Superfluid Phase Transitions in Disordered Systems

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Abstract

This thesis presents results from large scale Monte Carlo simulations of systems subject to a superfluid phase transition in the presence of disorder. The simulations are performed by state-of-the-art, collective Monte Carlo algorithms treating phase degrees of freedom in effective models with amplitude fluctuations integrated out.

In Paper I a model system for the possible solid to supersolid transition in $^4\text{He}$ is presented. The Wolff cluster algorithm is used to study how the presence of linearly correlated random defects is able to alter the universality class of the 3-dimensional XY-model. In the pure case the superfluid density and heat capacity have singular onsets, which are not seen in the supersolid experiments where instead a smooth onset is obtained. Using finite size scaling of Monte Carlo data, we find a similar smooth onset in our simulations, governed by exponents $\nu = 1$ for the superfluid density and $\alpha = -1$ for the heat capacity. These results are in qualitative agreement with experiments for the observed transition in solid $^4\text{He}$.

In Paper II a systematic investigation of the scaling result $z = d$ for the dynamic critical exponent at the Bose glass to superfluid quantum phase transition is performed. The result $z = d$ has been believed to be exact for about 20 years, but although it has been questioned lately no accurate estimate of $z$ has been available. An effective link current model of quantum bosons at $T = 0$ with disorder in $2D$ is simulated using highly effective worm Monte Carlo simulations. The data analysis is based on a finite size scaling approach to determine the quantum correlation time from simulation data for boson world lines without any a priori assumption on the critical parameters. The resulting critical exponents are $z = 1.8 \pm 0.05$, $\nu = 1.15 \pm 0.03$, and $\eta = -0.3 \pm 0.1$. This suggests that $z = d$ is not satisfied.
Preface

This thesis summarizes my academic work so far. The projects have been performed at the KTH Department of Theoretical Physics from fall 2008 until fall 2011. The thesis is divided into an introductory background part and a second part featuring the scientific articles that I contributed to.

Scientific Articles

Paper I
Superfluid Transition in a Correlated Linear Defect Network, Hannes Meier, Mats Wallin and Stephen Teitel, Manuscript [50]

Paper II

Comments on My Contribution to the Papers

Paper I
I wrote all the simulation code, performed the scaling analysis and wrote the necessary software and scripts for it. I contributed to writing the paper.

Paper II
I wrote all the simulation code, performed the scaling analysis and wrote the necessary software and scripts. I produced all the figures and contributed to writing the paper.
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Part I

Background
Introduction

Phase transitions are omnipresent fascinating physical phenomena with many applications in engineering, ranging from steam engines to superconducting magnetic coils. They describe collective changes in the macroscopic properties of many particle systems of atoms or molecules under variation of some control parameter, like temperature or pressure. A microscopic description of these systems is not possible as it requires solving about $10^{23}$ equations. In addition, such a detailed answer would be completely useless. Therefore, in statistical mechanics one is only interested in macroscopic properties, such as the magnetization, the pressure, and the density. Two important classes are continuous and discontinuous phase transitions, depending on the involvement of latent heat. In this thesis I only consider continuous, second-order phase transitions. For these, in the general framework of the renormalization group, it turns out that many presumably unrelated systems show the same, universal, critical behavior. Thermodynamic quantities then show power law behavior with the same critical exponents. This is a great help for us theoretical physicists studying critical properties, as we can ask questions on complex systems, and then only need to identify the easiest model expected to lie in the same universality class.

During the 20th century, even before the birth of quantum mechanics, many novel phases of matter have been discovered. Most relevant for this thesis are, the superfluidity in $^4$He, and the superconductivity in metals. Remarkably, even if their ordered phases can only be derived using quantum mechanics, the thermodynamic behavior at the transition itself is insensitive to quantum mechanical effects, and thus entirely classical.

This was believed to be true for all phase transitions, until the possibility of quantum phase transitions (QPTs) was discovered. There, the variation of some non-thermal parameter, such as the chemical potential $\mu$, magnetic field $H$ or the pressure $P$ leads to an abrupt change in the ground state of the system, driven by quantum fluctuations. For example, bosonic systems, which for one choice of the chemical potential $\mu$ are entirely insulating, with each boson occupying a certain position, can suddenly become superfluid. Then, all bosons delocalize and a large fraction participates in macroscopic exchange cycles. QPTs occur only at the experimentally strictly speaking inaccessible temperature of 0 K. However, as outlined later, they will have profound influence on the low temperature phase diagram if the
relevant parameter $K$ taking the system through the zero temperature transition is adjusted to its critical value $K_c (T = 0)$.

Even today, possible discoveries of novel phases of matter are published. In 2004 M.H.W. Chan and E. Kim reported evidence for a supersolid transition of $^4$He [25]. Their experiments suggested that, in a crystal of entirely solid $^4$He, a fraction of the atoms could decouple from the crystal and move without resistance through the lattice background. This is totally at odds with the naive picture of a solid crystal. In addition, heat capacity measurements were performed, which after subtraction of the phonon $T^3$ contribution, suggested the presence of a smooth, nearly parabolic maximum $[84]$. This would be a strong indication for the interpretation that the period drop not only is a dynamical effect. In the years after these discoveries it has become clear that impurities and disorder effects, such as dislocation lines and $^3$He foreign atoms, play a key role in the experiments $[22, 65, 23]$. Up to this day, there exists no theory explaining all the results obtained by different experimental groups. This leaves the mechanism at play as an open issue. In this thesis, in the spirit of universality, I present results achieved by exposing the simplest possible model to describe a superfluid phase transition, the $3D$ XY-model, to a network of isotropically linear correlated defects. This reproduces some qualitative effects of the experimental findings mentioned above.

Effects of disorder and impurities in crystals have many important implications on our everyday life. Plastic deformation of solids is solely due to the generation and mobility of dislocations. Smelting and forging hardened steel need dislocation lines that become immobile by pinning to impurities. In addition, the presence or absence of disorder can lead to a new critical behavior or even cause a quantum phase transition. A complicating issue is that, even the simplest available model, often lacks an exact solution. Therefore, exact analytical calculations of critical exponents are scarce. Introducing disorder further complicates this problem. To study such systems effective, large scale Monte Carlo simulation techniques are required. The dynamics of one such transition will be studied in the second part of this thesis. There, another working horse of theoretical physics is used to describe a superfluid to insulator transition at zero temperature, namely the boson Hubbard model. At certain choices of the chemical potential $\mu$, the pure system exhibits a phase transition from an insulating, incompressible Mott phase to a superfluid phase. Introducing disorder to the system, a new, compressible Bose glass phase shows a transition to a superfluid phase on increasing the hopping strength. This critical behavior is relevant for experiments on ultrathin, granular, superconducting films, Josephson junction arrays, superfluid helium films, and cold bosons in optical lattices with disorder $[28, 80]$. The original theory proposed the remarkable relation $z = d$, where $d$ is the number of spatial dimensions $[28]$, for the dynamic critical exponent $z$. This scaling result was long believed to be exact, but has been questioned recently both analytically and numerically $[78, 57]$. For the 2-dimensional case I will show, using an extensive finite size scaling analysis, that $z = 1.8 \pm 0.05$. This is close to, but clearly distinct from the original suggestion.
Chapter 1

Renormalization Group Theory and Scaling at Continuous Phase Transitions

This chapter briefly summarizes the theoretical background for the scaling analysis performed in paper I and II.

1.1 Continuous Phase Transitions

At the critical point of a second order phase transition the correlation length $\xi$ and the correlation time $\tau_c$ diverge according to the two power laws

$$\xi \propto |t|^{-\nu}$$

$$\tau_c \propto \xi^z \propto |t|^{-\nu z}$$

where $t = (T - T_c)/T_c$ and $T_c$ is the critical temperature. The exponents $\nu$ and $z$ are called correlation length exponent and dynamic exponent. Hence the microscopic degrees of freedom exhibit highly correlated, large scale fluctuations in space and time. The system looks the same under arbitrarily rescaling lengths and thus has to be self similar. The characteristic behavior becomes almost independent of its microscopic details and therefore universal, in the sense that seemingly unrelated different physical systems exhibit the same critical behavior. The respective Hamiltonians only need to share the same symmetries and need to be considered in spaces of equal dimensions [32]. Differences in the range of interactions also matter. In this spirit a renormalization group (RG) transformation amounts to a coarse graining procedure, that eliminates the short wavelength degrees of freedom by subsequently integrating them out on increasing length scales.
CHAPTER 1. RENORMALIZATION GROUP THEORY AND SCALING AT CONTINUOUS PHASE TRANSITIONS

Renormalization and Scaling Theory

To briefly elucidate the formalism, consider a system with Hamiltonian

\[ H = -\beta H_\Omega = \sum_n K_n \Theta_n \{ S \} \]  

(1.3)

where \( \{ K_n \} \) are coupling constants, \( \beta \) is the inverse temperature and \( \{ S \} \) the degrees of freedom. In classical systems such as the Ising or Heisenberg model the \( S \) usually are (vector valued) lattice variables defined on different sites. In general these systems can, via a Hubbard-Stratonovich transformation, be mapped on a functional field integral representation [32, 1]. This also is the natural representation of pure quantum systems. There, the corresponding quantity is the Landau Ginzburg Wilson (LGW) action functional \( S \), which essentially is derived by calculating the density matrix in a coherent state base. \( S \) usually takes the form

\[ S[\psi] = \sum_i g_i O_i[\psi] \]  

(1.4)

where \( \psi(x) \) are complex fields and the \( g_i \) are coupling constants. The operators \( O_i[\psi] \) commonly can be written as

\[ O_i[\psi] = \int d^d x (\partial^n \psi)^n \psi^m \]  

(1.5)

The RG procedure then usually involves the following steps. First one identifies and separates the fast fluctuating, high frequency microscopic fluctuations from the long wavelength, large scale fluctuations. In a block spin scheme, as considered by Kadanoff and Wilson [82], this corresponds to the grouping of single microscopic spins in a cubic volume of size \( \Delta L \) together to large blocks with a correspondingly averaged net spin and size \( \Delta L' = l \Delta L \) without altering the respective partition function

\[ Z = Tr e^{-H} \text{ or } Z = \int D\psi e^{-S[\psi]} \]  

(1.6)

Thus the correlation length \( \xi' \) measured in length units of the new system, which due to the choice of the transformation is identical to the first one, then is rescaled to

\[ \xi' = \xi / l. \]  

(1.7)

Self similarity of the system implies that the rescaled couplings are the same as the old ones. Thus

\[ R_l[\{ g_n \}] = [\{ g_n \}] \]  

(1.8)

meaning, that critical couplings need to be fixed-points of the mapping \( R_l \), which will be denoted by \( \{ g_n^* \} \). At these fixed-points the correlation length thus transforms as

\[ \xi (R_l[\{ g_n^* \}]) = \xi (\{ g_n^* \}) \], which using Eq. (1.7) only can be true if \( \xi = 0 \) or \( \xi = \infty \).
These two cases are called *trivial fixed-points* and *critical fixed-points*. Couplings that under $R_l$ "flow" towards a fixed point define its basin of attraction. If the fixed point is critical, its basin of attraction is called the critical manifold. The codimension of the critical point is defined by the difference between the total number of couplings minus the dimension of the critical manifold. Close to a fixed point for couplings \( g_n = g_n^* + \delta g_n \) the transformation can be approximated by

\[
g'_n = R' \left[ \{ g_n^* + \delta g_n \} \right] \approx g_n^* + \frac{\partial g'_n}{\partial g_j} \delta g_j = g_n^* + M_{nj}^l \delta g_j
\]

where $M_{nj}^l$ is the linearised RG transformation. In a diagonal representation $\{ \tilde{g} \}$ this relation becomes $\delta \tilde{g}_n = \lambda_n \delta \tilde{g}_n$. The RG transformation can be quite complex such that the Matrix $M_{nj}^l$ does not need to be symmetric. In general it is complex and left and right eigenvectors have to be distinguished [32]. If, however, its right eigenvalues are real, one can exploit that a repeated application of the transformation with scales $l, l'$ has to be equal to the application of the transformation only once rescaling lengths by $l \cdot l'$

\[
M_{n'u}^l M_{uj}^l = M_{nj}^{l'}
\]

\[
\Rightarrow \lambda_{n'u}^l \lambda_n^l = \lambda_{n'}^{l'} \lambda_n^l
\]

This means that the eigenvalues transform according to a power law $\lambda_{n'}^l = l^{y_n} \lambda_n^l$ [32], which is the basis for all the data analysis performed in this thesis. Depending on the value of $y_n$, the scaling fields $\tilde{g}_n$ are called:

1. *relevant*, if $y_n > 0$, as then the weight of the associated scaling field increases under renormalization.
2. *irrelevant*, if $y_n < 0$, as the weight of the associated scaling field decreases under renormalization.
3. *marginal*, if $y_n = 0$.

The number of relevant eigenvalues gives an indication for how many independent parameters need to be adjusted to hit the critical point in experiment or simulation [32]. The RG transformation leaves the partition function invariant. The free energy density $f = F/V k_B T = -L^{-d} \ln Z$ scales as

\[
f = b^{-d} f_s (\{ g' \}) + f_n (\{ g \})
\]

where $f_n (\{ g \})$ is the analytic part of the free energy density and $b$ an arbitrary rescaling factor [17]. This leads to the form

\[
f_s (g_1, g_2, \ldots) = b^{-d} f_s (b^{y_1} g_1, b^{y_2} g_2, \ldots)
\]
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heat capacity: \( c \sim |t|^{-\alpha} \implies L^{-\alpha/\nu}c_L = \tilde{c}(L^{1/\nu}t) \)

magnetization: \( m(t) \sim (-t)^\beta \implies L^{\beta/\nu}m_L = \tilde{m}(L^{1/\nu}t) \)

order parameter susceptibility: \( \chi(t) = \frac{\partial m}{\partial h} \bigg|_{h=0} \sim |t|^{-\gamma} \implies L^{-\gamma/\nu}\chi_L = \tilde{\chi}(L^{1/\nu}t) \)

order parameter at the critical isotherm: \( m(h)|_{t=0} \sim |h|^{1/\delta} \)

two-point correlation function: \( C(r) \sim \begin{cases} \frac{1}{r^{d-2+\eta}}, & \text{if } r \ll \xi \\ e^{-r/\xi}, & \text{if } r \gg \xi \end{cases} \)

Table 1.1: Asymptotic scaling forms for various quantities at the critical point for a magnetic system together with the corresponding finite size calling form [1].

Including only the reduced temperature \( t \), the reduced external field \( h \) conjugate to the order parameter and the finite system size \( L \) as relevant scaling fields yields

\[
 f_s(t, h, L) = \frac{1}{L^d} \tilde{f}_s \left( L^{1/\nu}t, L^{y_h}h, 1 \right) = \frac{1}{L^d} \tilde{f}_s \left( L^{y_h}h, 1 \right) \quad (1.14)
\]

where Eq. (1.1) has been used. From this relation the finite size scaling forms of all other quantities follow. The most prominent one out of these probably is the heat capacity relation

\[
 c_s \sim \frac{\partial^2 f_s}{\partial t^2} \sim L^2/\nu - d \propto |t|^{-\alpha} \quad (1.15)
\]

which implies the Josephson scaling relation

\[
 d\nu = 2 - \alpha \quad (1.16)
\]

central to the supersolid problem in [50]. Table 1.1 shows a collection of the critical behavior of other thermodynamic quantities.

1.2 Corrections to Scaling

Including irrelevant scaling fields \( v_i \) the singular part of the free energy of a finite system reads

\[
 f_s(t, h, L) = L^{-d} \tilde{f} \left( u_t L^{1/\nu}, u_h L^{y_h}, \{v_i L^{y_i}\} \right) \\
 \approx L^{-d} f \left( u_t L^{1/\nu}, u_h L^{y_h} \right) + v_\omega L^{-d-\omega} f_{\omega} \left( u_t L^{1/\nu}, u_h L^{y_h} \right) + \cdots \quad (1.17)
\]

The non-analytic correction-to-scaling exponent \( \omega \) corresponds to the RG dimension \( y_\omega \) of the leading irrelevant scaling field \( v_\omega = v_1, \omega = -y_\omega \). The scaling fields
are analytic functions of the system parameters. Respecting the symmetry of \( f_s \) under \( h \to -h \) they can be approximated by 
\[
\bar{u}_h(t) + O(h^3)
\]
where \( \bar{u}_h \) is a linear approximation close to the critical point \( h = t = 0 \) [35]. The fields \( u_h \) and \( u_t \) are independent of \( L \).

With these definitions corrections to all other quantities can be derived. Usually, to leading order, the overall effect of the irrelevant scaling field is that an operator \( O(T,H,L) = \tilde{O}(L^{1/\nu}t, L^\eta h) \) acquires a finite size dependent scaling corrections term
\[
O(T_c, H_c, L) = O_\infty \left(1 + c_1 L^{-\omega} + \cdots\right)
\]
Thus by a suitable nonlinear minimization procedure it is possible to determine the asymptotic value \( O_\infty \) of the operator for an infinite system and the corresponding corrections to scaling exponent \( \omega \). To perform this reliably, high quality data sets are needed.

1.3 Path Integral Formulation of Statistical Mechanics

Suppose that the Hamiltonian of a \( d \)-dimensional system is given by the expression
\[
\mathcal{H} = \mathcal{T} + \mathcal{V}
\]
(1.19)
where \( \mathcal{T} \) and \( \mathcal{V} \) are the kinetic and potential energy operators. Cutting \( \beta \) in \( M \) equidistant slices \( \Delta \tau = \beta/M \) the partition function \( Z = \text{Tr} e^{-\beta \mathcal{H}} \) can be written as the trace over a product of density matrices
\[
e^{-\beta \mathcal{H}} = \left[e^{-\Delta \tau \mathcal{H}}\right]^M.
\]
Inserting resolutions of unity and choosing an arbitrary complete set of states \( \{|\alpha\rangle\} \) the partition function becomes
\[
Z = \sum_{\alpha_0} \sum_{\alpha_1} \cdots \sum_{\alpha_{M-1}} \langle \alpha_0 | e^{-\Delta \tau \mathcal{H}} | \alpha_1 \rangle \langle \alpha_1 | e^{-\Delta \tau \mathcal{H}} | \alpha_2 \rangle 
\times \cdots \times \langle \alpha_{M-1} | e^{-\Delta \tau \mathcal{H}} | \alpha_0 \rangle
\]
(1.20)
and thus has the form of a sum over weighted trajectories in “state-space”. All these paths start and end at \( |\alpha_0\rangle \) and develop according to a transfer matrix. This exactly is the Feynman path integral, as it usually is introduced in elementary quantum mechanics if the \( |\alpha\rangle \)'s are replaced by position eigenstates [27, 66]. The transfer matrix elements couple two different time slices, which renders the system essentially \( d + 1 \) dimensional [26, 18]. For finite temperature \( T \) the extension in \( \tau \)-direction is limited. At zero temperature \( T = 0 \), the system truly is \( (d + 1) \)-dimensional. The sum then basically runs over the set of possible eigenvalues of the base \( \{|\alpha\rangle\} \), which makes \( Z \) equivalent to a partition function of a classical system in a by one higher dimensional space [69]. For high temperatures the corresponding time interval \( \beta \) is very small, if compared to the natural frequency scales of the system. Thus the system looks static in all time slices \( 0 \ldots M - 1 \) [69]. Thus the dynamics drops out and the path integral turns into an ordinary Boltzmann weight.
1.4 Quantum Phase Transitions

Quantum phase transitions (QPT) are changes between competing ground states of a system, as a function of some non-thermal control parameter $K$. From the above discussion zero temperature phase transitions in $d$-dimensional quantum mechanical systems and finite temperature phase transitions in their $(d + 1)$-dimensional counterparts are equivalent. This implies directly, that at a quantum critical point (QCP) the transition also will exhibit diverging length and time scales [69] as given in Eqs. (1.1) and (1.2). The corresponding divergencies of the thermodynamic quantities are discussed in Sec. 1.1. Equation (1.2) is directly related to a corresponding frequency and therefore energy scale [76]

$$\hbar \omega_c \propto |t|^\nu z$$  (1.23)
which can be applied as a measure to determine whether quantum or thermal fluctuations drive the transition. In the limit of a diverging \( \tau_c \) the typical frequency \( \omega_c \) vanishes. If \( \hbar \omega_c \ll k_B T \) the regime is purely classical which renders quantum fluctuations completely negligible for temperatures

\[
|t| < T_c^{1/z}
\]  

for any finite \( T_c \) [76]. In short this means: At finite temperatures the fluctuations of any physical system asymptotically close to a critical point are entirely classical [76, 69]. Only at zero temperature can a phase transition be entirely driven by quantum fluctuations. If it is continuous, the correlation length and time then diverge like

\[
\xi \propto |k|^{-\nu}
\]

\[
\tau_c \propto \xi^z \propto |k|^{-\nu z}
\]

where the non-thermal parameter \( k = (K - K_c) / K_c \) tunes the system through the quantum phase transition. Figures 1.1a and 1.1b show two important different cases. In Fig. 1.1a order at finite \( T \) is forbidden but at \( T = 0 \) order persists for values of \( K < K_c \). The situation looks completely different in Fig.1.1b where the order parameter is allowed to take nonzero values even for finite \( T \) at \( K < K_c \). In both phase-diagrams the quantum critical region is determined by

\[
k_B T > \hbar \omega_c \propto |K - K_c|^{\nu z}
\]

meaning that in this parameter regime \( K \) is close to its critical value, but the system is driven away from criticality by thermal fluctuations. The quantum critical behavior is cutoff for temperatures above some characteristic temperature, reflecting microscopic energy scales of the system. In the quantum critical region thermal excitations of the quantum critical ground state are of major importance [76]. The behavior in this region is normally non-universal except in the direct vicinity of the quantum critical point itself.

### 1.5 Scaling at a QPT

If the quantum dynamic exponent \( z \) is not unity, the correlation volume grows infinitely anisotropically on approaching the critical point. This often is observed in systems where isotropy is broken by introducing a symmetry breaking field or correlated disorder along a specified axis [73, 77]. The free energy density then fulfills the homogeneity law

\[
f(k, h, T) = b^{-(d+z)} f \left( kb^{1/z}, hb^{w}, Tb^2 \right)
\]

at finite temperature where \( k \) is the rescaled non-thermal coupling parameter mentioned above [76]. This is the same relation as Eq. (1.13) but with \( d \) replaced by

\[
D = d + z
\]
dimensions. An arbitrary finite temperature maps inversely onto the length $L_\tau$ of the imaginary time axis. Close to quantum criticality, crossover phenomena can occur which are intimately related to the correlation time $\tau_c$ and $L_\tau = 1/T$. In contrast to classical phase transitions where static and dynamic phenomena decouple, non-commutativity of the kinetic and the potential contribution to the Hamiltonian always couples the two in the quantum case [76]. When $t^{\nu z}$ exceeds $k_B T$ the $d$-dimensionality of the system becomes obvious again and leads to crossover scaling [76]. If both the temperature $T$ and the coupling parameter $K$ are simultaneously manipulated to reach the quantum critical point $\xi$ and $\tau_c$, diverge simultaneously and the scaling relations of the system become truly as those of a $d + z$ dimensional one. If the critical point satisfies hyperscaling the existence of $\xi$, as a single lengthscale and $\xi_z$ as a single timescale, apart from microscopic cutoff length scales important for anomalous scaling dimensions [32], implies that any static or dynamic observable scales as [76]

$$O(t, |k|, \omega, T) = \xi^{d/2} \tilde{O}_1 (|k|, \xi, \omega \xi^z, T \xi^z) = T^{-d\omega/z} \tilde{O}_2 (|k| T^{-1/z}, \omega T, T \xi^z)$$ (1.30)

At the quantum critical point $\xi = \infty$ so that the only length scale is set by the measurement wave vector $|k|$ and the only energy is $\omega$. The observable then scales as

$$O(t = 0, |k|, \omega, T = 0) = |k|^{-d\omega} \tilde{O}_3 \left( \frac{k \omega}{T} \right)$$ (1.31)

In case that $T$ is finite

$$O(t = 0, |k|, \omega, T) = T^{-d\omega/z} \tilde{O}_4 \left( \frac{\omega}{T} \right)$$ (1.32)

These relations are valid below the upper critical dimension $d_\up$, above which the critical behavior is given by the mean field solution. Finite size systems considered in simulations are usually hyper-cuboids of volume $L^d L_\tau$. Any equilibrium observable $O(K, L, L_\tau)$ with scaling dimension zero then will obey the scaling relation

$$O(K, L, L_\tau) = \tilde{O} \left( k L^{1/\nu}, \alpha_\tau \right)$$ (1.33)

where $\alpha_\tau = L_\tau / L^z$ is the aspect ratio of the system.

1.6 Effects of Disorder - Harris Criterion

In reality, phase transitions do occur in materials that are not free of impurities. Harris [34] gave a heuristic criterion to answer the question of whether the critical behavior of the impure system does differ from that of the ideal one. Depending on the disorder strength $p$ the critical temperature is potentially altered $T_c = T_c (p)$. The power law behavior of the correlation length then becomes

$$\xi \sim |T - T_c (p)|^{-\nu(p)}$$ (1.34)
where $\nu$ should depend continuously on the strength $p$ and approach its pure value for $p \to 0$. The net effect of the disorder is the occurrence of spatial variations in the transition temperature. Writing the local deviation as

$$\delta T_c(r) = T_c(r) - T_c(p)$$ (1.36)

the two-point correlation function is given by

$$W(r - r') \equiv \langle \delta T_c(r) \delta T_c(r') \rangle$$ (1.37)

Its exact form is needed in order to determine if the universality class of the pure system is altered through the disorder. Averaging the fluctuations in $T_c(p)$ over a correlation volume with linear dimension $\xi$ gives

$$\Delta T_c(p) = \left[ \int \frac{d^d r}{\xi^d} \int \frac{d^d r'}{\xi^d} W(r - r') \right]^{1/2}$$ (1.38)

For the transition to be well-defined these fluctuations need to be small compared to the distance to criticality $|T - T_c(p)|$ as $T \to T_c(p)$. Depending on the kind of disorder chosen the value of $\nu$ determines if the pure fixed point will survive. Here two examples shall be given.

1. **uncorrelated random disorder:** Using $W(r - r') \propto \delta(r - r')$ in Eq. (1.38) gives $\Delta T_c(p) \sim \xi^{-d/2}$. The general relation Eq. (1.35) implies the stability criterion

$$|T - T_c(p)|^{\nu d/2} \ll |T - T_c(p)|$$ (1.39)

as $|T - T_c(p)| \to 0$ yielding

$$\nu > 2/d$$ (1.40)

Point-disorder consequently is irrelevant to the critical fixed point for models obeying Eq. (1.40).

2. **rodlike disorder along a symmetry axis:** In this case $W(r - r') \propto \delta^{d-1}(r - r')$ forces only $d - 1$ components of the position vectors $r, r'$ to coincide for a nonzero contribution. Thus Eq. (1.38) gives $\Delta T_c(p) \sim \xi^{-(d-1)/2}$ yielding

$$\nu > 2/(d - 1)$$ (1.41)

Such relations set bounds on the possible value of $\nu$ at the phase transition in the disordered system. These arguments are frequently used in the research projects considered in this thesis and central to the Chayes inequality in [50].
Chapter 2

Superfluidity

This chapter provides concise theoretical and experimental background information on Bose-Einstein condensation (BEC) in interacting systems. Superfluid phenomena on the basis of liquid $^4$He are discussed. The characteristic observables related to superflow, which are important for numerical simulations are introduced. A brief overview on the recent experiments on solid helium, coining the name supersolid, is given.

2.1 Experimental Observations of Liquid Helium

At very low temperatures a many particle system of $^4$He atoms forms a quantum liquid [44]. In this regime the phase of the system is not only governed by the laws of quantum mechanics itself but also by the underlying elementary particle statistics of its constituents. This becomes important when the thermal wavelength

$$\Lambda = \frac{\hbar^2}{\sqrt{2\pi m k_B T}}$$ (2.1)

is comparable to the inter-particle separation [63]. In their ground state $(1s)^2$ or $^1S_0$ the $^4$He atoms behave as a system of interacting bosons without any internal degrees of freedom [46]. As a first approximation the interaction can be modeled by a Lennard-Jones potential

$$V(r) = 4\epsilon \left[ \left( \frac{}\sigma \right)^{12} - \left( \frac{\sigma}{r} \right)^{6} \right]$$ (2.2)

with a minimum of $\sim 11$ K at a nuclear separation of $\sim 2.3$ Å [46] but a more exact potential has been given by Aziz and is frequently used in first principle simulations [9, 18, 15].

As the second lightest element, and due to the weak attraction, helium does not solidify under its own vapor pressure. The solid phase is only stable above
26 atm (= 26.3458 hPa) [46, 68]. The particle density in liquid $^4$He varies from $\sim 0.02\text{Å}^{-3}$ at saturation vapor pressure to $\sim 0.023\text{Å}^{-3}$ at melting pressure. This implies that the typical interatomic separation is of the same order as the position of the potential minimum [46]. In most experiments on bulk samples the $^4$He is kept in a container but also free droplets containing of the order of $10^7$ particles can be produced [46]. Such a container mainly imposes yet another potential $U(r)$ on the liquid. It is vanishing everywhere inside the container except for positions close to the container walls. There van der Waals effects first attract the atoms until the wall itself acts strongly repulsive. The attractive part leads to an increasing density close to the wall. It is assumed that the first layers of $^4$He in such a container are solid like [46]. At saturated vapor pressure if there is enough free surface a liquid film will cover these layers and literally creep up the walls [46]. In contrast to all other atomic bosons that crystallize at temperatures far above a possible superfluid transition, $^4$He becomes superfluid at $T_\lambda = 2.17\text{K}$ [68]. The normal fluid and superfluid phases are referred to as He-I for the fluid phase with finite viscosity and He-II for the phase with vanishing viscosity respectively. The non-viscous flow properties of He-II below the lambda point where first discovered in 1937 by Pyotr Kapitsa in Moscow and independently around the same time by John F. Allen and Don Misener in Cambridge [40, 6]. Later Hess and Fairbank directly measured a decrease in the moment of inertia for helium in a rotating cylinder occurring at slow rim velocities if cooled through $T_\lambda$ [36]. These so called

**Figure 2.1:** The low temperature phase diagram of $^4$He including the modifications by Chan et al.[20]. The super solid line is however highly debated.
non classical rotation inertia (NCRI) maybe are the most direct signals of superflow and can be understood in a model of two intertwining fluids. These are often called the normal fluid following the boundary motion due to its viscosity and the superfluid whose constituents freely move through the normal background. Figure 2.1 illustrates the phase diagram of $^4$He. The correlation length critical exponent has been determined in high-precision measurements in zero gravity [48] with result $\nu = 0.6709 \pm 0.0001$. In the following two sections mostly following reference [46] the most important background information on the phenomenon of superfluidity will be given and some of its remarkable effects will be presented.

2.2 Bose-Einstein Condensation

Non-Interacting Bosons

Superfluidity is strongly related to the phenomenon of BEC. For pure, non-interacting, spinless bosons the average number of particles in state $i$ is given by

$$\langle n_i(T) \rangle = \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1}$$

(2.3)

where the chemical potential $\mu(T,N) < 0$ is implicitly defined by [46]

$$\sum_i \langle n_i(\mu,T) \rangle = N$$

(2.4)

This system will undergo a phase transition at

$$T_C \approx \left( \frac{2\pi\hbar^2}{mk_B} \right) \left( \frac{\langle n \rangle}{2.612} \right)^{\frac{2}{3}}$$

(2.5)

where $\langle n \rangle$ denotes the average particle density [63]. Below the critical temperature the single particle ground state becomes macroscopically occupied meaning that $\langle n_0 \rangle = O(N)$ and the chemical potential $\mu$ vanishes.

System of Interacting Bosons

The spin statistics theorem requires the total wave function describing a system of $N$ bosons to be totally symmetric under interchange of any two particles [68]. Any possible state can thus be written as a superposition of states

$$\Psi_N(t) = \Psi^s(r_1,\ldots,r_N,t)$$

(2.6)

where the index superscript $s$ denotes that the state is properly symmetrized [46]. To determine if BEC can occur in the interacting system one needs to investigate
the density matrix

\[
\rho_1 (r, r', t) = N \sum_s p_s \int dr_2 \ldots r_N \Psi^*_s (r, r_2 \ldots r_N, t) \Psi_s (r', r_2 \ldots r_N, t) \\
\equiv \langle \hat{\psi}^\dagger (rt) \hat{\psi} (r't) \rangle
\]

(2.7)

where \( \hat{\psi}^\dagger (rt), \hat{\psi} (r't) \) are Bose field operators. Due to its hermiticity it can be brought into diagonal form

\[
\rho_1 (r, r', t) = \sum_i n_i (t) \chi^*_{i} (r, t) \chi_i (r', t)
\]

(2.8)

where the functions \( \chi_k (r, r', t) \) form a complete orthonormal set. Penrose and Onsager [53] gave a very useful classification of whether or not BEC occurs in the interacting system [46]

1. If all eigenvalues \( n_i (t) \) of \( \rho_1 \) are of order unity, the system is said to be normal at time \( t \).

2. If there exists exactly one eigenvalue of order \( N \) and all the other eigenvalues are of order unity the system exhibits simple BEC.

3. If there are several eigenvalues of order \( N \) and the remaining ones are of order unity then the system is said to exhibit fragmented BEC.

Another possible definition is given by considering the off-diagonal elements of the two-point correlator \( \rho_1 (r, r', t) \). If these remain finite for \( r, r' \) arbitrarily far apart [46] the system is said to possess off-diagonal long range order (ODLRO), a concept first mathematically postulated by C.N. Yang [85].

The Order Parameter in a Many Body System of Spinless Interacting Bosons

For a system possessing simple BEC the condensate wave function

\[
\Psi (r, t) \equiv \sqrt{N_0 (t)} \chi_0 (r, t)
\]

(2.9)

encodes both the magnitude of BEC that has occurred and the corresponding single particle state involved. Using the normalization of Eq. (2.8) the order parameter is normalized to the number of condensed particles

\[
\int |\Psi (r, t)|^2 dr = N_0 (t)
\]

(2.10)

or equivalently the single \( \mathcal{O} (N) \) eigenvalue of \( \rho_1 \). The condensate wave function is a complex scalar. Writing the order parameter as

\[
\Psi (r, t) = |\Psi (r, t)| e^{i \Theta (r, t)}
\]

(2.11)
immediately provides the density of the condensate $\rho_c (r, t)$ together with its current $j_c (r, t)$ [46] through

$$\rho_c (r, t) = |\Psi (r, t)|^2 \quad (2.12)$$

$$j_c (r, t) = \frac{\hbar}{2mi} \{ \Psi^* (r, t) \nabla \Psi (r, t) - \nabla \Psi^* (r, t) \Psi (r, t) \} = |\Psi (r, t)|^2 \cdot \frac{\hbar}{m} \nabla \Theta (r, t) \quad (2.13)$$

Due to its dimension the ratio $j_c (r, t)/\rho_c (r, t)$ defines the condensate velocity or in the language of $^4$He systems the superfluid velocity

$$v_s (r, t) = \frac{\hbar}{m} \nabla \Theta (r, t) \quad (2.14)$$

Thus in any region where the eigenfunction $\chi_0 (r, t)$ is non-vanishing meaning that $v_s (r, t)$ is uniquely defined the irrotational condition

$$\nabla \times v_s (r, t) \equiv 0 \quad (2.15)$$

has to hold. The phase $\Theta (r, t)$ is however only defined up to integer multiples of $2\pi$. This leads to the Onsager-Feynman quantization condition [46]

$$\oint v_s (r, t) \cdot dl = n \cdot \frac{\hbar}{m}, \quad n = 0, \pm 1, \pm 2, \ldots \quad (2.16)$$

2.3 The Two Fluid Model

Static Phenomena

The two fluid model defines in addition to $v_s (r)$ a second additional velocity $v_n (r)$ called the normal velocity or the velocity of boundary conditions. The choice of names will be evident soon. The total density and current-density of the liquid then are given by

$$j (r) = \rho_s (r) v_s (r) + \rho_n (r) v_n (r) \quad (2.17)$$

$$\rho (r) = \rho_s (r) + \rho_n (r) \quad (2.18)$$

Denoting the energy of the state with $v_s (r) = v_n (r) \equiv 0$ by $\mathcal{E}_0$

$$\mathcal{E} (v_s (r), v_n (r)) - \mathcal{E}_0 = \frac{1}{2} \rho_s (r) v_s^2 (r) + \frac{1}{2} \rho_n (r) v_n^2 (r) \quad (2.19)$$

yields the excess energy due to the presence of superfluid and normal flow [46]. It is however important to realize that the superfluid and normal components cannot be identified with the condensate and non-condensate atoms in the liquid [46]. The superfluid velocity $v_s (r)$ is meaningless for temperatures above the $\lambda$-point as the superfluid density vanishes in that region. One expects that at absolute zero the
whole system is superfluid \( \rho_s (r) = \rho (r) \) and \( \rho_n (r) \equiv 0 \) regardless of being only partially condensed.

Now to one of the experimentally most important features concerning superfluidity. In a rotating container with toroidal shape the normal component moves, in phase with the boundaries, at the angular velocity \( \omega \). This implies

\[
v_n(r) = \omega R \hat{\Theta}
\]

where \( \hat{\Theta} \) is a unit tangent-vector to the torus at point \( r \). Defining the quantum of rotation [46]

\[
\omega_c = \frac{\hbar}{m R^2}
\]

and denoting the cross sectional area of the torus by \( A \), the classical total angular momentum of \( ^4\text{He} \) above the \( \lambda \)-temperature (\( \rho = \rho_n \)) is given by

\[
|L| = 2 \cdot \pi R^2 A \rho_n v_n = M R^2 \omega = I_{cl} \omega
\]

where \( M \) is the total mass of the liquid helium enclosed in the container and \( I_{cl} \) is the classical moment of inertia for a mass distribution on a ring with radius \( R \), valid if the inner radius of the torus tube is much smaller than the radius of the torus itself. This is the situation for He-I above the superfluid transition. Below \( T_\lambda \) however things look quite different as has been shown by the angular momentum measurements of Hess and Fairbank [36]. For this geometry Eq. (2.16) requires \( v_n \) to be quantized in integer multiples of \( \omega_c R \). Inserting this quantized velocity in Eq. (2.19) the system thus needs to minimize its effective free energy

\[
\mathcal{E}_{sf} = \rho_s (T) R^2 \left( \frac{1}{2} v_n^2 \omega^2 - n \omega \omega_c \right)
\]
with respect to the winding number $n$. The latter however is topologically conserved. If the system once has chosen its winding number the latter will remain constant. Minimizing $E_{s}$ means that $n$ has to be chosen to be the closest integer to the ratio $\frac{\omega}{\omega_c}$. If $\omega$ is chosen to be smaller than $\omega_c/2$ no superfluid can be set into rotation and after cooling through the $\lambda$-line the system will keep $n=0$ and not change this value. Fixing $n$ in this way $v_s$ is fixed to zero and the superfluid component does not contribute to the moment of inertia. The angular momentum decreases in the same way

$$|L(T)| = \frac{\rho_s(T)}{\rho} I_{cl}\omega = f_s(T) I_{cl}\omega$$ \hspace{1cm} (2.24)$$

If on the contrary $\frac{1}{2}\omega_c < \omega < 1$ the system will choose a value greater than the classical value. The total angular momentum is then given by

$$|L(T)| = I_{cl} (f_n(T) \omega + f_s(T) n\omega_c)$$ \hspace{1cm} (2.25)$$

where $f_s(T) = \rho_s(T)/\rho$ and $n$ is the integer part of $\left[\frac{\omega}{\omega_c} + \frac{1}{2}\right]$. The angular momentum for fixed $T < T_\lambda$ is therefore quantized and increases discontinuously in units of $\hbar$ as a function of $\omega$ at angular velocities $\omega_i = (2i+1)\cdot \frac{\omega_c}{2}$, where $i$ is a nonnegative integer. Another main defining phenomenon of superfluidity is the metastability of circulating supercurrents [46]. If an annular container that is rotating at a very high annular velocity $\omega$ is cooled through $T_\lambda$ the system will choose a very large value for the winding number. If after cooling through $T_\lambda$ the rotation is stopped the velocity $v_s(r)$ will equilibrate to zero. The winding number of the superfluid velocity however is still topologically conserved yielding

$$|L(T)| \cong \frac{\rho_s(T)}{\rho} I_{cl}\omega_0 = f_s(T) I_{cl}\omega_0$$ \hspace{1cm} (2.26)$$
where $\omega_0$ denotes the angular velocity that the container had while the whole system was cooled down.

### 2.4 Ginzburg-Landau Theory

Although the free energy in general is not an analytical function of the order parameter, in the vicinity of the critical temperature it is possible to define the so called Ginzburg-Landau (GL) free energy functional $F\{\psi(r), T\}$. This functional is defined as

$$F\{\psi(r), T\} = F_0(T) + \int dr \{ \alpha(T) \cdot |\psi(r)|^2 + \frac{1}{2} \beta(T) \cdot |\psi(r)|^4 + \gamma(T) \cdot |\nabla\psi(r)|^2 \}$$

and should give the actual free energy if minimized with respect to the order parameter [46]. Close to $T_c$ it is reasonable to assume that the coefficients have temperature dependencies such as

$$\alpha(T) = \alpha_0(T - T_c), \beta(T) = \text{const}, \gamma(T) = \text{const}$$

In more general cases the Ginzburg-Landau functional will also contain higher order terms in $|\psi(r)|^6$ or $|\psi(r)|^2$ and $\nabla|\psi|^2$. This form is applicable for the equilibrium or near equilibrium behavior of liquid $^4$He for temperatures below $T_c$.

### 2.5 The XY-Model

The classical planar spin model, most commonly known under the name XY-model, allows a clear separation in near and far zones for a system of vortex lines such as in $^4$He [43]. By only using the variables $|\Psi_i|$ and $\Theta_i$ and making the coarse grained assumption that the condensate wave function is fairly constant throughout the system, only the on site phase angles $\Theta_i$ remain as dynamical variables. The GL functional can now be written as

$$E = a_0 a^3 \sum_i \left\{ \sum_n \left[ \frac{\hbar^2}{2m} \frac{1}{a^2} |\nabla_n \Psi_i|^2 - U |\Psi_i|^2 + \frac{V_0}{2} |\Psi_i|^4 \right] \right\}$$

The index $i$ denotes the lattice site and $\mu$ denotes the bond direction pointing away from the site $i$. As the size of the order parameter is considered frozen throughout the whole system, the energy functional becomes

$$E = \frac{ah}{2m} |\Psi_i|^2 \sum_{i,\mu} \nabla_\mu e^{i\Theta_i \mu} |^2 - E_c$$
The constant $E_c$ contribution can be omitted leading to
\[
E = \frac{J}{2} \sum_{i,\mu} |\nabla_{\mu} e^{i\Theta_i}|^2 = \frac{J}{2} \sum_{i,\mu} |e^{i\Theta_{i+\mu}} - e^{i\Theta_i}|^2 \tag{2.31}
\]
\[
= J \sum_{i,\mu} (1 - \cos (\Theta_{i+\mu} - \Theta_i)) = J \sum_{i,\mu} (1 - \cos (\nabla_{\mu} \Theta_i)) \tag{2.32}
\]
Omitting the $\Theta_i$ independent part one is left with the standard Hamiltonian of the classical XY-model
\[
H = -J \sum_{\langle i,j \rangle} \cos (\Theta_i - \Theta_j) \tag{2.33}
\]
where $\langle i, j \rangle$ denotes nearest neighbor summation. The actual superfluid one wants to describe does not have any lattice structure. But in the now discretized version of the GL energy functional the lattice structure will essentially enter in the results obtained from this model. Therefore one should be rather careful with the physical results for $\beta \to 0$ and $\beta \to \infty$. In the critical regime, where by universality the correlation length and time diverge, the underlying lattice structure is assumed to be irrelevant [43]. In 3D the critical exponents have been calculated to very high precision using numerical simulation [16].

2.6 Superfluidity and Winding Numbers

As discussed before superfluidity is experimentally characterized by the different response of the normal and superfluid component to boundary motion. Pollock and Ceperly [55] showed, that in a path integral representation of a bosonic system with linear extension $L$, the winding number $W$ defined by
\[
LW = \sum_{i=1}^{N} (r_P_i - r_i) \tag{2.34}
\]
where $P$ denotes the permutation operator relates to the superfluid density in the straightforward manner
\[
\rho_s = \frac{m}{\hbar^2} \frac{\langle W^2 \rangle L^{2-d}}{p d \beta} \tag{2.35}
\]
which is extremely useful also for the linkcurrent representation presented in [77].

They considered in a gedanken experiment $^4$He enclosed between two cylindric walls with radii $R$ and $R + d$ that rotate at angular frequency $\omega$. For $d/R \ll 1$ the boundary motion then simply has velocity $v = \omega R$ and the system is periodic in one direction. The density matrix operator $\rho_s$ is then determined in a system $S'$, at rest with the moving walls. Its Hamiltonian becomes $\mathcal{H}' = \sum_j (p_j - m v)^2 / 2m + V$ with $V$ is chosen to be a translation invariant pair potential. The density matrix then looks like
\[
\rho' = \exp (-\beta \mathcal{H}') \tag{2.36}
\]
and has the property that it does not change if transformed to the lab frame \[55\]. The distribution of states, therefore, in both cases is exactly alike and \( \rho' = \rho_v \). Only the normal component is affected by the wall motion and can be defined by

\[
\rho_n N m v = \langle \hat{P}_v \rangle = \frac{\partial / \partial \nu \text{Tr} \{ \rho_v \}}{\text{Tr} \{ \rho_v \}} + \frac{\text{Tr} \{ N m v \rho_v \}}{\text{Tr} \{ \rho_v \}}
\]

(2.37)

where \( \nu \) is fixed, \( \hat{P} \) denotes the total momentum operator and \( N \) the particle number. Using

\[
\exp [-\beta F_v] = \text{Tr} \{ \rho_v \}
\]

(2.38)

Eq. (2.37) can be rewritten as

\[
\frac{\rho_n}{\rho} N m v = \frac{\partial}{\beta \partial \nu} \ln [\text{Tr} \{ \rho_v \}] + N m v = - \frac{\partial F_v}{\partial \nu} + N m v
\]

(2.39)

leading to

\[
\rho_s = \frac{\partial [F_v/N]}{\partial \left[ \frac{1}{2} m \nu^2 \right]}
\]

(2.40)

where \( \rho_s / \rho = 1 - \rho_n / \rho \) has been used. Expressing Eq. (2.40) in terms of finite differences yields the free energy increment due to sample wall motion

\[
\frac{\Delta F_v}{N} = \frac{1}{2} \nu^2 \rho_s \rho + O (\nu^4)
\]

(2.41)

which vanishes if no superfluid is present. Experiments usually probe the limit \( \nu \to 0 \). Periodic boundary conditions imply on \( \rho_v \)

\[
\rho_v (r_1, \ldots, r_N, r'_1, \ldots, r'_N; \beta) = \rho_v (r_1, \ldots, r_N, r'_1, \ldots, r'_N; \beta)
\]

(2.42)

Further \( \rho_v \) has to be a solution to the Bloch equation \[55, 26, 18\]

\[
-\hbar \frac{\partial \rho (u)}{\partial \beta} = \mathcal{H}_\beta (u)
\]

(2.43)

which now reads

\[
- \frac{\partial \rho_v (R, R'; \beta)}{\partial \beta} = \left[ \frac{1}{2m} \sum_j (-i\hbar \nabla_j - m \nu)^2 + V \right] \rho_v (R, R'; \beta)
\]

(2.44)

and can always be written as

\[
\rho_v (R, R', \beta) = \exp \left[ \frac{m}{\hbar} \nu \sum_j (r_j - r'_j) \right] \tilde{\rho} (R, R'; \beta)
\]

(2.45)
2.7 HELICITY MODULUS AND SUPERFLUIDITY

It is important to realize that
\[ \exp \left[ -\beta F_v \right] = \text{Tr} \{ \tilde{\rho} \} \]  
(2.46)
with \( \tilde{\rho} \) satisfying yet another Bloch equation
\[ -\frac{\partial \tilde{\rho}(R, R'; \beta)}{\partial \beta} = \left[ \frac{1}{2m} \sum_j (\mathbf{\tilde{v}} \nabla_j)^2 + V \right] \tilde{\rho}(R, R'; \beta) \]  
(2.47)
which is exactly the equation of motion for a density matrix of a system with fixed boundaries. Equations (2.42) and (2.45) then imply that
\[ \tilde{\rho}(r_1, \ldots, r_N, r'_1, \ldots, r'_N; \beta) = \exp \left[ im/\hbar \mathbf{v} \cdot \mathbf{L} \right] \tilde{\rho}(r_1, \ldots, r_N, r'_1, \ldots, r'_N; \beta) \]  
(2.48)
With the definition of the winding number \( W \) given in Eq. (2.34) the free energy change \( \Delta F_v \) can be calculated through the winding number distribution \([55]\)
\[ \exp \left[ -\Delta F_v \right] = \frac{\int \rho_v(R, R; \beta) dR}{\int \rho_v=0(R, R; \beta) dR} = \langle \exp \left[ im/\hbar \mathbf{v} \mathbf{W} \right] \rangle \]  
(2.49)
and is periodic under \( v \rightarrow v + h/mL \). Consequently Eq. (2.49) implies that the free energy change is the Fourier transform of the winding number distribution. Expanding for small velocities and using Eq. (2.41) yields
\[ \frac{\rho_s}{\rho} = \frac{m}{\hbar^2} \frac{(W^2) L^2}{3\beta N} + O(v^4) \]  
(2.50)
for a three dimensional cubic system. Using \( N = \rho L^d \) it is possible to generalize this relation for arbitrary dimensions \( d \) yielding Eq. (2.35). Thus the occurrence of large scale fluctuations in the winding number directly signals the onset of superfluidity. As a dimensionless quantity it also exhibits scaling invariance.

2.7 Helicity Modulus and Superfluidity

In 1973 Fisher et al. showed how to define a helicity modulus \( \Upsilon(T) \) which measures the free-energy increment associated with imposing a phase twist on the order parameter and showed that it is closely connected to the second order derivative of the free energy \([29]\). They achieved a microscopic definition of the superfluid density expressed only in equilibrium free energies, requiring only the calculation of the partition function of a system, under twisted boundary conditions without involving the calculation of correlation functions. More exactly, they argued by considering an isotropic system on a uniform cylindrical domain \( \Omega \), with a generally complex vector order parameter \( \Psi \) as in Eq. (2.9). In a system with an infinitely degenerate ground state, usually, a symmetry breaking field, coupling to the order parameter
\( \Psi = \langle \Psi (r, t) \rangle \) would be required to stabilize a specific thermodynamic phase. This, however, can be replaced by a set of wall potentials \( U_\Theta \) enforcing a certain angle on the system at the wall, while at the same time respecting the symmetry of \( \Omega \). On the top and bottom wall of the cylinder they either imposed periodic boundary conditions \( \Theta_{\text{top}} = \Theta_{\text{bottom}} \) or twisted boundary conditions \( \Theta_{\text{top}} = -\Theta_{\text{bottom}} \) where \(|\Theta_{\text{top}}| = |\Theta_{\text{bottom}}| < \frac{\pi}{2} \). In the periodic case, the system exhibits uniform bulk phases at which \( \langle \Psi (r, t) \rangle \) has a constant mean phase angle \( \phi (r, t) \) independent of position. The free energies of these phases are equal

\[
F (T; \Omega, U_\Theta^{\pm}) = F (T; \Omega, U_\Theta^{-})
\]

(2.51)

In contrast to this, if mixed boundary conditions are introduced, the system will have a phase twist \(|\Delta \Theta| = 2 |\Theta| \) along the axis of the cylinder. They then noted, that an isotropic system should have an approximate transverse translational symmetry, if the cross sectional area of the cylinder \( A(\Omega) \) is very large. Then the difference

\[
\Delta F (T, \Omega) = F (T; \Omega, U_\Theta^{+-}) - F (T; \Omega, U_\Theta^{++})
\]

(2.52)

simply becomes proportional to \( A \). The phase gradient of \( \phi (r, t) \) then would have to point along the axis of the cylinder with a magnitude of

\[
\langle \nabla \phi \rangle = \frac{\int [\nabla \phi (r)] || d^3r}{V (\Omega)} = 2 \frac{\Theta}{L (\Omega)}.
\]

(2.53)

The symmetry of the problem then requires \( \Delta F \) to be an even function of \( u = \langle \nabla \phi \rangle \) and using Eq. (2.51) \( \Delta F = 0 \) if \( u = 0 \). The gradient of \( \phi \) then introduces some strain energy density along the \( z \)-axis of the cylinder. The free energy density then should also be proportional to the length \( L (\Omega) \) of the axis. To lowest order Fisher et al. [29] therefore expected

\[
\Delta F (T, \Omega) \approx \frac{1}{2} \Upsilon (T) \langle \nabla \phi \rangle^2 A (\Omega) L (\Omega)
\]

\[
= 2 \Theta^2 \Upsilon (T) \frac{A (\Omega)}{L (\Omega)}
\]

(2.54)

where Eq. (2.53) has been used. If \( \Theta \) is held fixed the the limit \( u \to 0 \), where Eq. (2.54) is expected to become exact, is given for \( L \to \infty \). Solving for \( \Upsilon (T) \) then gives together with Eq. (2.53)

\[
\Upsilon (T) = \lim_{A(\Omega), L(\Omega) \to \infty} \left[ \frac{L (\Omega)}{2 \Theta^2 A (\Omega)} \right] \left[ F (T; \Omega, U_\Theta^{+-}) - F (T; \Omega, U_\Theta^{++}) \right]
\]

(2.55)

meaning that the helicity modulus \( \Upsilon (T) \) can be obtained as a second order derivative of the free energy density with respect to an infinitesimal phase twist. As outlined in previous sections, in a Bose system, the phenomenologically derived free energy density increment due to superflow is

\[
\Delta F / V (\Omega) = \rho_s c_s^2 (T) / 2.
\]

(2.56)
2.8. TOPOLOGICAL DEFECTS

Relating the phase gradient to the superfluid velocity finally leads to the relation

$$\rho_s(T) = \left( \frac{m}{\hbar} \right)^2 \Upsilon(T)$$

(2.57)

associating the superfluid density with the helicity modulus $\Upsilon(T)$. Its usefulness lies in the straightforward applicability to the classical lattice spin systems such as the XY-model [50].

2.8 Topological Defects

Many physical systems with broken continuous symmetry can sustain topological defects. These typically can be described by the variation of some elastic variable in some region of space. The proliferation of topological defects can destroy the ordered phase. Depending on the dimension of space of the problem considered topological defects can reside in points or lines and can be detected by measuring an appropriate field along a path enclosing the defect [19]. Again, Eq. (2.16) is such an example restricting the gradient field of the order parameter to a certain form. In superfluid Helium and the XY-model the topological defects described by an analogue of Eq. (2.16) are called vortices. The defects get different names depending on which symmetry they break [19]. Dislocations in solids are yet another example. A topological defect is stable if one cannot find a mapping that removes the defect by continuously deforming the order parameter.

Quantized Vortices in Liquid Helium

The vorticity $\omega$ is defined as

$$\omega(r,t) = \nabla \times \mathbf{v}(r,t)$$

(2.58)

where $\mathbf{v}$ is the mean fluid velocity [46]. It is possible that the vorticity vanishes nearly everywhere in space excluding only a particular line where it is singular. This defines the circulation $\kappa$ by taking

$$\kappa = \oint_C \mathbf{v}(r,t) \cdot dl \neq 0$$

(2.59)

along a contour $C$ enclosing the line. Depending on if this line of singularity has ends that terminate on the system boundaries or closes on itself, it is called a vortex line or vortex ring. Lines with open ends cannot exist as $\nabla \cdot (\nabla \times \vec{v})$ is zero for any vector field $\vec{v}$. The definition of vorticity given above is the same for any liquid. The circulation of the normal fluid can be any real number. The superfluid component however can only sustain circulations that are integer multiples of $\kappa_0 = \frac{\hbar}{m} \approx 10^{-7} \text{ m}^2 \text{ sec}^{-1}$ due to Eq. (2.16). In systems exhibiting BEC talking about vortices usually refers to these quantized ones associated exclusively with the superfluid component [46]. For vortices in superfluid helium the vorticity cannot be a smooth
CHAPTER 2. SUPERFLUIDITY

function of position on arbitrarily small scale. However if looked at from a coarse grained scale the differences between bulk vorticity of a classical fluid and the quantized one of He-II are not easily visible and thus \( \omega (r, t) \) seems smooth. If the contour in Eq. (2.59) is taken properly around the vortex, the circulation \( \kappa \) will be preserved unless strong dissipative effects are added. This corresponds to the criterion for topological stability stated in the introduction. If the vortices move through the system they will do this at the speed of the background fluid [46].

A single straight vortex line in \( z \)-direction can be modeled by setting

\[
\Theta (r) = \phi + \Theta_0
\]

\[
\Rightarrow \nabla \Theta (r) = \frac{1}{r} \epsilon \phi
\]

in cylindrical coordinates \( (r = \sqrt{x^2 + y^2}, z, \phi) \). The vorticity will then be given by

\[
\omega (r) = \nabla \times \nabla \Theta (r) = 2\pi \delta (r) \hat{z}
\]

where the \( z \)-direction has been chosen arbitrarily as the direction of the vortex line. The singularity can be removed by cutting out a small hole around the vortex core. The situation can also be remedied by forcing the magnitude of the order parameter \( |\Psi (r)| \) itself to vanish in this tiny region. The condensate wave function must be single valued after all. Every vortex will thus have a core region at the center whose dimensions are of the order of the Ginzburg-Landau coherence length \( \xi \) [47]. Any creation of a vortex will therefore lead to two contributions to the total energy, namely the core energy coming from the depletion of the magnitude \( |\Psi (r)| \) and an elastic part, coming from the gradient of the phase outside the core. Using the expression Eq. (2.19) for the elastic energy of the phase distortion the energy per unit length of a single vortex line at the center of a cylinder of radius \( R \) can be calculated as

\[
\mathcal{E} = \frac{1}{2} \rho \kappa^2 \ln \left( \frac{R}{\xi} \right)
\]

Using \( \xi \) is of the order of the interatomic distance, a scale where the continuum description already is invalid [46, 60]. For parallel vortex lines the calculation can be done analogously [19]. The potential energy and thus the force between them is

\[
\mathcal{E}_\parallel (r) = \frac{1}{2\pi} \rho \kappa^2 \ln \left( \frac{R^2}{\xi r} \right)
\]

where \( r \) is their separation and \( r \gg a \). It follows directly, that parallel vortex lines repel each other as an increase in distance means a decrease in potential energy. For antiparallel vortex lines the potential energy difference turns out to be

\[
\mathcal{E}_\perp \approx \frac{1}{4\pi} \rho \kappa^2 \ln \left( \frac{r}{\xi} \right)
\]

meaning that antiparallel vortex lines attract each other [19]. It follows further that a system, which only is required to have the total circulation fixed at some value
\[ \kappa, \text{ will successively break up single vortex lines with large circulation } \kappa \text{ into several vortices, each with a lower circulation. The vorticity will then become diffuse [46].} \]

For the quantized vortices in pure He-II this further implies that vortices with a winding number \(|n| > 1\) should not be found. Rotating cylinders containing superfluid He-II show the same surface profile as common fluids [46]. At a coarse scale this means that if the container is rotated at angular frequency \(\omega\) the velocity field is given by

\[ \mathbf{v}(\mathbf{r}) = \omega \times \mathbf{r} \quad (2.65) \]

which is impossible if Eq. (2.15) has to hold. If however \(2\omega / \kappa_0 \) vortex lines are present in the liquid with circulation parallel to the rotation axis, then the behavior looks the same at large scales while still being completely different on scales where the splitting in single vortex lines becomes visible.

### Crystal Defects

#### Point Defects

A region in a solid, where the microscopic arrangement of atoms differs drastically from that of a perfect crystal is called a defect [8]. The two most important kinds of point defects are vacancies and interstitials. If a vacancy occurs then a regular lattice position remains empty. In contrast to that, if an interstitial is present, an extra atom or ion is positioned at a site, which normally should remain unoccupied. Impurity atoms of a different element can also occupy a regular lattice site. If an atom leaves its site and replaces a vacancy, the vacancy itself travels in the opposite direction. One of the most important questions, regarding the possibility of a supersolid, was if vacancies could exist at zero Kelvin or need to be thermally excited (sec. 2.9).

#### Extended Defects

The basic mechanism for gliding and slip effects can be accounted for by the concept of extended line defects, the dislocations. These come in two standard types. An edge dislocation can be depicted by cutting into the crystal and inserting an extra lattice plane into the crystal (Fig. 2.4a). The dislocation line here is given by the lower edge of the inserted plane. Dislocations are classified by their Burgers vector \(\mathbf{b}\), which can be defined by considering the difference of a closed path in the perfect crystal vs. the same sequence of steps around the defect. It then can be read off as the difference between the starting point for both paths and the end point for the path enclosing the dislocation line. For an edge dislocation the Burgers vector is orthogonal to the inserted plane. A screw dislocation is produced by cutting into the crystal and displacing the two planes against each other by one lattice spacing. The dislocation line is marked by the cutting edge. The Burgers vector can be defined in exactly the same way as for the edge dislocation but this time it is parallel to the dislocation line. The name screw dislocation comes from the
Figure 2.4: a) Sketch of an edge dislocation. The burgers vector is obtained by comparing the closed path around the dislocation line to the non-closed path using the same sequence of steps in the ideal crystal [81]. b) Schematic representation of a screw dislocation with Burgers-vector $\vec{b}$ pointing normal to the surface along the dislocation line.

fact that encircling the dislocation line in an orthogonal lattice plane traces out a screw line. It is in principle possible that Burgers vectors with a length smaller than one lattice spacing occur [38]. These lead to a much higher energy than ordinary dislocations and are thus not stable. Ring dislocations occur more often than dislocations lines and can be thought of as a small plane inserted into the crystal lattice which does never reach the crystal boundaries [38]. Those however can never be built up by screw dislocations as for those the dislocation line always has to point along a straight line. Edge and screw dislocations can be considered as two special cases of the same kind of physical object that is classified by the angle it builds with the Burgers vector. The Burgers vector is constant along an arbitrarily shaped dislocation line. Edge dislocations can built a source or drain for vacancies and interstitials as e.g. the required binding energy is much lower if an interstitial moves from the end of the inserted plane down into the crystal as the crystal lattice already is favorably distorted. The picture of ideally straight dislocation line is also much too simplified. Dislocation lines can be rough due to the built-up of kinks. These are a subclass of the so called jogs which are defects in the plane ending with the dislocation line.
2.9 Search for Experimental Evidence of a Supersolid State of Matter

The possibility of a supersolid state was conjectured several decades ago. Penrose and Onsager had found that perfect crystals cannot exhibit ODLRO but did not use properly symmetrized wave functions [53, 11]. Conversely Legget suggested that NCRI in solid $^4\text{He}$ would be the signal to look for [45]. The originally proposed mechanism was the condensation of zero point vacancies. Although these cost an activation energy $E_0$ Andreev and Lifshitz [7] conjectured that if these vacancies at low temperatures could tunnel through the crystal with a sufficiently high exchange frequency, a quantum wave spanning across the whole crystal would be created. Delocalization then implies a low momentum uncertainty. For high enough exchange frequencies the vacancy gas energy contribution becomes negative leading to a finite density of vacancies even at absolute zero [10]. Bosonic vacancies in a $^4\text{He}$ crystal then possibly could Bose-Einstein condense and become superfluid. Thus the system would show the peculiarity of being both ordered in position space and momentum space. Prokof’ev argued that commensurate crystals cannot exhibit ODLRO and therefore are insulating [58]. In addition, Path integral Monte Carlo simulations of solid hcp helium found a very large activation energy $\approx 10$ K of vacancies and that these phase separate instead of condensing [14]. Today the naive vacancy supersolid scenario is widely refuted. The effects of the second class of defects mentioned, the dislocation lines are however still at the heart of the debate [10, 2, 71]. The following subsections guide through some experimental results and recent developments.

Early Experiments

In the beginning experiments investigated the plastic flow of objects moving in solid $^4\text{He}$ [72, 31]. Later studies targeted torsional oscillator and mass flow experiments but failed to observe any unusual behavior [33, 13]. The region probed was limited by $T > 25$ mK and $25$ bar $< P < 48$ bar partly overlapping with some of the work of Kim and Chan without finding NCRI [31, 25]. Only Goodkind et al. described that acoustic waves in solid $^4\text{He}$ where scattered by a non-phonon family of excitations [30]. $^3\text{He}$ impurities produce a sharp peak in the acoustic attenuation [37] which strangely was explained as a second order phase transition from a bose condensed state above around $160 – 180$ mK to a normal state below it [31]. It seems feasible to expect that these early findings and more recent observations in torsional oscillator experiments as well as mechanic anomalies for solid $^4\text{He}$ are related.

Torsional Oscillator Experiments

In a torsional oscillator experiment the expected resonance frequency $\omega_R = \sqrt{G/I}$ is given by the moment of inertia $I$ and the torsional spring constant $G$ of the torsion rod. An anomaly in this resonance frequency then is attributed to NCRI as
CHAPTER 2. SUPERFLUIDITY

suggested by Leggett [45]. In 2003 Kim and Chan reported a temperature dependent period drop in $\omega_R$ for a sample of solid $^4$He, confined to vycor glass, cooled below 175 mK [25]. Vycor is highly porous and contains a mesh work of channels $\approx 60 \text{ Å}$ in diameter requiring large pressures of $\approx 40 \text{ bar}$ for solidification [31]. As expected for a bulk superfluid the period drop was attenuated by increasing the amplitude and therefore rim velocity. The same effect is expected for a superfluid and attributed to vortex excitations. The subsequent observation of Kim and Chan of NCRI in bulk solid $^4$He opposed the claim that superflow only could have occurred due to disorder induced by the vycor [41]. Blocking the annulus with a magnesium barrier as a control experiment diminished the NCRI response [41]. Later similar experiments with $^4$He in porous gold were performed [42]. NCRI occurred below $T = 0.2 \text{ K}$ and higher oscillation amplitudes where again accompanied by a larger attenuation of the response signal. Gold has a larger pore size than vycor of about 490 nm [42]. Effects of disorder emerged as a likely source for the NCRI. Experiments of Rittner and Reppy showed, that the effect of NCRI is undetectable if the $^4$He is solidified under a procedure called annealing, delivering high quality crystals [64]. During annealing the sample is heated and cooled several times. In highly disordered samples of $^4$He the NCRI fraction might however exceed as much as 20% [65]. It has further been suggested that a superfluid like flow between grain boundaries can contribute to the phenomenon [67]. The NCRI measured are also dependent on the surface to volume ratio $S/V$ of the annular container increasing with $S/V$ proposing that more confining geometries freeze out disorder and suppress NCRI [65]. Clark et al. argued that even to obtain low NCRI fractions of 1% enormous geometries would be needed as well as completely interconnected grain boundaries [22]. By applying improved growth techniques at constant temperature or pressure (CT/CP) carried out at a specific point of the solid-liquid coexistence curve they claimed to get large single crystals still showing NCRI. The onset however is sharper. Above 40 mK all isotopically pure (CT/CP) $^4$He samples considered in their measurement collapsed on one single curve in the NCRI($T$) measurement and show a common, single onset temperature [22] (see also Fig. 6.1b). The container geometry, as well as its construction material and thermal properties of the sample cells, seem to effect the fraction of NCRI. As dislocation lines form an entangled web throughout each crystal and show large density variations they are mentioned as an important cornerstone in order to understand the NCRI [22]. It seems, that the annealing process can just reduce the number of certain dislocations. It remains questionable that these alone are responsible for the apparent supersolidity.

Heat Capacity Measurements

If the onset of NCRI really describes a solid-supersolid transition it should also leave its signature in different thermodynamic quantities. Lin et al. [84] observed a broad peak in the non-phonon contribution to the specific heat of a bulk helium sample confined to a silicon container (see also Fig. 6.1a). The specific heat of silicon is
about one order of magnitude smaller than that of $^4$He [31]. The peak occurred at
temperatures of 70 – 80 mK, comparable to the onset for the isotopically pure $^4$He
CT/CP samples mentioned in the preceding section. Missing linear contributions
in the specific heat, they ruled out a glassy origin of the NCRI as according to
their data a plot of the full specific heat per mole against $T^3$ extrapolates through
the origin [84]. Again the peak magnitude depends on the growth method and the
sample purity. Disordered samples do again show a higher peak. The glass scenario
still is a very interesting candidate [56].

Mass Flow Experiments
Another manifestation of superfluid behavior is DC mass flux inside the solid. Ex-
periments, in which the pressure to create this mass flow was directly applied to
the crystal lattice, failed to observe any signature [24]. Ray and Hallock reported
the observation of unusual mass flow in solid hcp $^4$He [61]. Their setup allowed the
direct addition of $^4$He atoms from the superfluid to the solid, using two vycor glass
rods filled with liquid $^4$He entering the cell containing the solid. Flow was observed
at samples grown by the more standard blocked capillary method (BC) and those
grown according to CT. The flow shows pressure and temperature dependencies
and vanishes close to 27 bar and above 800 mK. At small pressure and $T$ lower
than 400 mK flow is observed that is directly proportional to time as predicted for
a superfluid moving at a critical velocity [31]. The same group recently reported an
analogue to the fountain effect [5] between two superfluid reservoirs connected by
solid $^4$He appearing around 600 mK and increasing if the temperature is reduced
below 75 mK [62].

Mechanic Anomalies in Solid $^4$He
The discussion was once again revived when Day and Beamish [23] observed large
increases of about 10% in the shear modulus below 200 mK with a similar de-
pendence on measurement amplitude, $^3$He impurity concentration and annealing
as seen in the torsional oscillator measurements. At first sight a stiffening of the
solid seems add odds with a superflow scenario. Their first explanation was, that
the solid $^4$He sample contains a dislocation network that is pinned by $^3$He impu-
rities at the lowest temperatures. Above 100 mK the mobility of the dislocations
increased. In the experiments performed by Ray and Hallock mentioned before
pressure and density of supersolid samples reacted spatially uniform to alterations
of the chemical potential in the vycor electrodes [61]. Söyler, Kuklov et al. ex-
plain this by a super climb mechanism of edge dislocations with superfluid cores
[71]. At low temperatures they propose that the effect nearly is absent due to a
crossover to a smooth dislocation lines [71]. Being defects, themselves dislocation
lines may also carry defects. At higher temperatures kinks can lead to mobile and
rough dislocation lines. A resultant higher mobility of the dislocation lines leads
to mass currents which themselves are caused by phase gradients, thereby destroy-
ing superflow [10]. At $T = 0$ the dislocations are straight and do not fluctuate. Some experimental research is performed to verify if this roughening transition is possible in ultra pure crystals [10]. Other groups have recently shown that there is an interplay of the mechanical bulk crystal dynamics with the superflow [56]. They find that the same microscopic excitations influencing the torsional oscillator motions are independently created by thermal and mechanical stimulation without any signs of a critical temperature in the relaxation time.

2.10 Effective Model of a Supersolid

With its superior accuracy describing the superfluid transition in $^4$He the 3DXY-model is the natural candidate to model effects of superflow also in a crystal background. Due to $\nu \approx 0.671 > 2/d$ [16, 48] its fixed point is stable with respect to quenched, uncorrelated, random disorder. With the previous experimental discussion in mind, correlated defects have emerged as possibly aiding superflow. Assuming the dislocation network to be static and ignoring amplitude fluctuations of the order parameter field $\Psi(r) = |\Psi|e^{i\theta(r)}$, the phase fluctuations driving the superfluid transition can be modeled as

$$H = -\sum_{i,\mu} J_\mu^i \cos(\theta_{i+\mu} - \theta_i)$$

(2.66)

where $\theta_i$ is the phase of the superfluid (SF) order parameter at site $i$ of a simple cubic lattice of size $L^3$ with periodic boundary conditions in all directions. The index $\mu = x, y, z$ denotes bonds along the coordinate directions. The dislocation network is modeled by selecting the coupling constant to be $J_\mu^i = 1 \pm \delta$ with equal probability. Here $J_\mu^i = 1 + \delta$ describes a dislocation line and $J_\mu^i = 1 - \delta$ the bulk. The values of $J_\mu^i$ are assumed to be perfectly correlated along the coordinate axis directions. This model thus describes a network with linear SF channels in the coordinate directions for simplicity. It should be able to adequately grasp the essential features of the SF transition in an isotropic static dislocation system. Invoking the additional requirement of $\langle J_\mu^i \rangle = 1$, convergence of the MC disorder averages is improved. This choice reflects a coarse grained model with lattice spacing set to half the mean dislocation distance. Ideally $\delta = 1$ means that the superfluid density, locally, either is finite or zero, as can be seen in Eq. (2.30). However as this dramatically increased the convergence time for large system sizes in the Monte Carlo simulations, a value of $\delta = 0.95$ was chosen to obtain reliable scaling results for large system sizes and prevent that out of equilibrium expectation values ridicule the gains of smaller finite size corrections.

Needless to say, in real experiments there are other contributions to the results. For example any dislocation movement is ignored in this model, which is unrealistic since the He solid is soft and close to melting. However in the solid phase dislocation motion is stronger and stronger bounded with decreasing temperature. Thus assuming immobile dislocation loops can be correct to lowest order.
Chapter 3

The Dirty Boson Model

Following references [28, 79] the dirty boson Hamiltonian is introduced and its most important properties are described. General scaling relations are derived and the transformation to the for numerical simulations very important link current model are performed in detail.

3.1 The Bose Lattice Gas

For bosons in a random potential repulsive interactions are necessary to hinder the particles from condensing into the lowest, localized eigenstate [28]. The onset of superfluidity is due to an interplay of several factors. First, the kinetic energy trying to delocalize the particles by decreasing phase fluctuations of the bose field. Second, particle interactions together with the random potential favoring a localized state with small fluctuations in the number density. M. P. A. Fisher, Weichman, Grinstein and D. S. Fisher argued, that at $T = 0$ K in general three different phases can exist [28]. These are a superfluid phase, a commensurate, gapped and incompressible Mott insulator phase and a *bose glass*. In the latter there is no gap for particle-hole excitations and the compressibility is finite. It further is insulating as the random potential localizes the particles.

The Hamiltonian is given by

$$H = H_0 + H_1$$

$$H_0 = - \sum_i (\delta \mu_i + \mu) \hat{n}_i + \frac{1}{2} \sum_{i,j} V_{ij} \hat{n}_i (\hat{n}_j - \delta_{ij})$$

$$H_1 = - \frac{1}{2} \sum_{i,j} J_{ij} \left( \hat{\Phi}_i^\dagger \hat{\Phi}_j + \hat{\Phi}_j^\dagger \hat{\Phi}_i \right)$$

where $i$ denotes a site on a $d$-dimensional hyper cubic lattice, $J_{ij}$ is the hopping matrix element between two sites. The zero of the chemical potential $\mu$ is fixed by requiring $J_0 = \sum_j J_{ij} = 0$, which can always be achieved by a suitable choice of the diagonal elements $J_{ii}$ [79]. The average boson density is determined by the chemical
potential \(\mu\). The random on-site potential \(\delta\mu_i\) is symmetrically distributed around zero and bounded. The symmetric pair potential \(V_{ij}\) is taken to be translationally invariant and does not include any disorder effects. The boson field operators \(\Phi_i\) fulfill the usual commutation relation \([\Phi_i, \Phi_j^\dagger] = \delta_{ij}\). The particle number on site \(i\) is given by \(\hat{n}_i = \Phi_i^\dagger \Phi_i\). Omitting on-site disorder \(\delta\mu_i = 0\) this model nearly always describes a superfluid, except if hard core bosons with \(V_{ij} = \delta (r_i - r_j)\) are considered [28]. In this limit exactly one boson sits at each site. For large particle density the model in Eq. (3.1) can be mapped on the Josephson junction array considered [28]. In this limit exactly one boson sits at each site. For large particle densities the model in Eq. (3.1) can be mapped on the Josephson junction array [77, 79].

\[
H_J = -\sum n_{ij} \cos (\hat{\phi}_i - \hat{\phi}_j) - \sum \left(\delta \hat{\mu}_i + \hat{\mu}_i\right) \hat{n}_i + \frac{1}{2} \sum U_{ij} \hat{n}_i \hat{n}_j
\]  

(3.2)

with now canonically conjugate variables \(\hat{\phi}_i, \hat{n}_i\) and the associated commutator \([\hat{\phi}_i, \hat{n}_j] = i\delta_{ij}\). The lattice field operators have been redefined to \(\hat{\Phi}_i = (N_0 + \hat{n})^{1/2} e^{i\hat{\phi}_i}\) \(\approx N_0^{1/2} e^{i\hat{\phi}_i}\) and \(\hat{\Phi}_i = e^{-i\hat{\phi}_i} (N_0 + \hat{n})^{1/2} \approx N_0^{1/2} e^{-i\hat{\phi}_i}\), and thus \(\hat{n}_i = N_0 + \hat{n}_i\). Between Eq. (3.1) and (3.2) the correspondences \(\tilde{J}_{ij} = N_0 J_{ij}, U_{ij} = V_{ij}, \delta \tilde{\mu}_i = \delta \mu_i, \tilde{\mu} = \mu - N_0 \tilde{V}_0 + \frac{1}{2} \tilde{V}_0\) hold [79] where \(\tilde{V}_0 = \sum V_{ij}\) and \(V_0 = V_{ii}\). The Hamiltonian \(H_J\) incorporates two important symmetries. Consider for integer \(n_0\) the shift \(\hat{n}_i \rightarrow \hat{n}_i' = \hat{n}_i + n_0\). It only leads to an additive term in the free energy density \(f_J(\tilde{\mu}) = f_J(\tilde{\mu} - n_0 \tilde{U}_0) + e^0(n_0, \tilde{\mu}) = n_0(\frac{1}{2} n_0 \tilde{U}_0 - \tilde{\mu})\), and \(\tilde{U}_0 = \sum U_{ij}\) [79]. Thus the only effect of the alteration is an extra term containing neither \(\tilde{J}_{ij}\) nor \(\delta \tilde{\mu}_i\) and linear in \(\tilde{\mu}\). This symmetry is not present in the original Hamiltonian. Thus the phase diagram is invariant under shifts of \(k \tilde{U}_0\) with integer \(k\). The system then will be considered at a different density, but the physics will be the same. For the original system, this statement only is exactly valid for zero hopping \(J_{ij} = 0\). In addition \(\hat{n}_i' = -\hat{n}_i, \hat{\phi}_i' = -\hat{\phi}_i\) implies \(f_J(\tilde{\mu}, \{\delta \tilde{\mu}_i\}) = f_J(\tilde{\mu}, \{-\delta \tilde{\mu}_i\})\) [79]. Together these symmetries imply, that for zero disorder the Hamiltonian is particle-hole symmetric at the points \(\tilde{\mu} = \tilde{\mu}_k = \frac{1}{2} k \tilde{U}_0\) for integer \(k\). The combined transformation \(\hat{n}_i' = k - \hat{n}_i, \hat{\phi}_i' = -\hat{\phi}_i\) leaves everything unchanged. Particles and holes are equally likely to be added to the system. This symmetry is microscopically destroyed by the introduction of disorder. With the disorder potential chosen above the particle-hole symmetry is statistically conserved.

### 3.2 Zero Temperature Phase Diagram

Consider the zero temperature phase diagram of the system described by Eq. (3.2). In the \(\tilde{\mu} - J_{ij}\) plane and \(d\)-dimensions. The parameters are those given in the definition of \(H_J\). To match preceding numerical and theoretical work [77] I explicitly discuss the case of an on-site interaction potential \(U_{ij} = U_0 \delta_{ij}\) and a tridiagonal
3.2. ZERO TEMPERATURE PHASE DIAGRAM

a: In the pure case the phase diagram is periodic in \( \tilde{\mu} \) with period \( U_0 \). In each lobe the particle number per site is an integer constant \( n_0 \). The points \( \tilde{\mu}/U_0 = k + 1/2 \) with integer \( k \) are \( 2^N \)-fold degenerate, as here each site independently accommodates \( k \) or \( k + 1 \) particles. At these points the system is superfluid for arbitrarily small \( J_0 \). The MI to SF transition occurring at the tips of the Mott lobes lie in the universality class of the \((d+1)\)-dimensional XY-model [28, 78, 79].

b: If bounded random on-site disorder \( \delta \tilde{\mu}_i \) with \( \Delta \leq \tilde{\mu}_i \leq \Delta \) is introduced, a completely new phase, intervening between the MI and SF phases already shown in the left panel, appears. This is the bose glass phase. Now the Mott lobes have shrunk and, if the disorder is sufficiently strong, might even be absent [28, 78, 79]. It has been shown that there is no direct transition between the MI and SF phase [54].

**Figure 3.1:** Comparison of the phase diagrams for the pure and the disordered model in terms of the couplings \( J_0, \tilde{\mu} \) relative to the on site repulsion \( U_0 \).

hopping matrix \( J_{ij} \). Thus only nearest neighbor hopping can occur and the sum over the hopping matrix elements is modified from \( \sum_{ij} J_{ij} (\ldots) \rightarrow J_0 \sum_{\langle ij \rangle} (\ldots) \) where \( \langle ij \rangle \) denotes nearest neighbor pairs only.

**Pure System with On-Site Interaction**

Increasing the hopping strength \( J_0 \) will start to delocalize the bosons. In the limit of zero hopping \( J_0 = 0 \) the Hamiltonian \( H_B \) is diagonal in the occupation numbers. In the pure case the chemical potential fixes the density uniformly throughout the system. The energy per site then will be

\[
\epsilon_f(n) = -\tilde{\mu}n + \frac{1}{2}U_0n^2
\]
a: If $\tilde{\mu}$ is an integer multiple of the on-site repulsion potential the pure system exhibits particle-hole symmetry [28, 77, 79]. Superfluidity is achieved by the simultaneous buildup of large scale, boson world-line, particle and hole-fluctuations within the background of the system [79]. The particle number is fixed to an integer multiple of the number of sites. For other choices of $\tilde{\mu}$ within the same Mott lobe, the nature of the transition is different. Depending on the size of the respective excitation gap either particles or holes are added to the system [28].

Figure 3.2: Influence of Particle-hole symmetry on the nature of the phase transition in the pure case at different values of $\tilde{\mu}/U_0 = 3/4, 1, 5/4$. Data has been created by using the link current representation presented in Reference [77].

which has its global minimum at $n_0 = \frac{\tilde{\mu}}{U_0}$. Thus for

$$n_0 - \frac{1}{2} < \frac{\tilde{\mu}}{U_0} < n_0 + \frac{1}{2}$$

(3.4)

exactly $n_0$ bosons occupy each site. The loci $\tilde{\mu}/U_0 = k + 1/2$ for integer $k$ are $2^N$ fold degenerate as the energy costs are equal for $k$ and $k + 1$ particles. To illustrate the dependence on increasing $J_0$ imagine $\tilde{\mu}$ to be fixed at $\tilde{\mu}/U_0 = k + \alpha$ for $-1/2 < \alpha < 1/2$. Thus adding a particle means that an amount of $\delta E_p = \epsilon (k + 1) - \epsilon (k) = U_0(k + 1/2) - \tilde{\mu} = -U_0(\alpha - 1/2)$ has to be brought up by the system. Likewise removing a particle means that $\delta E_h = \epsilon (k - 1) - \epsilon (k) = U_0(\alpha + 1/2)$ has to be invested. So if the energy gained by letting the particle/hole hop around in the lattice does not exceed the lesser of the energies $\delta E_p, \delta E_h$ then
the system will, even for finite $J_0 < J_{0,c}(\tilde{\mu})$, remain in an insulating state with fixed particle number $n_0$ at each site. If the particle would be delocalized in such a region, it would win the energy $J_0$ for the price of $\delta E_{ph} = \delta E_p + \delta E_h$. Thus the probability for a boson of hopping a distance $r$ away from its original position decays exponentially $\propto e^{r/\xi}$ with $\xi \sim [\ln (\delta E_{ph}/J_0)]^{-1}$ [28]. Thus within certain lobe-like regions in the $\tilde{\mu}/U_0 - J_0/U_0$ plane the particle number is exactly fixed to $k$ particles per site. There the compressibility $\kappa = \partial \rho / \partial \tilde{\mu} = 0$ vanishes and a Mott-insulator is recovered. The characteristic property of this phase is exactly that there exists a finite energy gap for the creation of particle-hole excitations [28].

Starting out from a Mott insulating state in $\tilde{\mu}/U_0 - J/U_0$ space this gap energy can be seen to be the distance in $\tilde{\mu}$ direction at fixed $J_0$, from the upper boundary $\tilde{\mu}_+(J_0)$ (particles) or lower (holes) phase boundary $\tilde{\mu}_-(J_0)$. The extra particles added to the system are for $\tilde{\mu} \neq kU_0$ well described by a Bogoliubov model and travel as a dilute Bose fluid on the top of the virtually inert background density [79].

The onset of superfluidity is described by mean field like exponents. In the Mott phase the chemical potential is ambiguous and thus the correlation length $\xi(\tilde{\mu}, J_0)$ is independent of $\tilde{\mu}$ even at $J_{0,c}(\tilde{\mu})$ where it does not diverge and thus partly reminds of a first order transition [79]. If $\tilde{\mu}$ however is fixed to an integer multiple of the on site interaction $U_0$ the transition is a completely different one. Tuning $J_0$ through the value $J_0 = J_{0,c}(\tilde{\mu} = kU_0) = J_{0,c}(0)$ the correlation length diverges as $\xi \sim (J_0 - J_{0,c})^{-\nu_{XY}}$ where $\nu_{XY}$ is the critical exponent of the $(d + 1)$ dimensional XY-model [28]. The cardinal difference between the case of fixed density $\tilde{\mu} = kU_0$ and the previous one is, that at these points $H_J$ is exact particle-hole symmetric. The superfluid fluctuations come from within the background and off-diagonal long range order is established through particles and holes equally subduing the on site repulsion $U_0$ [79].

**Effects of Disorder**

Consider the case of, bounded uniform weak disorder $-\Delta \leq \delta \tilde{\mu}_i \leq \Delta$ where $\Delta < U_0/2$. The on-site energy

$$\epsilon(n_i) = -(\tilde{\mu} + \delta \tilde{\mu}_i) n_i + \frac{1}{2} U_0 n_i^2$$

becomes position dependent. The activation energies become

$$\delta E_{p,i} = \frac{2n_i + 1}{2} U_0 - \delta \tilde{\mu}_i - \tilde{\mu}$$

$$\delta E_{h,i} = \frac{1 - 2n_i}{2} U_0 + \delta \tilde{\mu}_i + \tilde{\mu}$$

for particles and holes respectively. In analogy to the case without disorder minimizing the energy at site $i$ yields the optimal occupation $n_{0,i} = \tilde{\mu}/U_0 + \delta \tilde{\mu}_i/U_0$. At $J_0 = 0$ one thus expects regions around the values $\tilde{\mu} = \tilde{\mu}_{2k} = kU_0$, in which the system is a Mott insulator and the particle number is fixed to some integer $k$. These
incompressible regions will however be smaller than in the case of a pure system. The disorder implies that at site \( i \) for \( \tilde{\mu} > (k + \frac{1}{2}) U_0 - \delta \tilde{\mu}_i \) the system becomes unstable for the creation of particles. In the same way for \( \tilde{\mu} < (k - \frac{1}{2}) U_0 - \delta \tilde{\mu}_i \) the system becomes unstable with respect to the creation of holes. The net effect after performing the disorder average and considering all sites is, that at \( J_0 = 0 \) the \( \tilde{\mu} \) axis splits up into intervals of width \( U_0 - 2\Delta \) centered around the positions \( \tilde{\mu}_i \) for integer \( k \). For any \( \tilde{\mu} \) within these intervals there are exactly \( k \) bosons occupying each site. As a result of the random disorder, gaps of width \( 2\Delta \) occur between these intervals for \( ((k - \frac{1}{2}) U_0 - \Delta) < \tilde{\mu} < ((k - \frac{1}{2}) U_0 + \Delta) \). There, the occupation number varies between \( k \) and \( k - 1 \) for different sites, depending on the value of \( \delta \tilde{\mu}_i \). If \( J_0 \) is increased to a finite positive value much smaller than \( U_0 \) the effect is again, that the energy gained by adding and delocalizing the particle cannot compensate the repulsive interaction contribution. Thus, again, there are finite regions in \( \tilde{\mu} - J_0 \) space, where the incompressible Mott insulating state strictly is conserved. Now, however, the transition between the isolating, incompressible Mott state and the superfluid state, always goes via the insulating but compressible Bose-glass \([54, 79]\). For nonzero \( \Delta \), particle-hole symmetry is locally broken everywhere even for \( \tilde{\mu} = \tilde{\mu}_k \). Nevertheless, it is statistically conserved in these points. Tuning \( J_0 \) through the critical value at these loci the superfluid onset is in the universality class of the \((d + 1)\) dimensional XY-model with columnar bond disorder \([79, 77]\).

### 3.3 Field-Theoretic Representation

To derive some scaling properties of the dirty boson Hamiltonian, it is most convenient to choose a functional integral formulation \([28]\). The dirty boson GLW functional is directly obtained by combining Eqs (3.1), (1.21) and replacing the lattice operators \( \hat{\Phi}_j, \hat{\Phi}_i^\dagger \) by their continuum counterparts \( \psi(x, \tau), \psi^\dagger(x, \tau) \). Then evaluation in a coherent state representation gives

\[
\mathcal{L}_B = \int d^d x \int_0^\beta d\tau \left\{ -J \psi^\dagger \nabla^2 \psi - K \psi^\dagger (\partial_\tau - \mu(x))^2 \psi + r_0 |\psi|^2 + u_0 |\psi|^4 \right\} \quad (3.7)
\]

where now for simplicity only \( \mu(x) = \mu + \delta \mu(x) \) includes quenched random disorder. It is a continuum approximation to the lattice Josephson Lagrangian

\[
\mathcal{L}_J = -\int_0^\beta d\tau \left\{ \sum_{i,j} \tilde{J}_{ij} \cos[\phi_i(\tau) - \phi_j(\tau)] \right. \\
+ \left. \frac{1}{2} \sum_{i,j} (U^{-1})_{ij} \left[ i\dot{\phi}_i(\tau) + \tilde{\mu} - \delta \tilde{\mu}_i \right] \left[ i\dot{\phi}_j(\tau) + \tilde{\mu} - \delta \tilde{\mu}_j \right] \right\} \quad (3.8)
\]

The procedure is outlined in detail in the appendix of reference \([79]\).
3.4 The Equality $z = d$

A widely discussed and numerically probed question was the exact value of the dynamic critical exponent $z$ in $d$ dimensions. It was motivated that in any dimension the critical exponent had to fulfill $z = d$ [28]. As discussed in section 1.4 the value of $z$ marks the relative divergence of the temporal and spatial correlation lengths

$$\xi_\tau \propto \xi^z$$  \hspace{1cm} (3.9)

In $d = 1$ this has been shown to be correct [28] but in $d = 2$ there have only been a series of arguments that equated $z$ to the number of spatial dimensions and some numerical work that in the majority of cases assumed $z = 2$ [70, 77]. With respect to the system-sizes considered there was a very good agreement with the prediction [3]. Recently different numerical work without a priori assumptions suggested $z = 1.40 \pm 0.02$ [57] by far smaller than predicted. Weichman and Mukhopadhyay argued that their might in fact not be any simple scaling argument restricting the value of $z$ [79, 78].

Scaling Arguments

As outlined in section 2.7 phase gradients $\nabla \phi$ in the order parameter imply an increment of

$$\Delta f_x = \left( \frac{\Upsilon}{2\beta V} \right) \int_0^\beta d\tau \int d^d x |\nabla \phi(x, \tau)|^2$$ \hspace{1cm} (3.10)

to the free energy. Since $\nabla \phi$ has dimensions of inverse length it should scale as $\xi^{-1} \propto |\delta|^\nu$. The singular part of the free energy scales as

$$f_s \sim \xi^{-d} \xi_\tau^{-1} \sim |\delta|^{\nu(d+z)} \sim \delta^{2-\alpha} \sim \Upsilon \delta^{2\nu} \Leftrightarrow \Upsilon \sim \delta^{2-\alpha-2\nu}$$ \hspace{1cm} (3.11)

where the hyperscaling relation $2 - \alpha = (d + z)\nu$ has been used. Thus

$$\Upsilon \sim \delta^{(d+z-2)\nu}$$ \hspace{1cm} (3.12)

Phase twists in the imaginary time direction are equally punished by an increase in the free energy. These twists couple to the chemical potential. It is thus possible to define the compressibility as a helicity modulus in the imaginary time direction [77]. Temporal twists contribute

$$\Delta f_\tau = \left( \frac{\kappa}{2\beta V} \right) \int_0^\beta d\tau \int d^d x (\partial_\tau \phi)^2$$ \hspace{1cm} (3.13)

to the free energy, leading to the scaling relation

$$\delta^{2-\alpha} \sim \kappa \delta^{2\nu} \Leftrightarrow \kappa \sim \delta^{(d-z)\nu}$$ \hspace{1cm} (3.14)

where the same hyperscaling argument as above has been exploited. If the system goes through a phase transition from a Bose glass to superfluid $\partial n/\partial \mu$ and therefore
the compressibility is finite and nonzero on either site of the critical point. The conjecture then was that this at $\delta = 0$ requires $z = d$.

For the above argument Weichman and Mukhopadhyay [79] pointed out that it only can be valid if the temporal or spatial phase twists contribute to the singular part of the free energy. Their suggestion was that the free energy increment $\Delta f$ shall only be included in the singular part if the corresponding twisted boundary condition breaks a fundamental symmetry of the model [79]. The superfluid transition as outlined before occurs with increasing hopping strength $J$ at a given $J_c(\mu)$ which makes it convenient to choose

$$\delta = (J - J_c(\mu))/J_c(\mu).$$

Time derivatives and chemical potential are included in the combination $\partial_\tau - \mu$. This is important for their arguments.

To derive the scaling properties of the superfluid density and the compressibility one needs to calculate the response of the Lagrangian (3.7) to twisted boundary conditions as discussed in section 2.7. Twisting the system in $\alpha$-direction implies that

$$\psi(x + L_\alpha \vec{e}_\alpha) = e^{i \Theta_\alpha} \psi(x), \quad |\Theta_\alpha| \leq \pi$$  

where $x = (\tau, x)$ and $\vec{e}_\alpha$ for $\alpha = 0, 1, \ldots, d$ are space-time unit vectors. As usually, the length in time direction is $L_0 = L_\tau = \beta$ and $L_\alpha, \alpha > 0$ denotes the dimension of the system along the unit vector $\vec{e}_\alpha$. Expressing the relative phase twists as $\omega_0 = \Theta_0/\beta$ and $k_0 = (\Theta_1/L_1, \ldots, \Theta_d/L_d)$ it is obvious that

$$\ddot{\psi}(x) = e^{-i k_0 x - i \omega_0 \tau} \psi(x)$$  

obeys periodic boundary conditions. If $\ddot{\psi}_0 = \langle \ddot{\psi}(x) \rangle$ is uniform then the order parameter becomes

$$\langle \psi(x) \rangle = e^{i k_0 x + i \omega_0 \tau} \ddot{\psi}(x)$$  

and has a uniform phase twist. The twisted Lagrangian becomes

$$\mathcal{L}^{\omega_0 k_0} [\ddot{\psi}; \mu, r_0] = \mathcal{L} [\ddot{\psi}; \mu - i \omega_0, r_0 + Jk_0^2] + k_0 \mathcal{P} [\ddot{\psi}]$$

where $\mathcal{P} [\ddot{\psi}] = -i J \int d^d x \int d\tau \left[ \ddot{\psi}^* \nabla \ddot{\psi} - \text{c.c.} \right]$ [79]. The free energy in presence of the phase twist is

$$\mathcal{F}^{\omega_0 k_0} = - (\beta V)^{-1} \left[ \ln \left( e^{-\mathcal{L}^{\omega_0 k_0}} \right) \right]$$

where $[\ldots]$ denotes disorder averaging with respect to realizations of $\delta \mu(x)$ and $V = \prod_{\alpha \neq 0} L_\alpha$. The key now lies in understanding the differences between the effects of a pure spatial phase twist and a pure temporal phase twist. Distorting along one
of the directions $\alpha = 1 \ldots d$ and using Eqs (1.6) and (3.19) yields

$$\Delta f_{\alpha} = f^{k_0} - f^0 = \left[ \ln \left( 1 + \frac{\delta Z}{Z} \right) \right]$$

$$= -\frac{1}{\beta V} \left[ \langle \delta L \rangle + \frac{1}{2} \langle \delta L^2 \rangle - \frac{1}{2} \langle \delta L \rangle^2 \right]$$

$$= \frac{1}{2} T k_0^2 + O(k_0^4) \quad (3.20)$$

where $\delta L = L^{k_0} - L$, $\delta Z = Z^{k_0} - Z$ and all statistical averages are evaluated under periodic boundary conditions. There are no terms linear in $k_0$ left in the free energy increment as $\langle P \left[ \bar{\psi} \right] \rangle$ vanishes under periodic boundary conditions. If $k_0 = 0$, then by using the dependence of $L^{\omega_0 k_0}$ on $\omega_0$ one has [79]

$$f^{\omega_0}(\mu) = f(\mu - i\omega_0) \quad (3.21)$$

as also outlined in section 3.1. Expanding around $\omega_0 = 0$ gives

$$\Delta f = i\omega_0 \rho + \frac{1}{2} k_0^2 + O(\omega_0^2) \quad (3.22)$$

Only in the case of $\mu(x) = 0$ is $L$ invariant under time inversion, which then is broken by the twist $\omega_0$. For non-vanishing $\mu$ this symmetry already has been broken by $\mu$ itself and a phase twist in the temporal direction only corresponds to a smooth variation of the chemical potential [78, 79].

### 3.5 Scaling at the Dirty Boson Critical Point

For $\mu = 0$ the classical $(d + 1)$-dimensional XY-model is obtained and $L$ is invariant under both time inversion and space inversion. The compressibility $\kappa$ should vanish in the disordered phase and be finite in the ordered phase. This can most easily be checked by the interpretation of $\kappa$ as the temporal helicity modulus $\Upsilon$, and the fact that the $(d + 1)$ dimensional XY-model is isotropic. The twists have dimensions of inverse length. For the singular part of the free energy one therefore can make the scaling ansatz [79]

$$\Delta f^{k_0 \omega_0} \approx \beta^{-1} L^{-d} \Phi_0^{k_0 \omega_0} \left( A_0 \delta L^{1/\nu_0}, B_0 \delta \beta^{1/\zeta_0} \right) \quad (3.23)$$

where $\nu_0, \zeta_0$ are the critical exponents of the pure $(d+1)$-dimensional XY-model. For nonzero helicity modulus one desires that the boundaries imply corrections of order $L^{-2}$ and $\beta^{-2}$. This can be achieved by requiring

$$\Phi_0^{k_0 \omega_0}(x, y) \approx x^{\nu_0} y^{\zeta_0} \left( Q_xx^{-2\nu_0} + Q_\tau y^{-2\zeta_0} \right) \quad (3.24)$$
CHAPTER 3. THE DIRTY BOSON MODEL

where the prefactor compensates for the $L^{-d} \beta^{-1}$ term in (3.23) without altering the scaling form. For large values of $x, y > 0$ resubstituting the above definitions and using $(k_0)_\alpha = \theta_\alpha/L_\alpha$ gives

$$\Upsilon \approx A_0^{(d-2)\nu_0} B_0^{\nu_0} \left( Q_x/\Theta_x^2 \right) \delta^{\nu_0}$$

(3.25)

$$\kappa \approx A_0^{d\nu_0} B_0^{-2\nu_0} \left( Q_0/\Theta_0^2 \right) \delta^{\nu_0}$$

(3.26)

where $\Theta_x^2 = \Theta_1^2 + \cdots + \Theta_d^2$ [79]. Thus the Josephson scaling relations in $D = d + z_0$ dimensions are received

$$\nu_0 = (d + z_0 - 2) \nu_0 = 2 - \alpha_0 - 2\nu_0$$

(3.27)

$$\nu_{\tau_0} = (d - z_0\nu_0) = 2 - \alpha_0 - 2z_0\nu_0$$

(3.28)

and $Q_{x0} \propto \Theta_x^2$ has to hold.

At the Bose glass to superfluid transition one comes across a different situation. Both $\rho$ and $\kappa$ are smooth functions of $\mu$ in each respective phase. At finite $\mu$ a temporal twist only minimally changes the particle-hole symmetry-breaking term included in $\mathcal{L}$. Spatial twists however enter in the very same way as above for $\omega_0 = 0$. The scaling form of Eq. (3.23) now implies

$$\Delta f^{k_0} \approx \beta^{-1} L^{-d} \Phi^{k_0} \left( A\delta L^{1/\nu}, B\delta^{1/\nu} \right)$$

(3.29)

where again in order to get the appropriate leading terms

$$\Phi^{k_0} (x, y) \approx R_x x^{(d-2)\nu} y^{\nu}$$

(3.30)

which for large $x, y > 0$ yields

$$\Upsilon \approx A^{(d-2)\nu} B^{\nu} \left( R_x/\Theta_x^2 \right) \delta^{\nu}$$

(3.31)

where $v = (d+z-2)\nu = 2 - \alpha - 2\nu$. Again $R_x \propto \Theta_x^2$ and all exponents are those of the dirty Boson critical point. As there are no twisted boundary conditions imposed along the time direction, no $O (\beta^{-1}, \beta^{-2})$ appear in the free-energy increment. Finally, including a temporal phase twist $\omega_0$ has the net effect of shifting $\mu \rightarrow \mu - i\omega_0$ and the occurrence of extra $\beta$-boundary conditions in (3.29). The free energy increment then turns out to be

$$\Delta f^{k_0} = \beta^{-1} L^{-d} \Phi^{k_0} \left( A\delta L^{1/\nu}, B\delta^{1/\nu} \right)$$

(3.32)

$$+ f_a \left( J, r_0 + Jk_0^2, \mu - i\omega_0 \right) - f_a \left( J, r_0, \mu \right)$$

where $\delta_\theta = J - J_x (\mu - i\omega_0) \approx \delta + i\omega_0 J_x^\prime (\mu)$ and $f_a$ denotes the analytic part of the free energy [79]. But $\Phi^{k_0}$ is still given by Eq. (3.29) and therefore is unable to give rise to $O (\beta^{-1}, \beta^{-2})$ corrections [78, 79]. So with the above reasoning Weichman et al. conclude that the only ways that $\rho$ and $\kappa$ can pick up these temporal corrections are:
3.6. DUAL REPRESENTATION OF THE JOSEPHSON LAGRANGIAN

1. through a possible $\omega_0$ dependence of $\delta_{0a}$ which couples derivatives with respect to $\mu$ or equally well $\omega_0$ to derivatives with respect to $\delta$ yielding the dominating singular behavior

$$\kappa_s \propto |\delta|^{-\alpha}$$  \hspace{1cm} (3.33)

which for $\alpha < 0$ becomes negligible at $\delta = 0$

2. through $f_a$

So far simulations of the problem including the one presented here seem to be well consistent with $z > 1$ and $\nu \geq 1$ [4, 77, 57]. Thus

$$\alpha = 2 - (d + z)\nu < 0$$  \hspace{1cm} (3.34)

for $d \geq 2$. This suggests strongly that $\kappa$ amounts from the analytic part of the free energy. Without any spatial phase twist the analytic part in the free energy therefore becomes [79]

$$f_a (J, \mu) = -\rho_c (J) [\mu - \mu_c (J)] - \frac{1}{2} \kappa_c (J) [\mu - \mu_c (J)]^2 + \ldots$$  \hspace{1cm} (3.35)

close to the transition line $\mu_c (J)$. This means that Eq. (3.32) leads to a finite $\kappa$ through the transition without imposing any restrictions on $z$.

### 3.6 Dual Representation of the Josephson Lagrangian

In the 1970’s Villain [75] came up with a transformation for the planar XY-model that mapped it onto a model of integer variables residing on a dual lattice. His method has been widely used for vortex systems as it integrates out the spin wave degrees of freedom leaving only the Coulomb gas [39, 77].

**Derivation**

Starting with the periodic potential $V (\theta_i - \theta_j) = -K [1 - \cos \theta_i - \theta_j]$ of the XY-model and using that any periodic and differentiable function $V (\theta)$ can be expressed as a Fourier expansion

$$f (\theta) := e^{V (\theta)} = \sum_{s = -\infty}^{\infty} c_s e^{is\theta}$$  \hspace{1cm} (3.36)

The coefficients are given by

$$c_s = e^{-\bar{V} (s)} = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{-is\theta} e^{-V (\theta)} = e^{-K I_s (K)}$$  \hspace{1cm} (3.37)

where $I_s (K)$ denotes a Bessel function. With the help of the Poisson summation formula [39] known from elementary Fourier analysis

$$\sum_{s = -\infty}^{\infty} g (s) = \sum_{m = -\infty}^{\infty} \int_{-\infty}^{\infty} d\Phi g (\Phi) e^{-2\pi im\Phi}$$  \hspace{1cm} (3.38)
and by defining $e^{V_0(\theta)} = \int_{-\infty}^{\infty} d\Phi e^{\tilde{V}(\Phi)} + i\Phi \theta$ as a Fourier integral. Eq. (3.36) now reads

$$
e^{V(\theta)} = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{\infty} d\Phi e^{i\Phi \theta + \tilde{V}(\Phi) - 2\pi m \Phi} = \sum_{m=-\infty}^{\infty} e^{V_0(\theta - 2\pi m)}$$

(3.39)

The good news now is that even if $V_0(\theta)$ itself is not periodic the summation over the index $m$ in (3.39) automatically ensures periodicity [39]. Villain [75] chose to approximate the $[1 - \cos \theta]$-term by its lowest order series expansion. Thus in his approximation $V_0(\theta)$ and $V(\Phi)$ are given by

$$V_0(\theta) = -\frac{1}{2} K \theta^2$$

(3.40)

and

$$\tilde{V}(\Phi) = -\frac{\Phi^2}{2K}$$

(3.41)

Duality Mapping of the Lattice Josephson Hamiltonian

With Eq. (3.39) and the Villain approximation Eq. (3.40) of the cos-term in the lattice Josephson Lagrangian $L_J[\phi]$ given by Eq. (3.8) we can define the Villain form $L_{JV}[\phi, \mathbf{m}]$ by

$$e^{-L_J[\phi]} = \sum_{\mathbf{m}} e^{-L_{JV}[\phi, \mathbf{m}]}$$

(4.42)

$$L_{JV}[\phi, \mathbf{m}] = \frac{1}{2} \sum_{\mathbf{r}, \alpha \neq 0} \left( \partial_\alpha \phi_\mathbf{r} - 2\pi m_\mathbf{r}^\alpha \right)^2$$

$$+ \frac{1}{2} \sum_{ij, \tau} (V^{-1})_{ij} \left( \partial_\tau \phi_{i\tau} - i\nu_i - 2\pi m_{i\tau}^0 \right) \times (\partial_\tau \phi_{j\tau} - i\nu_j - 2\pi m_{j\tau}^0)$$

(3.43)

where $\partial_\alpha \phi_\mathbf{r} = (\phi_{\mathbf{r}+\hat{\alpha}} - \phi_\mathbf{r})$ is the finite difference “derivative” and $\mathbf{m}_\mathbf{r} = (m_\mathbf{r}^1, m_\mathbf{r}^2, \ldots, m_\mathbf{r}^d)$ a $(d+1)$-dimensional integer vector field sitting at each lattice site $\mathbf{r} = (i, \tau)$. The index $\alpha = 0, 1, \ldots, d$ denotes the $(d+1)$-unit bond directions adjacent to each site, where $\alpha = 0$ is the $\tau$-direction. The coupling constants $K_\alpha$, $V_{ij}$ and $\nu_i$ correspond to $J_{ij} \Delta \tau$, $U_{ij} \Delta \tau$ and $\mu_i \Delta \tau$ in the original model Eq. (3.8). Substituting
\( \theta^a_r = \phi_{r+\hat{a}} - \phi_r \) the partition function is given by

\[
Z = \text{tr} \left\{ e^{-L_J[\phi]} \right\} = \int D\phi \left( \prod_{r, \alpha \neq 0} \sum_{\{m^\alpha_r = -\infty\}} e^{-\frac{1}{2} K^\alpha_r (\theta^a_r - 2\pi m^\alpha_r)^2} \right) \times \left( \sum_{\{m^\alpha_r = -\infty\}} e^{-\frac{1}{2} \sum_{i,j,r} (V^{-1})_{ij} (\theta^0_{ij} - i\nu_i - 2\pi m^0_{ij}) \times (\theta^0_{ij} - i\nu_j - 2\pi m^0_{ij})} \right)
\]

(3.44)

First consider \( I_r \) by a straightforward generalization of the Poisson sum rule Eq. (3.38)

\[
I_r = \prod_{r, \alpha \neq 0} \sum_{\{m^\alpha_r = -\infty\}} e^{-\frac{1}{2} K^\alpha_r (\theta^0_r - 2\pi m^0_r)^2} = \prod_{r, \alpha \neq 0} \sum_{\{m^\alpha_r = -\infty\}} \int d\Phi^\alpha_r e^{-2\pi i n^\alpha_r \Phi^\alpha_r - \frac{1}{2} K^\alpha_r (\theta^0_r - 2\pi \Phi^\alpha_r)^2}
\]

(3.45)

\[
= \sum_{\{m^\alpha_r = -\infty\}} \prod_{r, \alpha \neq 0} \frac{1}{\sqrt{2\pi K^\alpha_r}} e^{-i n^\alpha_r (\phi_{r+\alpha} - \phi_r)} e^{-\frac{1}{2} n^\alpha_r M^\alpha_r}
\]

Here the standard complex Gaussian integral

\[
\int_{-\infty}^{\infty} du e^{i m u} e^{-\frac{1}{2} K (u+i v)^2} = \frac{1}{\sqrt{2\pi K}} e^{-m v - m^2/2 K}
\]

(3.46)

has been used. In the same way the interaction part can be attacked

\[
I_r = \sum_{\{m^\alpha_r = -\infty\}} e^{-\frac{1}{2} \sum_{i, j, r} (V^{-1})_{ij} (\theta^0_{ij} - i\nu_i - 2\pi m^0_{ij}) (\theta^0_{ij} - i\nu_j - 2\pi m^0_{ij})} = \sum_{\{m^\alpha_r = -\infty\}} \int d\Phi^0_r e^{-2\pi i n^0_r \Phi^0_r} e^{-\frac{1}{2} \sum_{i, j, r} (V^{-1})_{ij} (\theta^0_{ij} - i\nu_i - 2\pi \Phi^0_r) (\theta^0_{ij} - i\nu_j - 2\pi \Phi^0_r)}
\]

(3.47)

\[
= \sum_{\{m^\alpha_r = -\infty\}} e^{-\frac{1}{2} n^0_r \sum_{i, j, r} (v_i + (\phi_{i+\hat{r}} - \phi_{i, r})) n^0_{i, r}}
\]

where the multivariate generalization of Eq. (3.46)

\[
\int \frac{du^n}{(2\pi)^n} e^{-\frac{1}{2} \sum_{i, j = 1}^{\infty} A_{i j} (u_{i, j - m_{ij}}) (u_{i, j - m_{ij}}) + \sum_{i = 1}^{\infty} B_i u_i} = \frac{1}{\sqrt{\det (2\pi A)}} e^{\frac{i}{2} B^T A^{-1} B + B^T m}
\]

(3.48)
has been applied. The total partition function thus can be written as

\[ Z = \frac{1}{\mathcal{M}} \sum_{n=\infty}^{\infty} \prod_{l} \int_{0}^{2\pi} d\phi l^{2} \pi e^{-\sum_{r,\alpha} n^{\alpha}_{r}(\phi_{r+\alpha} - \phi_{r}) - \tilde{\mathcal{L}}_{J}[n]} \]  

(3.49)

where the normalization factor is given by

\[ \mathcal{M} = \sqrt{\det(2\pi \mathbf{V})} \prod_{i,\tau,\alpha \neq 0} \frac{2\pi}{K_{i}^{\alpha}} \]  

(3.50)

and the dual Lagrangian

\[ \tilde{\mathcal{L}}_{J}[n] = \frac{1}{2} \sum_{i,\tau,\alpha \neq 0} \left( \frac{n^{\alpha}_{r}}{K_{i}^{\alpha}} \right)^{2} + \frac{1}{2} \sum_{i,j} V_{ij}n^{0}_{i\tau}n^{0}_{j\tau} - \sum_{ir} \nu_{i} n^{0}_{i\tau} \]  

(3.51)

has been defined. Integrating over the phases in Eq. (3.49) yields the divergence free condition

\[ \nabla \cdot n_{r} = \sum_{\alpha} (n^{\alpha}_{r} - n^{\alpha}_{r-\hat{\alpha}}) = 0 \]  

(3.52)

meaning that there is no net flow to or from any of the sites on the \((d+1)\)-dimensional lattice. The partition function then becomes

\[ Z = \frac{1}{\mathcal{M}} \prod_{n} \prod_{r} \delta \nabla \cdot n_{r} \delta \tilde{\mathcal{L}}_{J}[n] \]  

(3.53)

If all couplings \(K_{i}^{\alpha}\) are chosen to be isotropic and the interaction potential is set to on-site repulsive including disorder we can re-substitute the parameters \(K_{i}^{\alpha}, V_{ij}\) and \(\nu_{i}\) by the original ones \(J_{ij}\Delta \tau, U_{ij}\Delta \tau\) and \(\mu_{i}\Delta \tau\) from the original Hamiltonian the \(J\)-current model of Wallin et al. [77] emerges

\[ H_{V} = \frac{1}{K} \left[ \sum_{r,\alpha} \frac{1}{2} \left( J_{r}^{\alpha} \right)^{2} - \sum_{r} (\tilde{\mu} + \delta \tilde{\mu}) J_{r}^{\alpha} \right] \]  

(3.54)

\[ Z = \text{tr} \left\{ \delta \nabla \cdot J e^{-H_{V}} \right\} \]  

(3.55)

In this imaginary time representation \(J_{r}^{\alpha}\) represents the boson density of the problem which only treats the phase fluctuations of the underlying Hamiltonian \(H_{J}\). The random on-site potential is chosen to be uniformly bounded between \(-\tilde{\Delta} < \tilde{\nu}_{i} < \tilde{\Delta}\). The dual Lagrangian is entirely real. In addition the closed loop property makes it ideal for numerical investigation by means of the classical worm algorithm invented by Prokof’ev and Svistunov [59].
Chapter 4

Monte Carlo Methods

4.1 Classical Monte Carlo

In classical Monte Carlo simulations one normally is interested in the calculation of the equilibrium expectation value $\langle Q \rangle$ of some physical observable $Q$ [52]

$$
\langle Q \rangle = \frac{\sum_{\mu} Q_{\mu} e^{-\beta E_{\mu}}}{\sum_{\mu} e^{-\beta E_{\mu}}} \quad (4.1)
$$

The index $\mu$ denotes one of the possible configurations in the set $\{X_{\mu}\}$ of possible states that the system might be in and $E_{\mu} = E(X_{\mu})$ its energy. Simulations usually only can cover a subset of the theoretically accessible configurations. This set has to be chosen at random according to a probability distribution $P(X_{\mu})$. The estimator with respect to the subset of states sampled then is given by

$$
Q_M = \frac{\sum_{i=1}^{M} Q_{\mu_i} P(X_{\mu_i})^{-1} e^{-\beta E_{\mu_i}}}{\sum_{j=1}^{M} P(X_{\mu_j})^{-1} e^{-\beta E_{\mu_j}}} \quad (4.2)
$$

By increasing $M$, the number of states considered in the calculation of the estimator, one should obtain the limit $Q_M \xrightarrow{M \to \infty} \langle Q \rangle$. A proper and effective choice of this probability distribution is at the heart of any Monte Carlo algorithm. The sum giving $\langle Q \rangle$ is dominated by only a small fraction of the total number of theoretically accessible configurations. The remaining ones contribute only a negligible part to it, especially at temperatures close to zero. The technique of importance sampling accommodates for this.

Importance Sampling

In the canonical ensemble, the probability for a physical system to be in a certain state is Boltzmann distributed. So instead of choosing all $M$ states with equal
probability one chooses
\[ P(X_\mu) = \frac{e^{-\beta E_\mu}}{Z} \]  
(4.3)

Z in general is the canonical partition function given by Eq. (1.6) with \( H = \beta H \).

In the case that the Hamiltonian \( H \) is time independent \( Z \) becomes
\[ Z = \sum_\mu e^{-\beta E_\mu} \]  
(4.4)

The estimator \( Q_M \) then simply is given by
\[ Q_M = \frac{1}{M} \sum_{i=1}^{M} Q_{\mu_i} \]  
(4.5)

Any canonical Monte Carlo algorithm needs to pick the states in a way which ensures that they occur with their correct Boltzmann probability.

**Markov Processes and Ergodicity**

The generation of an appropriate set of states is a highly non trivial task. Choosing states randomly and accepting or rejecting them with the correct Boltzmann probability is highly inefficient as nearly all generated configurations would be rejected. Markov processes provide a mechanism that dictates how a system will do transitions between two states \( X_\mu \) and \( X_\nu \). Those transitions are random in a way that given \( X_\mu \), the system will, not necessarily always, create the same trial state \( X_\nu \). As the transition probabilities \( W(X_\nu | X_\mu) \) are classical probabilities they need to fulfill
\[ 0 \leq W(X_\nu | X_\mu) \leq 1 \]  
(4.6)
\[ \sum_\nu W(X_\nu | X_\mu) = 1 \]  
(4.7)

whereas \( W(X_\mu | X_\nu) \) does not necessarily need to vanish. In addition \( W(X_\nu | X_\mu) \) obeys

1. \( W(X_\nu | X_\mu) \) is time independent.
2. \( W(X_\nu | X_\mu) \) is only dependent on the current states \( \mu \) and \( \nu \) and not on any other states, the system eventually went through before.

The Markov chain used in Monte Carlo simulations is designed in such a way that it will eventually produce a sequence of states which appear with probabilities given by the Boltzmann distribution, thereby equilibrating the system. One condition that has to be imposed on all such possible Monte Carlo algorithms is the condition of ergodicity. This means that starting off from any possible state, the Markov
4.1. CLASSICAL MONTE CARLO

Process should be able to reach any other state of the system in finite time. This is a necessity in order for all states to appear with their respective Boltzmann probability. There is however a big freedom in how one can tweak the transition probabilities. Many of them can be chosen to be zero but there has to be at least one single path connecting any two states of the system.

Detailed Balance

In equilibrium the rate at which the system makes transitions into and out of any state \( \mu \) must be equal:

\[
\sum_{\nu} P(X_{\nu}) W(X_{\nu}|X_{\mu}) = \sum_{\nu} P(X_{\mu}) W(X_{\mu}|X_{\nu})
\]  

Using the normalization condition from Eq. (4.7) this is equivalent to

\[
P(X_{\mu}) = \sum_{\nu} P(X_{\nu}) W(X_{\mu}|X_{\nu})
\]  

The probability distribution \( P(X_{\mu}) \) will be an equilibrium distribution of the dynamics of the Markov process for any set of transition probabilities satisfying Eq. (4.9). This is however not enough to ensure that the generated states are distributed according to the Boltzmann distribution. It would be possible that the process reaches a dynamical equilibrium where the same probability distribution is obtained in a limit cycle after a certain number \( n \) of steps. By imposing the detailed balance condition

\[
P(X_{\mu}) W(X_{\nu}|X_{\mu}) = P(X_{\nu}) W(X_{\mu}|X_{\nu})
\]  

this problem is avoided and Eq. (4.9) is still fulfilled. By imposing the detailed balance condition on the Markov process this process can be made to tend to any distribution \( P(X_{\mu}) \) simply by adjusting the transition probabilities satisfying (4.10). In the Boltzmann case this leads to

\[
\frac{W(X_{\nu}|X_{\mu})}{W(X_{\mu}|X_{\nu})} = \frac{P(X_{\nu})}{P(X_{\mu})} = e^{-\beta (E_{\nu} - E_{\mu})}
\]  

For an equilibrium simulation the constraints on the transition probabilities \( W(X_{\nu}|X_{\mu}) \) finally are given by Eqs. (4.7), (4.11) and ergodicity.

Acceptance Probabilities

The constraints discussed in the last section leave a lot of freedom to the actual design of the Monte Carlo algorithm. By breaking down the transition probabilities into two parts one can tremendously improve the efficiency of the algorithm. First of all \( W(X_{\mu}|X_{\nu}) \) can be set to a nonzero value. This gives further freedom to
adjust all the other transition probabilities. Principally one can for any two states \( X_\mu, X_\nu \) adjust \( W(X_\nu | X_\mu) \) and \( W(X_\mu | X_\nu) \) in such a way that they stay in the allowed parameter range \( W(X_\nu | X_\mu) \in [0,1] \) and that the changes compensate each other in the constraint of Eq. (4.7). Similarly \( W(X_\nu | X_\mu) \) and \( W(X_\mu | X_\nu) \) can be adjusted in a way that their ratio is preserved. This gives enough freedom to make the transition probabilities take any desired values by proper selection of \( W(X_\mu | X_\mu) \).

Writing

\[
W(X_\nu | X_\mu) = g(X_\mu \to X_\nu) \cdot A(X_\mu \to X_\nu) \quad (4.12)
\]

the selection probability and acceptance probability, \( g(X_\mu \to X_\nu) \) and \( A(X_\mu \to X_\nu) \), are defined. So generating a Monte Carlo algorithm can actually be seen as creating an algorithm that generates random new states \( X_\nu \) given old ones \( X_\mu \) according to the distribution of \( g(X_\mu \to X_\nu) \) and then accepts those states with the acceptance probability \( A(X_\mu \to X_\nu) \). Here one of the most important catches considering efficiency comes into play. In order to have an efficient program, the acceptance probabilities should be designed as close to unity as possible while the correlation between subsequent configurations are minimized. Otherwise the simulation just generates trial states that are rejected and do not enter the estimator calculation or states that are highly dependent. The condition (4.11) does only fix the ratio

\[
\frac{W(X_\nu | X_\mu)}{W(X_\mu | X_\nu)} = \frac{g(X_\mu \to X_\nu) A(X_\mu \to X_\nu)}{g(X_\nu \to X_\mu) A(X_\nu \to X_\mu)} \quad (4.13)
\]

meaning that \( A(X_\mu \to X_\nu) / A(X_\nu \to X_\mu) \) can take any desired positive value as well as both \( g(X_\mu \to X_\nu) \) and \( g(X_\nu \to X_\mu) \) can take any desired value. So multiplying the larger value of \( A(X_\mu \to X_\nu) \) and \( A(X_\nu \to X_\mu) \) by a positive number in such a way that the product becomes unity and adjusting the other acceptance ratio by the same multiplication, the acceptance ratios are made as large as possible while still obeying all constraints. The best thing to do in order to keep the acceptance ratios large is on the other hand to implement as much as possible of the dependence of \( W(X_\nu | X_\mu) \) on the states \( X_\mu, X_\nu \), in the selection probabilities \( g(X_\mu \to X_\nu) \) of the trial states. An ideal Monte Carlo algorithm is one that in a state \( X_\mu \) selects the states with exactly the right transition probability \( W(X_\nu | X_\mu) \) making the acceptance probability unity.

### 4.2 The Metropolis Algorithm

This is probably the most widely used Monte Carlo algorithm [52, 51]. Usually it is used for systems in which the interesting parameters are variables that live on a lattice such as Ising spins or continuous angles. The Metropolis approach is to choose all selection probabilities equal such that \( g(X_\mu \to X_\nu) \) becomes \( \frac{1}{N} \) on a lattice of \( N \) sites. As for many systems of interest the actual possible energies lie in a rather narrow region, the Metropolis method uses local updates of the site variables.
As the state of the whole system is characterized by the ensemble of the local site variable states, ergodicity is easily fulfilled. With the selection probabilities being constant the probability ratio simply becomes

\[
\frac{W(X_\nu|X_\mu)}{W(X_\mu|X_\nu)} = \frac{A(X_\mu \rightarrow X_\nu)}{A(X_\nu \rightarrow X_\mu)} = e^{-\beta(E_\nu - E_\mu)} \tag{4.14}
\]

For maximum efficiency the acceptance probability has to be maximized. For the Boltzmann distribution if \(E_\mu > E_\nu\) then \(W(X_\nu|X_\mu) > W(X_\mu|X_\nu) \Rightarrow A(X_\mu \rightarrow X_\nu) > A(X_\nu \rightarrow X_\mu)\). By setting \(W(X_\nu|X_\mu) = 1\) and adjusting \(W(X_\mu|X_\nu)\) such that (4.14) is obeyed the optimal Metropolis choice of the acceptance probabilities is

\[
A(X_\mu \rightarrow X_\nu) = \begin{cases} e^{-\beta(E_\nu - E_\mu)} & \text{if } E_\nu - E_\mu > 0 \\ 1 & \text{else} \end{cases} \tag{4.15}
\]

### 4.3 The Wolff Algorithm

The problem for local update schemes like the Metropolis algorithm is that they suffer from critical slowing down. The number of effectively sampled independent measurements is \(N_{\text{eff}} = \frac{N_{\text{samples}}}{2\tau}\) where \(\tau\) is the autocorrelation time. In local schemes \(\tau\) grows as the transition temperature is approached according to the power law

\[
\tau \sim \xi^z \sim t^{-\nu z} \tag{4.16}
\]

In 1989 Wolff showed that critical slowing down can be nearly eliminated by using a percolation inspired algorithm that allows the simulation of spin models with standard actions [83]. Consider for simplification a \(O(n)\) \(\sigma\) model like the Ising \((n = 1)\), XY \((n = 2)\) and Heisenberg \((n = 3)\) restricted to a cubic lattice with periodic boundary conditions. The algorithm can be sketched as follows. The partition function in those models is

\[
Z = \left\{ \prod_i \int \! d\sigma_i \right\} e^{\beta \sum_{\langle i,j \rangle} \sigma_i \cdot \sigma_j} \tag{4.17}
\]

where \(i\) denotes all lattice sites. The spin flip operation is generalized to a reflection with respect to a hyperplane orthogonal to some vector \(\mathbf{r}\) on the respective \(n\) dimensional unit sphere.

\[
R(\mathbf{r}) \sigma_i = \sigma_i - 2 (\sigma_i \cdot \mathbf{r}) \mathbf{r} \tag{4.18}
\]

The action in \(Z\) is of course invariant under a global application of this operation. The cluster update is now done as follows.

1. Choose a random lattice site \(i\) and a random reflection vector \(\mathbf{r}\).
2. Flip the seed spin \(\sigma_i\) according to Eq. (4.18).
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3. Check all bonds connecting site $i$ to its nearest neighbors $\{j\}$. The bond $\langle i,j \rangle$ is activated with probability

\[ P(\sigma_i, \sigma_j) = 1 - \exp\left(\min\{0, \beta J \sigma_i [1 - R(r) \sigma_j]\}\right) \]

\[ = 1 - \exp\left(\min\{0, \beta J (r \sigma_i)(r \sigma_j)\}\right) \] (4.19)

In case of activation the spin $j$ is flipped. All sites that have been joined to the cluster are saved in a list.

4. Consider the last saved element on the list and continue with step 3 until the list is empty.

This update scheme clearly obeys ergodicity as there is a finite probability that just one $\sigma_i$ is flipped. This would be the limiting case of a Metropolis scheme. The transition probabilities obey [83]

\[ \frac{W(\{\sigma'_i\} | \{\sigma_i\})}{W(\{\sigma_i\} | \{\sigma'_i\})} = e^{\beta J \sum_{\langle i,j \rangle} (\sigma'_i \sigma'_j - \sigma_i \sigma_j)} \] (4.20)

Hence detailed balance is fulfilled.

4.4 The Worm Algorithm

If the configuration space of the considered model admits a “closed path” (CP) representation, the worm algorithm is an effective tool whose efficiency is similar to the best cluster methods at the critical point [59]. For the classical Ising, XY and Potts models, such a representation arises by performing a high temperature expansion. Elementary updates like removing or adding single plaquettes to the CP have the strong drawback that they cannot change loops winding around the system if periodic boundary are applied. Trying global updates proposing to add or remove a large loop stretching across the whole system suffers from the exponentially suppressed acceptance probability. The Worm algorithm has the big advantage that though being a local Metropolis scheme it is perfectly able to produce loops spanning across the whole system if the physical situation is favorable. The basic strategy of this updating scheme can be described as follows:

1. Disconnected loops CP$_g$ are added to the configuration space. If the two ends of such a graph happen to coincide a CP configuration is obtained. The CP$_g$ configurations are important to calculate correlation functions.

2. The CP$_g$ configurations are exclusively altered by local updates of the end points. No elementary loops or global lines are added.
4.4. THE WORM ALGORITHM

Implementation for the Classical Linkcurrent Model

Consider again a classical linkcurrent model of the dirty boson Hamiltonian \[77\]

\[
H_V = \frac{1}{K} \left[ \sum_{r,\hat{\alpha}} \frac{1}{2} (J_{\hat{\alpha}}^r)^2 - \sum_r (\tilde{\mu} + \delta\tilde{\mu}_i) J_{\hat{\alpha},\tau}^r \right] 
\]

(4.21)

\[
Z = \text{tr} \left\{ \delta \nabla \cdot J, 0 e^{-H_V} \right\} 
\]

(4.22)

There exist two different Monte Carlo updates.

1. **jump**: Beginning from a zero divergent configuration a site \( r \) on the \((d+1)\) dimensional lattice is randomly selected and the head and tail coordinate of the worm are simultaneously set to \( r \).

2. **move** A random bond direction \( \hat{\alpha} \) is chosen. The worm head is moved from its current position \( r \) to the corresponding neighboring site on the space time lattice. The current on the bond has to be "increased" by one according to the rules

- \( J_{\hat{\alpha}}^r + 1 \) if an update in direction \( \hat{\alpha} \) is suggested
- \( J_{\hat{\alpha}}^r - 1 = -(J_{\hat{\alpha}}^{r-\hat{\alpha}} + 1) \) if an update of the current variable flowing along the bond pointing in the opposite direction \(-\hat{\alpha}\) of the unit lattice vector \( \vec{e}_\alpha \) is suggested

The update procedure obviously ensures ergodicity as any current configuration can be obtained.

The sampling algorithm will then work in the following way.

1. Start from a random site \( r \) and set the worms head and tail coordinates equal to the site’s coordinates. Select randomly one direction \( \hat{\alpha} \) of the \( 2(d+1) \) bonds adjoined to the site.

2. Accept moving the worms head coordinates to \( r + \hat{\alpha} \) with probability \( p = \exp[-\Delta H_r^\alpha] \) and adjust the link currents according to the description in the move update above. The energy difference

\[
\Delta H_r^\alpha = \frac{1}{K} \left\{ \text{sign} (\hat{\alpha}) \left( J_r^\alpha - \delta_{\hat{\alpha},\pm\tau} (\tilde{\mu} + \delta\tilde{\mu}_i) \right) + \frac{1}{2} \right\} 
\]

(4.23)

between the initial state and the energy of the trial state.

3. Choose a new random direction \( \hat{\alpha} \).

4. Repeat from 2, until the coordinates of the worm head and tail coincide again.

5. Perform a measurement on the system and start over from 1 until the desired number of Monte Carlo moves has been done.
The above procedure so far covers only the closed CP region of the configuration space. However, the open CP$_g$ configurations contribute to the Greens function [59]. For the lattice Josephson model, the Greens function is given by

$$ C(x, x', \tau, \tau') = \langle e^{i(\theta_x(\tau) - \theta_{x'}(\tau'))} \rangle $$

and is translationally invariant $C(x, x', \tau, \tau') = C(x - x', \tau - \tau')$ [4, 77]. Expressed in the link current picture, this two-point correlator corresponds to open world lines going from $(x, \tau)$ to $(x', \tau')$. More exactly

$$ C(x, \tau) = \prod_{r_i = x_i, \tau_i \in \text{path}} \exp(-\Delta H_{r_i}) $$

meaning that the updating scheme automatically samples the Greens function with the right statistical weight. Thus every time the world line has its head at $(x', \tau')$ and its tail at $(x, \tau)$, the elements $C(x - x', \tau - \tau')$ have to be increased by one, and periodic boundary conditions need to be taken care of. After the sampling process is completed, the entries only need to be normalized by the total number of world lines created in order to obtain the correct expectation value for $C(x - x', \tau - \tau')$.

**4.5 Warmup and Convergence**

Independently of the Monte Carlo algorithm used starting from any initial configuration, it will take a finite time for the system to reach equilibrium. This means that the algorithm samples and transits between configurations according to their correct Boltzmann weight. In order to not violate detailed balance, it is vital that the estimators are updated after a constant number of elementary Monte Carlo moves. Calculating the expectation value $\langle A \rangle$ of some quantity $A$ as a function of non-overlapping time intervals

$$ \langle A \rangle_{N_t} = \frac{1}{N_t} \sum_{t=N_t+1}^{2N_t} A_t $$

is a good measure for convergence. Here $N_t$ is the number of sampling steps. The term MC sweep usually is defined as a single attempted update per degree of freedom. The equilibration can vary strongly between different quantities. The slowest quantity of interest should therefore be considered when deciding how many MC sweeps need to be run.

**4.6 Scaling Analysis of the MC Data**

The numerical results were obtained by simulating finite systems of extension $L^2 \times L_\tau$. In the finite size scaling form of any operator $\mathcal{O}(K, L, L_\tau)$ with scaling dimension zero, these system sizes then only enter in terms of the ratios $L/\xi$. 

4.7. SCALING OF MAXIMA

and $L_\tau/\xi$. Here $K$ is a parameter tuning the system through a phase transition. Thus $O(K, L, L_\tau)$ becomes a function of the two scaling variables $L^{1/\nu} k = L^{1/\nu} (K - K_c) / K_c$ and $\alpha_\tau = L_\tau/L^z$ leading to the finite size scaling ansatz

$$O(K, L, L_\tau) = \tilde{O}(k L^{1/\nu}, L_\tau/L^z)$$

(4.27)

leaving several options to find $K_c, z$ and $\nu$. In isotropic systems, as the supersolid model in paper I [50], $z = 1$ and thus the scaling function only depends on $k L^{1/\nu}$. Likewise, at criticality $\tilde{O}(L^{1/\nu} k, \alpha_\tau) = \tilde{O}(0, \alpha_\tau)$ becomes a function of $\alpha_\tau$ only. Fitting the MC data at each simulated coupling $K$ to this scaling ansatz yields an estimate of $K_c, z$, and $\nu$. In fact this is also a good method to see if the choice of $K_c$ is consistent. Another method is to Taylor expand $\tilde{O}(L^{1/\nu} k, \alpha_\tau)$ as a bivariate polynomial and find the best choice of $K_c, \nu$ and $z$ making the data collapse on a single surface.

4.7 Scaling of Maxima

It has been shown before [74] that if an observable obeys a scaling law of the form given by Eq. (4.27) its extreme values are suitable scaling quantities. If, for instance, $O(K, L, L_\tau)$ when viewed as a function of $L_\tau$, for fixed $K$ and $L$, has a maximum at a particular value $L_\tau^*$ the scaling law Eq.(4.27) dictates that this value must occur when

$$\alpha_\tau^* = L_\tau^*/L^z = \tilde{\gamma}(L^{1/\nu} k)$$

(4.28)

where $\tilde{\gamma}$ is a scaling function of the single variable $k L^{1/\nu}$. Defining the $K$ dependent value of the maximum at fixed $L$ of $O(K, L, L_\tau^*)$ as

$$O^*(K, L) \equiv \tilde{O}(L^{1/\nu} k, \tilde{\gamma}(L^{1/\nu} k)) \equiv \tilde{O}^*(L^{1/\nu} k)$$

(4.29)

yields a set of graphs intersecting at $K = K_c$ (i.e. $k = 0$). There, the respective slopes, can be fitted to a power law in $L$, yielding $\nu$. 
Chapter 5

Results

This chapter aims at providing additional information on the numerical results obtained, which could not be included in the articles [50, 49] due to length restrictions.

5.1 Supersolid Model

The helicity modulus $\Upsilon \propto \rho_s$ for the model in Eq. (2.66) can be straightforwardly calculated. Imposing an infinitesimal phase twist $(\nabla \theta)$ along the $\hat{x}$-direction yields

$$\Upsilon (T) = \frac{\partial^2 f}{\partial (\nabla \theta)^2} \bigg|_{\nabla \theta = 0}$$

(5.1)

$$= \left[ \frac{\beta}{L^3} \left( \left\langle \sum_i J_i \sin (\theta_i - \theta_{i+\hat{x}}) \right\rangle \right)^2 - \left\langle \left( \sum_i J_i \sin (\theta_i - \theta_{i+\hat{x}}) \right)^2 \right\rangle \right]$$

Here $\langle \cdots \rangle$ denotes thermal average, and $\langle \cdots \rangle$ denotes the average taken over different realizations of the columnar disorder. For finite systems of size $L^3$ Eq. (2.35) implies

$$L \Upsilon (T) = \tilde{\Upsilon} (L^{1/\nu} t),$$

(5.2)

where $\tilde{\Upsilon}$ is a scaling function. It allows to determine the critical exponent $\nu$ and $T_c$ through a suitable optimization procedure. Binder discovered the excellent scaling properties of the moments of $M = \left| \sum_j e^{i\theta_j} / L^3 \right|$ as an order parameter [12]. The Binder cumulant is defined as

$$U = \frac{\langle M^4 \rangle}{\langle M^2 \rangle^2}$$

(5.3)
and scales as \( U(T) = \tilde{U}(L^{1/\nu} t) \).

For planar spin models, in a magnetic analogy of the XY-model, \( M \) corresponds to the absolute magnetization. In such systems it is therefore also experimentally accessible. Derivatives of these quantities also provide valuable information. At \( T_c \) they scale according to power laws in the system size

\[
\frac{\partial U}{\partial T}\bigg|_{T=T_c} \propto L^{1/\nu}.
\]  

which is shown in Fig. 5.2. With \( \nu, T_c \) determined, the static equilibrium properties of the phase transition are fully determined, by only calculating one out of the remaining exponents \( \beta, \gamma, \eta \) [32]. Using \( L^{\beta/\nu} M = \tilde{M}(L^{1/\nu} t) \) (Fig. 5.1) and \( L^{-\gamma/\nu} \chi_L = \tilde{\chi}(L^{1/\nu} t) \) (Fig. 4 in [50]) the optimal parameters obtained by scaling independent quantities can be checked for consistency. The Rushbrooke scaling law [32] \( 2\beta + \alpha + \gamma = 2 \) is well fulfilled within error bars.

Figure 5.1: Scaling plot of \( L^{\beta/\nu} M \) with \( T_c = 2.4755, \nu = 1.0 \) and \( \beta = 0.55 \) in the critical region. Insets: Trends for the critical parameters determined by solely scaling the Binder parameter \( U \) and the rescaled spin stiffness \( L\chi \propto \rho_s \). These were obtained by fitting Eq. (5.2) to a polynomial using quadruplets of system sizes \( L = \{10, 12, 16, 20\}, \ldots, \{40, 60, 80, 100\} \).
5.1. SUPERSOLID MODEL

Figure 5.2: The rescaled derivative of the Binder parameter $L^{-1}\partial U/\partial T$ at different temperatures $T$ as a function of $L$. It shows a trend towards a power law $\sim L^0$ (dashed orange line) around $T \approx 2.475$. This is in very good agreement with the trends observed in the scaling analysis of $\Upsilon$ and $U$, obtained using least squares minimization. Inset: The maximum $\chi^\ast$ of the susceptibility $\chi$ scales over a very large range of system sizes as $\chi^\ast \sim L^{\gamma^\ast}$ where $\gamma^\ast = \gamma/\nu \approx 1.82$. 
CHAPTER 5. RESULTS

5.2 Dirty Bosons

From now on consider a discretized system of integer size $L \times L \times L$ under periodic boundary conditions. The free energy density of the $(2+1)$D equivalent classical problem Eq. (3.54) is given by

$$f = -\frac{1}{L^2 L_\tau} \ln \text{Tr} \left\{ e^{-H_V} \right\}$$

(5.5)

where $\beta$ has been identified with $L_\tau$ [77]. All microscopic lengths and times as well as $\hbar$ and $k_B$ have been set to unity. As introduced in the last chapter, the disorder only is correlated along the $\hat{\tau}$-direction and uniformly distributed according to $-\tilde{\Delta} < \delta \mu < \tilde{\Delta}$ where $\Delta = 1/2$. Therefore the system is not isotropic. Space and time are not equivalent and diverge according to Eqs (1.1) and (1.2) with $z \neq 1$, unless the disorder introduced is irrelevant to the critical fixed point. The chemical potential is adjusted to the statistically particle-hole symmetric choice of $\tilde{\mu} = 1/2$.

In the world line representation Eq. (4.21) the uniform stiffness can be calculated by introducing a vector potential of the form

$$A_i^\mu = \hat{\partial}_\mu \delta_{\mu, \hat{\delta}} \Theta L_\delta$$

(5.6)

giving rise to an additional coupling term $-i \sum_{\hat{\mu} = \hat{x}, \hat{y}} J^\mu_i A^\mu_i$ in Eq. (4.21) [77]. The mean square winding number is defined as

$$W^2_\delta = \left\langle \left( \frac{1}{L_\delta} \sum_i J^\delta_i \right)^2 \right\rangle$$

(5.7)

and is the natural quantity to detect superflow in this representation. The helicity modulus then simply becomes

$$\Upsilon(K) = L^d \frac{\partial^2 f}{\partial \Theta^2} \bigg|_{\Theta = 0} = \frac{1}{L_\tau L^d - 2} \left[ \langle W^2_\delta \rangle \right]$$

(5.8)

The winding number then scales according to Eq. (4.27) as

$$W^2(K, L, L_\tau) = \tilde{W}^2(L^{1/\nu} k, \alpha_\tau)$$

(5.9)

However, it proved to be advantageous to construct a new scaling function

$$\Phi(K, L, L_\tau) \equiv \frac{W^2}{\alpha^2} = \hat{\Phi}(L^{1/\nu} k, \alpha_\tau)$$

(5.10)

which has a maximum for the reasons described in the finite size scaling analysis section of [49]. Using the techniques described in section 4.7 then $K_c, \nu$ and $z$ can be extracted as shown in Fig. 5.4. In addition the Green’s function

$$G(r, t; r', t') = \langle \Phi^\dagger(r, t) \Phi(r', t') \rangle \sim r^{-(d+z-2+\eta)} g(r/\xi, \tau/\xi^z)$$

(5.11)
defined in Eqs (4.24) and (4.25) is related to the order parameter susceptibility

\[ \chi = \sum_{r, \tau} G(r, \tau) \sim \int_0^L d^d r \int_0^{L^z} d\tau \, G(r, \tau) \sim L^{2-\eta} \]  

(5.12)

and was used to calculate the critical exponents \( z, \eta \) and \( \nu \) together with the critical coupling \( K_c \).
Figure 5.4: Considering quadruplets of system sizes, the critical coupling can also be calculated by systematically determining the best possible power law fit to the maxima in $W^2/\alpha^2$ for each available coupling $K$. Insets: The $\chi^2(K)$ plot shows a nice minimum close to $K_C \approx 0.2477$ (left). The derivative of the scaling function shows a power-law divergence with system size (right).

Figure 5.5: In the very same way as for the winding number fluctuations, a non-linear least-squares optimization for the scaled susceptibility $\chi/L^{2-\eta}$ yields finite size dependent trends in the exponents. The overall agreement is good. The determination of the extra exponent $\eta$ is however quite shaky. Here only data with $0.5 \leq L_r/L^{1.8} \leq 1.0$ has been used as smaller aspect ratios show larger corrections to scaling.
Chapter 6

Conclusions

6.1 Defect Mediated Supersolid

The main intention was to test if, by introducing correlated disorder, a new universality class for the 3D XY-model could emerge, which qualitatively is in accordance with the findings of smooth onsets of NCRI and heat capacity by Lin, Clark, Kim and Chan [25, 84]. The basic assumption underlying the modification of the XY Hamiltonian is that boson degrees of freedom condense into a superfluid state at a transition from a normal solid phase to a supersolid phase. The presence of the solid was assumed to only affect this transition by coupling the superfluid bosons to its lattice defects. These include, apart from the for the 3DXY critical point irrelevant point defects, such as vacancies and interstitials, also correlated defects, such as dislocation lines. The model presented should describe the main properties of superflow in a correlated defect network on the level of a Ginzburg-Landau free energy. It could also be used to describe cold atoms in optical lattice potentials and superconductors containing an isotropic distribution of linear defects.

Using the power law behavior of the derivative of the Binder parameter at criticality and finite size scaling techniques the correlation length exponent could be determined to be \( \nu = 1 \pm 0.05 \). The analysis showed substantial finite size effects for smaller system sizes. This value is consistent with the lower boundary of a generalized Chayes inequality \( \nu \geq 1 \) obtained using the Harris criterion.

The exponent \( \nu \) here serves several purposes. It opens the possibility to indirectly calculate the heat capacity exponent \( \alpha = (2 - \nu d) \), which is hard to compute from the heat capacity due to analytic background contributions. The value of \( \alpha \) determines the shape of the singular part of the heat capacity \( c \) by \( c \sim |t|^{-\alpha} \) at criticality. If \( \nu < 1 \), the heat capacity critical exponent predicts a peaked maximum around \( T_c \) in the thermodynamic limit. Smooth shapes in simulations then only are finite size effects. Further, \( \nu \) also determines the sharpness of the NCRI onset, as \( \rho_s \sim |t|^{(d-2)\nu} \) at the transition.

As illustrated in Fig. 1 in paper I [50] the results differ quite substantially
Figure 6.1: a) The heat capacity measured by Lin et al. shows a smooth maximum centered around $0.25 \pm 0.025 \text{K}$ [21] which is strikingly different from the $\lambda$-transition in liquid $^4\text{He}$. b) The onset of NCRI measured is also much smoother than for the 3DXY case which starts off with a vertical tangent at $T = T_c$ (dashed line) [22]. The shaded area indicates the trend of several samples containing 300 ppb $^3\text{He}$. The red dots are a collection of different measurements of isotopically pure $^4\text{He}$ with 1ppb $^3\text{He}$, sharing a common onset and falling on a single curve.

from the superfluid $\lambda$-transition. The main experimental features are reproduced suggesting that defect carried superflow might have been observed. The model can be straightforwardly generalized to include fluctuating dislocation lines, which might lead to a more detailed quantitative agreement.

6.2 Quantum Critical Dynamics of the 2-Dimensional Boson Hubbard Model

With the estimate of the dynamic critical exponent $z = 1.8 \pm 0.05$, the long standing claim that $z = d$ apparently is invalid in $d = 2$. This is a very interesting result as exact solutions in statistical mechanics problems are rare and therefore have a special status. Due to the use of far too limited system sizes, most previous simulations were consistent with the a priori choice of $z = 2$. In the finite size scaling analysis of the MC data the relevance of corrections to scaling for small systems is revealed. It might then be tempting to think that, due to the fact that $z = 1$ holds in 1D, the general argument that $z$ is not restricted by any easy accessible hyperscaling argument would be too much of a coincidence. However, $z = 1$ does first and foremost mean that the correlation volume grows isotropically upon approaching the transition. In fact, the transition at the statistical particle-hole symmetric choice of $\mu = 1/2$ in one dimension is presumably in the Kosterlitz Thouless universality class. The exponent $z = 1$ then naturally emerges independently of the relation $z = d$. The result presented here is of basic importance for the theory of disordered quantum phase transitions and encourages further experimental and analytic work.
Bibliography


Part II

Scientific Papers