be closer than the distance \(r_0\). This is the method used in the renormalization equations, Secs. 2.2.2 and 2.2.3.

It is also convenient to introduce a large-distance cutoff \(\lambda_c\), in the interaction:

\[ (\nabla^2 - \lambda_c^{-2})V_c(r) = -2\pi \delta_r. \tag{13} \]

and take the limit \(\lambda_c \to \infty\) as the last step. The interaction becomes

\[ V_c(r) = K_0(r) = \begin{cases} \text{const} - \ln r, & r_0 < r \ll \lambda_c, \\ \sqrt{\pi \lambda_c/2r} \exp(r/\lambda_c), & \lambda_c \ll r, \end{cases} \tag{14} \]

where \(K_0\) is the modified Bessel function of zeroth order.

The 2D CG is defined in the grand canonical ensemble, which means that the number of Coulomb gas particles fluctuates, with the mean value determined by the chemical potential. Restricting ourselves to the neutral Coulomb gas, the partition function may be written

\[ Z = \sum_{N=0}^{\infty} \frac{1}{([N/2]!)^2} \int \prod_i \frac{dr_i}{r_0^2} e^{-H_N/T_{\text{CG}}}, \]

where \(i\) runs over the \(N\) particles and \(r_i\) is the position of particle \(i\). Since all particles with the same charge are identical, each distinct configuration will occur \([N/2]!\) times. The prefactor is included to compensate for this multiplicity.

The Hamiltonian for a configuration with \(N\) particles is

\[ H_N = \frac{1}{2} \sum_{i \neq j} q_i q_j [V_c(r_{ij}) - V_c(r_0)] + NT_{\text{CG}} \ln z, \]
where the summation runs over all the particles in the system, \( q_i \) is the charge of particle \( i \), and \( r_{ij} = |r_i - r_j| \). The \( z \) in the last term is usually called fugacity.

### 2.2.1 The Kosterlitz-Thouless transition

In Sec. 2.1.2 the existence of a finite resistivity in a thin type-II superconducting film led us to consider the possibility of free vortices, or, in the Coulomb gas picture, the possibility of free CG particles. The unbinding of CG charges may be considered as an escape over a barrier problem. This means that there only can be free charges if the barrier is finite. But in the limit of infinite \( \lambda_c \), which is the case of interest as far as phase transitions is concerned, the interaction in the 2D Coulomb gas is logarithmic for all \( r \), the potential barrier is infinite, and the possibility of free particles is excluded. This is the case for a single pair in the absence of other CG charges.

The situation when other charges are included was examined by Kosterlitz and Thouless[28] (KT). They studied how the presence of other CG charges affect the effective interaction. The essence of their analysis is that a pair with large separation polarizes smaller pairs in between. The CG may then be considered as a polarized medium which may be described by means of a length-dependent dielectric constant \( \varepsilon(r) \), and the effective interaction may be written

\[
V_{\text{eff}}(r) = \frac{V_c(r)}{\varepsilon(r)}.
\]

At low temperatures \( 1/\varepsilon(r) \) decreases slowly with increasing \( r \), but approaches a finite constant in the limit of large \( r \). The effective interaction is therefore, just as in the case of an isolated pair, a logarithmic function of distance. It is only the prefactor that is smaller. The conclusion is, again, that there is no free charge present in the system.

The remarkable finding by KT is that this behavior becomes different above a certain temperature, the Kosterlitz-Thouless temperature. Above this temperature the effective interaction approaches a constant in the large-\( r \) limit. This means that the potential barrier against breaking a pair is finite which, in turn, implies that there is a certain density of free particles in the system.

The existence of the phase transition, and actually also the transition temperature, may be obtained through a simple argument based on the energy entropy balance[28]. In a system with linear extension \( L \) characterized by the dielectric constant \( \varepsilon \), the self-energy for a single charge is \( \approx \frac{1}{2\varepsilon} \ln L/r_0 \), the entropy is \( \approx \ln(L/r_0)^2 \), and the free energy becomes

\[
F \approx \frac{1}{2\varepsilon} \ln L/r_0 - T^{\text{CG}} \ln(L/r_0)^2 = \left( \frac{1}{4\varepsilon} - T^{\text{CG}} \right) \ln(L/r_0)^2.
\]
2.2 The two-dimensional Coulomb gas

Figure 7: Flow diagram for the Kosterlitz RG equations. The arrows indicate the flow direction under integration. The thick line shows the position of the phase transition.

This shows that the free energy for inclusion of a free charge in the system changes sign at the temperature \( T_{CG}^{c} = 1/4\tilde{\varepsilon} \). In the \( L \to \infty \) limit we conclude that the CG has no free charges below \( T_{c}^{CG} \), whereas free charge is present above this temperature. Despite the crudeness of the argument, this result remains true for theoretical treatments so far, as long as the fugacity is below a certain threshold value[39].

2.2.2 Kosterlitz' renormalization group equations

Since the analysis by KT is based on the pairs, their interaction and polarizability, their results are not suitable for the high-temperature phase where free charge is present. The same is true for the Kosterlitz renormalization group (RG) equations. Kosterlitz showed that if one starts with a partition function for the CG based on the logarithmic interaction and certain values for \( T_{CG}^{c} \) and \( z \), and integrates out the shortest wave lengths in the charge distribution, one recovers a partition function with the same form, but now with a new set of values for \( T_{CG}^{c} \) and \( z \). This means that one has obtained an effective interaction which is also logarithmic, but now with a slightly different prefactor. The Kosterlitz RG equations describe how this set of parameters \((T_{CG}^{c}, z)\) change in the rescaling process. The equations are, however, only expected to be valid in the limit of small \( z \).

The reason for the interest in this kind of rescaling, is the renormalization group theory suggested by Wilson[60,61]. The idea is, basically, that the presence of a
fixed point – a point for which the output parameters are the same as the input parameters – signals the absence of a characteristic length and, therefore, a phase transition. The 2D CG is exceptional since the $T_{CG}$ axis for $T_{CG} < 1/4$ is a line of fixed points. The phase transition is associated with the point where this line terminates.

Figure 7 shows some RG trajectories in $(T_{CG}, z)$ space. For all points below the thick line, a rescaling leads to decreasing $z$, and thereby a decreasing density of charge. For the points on the upper right side of the thick line, the density of charge eventually increases in the rescaling process. This is a signal of the presence of free charge. The thick line is the last trajectory that terminates at the $T_{CG}$ axis, and is therefore the line for the phase transition.

In the low-temperature phase this rescaling may be continued indefinitely, since the effective interaction in this case is logarithmic for all $r$. Above the critical temperature, on the other hand, the rescaling may only be continued up to a certain length. This may be considered as a result of the fact that the effective interaction no longer is logarithmic when an appreciable amount of free charge is integrated out.

From an analysis of the length where the renormalization breaks down, it was possible for Kosterlitz to extract the behavior of the characteristic length $\xi$. The result is

$$\ln \xi = B + \frac{C}{\sqrt{T_{CG} - T_c}},$$

(16)

where $B$ and $C$ are constants. This temperature dependence of the characteristic length should also be present in the correlation length from the spin-spin correlation in the 2D XY model. This is further discussed in Sec. 2.2.4.

### 2.2.3 Minnhagen’s self-consistent renormalization equations (I)

An improved set of renormalization equations for the 2D CG have been constructed by Minnhagen[38]. These equations are self-consistent and reduce to the Kosterlitz RG equations in the limit of low density in the low temperature phase. In contrast the latter, they are, however, valid in both the low- and high-temperature phases.

The key quantity in the self-consistent equations is the linearly screened potential $V_L$, which is the potential per unit charge outside an infinitesimal test charge inserted into the system. It is also an approximation of the effective interaction, Eq. (15). $V_L$ is related to the bare interaction through

$$V_L(k) = \frac{V_c(k)}{\epsilon(k)},$$

(17)
2.2 The two-dimensional Coulomb gas

where $\epsilon(k)$ is the linear-response dielectric function. $\epsilon(k)$ may be related to the charge density correlation function $\langle n(r)n(0) \rangle$ through

$$\frac{1}{\epsilon(k)} = 1 - \frac{V_c(k)}{\Omega T_{CG}} \langle n(k)n(-k) \rangle,$$

(18)

where $\Omega$ is the area (cf. Appendix D in Paper IV).

The third equation derives from an exact expression for the pair correlation function, which can be systematically expanded in the linearly screened potential $V_L$. To lowest order one obtains[38]

$$\langle n(0)n(r) \rangle = -\frac{2z^2}{r^4} e^{-V_L(r_0)/T_{CG}} \sinh[\frac{V_L(r)}{T_{CG}}].$$

(19)

The three above equations constitute a self-consistent set of equations for $V_L$.

Previous analyses of Minnhagen's self-consistent renormalization equations, have been performed with no large-distance cutoff[43,44]. Paper I describes a reformulation of the self-consistent equations with the cutoff explicitly introduced into the bare interaction, Eq. (14). There are several advantages with this approach:

- The infinities associated with the logarithmic interaction at large distances are removed.
- The low- and high-temperature phases are described by the same equations. The low-$T_{CG}$ phase is characterized by $\lambda = \lambda_c$.
- It is possible to study the effect of a finite cutoff in the interaction, as is, e.g. the case in superconductors when the magnetic effects are included.

As shown in Paper I, it is possible to perform several integrations analytically and obtain a manageable expression for $V_L(r)$

$$V_L(r)/T_{CG} = -\left(1 - \frac{1}{\alpha^2}\right)^2 \int_{r'}^\infty \frac{dr'}{\lambda_c} \tilde{K}(r/\lambda_c, r'/\lambda_c) \sinh[V_L(r')/T_{CG}].$$

(20)

This equation may be solved with different values for the parameters $\alpha = \lambda/\lambda_c$ and $\lambda$. The latter parameter is used to specify the boundary condition on $V_L(r)$ for large $r$:

$$V_L(r)/T_{CG} = AK_0(r/\lambda), \quad r \to \infty.$$

Since the function $\tilde{K}$ is equal to zero for $r = r'$, and $V_L$ for large $r$ is given by the above expression, it is possible to iterate Eq. (20) down to successively smaller values for $r$. It is then possible to determine $z$ and $T_{CG}$ as functions of $r$ from the
Figure 8: Some renormalization trajectories. Panel a) is for the low-temperature phase $\alpha = 0.99$, and, from right to left, $A = 3.5, 4.0$, and $6.0$. Panel b) is for the high-temperature phase, $\alpha = 0.001$. The values for $A$ are, from right to left, $A = 3.3, 3.375, 3.5, 4.0, 4.5, 5.0, 6.0, 8.0$, and $10.0$. The dashed line in panel b) corresponds to an attempt to determine the trajectory in $(T_{CG}, z)$ space for the $XY$ model, Sec. 2.3.7. The circle corresponds to $T_c \approx 0.893J$. 


2.2 The two-dimensional Coulomb gas

linearly screened potential. This gives one trajectory in the \((T_{CG}, z)\) plane for each set of parameters \(\alpha\) and \(\Lambda\).

Figure 8 shows some trajectories from the self-consistent equations. Panel a) is some trajectories in the low-temperature phase, \(\alpha = 0.99\), and panel b) is for the high-temperature phase with \(\alpha = 0.001\).

An important quantity which is available through Minnhagen’s equations is the screening length \(\lambda\). Since it is a characteristic length it should be proportional to \(\xi\) in the previous section and the behavior in the critical region should be governed by an identical expression, cf. Eq. (16).

The relation between \(\lambda\) and the density of free vortices \(n_F\), may be obtained through a Poisson-Boltzmann description\[40\]. The potential due to an infinitesimal test charge \(t\), at the origin, may be written

\[
t \nabla^2 V_L(r) = -\frac{2\pi}{\xi} \left( t \delta(r) + n_F^+ e^{-t V_L/T_{CG}} - n_F^- e^{t V_L/T_{CG}} \right) = -\frac{2\pi}{\xi} \left( t \delta(r) + \frac{tn_F}{T_{CG}} V_L \right),
\]

where \(n_F^\pm\) are the densities of free positive and negative CG charges, respectively. From \((\nabla^2 - \lambda^{-2})V_L = -2\pi \delta(r)/\xi\), the density of free charge is obtained as

\[
n_F = \frac{\xi T_{CG}}{2\pi \lambda^2}. \tag{21}
\]

In the case of a superconductor, the density of free vortices is related to the flux-flow resistance through the Bardeen-Stephen formula, Eq. (4). This implies a relation between the flux-flow resistance and the screening length \(\lambda\),

\[
\frac{R}{R_N} = \frac{\xi T_{CG}}{2\pi \lambda^2} \left( \frac{\lambda}{\xi_{GL}} \right)^{-2}.
\]

From Eq. (16) we conclude that the main temperature dependence is given by

\[
\ln \frac{R}{R_N} \sim \frac{1}{\sqrt{T_{CG} - T_{CG}}} \approx \frac{1}{\sqrt{T - T_c}}, \tag{22}
\]

where the second step is justified in a temperature region close to \(T_c\) where the temperature dependence of \(\rho_0\) may be neglected.

2.2.4 Size of the critical region (II)

The most important result, in this thesis, from the solution of Minnhagen’s renormalization equations, is the estimate of the size of the critical region – the region where the screening length and the flux-flow resistance are described by Eqs. (16)
and (22). It is found that the critical region is very narrow, indeed. The relevant equations only hold in the temperature region $1.0 < T_{CG}/T_{CG}^{c} < 1.05$.

In the case of a thin superconducting films one finds, from a comparison with Fig. 6 that this corresponds to $\ln R/R_{N} < -15$, resistances that are very difficult to resolve experimentally. This is corroborated by the observation that there is no resistance data in the 2D resistance scaling function at these low values. The conclusion is that the KT critical region is too narrow to be observed in superconducting films.

This finding, at first, seems to be in conflict with several results from both experiments and MC calculations. It has become standard to fit both resistivity data from experiments and MC data for the correlation length in 2D $XY$-type models to the square root behavior of Eqs. (16) and (22), with $B$, $C$, and $T_{CG}^{c}$ (or $T_{c}$) as free parameters. The often excellent fits have been taken to show that the critical region in these systems actually is quite large.

The very appealing solution to this conflict that is suggested in Paper II is based on the observation of an extended region with a pseudo-critical behavior in the 2D CG, at temperatures well above the true critical region. In this region Eq. (16) is obeyed to a good approximation but with different values for the parameters $B$ and $C$. This behavior has nothing to do with the critical region; it is only a reflection of the properties of the Coulomb gas per se.

A further observation (Paper IX) is that the fit to Eq. (16) becomes even more convincing if $T_{CG}^{c}$ is used as a free parameter as is usually done in the analysis of experiments or MC data. Figure 9 shows that the pseudo-critical behavior then holds over more than three decades. This is for a critical temperature which is about five percent too high.

Similar results – that the critical region is very small – have earlier been obtained from some RG equations for melting in two dimensions[21]. A weak point with that analysis is, however, that the RG equations, which are closely related to the Kosterlitz RG equations, are used in a region where their validity is questionable.

### 2.3 The two-dimensional $XY$ model

This section opens with a general introduction to the 2D $XY$ model. Then follows a brief introduction to three different ways to analyze the two-dimensional $XY$ model with MC calculations.

The first of these, which is also the most common, is through the spin-spin correlation function. This method is briefly discussed in Sec. 2.3.2.

The second way to analyze the 2D $XY$ model is through the helicity modulus, Sec. 2.3.3. Since the helicity modulus measures the current obtained through an
2.3 The two-dimensional XY model

Figure 9: Pseudo-critical behavior well above the true critical region with the critical temperature as a free parameter.

external twist in the system, this quantity is very directly related to superconductivity. The transition to the non-superconducting phase is seen as a rapid decrease to zero of the helicity modulus as the temperature is increased above $T_c$. In Paper III, (Sec. 2.3.4), the same quantity is used for a determination of $T_c$ for the 2D XY model.

The third way to analyze the 2D XY model is based on the concept fractional vortices. Through use of this concept it is straightforward to derive correlation functions for the effective vortex interaction $V_i$, Sec. 2.3.5. As discussed above, this function gives an excellent characterization of the Coulomb gas. We might therefore say that whereas the first two methods deal with the spins or the current, this third method focuses on the vortices.

The crucial step in the analysis of the 2D superconductor in Sec. 2.1.3 was the separation of the current into two parts. In Sec. 2.3.6 the same kind of separation is discussed for the 2D XY model. The result turns out to be a more direct and precise analogy to the 2D CG. One of the aspects of this analogy is an expression for the 'bare superfluid density' in the $XY$ model. Some consequences of this expression are discussed in Sec. 2.3.7.

The last section discusses the successful use of Coulomb gas scaling in some XY-type models.
2.3.1 General

The $XY$ model is defined through the partition function

$$Z = \prod_i \int \frac{d\theta_i}{2\pi} e^{-H_{XY}/T},$$

where $i$ runs over all the lattice points and $\theta_i$ is the angle associated with lattice point $i$. The integrations are from zero to $2\pi$. The Hamiltonian, already given in Sec. 2.1.5, is

$$H_{XY} = -J \sum_{(ij)} \cos(\theta_i - \theta_j),$$

where the notation $(ij)$ signifies that $i$ and $j$ are nearest neighbors.

The ground state of the 2D $XY$ model is trivial, it is the state with all spins pointing in the same direction. This common direction is, however, arbitrary. The $XY$ model is therefore said to possess 'continuous symmetry', which has important consequences for models with no more than two dimensions.

With a temperature closely above zero, only the configurations with very low energy are important. The angular differences $\theta_i - \theta_j$ are therefore small, and the cosinus interaction may be approximated by a harmonic interaction $\frac{1}{2}(\theta_i - \theta_j)^2$. Due to the harmonic interaction, the system may be considered to be excited by a lot of independent 'spin waves', Fig. 10a. The average energy for each spin wave is equal to $T/2$, in accordance with the equipartition principle.
2.3 The two-dimensional XY model

At higher temperatures it becomes possible to have vortex excitations. A vortex is normally defined by means of the angular differences between nearest neighbors. We have a vortex at a certain plaquette if the sum of the angular differences around it is non-zero. The vorticity is given by a summation over the four links around a plaquette,

\[ n = \frac{1}{2\pi}(\theta_{21} + \theta_{32} + \theta_{43} + \theta_{14}) \]  

(24)

where the angular differences \( \theta_{ij} = \theta_i - \theta_j \) are restricted to the interval \(-\pi \) to \( \pi \). A vortex pair is shown in Fig. 10b.

It was Berezinskii[5] and Kosterlitz and Thouless[28] who showed that the vortices are responsible for the phase transition, Sec. 2.2.1. At low temperatures the vortices are bound closely together into neutral pairs. As the temperature is increased the vortices become able to move at gradually larger distances from each other, and above the critical temperature a tiny fraction of the vortex pairs breaks, giving free vortices in the system. This intuitive picture is very appealing but, nevertheless, somewhat misleading. It is in practice not possible to identify vortex pairs which have become free. The density of free vortices is rather a collective property of the whole system.

2.3.2 Spin-spin correlation

An important function that helps to characterize the 2D XY model is the spin-spin correlation function \( g(r) = \langle \cos(\theta_0 - \theta_r) \rangle \), where \( \theta_r \) is the value of the phase at the discrete lattice position \( r \).

The spin-spin correlation at low temperatures may be calculated analytically in the spin wave approximation[59,5]. The result is that the correlation decays algebraically

\[ g(r) = e^{-G(r)/J} \sim r^{-T/2\pi J} , \]

which implies that it approaches zero in the limit of large \( r \) for all \( T > 0 \). The algebraic decay at temperatures up to \( T_c \approx 0.9J \) is shown in Fig. 11a. \( G(r) \), the lattice Green's function in two dimensions, is discussed in Paper IV.

This behavior is different from the ordinary behavior in spin models with a phase transition. An ordinary low-temperature phase has a finite spin-spin correlation in the limit of large \( r \), and therefore a finite magnetization. The absence of a finite magnetization in the 2D XY model is a manifestation of the Mermin-Wagner theorem[35], which excludes the possibility of long range order in 2D models with continuous symmetry.

The above expression for the spin-spin correlation is only valid in the \( T \to 0 \) limit. At temperatures up to \( T_c \) it is valid if a (slightly \( r \)-dependent) renormalized coupling constant \( J' \) is substituted for \( J \). The large-\( r \) limit of this renormalized
Two Dimensions

Figure 11: The spin-spin correlation in the 2D XY model for the temperatures, from top to bottom, $T/J = 0.6, 0.8, 0.9, 1.0, 1.1$.

Constant is equal to the helicity modulus $\gamma$, discussed in the next section. The universal jump condition for the helicity modulus, Sec. 2.3.3, gives $-1/4$ for the exponent at $T_c$, a value which is only obtained in the limit of large $r[27,55,18,22]$. A consequence of the algebraic correlations in the low-temperature phase, is the absence of any characteristic length. This is the same kind of behavior as in the 2D CG, Sec. 2.2.2. The appearance of a characteristic length is therefore one of the attributes of the high-temperature phase. In the spin-spin correlation function this is seen through an exponential decay of the correlations with the characteristic length $\xi$

$$g(r) \propto e^{-r/\xi},$$

which is true at least for distances large compared to $\xi$. Figure 11b shows the exponential decay for $T/J = 1.0$ and 1.1.

2.3.3 The helicity modulus

A superconductor becomes normal as the temperature is increased above $T_c$, and the same behavior should be present in any acceptable model of superconductivity. In the superconducting state one gets a current $I$, through the system by introducing a twist of the phase over the sample. The helicity modulus is the proportionality constant between the externally introduced twist per link $\delta$, and
2.3 The two-dimensional XY model

the average current per link \( \langle I \rangle \) in the limit of small \( \delta \). We may write

\[
\gamma = \lim_{\delta \to 0} \frac{\langle I \rangle}{\delta},
\]

and since the current per link, for a \( N \times N \) lattice, is related to the total free energy through

\[
\langle I \rangle = \frac{1}{N^2} \frac{\partial F}{\partial \delta},
\]

the ordinary expression for the helicity modulus follows:

\[
\gamma = \frac{1}{N^2} \left. \frac{\partial^2 F}{\partial \delta^2} \right|_{\delta=0}.
\]

Nelson and Kosterlitz\[47\] showed that the approach to zero of the macroscopic superfluid density \( \rho_s \) at the critical temperature is discontinuous. From the analogy between the helicity modulus and the superfluid density\[20\], one obtains that this discontinuity in the helicity modulus – the universal jump – is from \( 2T_c/\pi \) at \( T_c \) to zero right above. This result has also been shown in a calculation of the helicity modulus directly in the 2D XY model\[48\].

It was later shown by Minnhagen\[45\] that the starting point for the derivation by Nelson and Kosterlitz was in error, but that the result nevertheless was correct. The correct equation for the superfluid density used by Minnhagen is

\[
\rho_s = \frac{1}{T} \int dr \left( \langle g_{\parallel}(0) \cdot g_{\parallel}(r) \rangle - \langle g_{\perp}(0) \cdot g_{\perp}(r) \rangle \right).
\]

Figure 12 shows the helicity modulus as determined by MC calculations at several different temperatures and lattice sizes. The rounding of the jump is due to the finite lattice sizes.

2.3.4 Determination of \( T_c \) (III)

Since a phase transition is characterized by singularities in some quantities it is natural to determine the critical temperature through the position of such an abrupt change. This is quite possible in the three-dimensional XY model (even though there are better methods) but as shown in Fig. 12, it is not possible in the 2D XY model, because of the finite-size rounding of the jump.

The method that has been most widely used for determinations of the critical temperature from MC data in XY-type models is to extract the correlation length from the spin-spin correlation and fit it to Eq. (16) with \( T_c \) as a free parameter\[22, 12\]. But in the light of the results in Paper II – that the critical region is very small
and that there exists an extended pseudo-critical region – it is no longer justified to draw conclusions about the critical properties in this way.

An appealing alternative to the above method is to make use of some knowledge of the behavior of the system precisely at $T_c$. It is the same kind of approach which has been used in three dimensions[10]. Beside the well-known universal jump for the helicity modulus it is possible to extract the finite-size dependence of the same quantity from the length-dependent dielectric constant in equations for the 2D CG. The first analysis of this kind was done by Minnhagen and Weber[58], but since they used lattices with $N$ ranging from 3 to 12 their result, $T_c = 0.887J$, was affected by the too small lattices use in their analysis. This is shown in Fig. 10 in Paper III which shows both the excellent fit for small lattices and the deviation from the expected behavior for larger lattices.

The analysis in Paper III differs from Ref.[58] in two respects. Firstly, the analysis is made on larger lattices. The best results are obtained with lattice sizes in the range 24 through 64. Secondly, two different scaling functions are used. With the scaling function used in Ref.[58], which may be derived from the Kosterlitz RG equations, we get $T_c \approx 0.892J$. The second scaling function, is obtained from the self-consistent equations (Paper I) and contains the leading as well as the next leading $N$-dependence for large $N$. Fitting to this function gives $0.891J$ as a lower bound at $T_c$. 

Figure 12: The helicity modulus from MC calculations on $N \times N$ lattices with $N = 4, 8, 16, 32, 64, 128$. Also shown is the universal jump criterion (dashed line), and the jump itself at $T_c = 0.893J$ (Paper III).
Together with a tentative determination of an upper bound for $T_c$, it was concluded that the critical temperature is $T_c/J = 0.893 \pm 0.002$.

### 2.3.5 Effective vortex interaction in the 2D XY model (IV)

Since the 2D XY model undergoes a KT transition and this transition is conveniently described in terms of the linearly screened interaction, Sec. 2.2.3, it is desirable to be able to determine this quantity in the 2D XY model. The idea in Paper IV is to introduce a pair of fractional vortices at distance $r$ with vorticity $\pm q$, $0 < q < 1$ in the Hamiltonian, and to express the free energy in terms of $q$. The linearly screened potential $V_i$, is then obtained from the expression

$$V_i(r) = \frac{1}{2} \left. \frac{\partial^2 F(q,r)}{\partial q^2} \right|_{q=0} .$$

Paper IV contains derivations of correlation functions for this quantity in both ordinary space and Fourier space.

It is further shown that $V_i$ is in accordance with known results for the effective vortex interaction in the two limits $T \rightarrow 0$ and $k \rightarrow 0$. Firstly, in the $T \rightarrow 0$ limit the expression for $V_i$ is in accordance with the result by KT:

$$V_i(r) = 4\pi^2 JG(r),$$

where $G(r)$ is the lattice Green’s function. Secondly, in the $k \rightarrow 0$ limit, for general $T$, $V_i$ is directly related to the helicity modulus[45]. Taken together, these two agreements constitute a strong confirmation of the soundness of the approach in Paper IV.

The vortex unbinding is nicely illustrated through measurements of $V_i(r)$ in MC calculations. Figure 13 shows the linearly screened potential at temperatures from zero to $1.2J$. At temperatures up to $T_c$ (the three uppermost solid lines in Fig. 13) the effective vortex interaction depends logarithmically on distance. The potential barrier is therefore infinite and it is impossible to break a vortex pair. At temperatures above $T_c$, on the other hand (the lines below the thick line), the interaction energy approaches a constant for large separations. The potential barrier is finite and the bonds between the vortices may therefore be broken.

### 2.3.6 Formal separation of the current (IV)

Crucial for most analyses of the 2D XY model is the separation of spin waves and vortices[28,25,57]. The idea is that the spin waves only contribute to a kind of background, analogous to the bare superfluid density, whereas the vortices behave
as Coulomb gas charges, polarizes the medium and give rise to the phase transition. With the ordinary XY-Hamiltonian this separation is, however, rather artificial. This is seen if we first consider a vortex free configuration and then increase the amplitude of the spin waves. The effect will be to create vortices.

From this kind of reasoning we also expect that what we normally call spin waves also contribute to the dielectric constant. Since it is often enough to make only a minute change of an angle to annihilate (or create) a vortex pair at unit distance, we have to assume that the configuration with the annihilated vortex pair (only spin waves) gives close to the same contribution to the dielectric constant as the vortex pair. This certainly calls for a different definition of vorticity, and this is also one of the results of Paper IV.

In Sec. 2.1.3 the 2D superconductor was analyzed by separating the mass current density into two parts, one divergence-free and one rotation-free. The vortices were found in the divergence-free part $g_\perp$. The idea in Paper IV is to perform the same kind of separation of the current $j$ in an expression for $V_i(k)$. The result may be written

$$\frac{V_i(k)}{4\pi^2 G(k)} = J_0 - \frac{4\pi^2 \beta J_0^2}{k^2 N^2} \langle n(k)n(-k) \rangle,$$

where the first term at the right-hand side is due to $j_\parallel$ and the second to $j_\perp$. This means that the contribution from the vortices are in the second term. In the above
2.3 The two-dimensional XY model

expression we have used

\[ J_0 = J \langle \cos \phi \rangle, \]  

and \( n(k) \), which is the Fourier transform of

\[ n(r) = \frac{1}{2\pi \langle \cos \phi \rangle} D \times j_r, \]  

where \( D \) is the difference operator.

Beside the factor \( J_0 \), the right-hand side of Eq (29) is identical with Eq. (18) for the 2D CG with the bare interaction given by \( 4\pi^2 J_0/k^2 \). This suggests firstly, the identification of \( J_0 \) with the bare superfluid density, and, secondly, the identification of \( n(r) \) with the vorticity. To strengthen the conclusion that \( J_0 \) corresponds to the bare superfluid density, we note that the above equations also suggest writing

\[ \frac{V_l(k)}{4\pi^2 G(k)} = \frac{J_0}{\epsilon(k)}, \]

where the reduction of \( V_l \) from its zero-temperature form is separated into two parts. The vortex part is obviously in the \( k \)-dependent \( \epsilon(k) \), so the spin wave part – the bare superfluid density – is contained in \( J_0 \).

It should also be noted that the identification of \( n(r) \) with the vorticity is intuitively very reasonable since \( n(r) \) measures the rotation of the current around the plaquettes. The prefactor in Eq. (31) ensures that the total vorticity measured at a large distance from an isolated vortex is equal to one. In contrast to the ordinary definition of vorticity, Eq. (24), this vorticity is spread over several plaquettes. The area over which the vorticity is spread is a measure of the vortex core.

A further consequence of the separation of the current into two parts is that it is possible to rederive an expression analogous to Eq. (27) for the helicity modulus. This is certainly not surprising[45], but serves as yet another confirmation of the calculations.

2.3.7 The bare superfluid density in the XY model

As shown in Sec. 2.1.3 the bare superfluid density \( \rho_0 \) is very important in the analogy between the 2D superconductor and the 2D CG. The corresponding quantity in the ordinary \( XY \) model is, as shown in the previous section, \( J_0 = J \langle \cos \phi \rangle \). \( J_0 \) as a function of temperature is shown as a solid line in Fig. 14.

We are now in the position to determine the Coulomb gas temperature for the phase transition in the 2D \( XY \) model. With \( T_c \approx 0.893J \) (Paper III) and \( \langle \cos \phi \rangle \approx 0.7228 \) from MC calculations, we get

\[ T_c^{CG} = \frac{T_c}{2\pi J_0} \approx 0.197. \]
To obtain a more complete comparison between the $XY$ model and the 2D CG one would also like to determine the fugacity $z$ and plot $z(T_{CG})$ for the $XY$ model in the phase diagram for the CG. One way to do this is to determine $E_c$ from the bare interaction at unit distance, $2E_c = 4\pi^2 J_0 G(1)$, and make use of $z = e^{-E_c/T}$.

The dashed line in Fig. 8b shows this trajectory for the $XY$ model in $(T_{CG}, z)$ space. The dot corresponds to the critical temperature $T_c \approx 0.893J$. The crossing with the critical line is at $T = 0.928J$.

This determination of $z$ is, however, not quite correct. The reason is that the real vortices, as discussed above, have their vorticity spread over several plaquettes whereas $E_c$ is calculated with the vorticity concentrated to a single plaquette. The problem is related to the different kind of CG particles. In the CG equations the particles are point charges with hard spheres around, but in the $XY$ model the charge associated with a vortex is spread over several plaquettes. A detailed comparison between the $XY$ model and the 2D CG is only possible after a new treatment of the latter model with a single-particle charge distribution[7].

The calculations in Paper IV are restricted to the ordinary $XY$ model with cosinus interaction. To get an expression for $J_0$ for a general potential $V(\phi)$, one notes from the derivations in Paper IV that $J_0$ in Eq. (30) is the second derivative of $V$,

$$J_0 = \left\langle \frac{d^2V}{d\phi^2} \right\rangle.$$  

(32)
2.3 The two-dimensional XY model

It is interesting to note that this has a direct intuitive interpretation as the effective strength of the harmonic behavior of the model. This means that the system, as far as the vortices are concerned, behaves as if the potential was harmonic with the coupling constant $J_0$:

$$V_{\text{harm}}(\phi) = J_0 \frac{\phi^2}{2}.$$ 

This may be considered as an improvement of the self-consistent harmonic approximation for the $XY$ model[40,33]. Note that this is consistent with the change in the interaction potential in the motivation for the $XY$ model as a model of superconductivity, Sec. 2.1.5.

The bare superfluid density was estimated in some other ways before the above expression for $J_0$ was found. Two different methods were used:

In Paper VIII it was assumed that the bare superfluid density $\gamma_0$ in that paper may be obtained from measurements of the helicity modulus in MC calculations where the (ordinary) vortices are excluded. $\gamma_0$ is shown as a dashed line in Fig. 14. Up to $T \approx 1.0J$ this quantity falls slightly below $J_0$. This is readily understood from the fact that this is a measurement of the helicity modulus where a large part, but not all, of the vorticity is removed. $J_0$ may, on the other hand, be thought of as the helicity modulus in the absence of vorticity. Since the vortices always have the effect to reduce the helicity modulus, $\gamma_0$ falls below $J_0$. At higher temperature $\gamma_0$ lies above $J_0$. The reason is that the exclusion of (ordinary) vortices also affects the spin waves, and that $\gamma_0$ becomes larger when the magnitude of the spin waves is reduced.

In Paper V the bare superfluid density was estimated by means of the spin wave approximation. This crude estimate, $\gamma_{\text{sw}} = J - T/4$, is shown as a dotted line in Fig. 14.

2.3.8 Coulomb gas scaling in the 2D XY model (V)

The subject of Paper V is the examination of a class of $XY$ models. These models are constructed by inserting spin chains between the original spins. The original motivation for the study was the search for a model with a higher vortex density, and thereby, possibly, a first-order transition[39].

It was, however, found that this class of $XY$ models had lower vortex density, and certainly not any first-order transition. The examination of these models instead turned into a nice demonstration of the CG scaling concept in $XY$-type models. The assumptions are that $T_c^\text{CG}$ is closely the same for the various $XY$ models, and that the bare superfluid density is given by $\gamma_{\text{sw}}(T)$, which is easily calculated analytically for the different models. From these assumptions and
$T_c = 0.893J$ for the ordinary $XY$ model on the square lattice, it should be possible to estimate the critical temperature for the other $XY$-type models.

Figure 15 demonstrates the success of this approach. The figure shows $T_c$ against average number of nearest neighbors for several models. The solid circle is the input value, $T_c$ for the $XY$ model with four nearest neighbors. The solid line is the calculated critical temperatures for the chain models. The critical temperatures from MC calculations, shown as open circles, are found to agree well with these values.

The filled squares are determinations of $T_c$ from MC data for the $XY$ model at hexagonal and triangular lattices while the critical temperatures estimated by means of the CG scaling concept are shown with the dashed line. The agreement is again very good.

The successful use of the CG scaling idea in this paper in spite of the crude approximation for the bare superfluid density, suggests that the ratio $\gamma_{sw}(T_c)/J_0(T_c)$ is closely the same for the different models in the analysis.
3 Layered systems — three dimensions

This last section is devoted to high-$T_c$ superconductors and the anisotropic 3D $XY$ model. After a short introduction to high-$T_c$ superconductors the two-dimensional behavior in these materials is discussed. This is the main characteristics of the high-$T_c$ materials of relevance for this work. The anisotropic 3D $XY$ model is then motivated as a model for high-$T_c$ superconductors, and, finally, the arguments from Papers VII and VIII for two-dimensional behavior above $T_c$ in this model, are presented.

3.1 High-$T_c$ superconductors

The notation for the highest critical temperature in a superconductor had since 1911, when Kammerlingh Onnes discovered superconductivity at 4.2 K in mercury, grown very slowly up to 23.3 K, the critical temperature for a compound with Nb and Ge, discovered in 1973. The discovery of ‘possible superconductivity’ at about 35K by Bednorz and Müller[4] in January 1986, was therefore a large and unexpected jump, which triggered an intense burst of activity among physicists all over the world. As a result of this work, a compound with a transition temperature as high as 91 K – YBa$_2$Cu$_3$O$_7$ – was discovered about a year later[9,63]. This is quite a bit above 77 K, which is kind of a magical temperature for practical applications, since it is the temperature available through cooling by means of liquid nitrogen. Other methods for cooling are much more expensive.

A large number of superconducting compounds with fairly high transition temperatures have now been discovered. One may well say that they constitute a new class of superconductors. But in spite of the enormous effort by physicists all over the world to come to grips with the microscopic mechanism behind high-$T_c$ superconductivity, there is still no generally accepted theory for these materials.

A common feature for this new class of superconducting materials is the layered structure; they all consist of Cu-O layers stacked upon each other. From measurements on single crystals of these compounds one have, accordingly, found a large anisotropy – properties measured parallel to the planes are very different from the corresponding ones in the perpendicular direction[13,62,56].

In the following, only two different superconducting compounds will be discussed, Bi$_2$Sr$_2$CaCu$_2$O$_8$ (BSCCO) and YBa$_2$Cu$_3$O$_7$ (YBCO). The values of some important parameters for these two materials are shown in Table 1.

This work describes a phenomenological approach to high-$T_c$ superconductivity. The working hypothesis is that the superconductivity in these materials – just as in the ordinary superconductors – may be described with Ginzburg-Landau theory.
3.1.1 Two-dimensional behavior

The layered structure of the high-$T_c$ superconductors suggests that 2D fluctuations are important for their behavior, and one therefore expects that these materials, to at least some extent, should behave as the 2D superconducting films described in Sec. 2.

The method to test for two-dimensionality used in several papers[53,52,34,64] is to fit resistance data to the behavior predicted for a KT transition, Eq. (22). A good fit to this equation is taken as evidence for a KT transition. As discussed in Sec. 2.2.4 there are, however, reasons to question this conclusion. Beside these arguments, the three-dimensionality of these materials strongly suggest that the transition is 3D in character, and not of the two-dimensional KT type. This does, however, not preclude the existence of 2D fluctuations at temperatures somewhat above the phase transition.

In the case of BSCCO, which has a very weak interplane coupling, it has been shown by Minnhagen[41] that the resistive tail just above the transition is in good agreement with the 2D resistance scaling curve discussed in Sec. 2.1.4. In this case the two parameters $T_c$ and $T_{c0}$ are determined independent of the CG scaling, which means that there are no free parameters in the comparison.

3.1.2 YBCO/PBCO superlattices (VI)

It is not possible to analyze YBCO in the same way as BSCCO. The reason for this is presumably the larger interplane coupling in YBCO. The fabrication of superlattices has, however, provided a new possibility.

The YBCO/PBCO superlattices consist of alternating layers of $\text{YBa}_2\text{Ca}_3\text{O}_{7-x}$ and $\text{PrBa}_2\text{Ca}_3\text{O}_{7-x}$. The latter material is an insulator at the relevant low temperatures[30,32]. The thickness of these layers, $N_Y$ and $N_P$ unit cells, may be varied independently.

Because of the relatively strong interplane coupling in YBCO, one expects each such layer, several unit cells thick, to act as a thin superconducting film. This means that the two-dimensional density of superconducting electrons becomes

<table>
<thead>
<tr>
<th></th>
<th>$\xi_{\parallel}^G(0)$ (Å)</th>
<th>$d$ (Å)</th>
<th>$m_\perp/m_\parallel$</th>
<th>$T_c$ (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bi$_2$Sr$_2$CaCu$_2$O$_8$</td>
<td>32[46]</td>
<td>15[54]</td>
<td>3000[15]</td>
<td>$\approx$ 84</td>
</tr>
</tbody>
</table>

Table 1: The Ginzburg-Landau coherence length, the interplane distance, the effective mass anisotropy, and the critical temperature for BSCCO and YBCO.
3.1 High-$T_c$ superconductors

Figure 16: Comparison between the YBCO/PBCO resistance data and the 2D resistance scaling function. The scaling function is given by the solid curve. The circles, diamonds, triangles, and asterisks correspond to $(N_Y, N_P) = (1,16), (2,16), (3,16)$, and $(3,4)$, respectively.

larger with more unit cells of YBCO. It is also possible to change the coupling between the YBCO layers. The coupling becomes smaller if $N_P$, the number of PBCO unit cells, is increased.

Just as for ordinary high-$T_c$ materials, the superlattices have been analyzed by fitting resistance data to the behavior for the KT critical region[50]. The fit is good over about three decades, which the authors take to be evidence for a KT transition.

However, analysis of the same resistance data by means of CG scaling and the 2D resistance scaling function, Sec. 2.1.4, turns out to yield more information:

Firstly, as shown in Fig. 16, the resistance data for the superlattices with small coupling between the YBCO layers, $(N_Y, N_P) = (1,16), (2,16)$, circles and diamonds, are very well described by the 2D resistance scaling function. This agreement is strong evidence that the resistivity close to the transition is caused by 2D vortex fluctuations. We may also conclude that YBCO, as far as the vortices are concerned, are very similar to ordinary type-II superconductors.

Secondly, in the superlattices with a slightly stronger coupling, the effect of the interlayer coupling is seen as a deviation from the 2D scaling function as the temperature approaches $T_c$ from above. This effect is systematically dependent on the interlayer coupling. The region with a deviation from the 2D scaling function
increases with the interlayer coupling. This is clear evidence that the phase transition itself is three-dimensional rather than of the 2D Kosterlitz-Thouless type. The triangles and asterisks in Fig. 16 show this behavior for $(N_Y, N_P) = (3, 16), (3, 4)$, respectively.

3.2 The layered $XY$ model

The Lawrence-Doniach model[29] is often used as a model for high-$T_c$ superconductors[14,24]. This is based on three assumptions: The first is that these superconductors – just as the ordinary ones – may be described by a complex order parameter $\psi(r)$. The second assumption is that the superconducting planes are coupled by means of a Josephson coupling – quantum tunneling between two superconductors. The third assumption is that the magnetic coupling between the layers may be neglected. This assumption is, however, not without controversy. The, in some sense, opposite approach, to neglect the Josephson coupling and only include the magnetic coupling, has sometimes been used.

Through the same steps as in Sec. 2.1.5 we arrive at the anisotropic 3D $XY$ model – the layered $XY$ model. There is, however, an additional complication which is related to the different length scales in the parallel and perpendicular directions. Whereas the transverse lattice constant is given by the interplane distance, the in-plane lattice constant is related to the GL coherence length, which varies with temperature. The effect will be that the anisotropy $J_\perp/J_\parallel$ in the layered $XY$ model depends on temperature.

With the coupling constants $J_\parallel$ and $J_\perp$ for the in-plane and interplane couplings, respectively, the Hamiltonian for the anisotropic three-dimensional $XY$ model may be written

$$H_{XY}^{3D} = - \sum_{(ij)\parallel} J_\parallel \cos(\theta_i - \theta_j) - \sum_{(ij)\perp} J_\perp \cos(\theta_i - \theta_j),$$

where $(ij)\parallel$ and $(ij)\perp$ denote nearest-neighbor pairs in the same plane, and in two adjacent planes, respectively.

The two following subsections describe two different approaches to the anisotropic model. The first is to consider the similarities with the isotropic model, and the second is to consider the vortices in a single plane and examine the effect of the third dimension on the vortex interaction.

3.2.1 The isotropic model

The phase transition properties for the anisotropic 3D $XY$ model are from general considerations expected to be identical with those for the isotropic model. The
properties of this model are well known from analyses of high-temperature series\cite{17, 51}, as well as from MC calculations\cite{23,10}.

The 3D XY model has a phase transition of the second order at the temperature $T_c \approx 2.203J\cite{10,17}$. The determination of $T_c$ from MC data is made by means of finite size scaling of the helicity modulus precisely at $T_c$. This is analogous to the method used in Sec. 2.3.4 for the two-dimensional model. The phase transition is most nicely seen in the heat capacity. Figure 17 shows the heat capacity as a function of temperature from MC calculations on a $64^3$ lattice.

The anisotropic model may be seen as a discretization of a continuous field with a larger distance between the lattice points in one direction than in the other. Starting from an expression for the energy in terms of the gradient of the phase squared, one finds a relation between the anisotropy and the fraction of the distances between the lattice points in the different directions

$$\sqrt{J_\perp/J_\parallel} = a_\perp/a_\parallel,$$

where $a_\parallel$ and $a_\perp$ are the two different lattice constants. This is the basic reason why it is often the square root of the anisotropy that appears in various expressions for the anisotropic 3D XY model.
3.2.2 Analysis in terms of coupled layers (VII)

The second approach to the anisotropic 3D $XY$ model is to start from the two-dimensional model and examine how the vortex interaction is modified by the neighboring layers. This is the subject of Paper VII.

The interaction between two vortices in a plane is, however, not as easily calculated in three dimensions as in 2D. The reason is that there now is a vortex loop associated with a vortex pair, and that this loop may take a lot of different paths through the lattice. In a proper calculation of the vortex interaction, the contributions from all these different vortex loops should be included. This is, however, rather involved.

The approach has therefore instead been to calculate the energy for a vortex loop which only goes through one plane. This is a good approximation to the vortex interaction at least at low temperatures. The kind of vortex loops used is shown in Fig. VII:2.

The first estimate of the vortex loop energy was a variational calculation in the zero temperature limit \([6]\). This showed that the vortex loop interaction has a linear term with a magnitude proportional to $\sqrt{\gamma}$.

Paper VII contains a generalization of this result to finite temperatures. The method employed is basically the same as in Paper IV, which means that it is the linearly screened vortex loop interaction $V_l(r)$, which is determined. The main result here is that the magnitude of the linear term decreases with increasing temperature and approaches zero at $T_c$, Fig. VII:7.

The MC results suggest that the magnitude of the linear term is proportional to $\gamma \sqrt{m}$, where $\gamma$ is the helicity modulus in the plane and $m$ is the magnetization. Both $\gamma$ and $m$ approach zero as $T \to T_c$ from below.

Since $V_l(r)$ at and above $T_c$, approaches a constant in the limit of large $r$, the vortex loops start to dissociate at $T_c$. This shows that the phase transition may be considered as a vortex loop unbinding transition, analogous to the KT transition in two dimensions.

The vanishing of the linear term has important implications for the high-$T_c$ superconductors. In terms of the vortices, the most important difference between the $XY$ model in two and three dimensions is the linear term in the interaction below $T_c$. The vanishing of this term above $T_c$ suggests that the effect of the neighboring layers is much smaller above $T_c$, and that each layer behaves more or less independently. This suggests that the crossover from 3D to 2D behavior found closely above $T_c$ in both BSCCO and the YBCO/PBCO superlattices, is also present in the layered $XY$ model.
3.2.3 Vortex density (VIII)

Since the 3D to 2D crossover in the high-$T_c$ superconductors is observed in resistivity data, one would like to examine the layered $XY$ model for the same kind of crossover in the closely related density of free vortices $n_F$, cf. Eq. (4).

The density of free vortices was determined in Paper IV from the vortex interaction for the 2D case, but since it is quite difficult to determine the vortex interaction in the layered model (as opposed to the vortex loop interaction), $n_F$ is not readily available either. A comparison between $n_F$ in these two models is therefore not feasible.

The best one can do is to make comparisons for another Coulomb gas quantity. One such quantity that is directly available in MC calculations is the vortex density. The idea behind Paper VIII is therefore to compare the vortex density in the layered $XY$ model and the ordinary 2D $XY$ model. The results are shown in Fig. VIII:2. The solid dots are MC results for the 2D model and the open circles and squares for the layered model with $J_\perp/J_\parallel = 0.02$ and 0.1, respectively. The corresponding critical temperatures are indicated by arrows.

The figure shows clearly that the density of thermally excited vortices for $J_\perp/J_\parallel = 0.02$ and 0.1, above their respective critical temperatures is nearly equal to the vortex density for the 2D $XY$ model. The conclusion is obvious: at temperatures above $T_c$ the layers in the layered $XY$ model are effectively decoupled; each layer behaves as a single plane.

Since this is yet another example of Coulomb gas scaling, the data should properly be plotted versus the Coulomb gas temperature $T_{CG}$. The crucial step in a determination of the Coulomb gas temperature is the determination of $\gamma_0(T)$ -- the analogue of $\rho_0(T)$ in Eq. (10). In Paper VIII this quantity was determined by measurements of the helicity modulus in MC runs where the vortices were excluded. It turns out that this quantity depends slightly on the interlayer coupling, which means that the curves in Fig. VIII:2 become displaced as shown in Fig. VIII:4 when the vortex density is plotted versus $T_{CG}$. The two-dimensional behavior is now even more striking.

As discussed in Sec. 2.3.7 the bare superfluid density used in Eq. (10) is better determined through $J_0 = J \langle \cos \phi \rangle$. It is therefore interesting to check how the conclusions of Paper VIII are affected by this more correct determination of $T_{CG}$. Figure 18 shows vortex density against $T_{CG}$ determined from $J_0$, for both the 2D model and the layered model with $J_\perp/J_\parallel = 0.1$. The arrow indicates the position for the phase transition in the layered model. The general features are the same as in Fig. VIII:4, and the conclusion is, again, that the layered $XY$ model to a very good approximation exhibits two-dimensional behavior above $T_c$.

In this context it might be interesting to note that it is possible to calculate
the vortex density in the high-temperature limit analytically. Consider a plaquette with the four spins numbered 1 through 4 as shown in Fig. 19. With certain fixed values for $\theta_1$ and $\theta_3$, there is a vortex at the plaquette if $\theta_2$ and $\theta_4$ have values such that the spins rotate in opposite ways along the path 1-2-3 as compared to the path 1-4-3. Figure 19 shows the sectors for $\theta_2$ and $\theta_4$ which will give a clockwise rotation of the spins. Since the spins point in random directions independent of each other in the high-temperature limit, the probability for a clockwise rotation along the path 1-2-3 is $\Delta = (\theta_1 - \theta_3)/2\pi$. The probability for the opposite rotation along the path 1-4-2 is $1 - \Delta$, and the probability for a vortex at the plaquette becomes

$$2\int_0^1 d\Delta \Delta (1 - \Delta) = \frac{1}{3}. $$

The factor of two is due to the two different orientations, corresponding to positive or negative vorticity.
Figure 19: A positive vortex is obtained if $\theta_2$ and $\theta_4$ are within the shaded sectors.
4 Conclusion

The results from this work fall naturally in three categories:

2D Coulomb gas (I,II)

The main results for the 2D CG are:

- A new formulation of Minnhagen’s self-consistent renormalization equations for a Coulomb gas with a large-distance cutoff in the interaction.
- A determination of the width of the critical region above the Kosterlitz-Thouless transition.
- The discovery of a large ‘pseudo-critical’ region above $T_c$. In this region the characteristic length may, to a good approximation, be fitted to the same functional form as in the critical region. This is put forward as the explanation behind the often reported observation of KT critical behavior in two-dimensional systems.

2D XY model (III, IV, V)

There are several results for the 2D XY model:

- Determination of the critical temperature by means of finite-size scaling of the helicity modulus precisely at $T_c$.
- Derivation of expressions for the linearly screened potential in the XY model.
- A derivation of an expression for the bare superfluid density and thereby the Coulomb gas temperature for the XY model.
- A new expression for vorticity in terms of the current rotating around the plaquette.
- The Coulomb gas scaling concept was shown to be applicable to XY-type models.

High-$T_c$ superconductors – the layered XY model (VI, VII, VIII)

The first part of the high-$T_c$ section is the analysis of experiments on YBCO/PBCO superlattices.
• It was shown that resistance data from YBCO/PBCO superlattices may be analyzed by means of the 2D resistance scaling function, and, furthermore, that this kind of analysis gives more information than the often-used fitting to the KT critical behavior.

The aim with the second part was to examine whether the layered $XY$ model has the same kind of two-dimensional behavior above $T_c$.

• The effect of the third dimension in the layered $XY$ model is, below $T_c$, that the vortex loop interaction has a linear term. It was shown that this linear term vanishes above $T_c$. This was taken to suggest that the effect of the neighboring planes is very small above $T_c$ and that the individual planes are effectively decoupled.

• This two-dimensional behavior was then examined through an analysis of the vortex density. The vortex density for the layered and the 2D $XY$ models turned out to be nearly the same for temperatures above $T_c$.

The main conclusion in the high-$T_c$ section is therefore that the working hypothesis stated in Sec. 3.1 is correct. The dissipation in the high-$T_c$ materials (in the absence of external magnetic fields) is caused by vortices in the complex order parameter, and these vortices are well described by a standard Ginzburg-Landau theory.
References


REFERENCES


Acknowledgement

First of all I would like to thank my supervisor Professor Petter Minnhagen. Without his persistent support this thesis would never have been written. We have also had a lot of fun discussing both the research and his never-ending stream of new ideas.

I would also like to express my thanks to:

- Mats Nylén for many fruitful discussions about physics in general, and the research, in particular.
- The computer gurus, 'chief guru' Mats Nylén and 'assistant guru', Olof Westman. The access to a handy and efficient computer system is indispensable for the kind of research presented in this thesis.
- Mats Wallin and Hans Weber, for friendship and for providing contact with a wider world of physics.
- Jens Houlrik and Henrik Jeldtoft Jensen for giving me numerous opportunities to practise listening to Danish.
- All members of the theory groups in Umeå for providing a good working atmosphere and Journal Club meetings with an exquisite mixture of valuable and worthless knowledge.
- My family for providing a rich leisure time and plenty of opportunities to forget about physics.