Emergent Critical Properties in Liquid-Gas Transition and Single Dislocations in Solid He4

Max Yarmolinsky

Graduate Center, City University of New York

How does access to this work benefit you? Let us know!
Follow this and additional works at: https://academicworks.cuny.edu/gc_etds

Part of the Condensed Matter Physics Commons, and the Statistical, Nonlinear, and Soft Matter Physics Commons

Recommended Citation
https://academicworks.cuny.edu/gc_etds/2974

This Dissertation is brought to you by CUNY Academic Works. It has been accepted for inclusion in All Dissertations, Theses, and Capstone Projects by an authorized administrator of CUNY Academic Works. For more information, please contact deposit@gc.cuny.edu.
EMERGENT CRITICAL PROPERTIES IN LIQUID-GAS TRANSITION AND SINGLE
DISLOCATIONS IN SOLID HE4

by

MAX YARMOLINSKY

A dissertation submitted to the Graduate Faculty in Physics in partial fulfillment of the
requirements for the degree of Doctor of Philosophy, The City University of New York

2019
Emergent critical properties in liquid-gas transition and single dislocations in Solid He4

by

Max Yarmolinsky

This manuscript has been read and accepted by the Graduate Faculty in Physics in satisfaction of the dissertation requirement for the degree of Doctor of Philosophy.

Supervisory Committee:

Roman Kezerashvili
Alfred Levine
Vadim Oganesyan
David Schmeltzer
Boris Svistunov

THE CITY UNIVERSITY OF NEW YORK
Abstract

Emergent critical properties in liquid-gas transition and single dislocations in Solid He4

by

Max Yarmolinsky

Adviser: Professor A. Kuklov

My research focuses on the analytical and numerical study of seemingly completely different systems – the classical critical point of the liquid-gas transition and a quantum topological defect (dislocation) in solid Helium-4. The unifying theme, though, is Emergence – the appearance of unexpected qualities at large distance and time scales in these systems. Our results resolve the long standing controversy about the nature of the liquid-gas criticality by showing with high confidence that it is the same as that of Ising ferromagnet. In solid $^4$He, a quantum superclimbing dislocation, which is expected to be violating space-time symmetry according to the elementary textbook assessment, shows emergence of this symmetry in our numerical simulations.
Acknowledgments

I want to acknowledge the Graduate Center and the City University of New York as a whole for providing me the opportunity to pursue my doctoral studies. In particular, I want to thank Mr. Moy of the Graduate Center physics department as well as the executive directors Professors Kusovsky and Greenbaum. I also want to thank the members of my doctoral committee for taking the time out of their busy schedules to listen to my proposal and defense.

All simulations were performed on the CUNY High Performance Computing Center at the College of Staten Island, for which I am grateful.

Most of all I want to thank my advisor Prof. Kuklov for generously giving a large amount of his time over the years to help me understand the many ideas occurring in the investigation of critical phenomena. Prof. Kuklov was very helpful not only in guiding my understanding of the physics but also in explaining practical matters such as the ways to practice and present talks and in matters of general professionalism regarding coding, data handling and presentation and countless other small details that are required to do proper scientific work.

Thanks to Prof. Kuklov, I was honored to have the opportunity to work with the truly legendary Prof. Alexander Patashinskii on the project regarding geometrical percolative transitions.

Finally, I would like to thank family (my mother Rachel, father Ben, brother David) and of course my lovely wife Qiongge.
# Table of Contents

List of Figures ix

1 Overview 1
   1.1 Emergence .................................................. 1
   1.2 Universality of Liquid Gas Criticality in 2D .................. 2
   1.3 Emergence of LL in superclimbing dislocation ............... 5
   1.4 Thesis Organization ......................................... 8

2 Metropolis and Quantum Monte Carlo 9
   2.1 Introduction .................................................. 9
   2.2 Quantum Monte Carlo ........................................ 11
   2.3 Effect of finite timestep: quantum harmonic oscillator .... 12

3 Finite Size Scaling and Numerical Flowgram 16
   3.1 Finite Size Scaling .......................................... 16
   3.2 General Flowgram Method ................................... 17

4 Criticality of the $\phi^4$ field model with $\phi^5$ term 21
   4.1 Introduction .................................................. 21
   4.2 Model Description .......................................... 24
   4.3 Duality Transformation ...................................... 27
### TABLE OF CONTENTS

#### 4.4 Worm Algorithm and Acceptance Ratios ........................................ 29

#### 4.5 Critical behavior at $g_5 = 0$ by the flowgram method .................... 32

#### 4.6 Critical behavior at finite $g_5$ ............................................. 38

#### 5 Criticality of the square well fluid ............................................. 43

##### 5.1 Introduction ................................................................. 43

##### 5.2 The mixing effect in the LG criticality ..................................... 45

##### 5.3 Strong and weak field domains for LG transition in free space .......... 47

- **5.3.1** Scaling in the strong field domain ..................................... 51
- **5.3.2** Scaling in the weak field domain ..................................... 52
- **5.3.3** Scaling along the coexistence line ..................................... 53
- **5.3.4** Non-analytical contributions to density ............................... 54

##### 5.4 The Square Well Fluid Model ............................................. 55

- **5.4.1** Determination of critical point ....................................... 58
- **5.4.2** Critical behavior in the strong field ................................ 61
- **5.4.3** Critical behavior in the Weak field ................................ 67
- **5.4.4** Order Parameter beta exponent ....................................... 70

#### 6 Luttinger transition in superclimbing dislocation ............................ 74

##### 6.1 Introduction ................................................................. 74

##### 6.2 Luttinger Liquid ............................................................ 77

##### 6.3 Response to Gauge Fields and Winding Numbers ......................... 78

##### 6.4 Superclimb and the giant isochoric compressibility ...................... 81

- **6.4.1** Giant isochoric compressibility ...................................... 85
- **6.4.2** Collective effects ....................................................... 87
- **6.4.3** Compressibility and dislocation excitation spectrum ................ 88

##### 6.5 Superclimb beyond the gaussian approximation ........................... 88
# TABLE OF CONTENTS

6.5.1 Dual representation ............................................. 89
6.5.2 Emergence of the LL behavior ................................. 91
6.5.3 Quantum phase transition (QPT). ......................... 94
6.6 Roughening induced by chemical potential .................... 97
   6.6.1 The smooth-rough crossover ............................... 98
   6.6.2 Hysteretic behavior of the smooth-rough dislocation .... 102
   6.6.3 Emergent LL in Solid He ................................. 102
6.7 Dynamics .......................................................... 103
   6.7.1 Metastability of the biased dislocation .................... 106
   6.7.2 Linear approximation for the superfluid phase ............ 106
   6.7.3 Bardeen-Herring loop generation .......................... 107

7 Summary and Future Work ................................. 110
   7.1 Conclusions .................................................. 110
   7.2 Future Work ................................................ 111
      7.2.1 Scaling of the LG diameter ............................ 111
      7.2.2 Stress anisotropy induced by superclimb. ............... 112
      7.2.3 Threshold for superclimb ............................... 113
      7.2.4 Sudden stopping of the pressure evolution in the supersolid 114
      7.2.5 Equilibrium syringe fraction. .......................... 114

A Universality of transition to insulating state .............. 116

References ......................................................... 120
List of Figures

1.1 The liquid-gas phase diagram ........................................... 3
1.2 The supersolid phase diagram ........................................... 6
1.3 Temperature dependence of the super flow rate ..................... 7

2.1 QHO error as function of timestep, \( \beta = 2 \) ......................... 14
2.2 QHO error as function of timestep, \( \beta = 5 \) ......................... 14
2.3 QHO error as function of timestep, \( \beta = 10 \) ....................... 15

3.1 General flowgram schematic ............................................. 20
3.2 Self-similar curves in the NF ............................................ 20

4.1 Gyration radius vs \( t \) at \( g_5 = 0 \) ....................................... 33
4.2 \( dU_r/dt \) vs \( U_r \) at \( g_5 = 0 \) ............................................. 34
4.3 \( dU_r/dt \) vs \( U_r \), the master curve .................................... 35
4.4 Correlator sum \( f(L) \) versus \( U_r \) ........................................ 36
4.5 Log-log of rescaling factor \( \lambda_n(L) \) versus \( L \) .................... 37
4.6 \( U_2^{-1} \) vs \( g_5 \) in the truncated model .............................. 39
4.7 \( dU_2^{-1}/dg_5 \) vs \( U_2^{-1} \) in the truncated model ............... 40
4.8 \( dU_2^{-1}/dg_5 \) vs \( U_2^{-1} \) master curve, inset: log-log \( \lambda \) versus \( L \) 41
4.9 Deviation from scaling for \( dU_2^{-1}/dg_5 \) ............................ 42
### List of Figures

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1</td>
<td>Sketch of a generic path toward the critical point ((h = 0, \tau = 0))</td>
<td>48</td>
</tr>
<tr>
<td>5.2</td>
<td>Schematic of the polar representation of the system parameters</td>
<td>57</td>
</tr>
<tr>
<td>5.3</td>
<td>Sketch for (U_4(\mu, L)) dependence. The arrows indicate the evolution of the maximum as (L \to \infty) at (T &lt; T_c) (upper), (T &gt; T_c) (lower) and (T = T_c) (horizontal)</td>
<td>59</td>
</tr>
<tr>
<td>5.4</td>
<td>Separatrix of (U_4(L)) maxima versus (L) at different (T)</td>
<td>60</td>
</tr>
<tr>
<td>5.5</td>
<td>The master curve of the strong field specific heat (C) vs (U_4)</td>
<td>62</td>
</tr>
<tr>
<td>5.6</td>
<td>Rescaling factor (\lambda_C(L)) versus (L)</td>
<td>63</td>
</tr>
<tr>
<td>5.7</td>
<td>The remainder (C_r) of (C) and the solid fit line</td>
<td>63</td>
</tr>
<tr>
<td>5.8</td>
<td>The master curve of (\frac{dU_4}{dl}, \phi = \pi/2), vs (U_4)</td>
<td>64</td>
</tr>
<tr>
<td>5.9</td>
<td>The log-log plot of the rescaling parameter (\lambda_{\mu}(L)) versus (L)</td>
<td>64</td>
</tr>
<tr>
<td>5.10</td>
<td>Strong field compressibility (\delta N^2) versus (U_4)</td>
<td>66</td>
</tr>
<tr>
<td>5.11</td>
<td>Log-log (\lambda_{\gamma/\nu}(L)) versus (L)</td>
<td>67</td>
</tr>
<tr>
<td>5.12</td>
<td>“(C)” versus (\phi) close to minimum at (\phi = \phi_V) for various sizes (L)</td>
<td>68</td>
</tr>
<tr>
<td>5.13</td>
<td>Histograms of density along straight paths near (\phi = \phi_V)</td>
<td>69</td>
</tr>
<tr>
<td>5.14</td>
<td>Master curve of (\frac{dU_4}{dl}) vs (U_4) at (\phi = \phi_V = (69.5 + 180))°. Inset: original curves</td>
<td>71</td>
</tr>
<tr>
<td>5.15</td>
<td>Log-log plot of the rescaling parameter (\lambda_{\nu}(L)) of (dU_4/dl)</td>
<td>72</td>
</tr>
<tr>
<td>5.16</td>
<td>The distribution of the density, (P(\rho, L)), for different system sizes (L)</td>
<td>72</td>
</tr>
<tr>
<td>5.17</td>
<td>Log-Log plot of the difference in the peaks (\rho_l(L) - \rho_g(L)) vs (L)</td>
<td>73</td>
</tr>
<tr>
<td>6.1</td>
<td>Forest of edge and screw dislocations with Burgers vector along the (hcp) axis</td>
<td>82</td>
</tr>
<tr>
<td>6.2</td>
<td>Schematic of the superclimbing dislocation in the crystal</td>
<td>83</td>
</tr>
<tr>
<td>6.3</td>
<td>One block of the dislocation network built by dislocations with superfluid core</td>
<td>85</td>
</tr>
<tr>
<td>6.4</td>
<td>Compressibility (\kappa) versus (\beta = T^{-1}). Inset: (\kappa) vs the number of time slices, (N_T)</td>
<td>92</td>
</tr>
<tr>
<td>6.5</td>
<td>(\kappa) vs (\beta = T^{-1}). Inset: superfluid stiffness vs (T^{-1})</td>
<td>93</td>
</tr>
<tr>
<td>6.6</td>
<td>Compressibility (\kappa) vs (L = 1/T) for various values of (G)</td>
<td>94</td>
</tr>
</tbody>
</table>
### LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>6.7</td>
<td>The inverse crossover temperature $T_L^{-1}$ and the width $\Delta_L^{-1}$ vs $L$</td>
<td>95</td>
</tr>
<tr>
<td>6.8</td>
<td>Asymptotic values $\kappa_{eff}$ of $\kappa$ in the limit $L \to \infty$</td>
<td>96</td>
</tr>
<tr>
<td>6.9</td>
<td>Phase diagram of the superclimbing edge dislocation model</td>
<td>97</td>
</tr>
<tr>
<td>6.10</td>
<td>$\kappa_1$ vs $\mu$ for several system sizes $L$</td>
<td>99</td>
</tr>
<tr>
<td>6.11</td>
<td>The log-log plot of the crossover value of $\mu_{0.5}$ vs $L$</td>
<td>100</td>
</tr>
<tr>
<td>6.12</td>
<td>Hysteretic behavior of the compressibility $\kappa_1$</td>
<td>100</td>
</tr>
<tr>
<td>6.13</td>
<td>Width $\Delta\mu$ of the hysteretic loop vs $1/T$</td>
<td>101</td>
</tr>
<tr>
<td>6.14</td>
<td>Schematic of the geometry of the sc-dislocation</td>
<td>104</td>
</tr>
<tr>
<td>6.15</td>
<td>Threshold for instability $\mu_c$ versus linear system size $L$</td>
<td>106</td>
</tr>
<tr>
<td>6.16</td>
<td>Numerical instability time versus system size $L$</td>
<td>107</td>
</tr>
<tr>
<td>6.17</td>
<td>Numerical instability time versus system size $\mu$.</td>
<td>108</td>
</tr>
<tr>
<td>6.18</td>
<td>Numerical instability time versus system size $G/\rho_0$</td>
<td>108</td>
</tr>
<tr>
<td>6.19</td>
<td>Bardeen-Herring overhang generation time $t_{FR}\mu^{1/2}$ versus $L$</td>
<td>109</td>
</tr>
<tr>
<td>A.1</td>
<td>The parameter $\sqrt{-C}$ versus $G$</td>
<td>117</td>
</tr>
</tbody>
</table>
Chapter 1

Overview

1.1 Emergence

This report reveals several cases of emergence in strongly correlated condensed matter systems – both classical and quantum. Economist Jeffrey Goldstein describes emergence as “the arising of novel and coherent structures, patterns and properties during the process of self-organization in complex systems”. For a simple example of emergence, think of a hurricane. A hurricane is a fast rotating storm system, with a spiral pattern of clouds that creates strong winds and heavy rain. Somehow, from the interactions of large numbers of microscopic particles, a new macroscopic entity, the hurricane, emerges. Note that hurricanes are consistent with, but (so far) cannot be predicted by the fundamental laws of physics using purely analytical means. However, it is possible to study and better understand hurricanes by setting up models and simulating them on a computer. To great extent the numerical approach gives important insights for formulating a proper analytical description (in addition to providing quantitative results). In my thesis I will be presenting several examples of systems where the numerical simulations provide such crucial insights.

Connected with emergence is the theory of phase transitions as a phenomenon of sponta-
neous symmetry breaking [1]. To illustrate this idea, consider magnetism. Most materials
are not magnetized because spins are randomly oriented and the average effect is zero. Magnetization occurs when somehow a macroscopic number of the tiny spins spontaneously “decide” to line up in the same direction. The temperature at which this occurs is called the Curie point (or critical point). The tendency of spins to orient in the same direction instead of random directions is an example of order. The key point is that whenever such order is established the underlying symmetry must be broken. In a material’s highest symmetry state there is no macroscopically detectable magnetism because all the spins point randomly. Thus, no matter in which direction you look at the material, it appears to be the same. In the Ising ferromagnet, the symmetry is lowered ($\mathbb{Z}_2$ is broken) when the magnetic phase emerges.

Based on this idea, it was suggested [2] that our world as we see it now is the result of the spontaneous symmetry breaking too, with the symmetry group determined by the Standard Model of the Universe and the Big Bang signifying the very moment of symmetry breaking – as a sort of the point of phase transition from a complete chaos (highest symmetry) to a state (of broken symmetry) with emerging different scales of interactions and particle masses.

It turns out that the rules that govern behavior at the critical point do not depend on the microscopic details of the particular system being studied [3, 4]. They depend on the underlying symmetries and dimensionality of space. This unexpected result is called universality, and it explains why systems such as magnets and fluids may have exactly the same critical properties despite seemingly having nothing to do with each other. In this sense, studying a glass of water at the critical point may give insight into the Big Bang.

### 1.2 Universality of Liquid Gas Criticality in 2D

A critical point occurs in fluids when two (coexisting) phases, liquid and gas emerge from a single high symmetry state known as the supercritical fluid (Fig. 1.1). The theory
of spontaneously broken symmetry appears to be not applicable to the critical point of the liquid-gas (LG) transition because there is no order in both phases and each phase can be viewed as a completely chaotic state of matter. Despite that, the textbook conjecture [3, 4] is that the LG criticality is the same as that of Ising magnet. In other words there is an emergent $\mathbb{Z}_2$ symmetry at the critical point which controls the collective behavior. As a matter of fact, this conjecture has never been convincingly verified either experimentally or numerically for the last almost 60 years. This has created a controversy about the nature of the liquid-gas criticality. There are suggestions [5] that this transition forms its own universality class. To great extent a lack of clarity is due to significant technical difficulties both in analytical and numerical approaches. The analytical methods are mostly based on the renormalization group, a powerful theoretical tool [3]. Several papers were published using this technique to analyze the LG critical point [6]. These approaches, however, are based on certain assumptions and approximations which are not well controlled.

Figure 1.1: Phase diagram showing a line of first order liquid-gas transitions terminating at the critical second order transition point.
A far more practical and effective approach is to use computer simulation. Several attempts [7, 8, 9] were made to understand the LG criticality but they were unable to achieve meaningful results because of inability to find the position of the critical point with controlled accuracy.

The first part of my thesis (Chapters 4 and 5) is devoted to applying the numerical flowgram method (NF) [10, 11] to the LG criticality. The crucial advantage of the method is that it does not require knowledge of where the critical point is. Instead its position can be found as a byproduct of the analysis with any desired accuracy - limited only by size of a simulated system. We applied the NF to the square well fluid model with large scale grand canonical monte carlo simulation methods. Our finding is that the critical behaviors of LG systems and Ising magnets in 2D belong to the same universality class. The work is contained in chapter 5.

The standard $\phi^4$ model is the simplest classical field theory that belongs to the Ising universality class as well. In the sense that the $\phi^4$ model is a continuum version of the Ising model, there existed speculations that inclusion of higher order odd terms might produce a critical point distinct from the Ising class, as these terms are renormalization group (RG) relevant, or marginal in three and two dimensions. By direct simulation, and again applying the NF, we checked to see if the term $\sim \phi^5$ induces any new critical behavior. As it appears now, the scaling dimension of the $\phi^5$ terms is the same as of the linear one $\phi$. This means that the higher order odd term does not modify the criticality. Thus, the conjecture can be formulated that all odd terms simply generate linear term at the critical point. The details of this work are described in chapter 4. This work, along with our findings from the square well fluid, was recently published in Physical Review E [12].
1.3 Emergence of LL in superclimbing dislocation

The quantum realm provides a rich playground for the emergence of unusual, exotic and unfamiliar behaviors. One example is superfluidity, a zero viscosity, friction free flow which occurs in liquid helium at temperatures below 2.18 Kelvins. When restricted to 1D, a superfluid may acquire the Luttinger Liquid (LL) structure [13]. The LL describes a wide class of 1D quantum systems. For our purposes, the relevant characteristics of the LL model are a sound like dispersion for low energy excitations at long wavelengths, power law decay of correlation functions at $T = 0$ and display of Berezinskii–Kosterlitz–Thouless (BKT) transition if there is an external lattice (see in Ref.[14]).

Chapter 6 of this thesis describes emergent properties of quantum dislocations in solid $^4$He. A “dislocation” refers to a one dimensional line defect — the most typical topological structural defect in crystal structures. The motivation for this study comes from the recent discovery of the superflow–through–solid effect by the experimental group at UMASS [15]. The superflow was found to be accompanied by the so called syringe effect — an unusually large accumulation of matter inside the solid. This effect has been recently confirmed in the Univ. of Alberta [16] as well as by the group led by Moses Chan at Penn State Univ. The phase diagram in Fig. 1.2 shows the boundaries of this “supersolid” regime to the extent that the current experimental data from 2017 provides.

It is important to realize that no existing theory based on purely classical approaches can explain how these two effects - the superflow through the solid and the syringe - can become stronger at lower temperature - as shown in Fig. (1.3). This effect was first observed by Ray and Hallock at UMASS in 2010 [18], and later confirmed by Cheng and Beamish[19]. This effect has been independently observed by all 3 research groups. The flow vanishes at pressures above 30 bar. The proposed mechanism for this phenomenon is associated with the superclimb of dislocations which have been found (in ab initio simulations) to possess
superfluid core in solid $^4$He [20]. In its essence, *superclimb* is the non-conservative motion of dislocations assisted by superflow along the dislocation core.

In this project, I study a single *slanted superclimbing* dislocation [“slanted” refers to a generic situation when dislocations are spread through several Peierls potential valleys so that this potential becomes irrelevant]. The standard dimensional analysis suggests [20] that such a dislocation must violate space-time symmetry – because the variation of the action in the long wavelength limit gives a parabolic spectrum. However, despite this theoretical prediction, the result of our simulations shows that, as the dislocation length increases and as temperature decreases as well, the LL state characterized by space-time symmetry and linear dispersion emerges. In our paper [21], we propose a way for this numerical result to be tested in experiment.

It was also found that the LL state of the dislocation is fragile: the imposition of an external bias by chemical potential results in a roughening transition of the dislocation –
Figure 1.3: Temperature dependence of the flow rate as observed by a) UMASS 2010 Ref. [18]. Reprinted figure with permission from M Ray and R Hallock, Physical Review Letters, 105, 145301 2010. Copyright 2010 by the American Physical Society. and b) Alberta 2016 in Ref. [19]. Reprinted figure with permission from Z Cheng and J Beamish, Physical Review Letters, 118(23), 235301 2016. Copyright 2016 by the American Physical Society.

when its shape becomes ragged. This leads to a breaking of space-time symmetry and to a subsequent restoration of the non-LL behavior. The key point is that the threshold value of the chemical potential above which the restoration occurs turns out to be macroscopically small – it decreases as some negative power of the dislocation length. This work was recently published in Physical Review B [21].

It is not an exaggeration to say that the superclimbing dislocation represents a unique system with no analogy in other condensed matter systems. I hope that my research will advance understanding of this object toward creating a consistent theory of the superflow through the solid and the syringe effect [15, 16].
CHAPTER 1. OVERVIEW

1.4 Thesis Organization

In order to give some background and context to the work presented so that this document is self-contained, we provide in Chapter 2 a short and simple description of the Monte Carlo methods we employed. The one dimensional simple harmonic oscillator illustrates both the general method as well as a simple example of the Worm Algorithm (WA) [22]. The WA is used throughout this work in both the \(\varphi^4\) field theory and in the dislocation model. The main advantage of the WA is the avoidance of the critical slowing down as a transition is approached.

In Chapter 3 we introduce the finite size scaling (FSS) theory and the NF method within FSS. We rely heavily on the NF to obtain critical exponents to high accuracy across all projects described in this thesis. In Chapter 4 we delve into the topic of the LG transition from the perspective of the \(\varphi^4\) field theory and then in Chapter 5 we directly simulate the fluid by grand canonical Metropolis Monte Carlo. In Chapter 5 we also put our Monte Carlo result in perspective by going into the theory of linear mixing and complete scaling which has important implications for our FSS analysis. In Chapter 6 we give some background on the LL and the BKT transition and then we describe the superclimbing dislocation and report our numerical results there. Finally, in Chapter 7 we draw conclusions and propose ideas for future work.
Chapter 2

Metropolis and Quantum Monte Carlo

2.1 Introduction

Monte Carlo may be used to calculate quantities from a known probability distribution $p(x)$, that would be difficult or impossible to calculate analytically or by other numerical techniques. Here, $x$ is a vector representing the degrees of freedom of our system in some statistical ensemble. Expectation values of physical quantities $Q$, are given by

$$\langle Q \rangle = Z^{-1} \sum_{\{x\}} Q(x)W(x), \quad Z = \sum_{\{x\}} W(x)$$  \hspace{1cm} (2.1)$$

where the sum is over all the possible microstates $x$ each having probability $p(x) = W(x)/Z$. $W(x)$ is the Boltzmann configuration weight which depends on the system energy, $E_x$, as $W(E_x) = e^{-E_x}$.

The idea of the Metropolis algorithm [23] is to use random numbers to drive the evolution of a system with respect to time. Here “time” refers to the number of iterations of an
algorithm that updates the configuration from one microstate to the next starting from some condition at $t = 0$. As long as the update scheme that we choose is both ergodic, meaning that it is capable of sampling the entire phase space, as well as meeting the detailed balance criterion, then it is guaranteed (for most cases) that the algorithm will eventually converge to the equilibrium of probability distribution. Detailed balance requires that the transition rates $P(x \to x')$ from one microstate $x$ to some other microstate $x'$ satisfy

$$\frac{P(x \to x')}{P(x' \to x)} = \frac{p(x')}{p(x)}. \quad (2.2)$$

A burn-in or thermalization time is usually required since the system may be initialized in states with low probability density. This initial data is thrown away.

It is useful to breakdown the transition rate $P$ into two pieces. Starting in some state $x$, updates are implemented by selecting a candidate state, $x'$, according to some probabilistic selection rule $g(x \to x')$. Then the transition is either made, or not made (in which case the system remains in the state $x$) according to the acceptance ratio $A(x \to x')$. These quantities must satisfy the same detailed balance condition which now reads as

$$\frac{P(x \to x')}{P(x' \to x)} = \frac{g(x \to x') A(x \to x')}{g(x' \to x) A(x' \to x)} = \frac{p(x')}{p(x)} \quad (2.3)$$

The important point is that, so long as detailed balance is maintained, there is some flexibility in choosing the values of $A$ such that the acceptance ratios are large. In this way, the system rapidly thermalizes and achieves equilibrium. The metropolis method is defined by the choice

$$A(x \to x') = \begin{cases} e^{-\beta(E_{x'} - E_x)} & \text{if } E_{x'} - E_x > 0 \\ 1 & \text{otherwise} \end{cases} \quad (2.4)$$
2.2 Quantum Monte Carlo

In quantum mechanics the quantity $e^{-\beta H}$ is an operator and in general we don’t know how to calculate it, nor do we know the energy eigenstates of the system that diagonalize the hamiltonian. One approach to simulating quantum systems is to map the $d$-dimensional quantum system to a $(d + 1)$-dimensional classical system. To show how this may be done, suppose, for simplicity, that we have a single particle hamiltonian in one spatial dimension so that in the coordinate representation the hamiltonian ($\hbar = 1$) is

$$H = -\frac{1}{2m} \left( \frac{d}{dx} \right)^2 + V(x)$$

(2.5)

Now consider the partition function, where the factor $\beta = N_t \Delta t$ is split into a number of pieces $N_t \to \infty$,

$$Z = Tr(e^{-\beta H}) = Tr(e^{-\Delta t H} e^{-\Delta t H} ... e^{-\Delta t H})$$

(2.6)

Note that the trace is independent of basis. In the energy eigenstate basis, the quantum problem reduces to the classical one. If we do not know the eigenstates, then it is useful to represent the partition function as an imaginary time path integral $[24]$ where the paths must return to the same state after some imaginary time interval $\beta$. Explicitly this can be shown by inserting an infinite number of resolutions of the identity in the position basis, and also integrating over momenta, then, in the limit $\Delta t \to 0$ into the RHS of Eq. 2.6.

$$Z = \int Dx(t) \exp \left\{ - \int_0^\beta dt \left[ \frac{m}{2} \dot{x}^2 + V(x) \right] \right\}$$

(2.7)

If we then discretize time we get
\[ Z = \lim_{N_t \to \infty} \int \left[ \prod_{i=1}^{N_t} \frac{dx_i}{\sqrt{2\pi\Delta t/m}} \right] \exp \left\{ -\frac{N_t}{\Delta t} \sum_{i=1}^{N_t} \Delta t \left[ \frac{m}{2} \left( \frac{x_{i+1} - x_i}{\Delta t} \right)^2 + V(x_j)\Delta t \right] \right\} \quad (2.8) \]

The measure is chosen to normalize \( Z \) and is usually not important for the purpose of Monte Carlo, where only ratios of the configuration weight matter.

This representation of the partition function reveals the added dimension. Instead of dealing with a single degree of freedom, we now have a closed string with \( N_t \) degrees of freedom. More generally, we can make the Trotter-Suzuki decomposition [25] \( e^{-\beta H} = e^{-\Delta t K} e^{-\Delta t V} + \mathcal{O}(\Delta t^2) \) where \( K \) is some quadratic term that can be handled exactly, and then proceed with the same procedure as described above as a method to transform any quantum problem into a one higher dimensional classical problem.

### 2.3 Effect of finite timestep: quantum harmonic oscillator

In Eq. (2.8) the discreteness of the time step introduces an error. As an illustrative example, a single quantum harmonic oscillator was simulated with the worm algorithm [22] (see sections 4.3 & 4.4 for a detailed explanation of the worm algorithm) to check the error as a function of time-step on the \( 0+1 \) dimensional lattice. Since the system is exactly solvable, we can compare our numerical result to the exact solution.

Plugging the potential harmonic potential \( V(x) = \frac{1}{2}m\omega^2 x^2 \) into Eq. (2.5), the partition function (2.8) can be written compactly with the discrete action

\[
S = -\sum_{(ij)} x_i x_j + \sum_{i=1}^{N_t} a_0 x_i^2 \quad (2.9)
\]
with periodic boundary conditions taken on the 1D lattice, where \( a_0 = \frac{1}{2} \Delta t^2 \omega^2 + 1 \). I have rescaled each \( x_i \to \sqrt{\frac{\Delta t}{m}} \) and chosen \( m = 1 \). The partition function

\[
Z = \int \mathcal{D}x \left( \prod_b e^{+x_i x_j} \right) \left( \prod_i e^{-a_0 x_i^2} \right)
\]

(2.10)

may be expanded over the exponentials defined on the bonds \( \langle ij \rangle \equiv b \), each with powers \( n_b \). This leads to the standard duality transformation of the worm algorithm (see Section 4.3), where the integer valued bond variables \( n_b \) are the new degrees of freedom.

At high temperatures, quantum fluctuations may be ignored and there is not much error introduced by large time-steps, e.g. we can take \( N_t = 1 \) in the classical limit. At lower temperatures, we will collect statistics on the quantity \( \langle x_i^2 \rangle \). The exact solution in the limit \( N_t \to \infty \) is

\[
\langle x_i^2 \rangle = \frac{1}{2\omega} \left( 1 + \frac{2}{e^{\beta \omega} - 1} \right).
\]

(2.11)

It is to be compared with the numerical result obtained by Worm Algorithm.

In simulations, the choice of inverse-temperature \( \beta \) was selected to stay in regime where quantum fluctuations play some role. At higher temperatures, simulation performance drops off at large \( N_t \) due to the classical limit; quantum fluctuations are accepted with very low probability. Still, the time step should be \(< 0.1 \) to reduce the time discretization error for \( \beta = 2 \) (as shown in Fig. 1). Shown in Figs. 2,3 is the dependence of the time discretization error on \( \Delta t \) for \( \beta = 5, 10 \).

Generally, most of the time when we are simulating a quantum system, we don’t know the exact solution. The values of \( \Delta t \) that control the error will vary from system to system. The only way to determine whether discretization error is controlled is to check that expectation values no longer depend on the time-step. E.g. we must decrease \( \Delta t \) to a sufficiently small number. Thus, this study only serves as a guide to the types of values we might start with as guesses when simulating systems which have no analytical solutions. This method will be
Figure 2.1: $\langle x_i^2 \rangle$ vs $N_t$ for $\beta = 2$. Systematic error is controlled for $N_t \gtrapprox 40$, or $\Delta t \lesssim \frac{\beta}{N_t} = \frac{2}{40} = 0.05$

applied to our model of the superclimbing dislocation in Chapter 6.

Figure 2.2: $\langle x_i^2 \rangle$ vs $N_t$ for $\beta = 5$. Systematic error is controlled for $N_t \gtrapprox 100$, or $\Delta t \lesssim \frac{\beta}{N_t} = \frac{5}{100} = 0.05$
Figure 2.3: $\langle x_i^2 \rangle$ vs $N_t$ for $\beta = 10$. Systematic error is controlled for $N_t \gtrsim 100$ or $\Delta t \lesssim \frac{\beta}{N_t} = \frac{10}{100} = 0.1$
Chapter 3

Finite Size Scaling and Numerical Flowgram

3.1 Finite Size Scaling

At the critical point, the non-analyticity in the free energy and the divergence of the correlation length occur only in the thermodynamic limit where the system size $L \to \infty$. One can think of a computer simulation of a system model on a finite size lattice or continuum as a kind of window that peers in on a potentially infinite system. Finite size scaling (FSS), is a systematic way of understanding the implications of a finite system size. Thus, if the model is at the critical point we expect the correlation length, $\xi$ to be cut off by the linear system size $L$. This rather useful fact can be exploited by running simulations at many different system sizes and observing the behavior of various statistical quantities. If they have a generalized homogeneous functional dependence [26] on the parameters at the critical point (this is the scaling ansatz), then this will be observed by power law scaling in the curves for different sizes [27].

Specifically, the critical exponents $\nu$ and $\mu$ are defined by the relationship between the
correlation length and the thermal \( \tau \) and magnetic field \( h \) primary operators by the relationship

\[
\xi \sim \begin{cases} 
|\tau|^{-\nu} & \text{if } h = 0 \\
|h|^{-\mu} & \text{if } \tau = 0
\end{cases}
\]  

(3.1)

When the critical divergent \( \xi \) is cut off by \( L \) in the finite system simulations, then \( \tau \sim L^{-1/\nu} \) and \( h \sim L^{-1/\mu} \). We shall also measure several other quantities including the susceptibility, order parameter and specific heat which have the following definitions for critical exponents and scaling behavior

\[
\chi \sim \tau^{-\gamma} \sim L^{\frac{\gamma}{\nu}}, \quad m \sim \tau^\beta \sim L^{\frac{\beta}{\nu}}, \quad C_V \sim \tau^{-\alpha} \sim L^{\frac{\alpha}{\nu}}.
\]  

(3.2)

It should be noted that corrections to the leading order scaling exist in any finite system, both power law and logarithmic. One must proceed with caution in making any statements from finite simulations without considering sufficiently large system sizes.

3.2 General Flowgram Method

One of the general difficulties in conducting FSS analysis of critical behavior is that the location of the critical point is unknown or is known only to limited accuracy. Here we describe the flowgram method [10, 11] which is a quite general way of conducting FSS in a controlled aproach to the critical point. The method relies on a quantity with zero scaling dimension at the critical point. We will refer to this quantity as the Binder cumulant [7]. So long as such a quantity can be defined and measured, then the scaling dimension of any critical parameter can be found by the algorithm described below. We shall consider the case where the critical parameter is the thermal one \( \tau = \frac{T-T_c}{T_c} \) however, it should be
emphasized that any model parameter that takes the system across the phase transition may be substituted in the place of $\tau$.

The idea of the flowgram method is based on constructing the FSS flow (with respect to the system size $L \to \infty$) by adjusting some critical parameter $\tau$ so that some Binder cumulant $U_B$ is tuned to a value within its critical range. Conversely, if $U_B$ is kept to be equal to a value within its critical range as $L \to \infty$, it is guaranteed that $\tau \to \tau_c$. Then, a quantity $Q$ characterized by scaling behavior will exhibit self-similar dependence versus $U_B$ with respect to $L$. In other words, if $U_B$ is kept in the critical range for large enough $L$, the plot $Q$ versus $U_B$ can be represented by some universal function multiplied by the factor $L^{-\Delta Q}$ with some exponent $\Delta Q$ determining scaling dimension of $Q$.

More specifically, far from the criticality $U_B$ takes some fixed values, say, $U_B = B_0$ in the disordered phase and $U_B = B_1$ in the ordered phase. At the critical point, $\tau = \tau_c$, it takes a value $U_B = B_c$ independent of the system size $L$ as long as $L \to \infty$ and such that $B_0 < B_c < B_1$ (where for the sake of argument we assume $B_1 > B_0$). It is important to note that for any finite $L$ the function $U_B(\tau)$ changes smoothly from $B_0$ to $B_1$ as $\tau$ passes from $\tau < \tau_c$ to $\tau > \tau_c$. However, as $L$ is taken larger and larger, the domain $\delta \tau$ around $\tau = \tau_c$ over which this change happens becomes smaller and smaller. Thus, in the thermo-limit ($L \to \infty$) the cumulant exhibits a jump from $B_0$ to $B_1$ at exactly $\tau = \tau_c$ because $\delta \tau \sim L^{-1/\nu}$ in accordance with the FSS.

This strategy is guaranteed to access a critical point in progression of growing sizes $L$ – as long as $U_B$ is tuned to any value within the critical range $B_0 < U_B < B_1$. Accordingly, the system is always in the critical range of $U_B$ (and of any other scaling quantity). In particular, the family of curves $dU_B/d\tau$ vs $U_B$ for various $L$ must be self-similar for large enough $L$ because $dU_B/d\tau \approx (B_1 - B_0)/\delta \tau \propto L^{1/\nu}$. Thus, constructing such a family and then rescaling them into a single master curve by a scaling factor $\lambda(L)$ gives the exponent $\nu$ by plotting $\ln \lambda$ vs $\ln L$. Similarly, other exponents can be found by choosing the appropriate
quantity $Q$ to plot versus $U_B$ and to perform the rescaling of the family of the curves (for various $L$) into a single master curve. Formally we may write,

$$U_B = U(L^{1/\nu} \tau, L^{1/\mu} h),$$

where $U(X,Y)$ is an analytical function of $X = L^{1/\nu} \tau$, $Y = L^{1/\mu} h$, and the critical domain of $U_B$ is given by $X \sim 1$ or $Y \sim 1$. Then, along the critical isochore, $h = 0$, $dU_B/d\tau = L^{1/\nu} dU(X,0)/dX$, where $X \sim 1$, and thus $dU(X,0)/dX \sim 1$. Similar logic can be used when $X \rightarrow 0$, $Y \sim 1$, which yields $dU_B/dh = L^{1/\mu} dU(0,Y)/dY \sim L^{1/\mu}$. Clearly, within this approach the values of $\tau_c$ and $h_c$ play no explicit role in the fitting procedure, with the only one fitting parameter being the scaling dimension.

The idea of the method is illustrated in Fig. 3.1 for the case of the the Ising model $U_B(\tau)$, shown schematically, for some increasing system sizes $L_1$, $L_2$, $L_3$, $L_\infty$. If $dU_B/d\tau$ vs $U_B$ for different $L$ are self similar, as shown schematically in Fig. 3.2, then we attempt to collapse by a single rescaling factor $\lambda(L) \propto L^{\xi}$. Later we will show the results of applying this method to the square well fluid and $\phi^4$ lattice field systems.
Figure 3.1: Schematic of Binder Cumulant $U_B$ vs $\tau$ of the flowgram method, the crossover width between $B_0$ and $B_1$ shrinks like $\delta\tau \sim L^{-1/\nu}$ where $L_3 > L_2 > L_1$.

Figure 3.2: Schematics of the self similar curves $\frac{dU_B}{d\tau}$ vs $U_B$ generated by the flowgram method, where $L_3 > L_2 > L_1$. 
Chapter 4

Criticality of the $\phi^4$ field model with $\phi^5$ term

4.1 Introduction

It was realized by Lev Landau that continuous phase transitions are generically characterized by spontaneous symmetry breaking and, accordingly, by a diverging correlation length [1]. Real fluids are asymmetric in that the free energy is not invariant under inversion of the order parameter $\rho_l - \rho_g \rightarrow -(\rho_l - \rho_g)$, where $\rho_l$, $\rho_g$ are the densities of the liquid and gas phases. Formally speaking, however, neither liquid nor gas can be characterized by a symmetry breaking order parameter simply because there is no order in both phases.

The two dimensional nearest neighbor Ising model with $h = 0$ can be mapped onto a lattice gas [28] which possesses an exact particle-hole symmetry. Real fluids are the continuum limit of the lattice gas. In the continuum limit, the particle-hole symmetry is lost. Thus, odd terms in the free energy expansion in the order parameter cannot be neglected in the liquid gas.

Absence of any underlying symmetry breaking raised the question about the universality
of the transition at the critical point. The standard conjecture is that this transition belongs to the $Z_2$ universality class, that is, of the Ising transition (see in Refs. [1, 29, 4]). This question have a straightforward answer for the lattice gas where a direct mapping to the Ising model exists [28]. It is formally possible to consider a free space fluid on a lattice with spacing being much smaller than any typical distance determining interaction. In this case the lattice and free space models should be equivalent. Thus, in general, no underlying $Z_2$ symmetry can be found in such a lattice. Accordingly, lattice models explicitly violating $Z_2$ symmetry have been considered [30]. It was further suggested that the asymmetry does not change the $Z_2$ universality of the LG criticality, and its role is reduced to mixing of the primary scaling operators which results in the non-analytical corrections to the position of the critical point [31, 32, 4, 33, 34]. The extended mixing scenario has been suggested in Ref.[35, 36, 37, 38] in relation to the Yang-Yang anomaly.

The conjecture that LG criticality is $Z_2$ is closely related to the question about the role of higher order odd terms in the field theory. As shown in Ref. [6], the LG transition characterized by quite generic two-body interactions in free space can be mapped on a field theory of a continuous scalar real field $\varphi$ with some effective Hamiltonian which, in addition to even terms $(\vec{\nabla}\varphi)^2, \varphi^2, \varphi^4, ...$, contains odd ones $\varphi^1, \varphi^3, \varphi^5, \varphi^7, ...$. Thus, there is a possibility that higher order odd terms $\varphi^5, \varphi^7, ...$ change the universality (the term $\varphi^3$ can be eliminated by a uniform shift $\varphi \rightarrow \varphi + \varphi_0$ with $\varphi_0$ being some constant) [39]. The analysis [5] based on the renormalization group (RG) approach found that there is a novel fixed point in dimensions $d = 10/3$ induced by the term $\varphi^5$, provided, $\varphi^1$ and $\varphi^3$ are tuned to zero. This result, however, was challenged in Ref. [40] based on the $\varepsilon$-expansion around $d = 4$ showing that all odd operators of higher order are strongly irrelevant at the symmetric fixed point, so that this point is stable with respect to the odd perturbations.

It is important to note that the argument [40] cannot be used in 2D. Thus, the question about the role of the higher odd terms in 2D remains open. More recently, the analytical
solution for the critical exponents of 3D LG transition has been found under quite general assumptions [41]. These exponents turn out to be different from the values obtained numerically. The same method can also be used in 2D and it gives the exponents which are different from the Onsager values [42].

Some early attempts to measure critical exponents experimentally have claimed significant deviations from the 3D Ising universality [43, 44], while others [45, 46] find an acceptable agreement with the Ising universality, provided the fitting procedure included subcritical corrections (with several adjustable parameters). The main problem turns out to be due to gravity which does not allow to approach the critical point close enough so that the corrections to the leading scaling can be ignored. The experiments in microgravity (see in Ref. [47]) didn’t improve the situation much.

Measurement of the LG criticality in 2D has been conducted in Ref.[46]. The value of the $\beta$-exponent was reported to be consistent with the Onsager result $\beta = 1/8$ within 15-20\% accuracy. This result was achieved within 3-parametric fitting procedure requiring knowledge of accurate values of the critical temperature and density. At this point we note that the value of $\beta = 1/8$ is also characterizing other universalities, e.g., XY and three-state Potts model. Thus, by itself it is not a “smoking gun” for the Ising criticality.

This chapter is organized as follows. First we introduce the modified $\phi^4$ field theory with the added term $g_5\phi^5$. Then we study the behavior at $g_5 = 0$ as a check. Finally, the critical behavior at finite $g_5$ is revealed. Using the numerical flowgram method we have determined the scaling dimension $\Delta_5$ of the $\phi^5$ term in the $\phi^4 + \phi^6$ model in the context of the correspondence between the LG and the field ensembles. Our finding is that $\Delta_5$ coincides with that of the linear term in the $Z_2$ class.
4.2 Model Description

As discussed above, there is a formal mapping between a gas of particles undergoing the LG transition and the field theory [6]. This mapping, however, unavoidably contains odd terms in the field. The proposal [5] of the asymmetric fixed point is based on the assumption that the operator \( Q_5 = \int d^d x \varphi^5 \) in the field model is relevant at the symmetric fixed point in \( d < \frac{10}{3} \)-dimensional space. Then, the symmetric point may become unstable and the system finds another (asymmetric) fixed point characterized by critical indices different from those of the Ising model [5]. The alternative view based on the \( \epsilon \)-expansion around \( d = 4 \) renders \( Q_5 \) and all higher terms as (dangerously) irrelevant [40]. This argument, however, cannot be used in 2D. Thus, the issue of the odd terms remains quite controversial, and our goal here is to resolve it by simulations.

Here we will specifically focus on the critical dimension \( \Delta_5 \) of the \( Q^5_5 \) term in the potential part of the action \( V(\varphi) \) characterized by the symmetry \( \varphi \rightarrow -\varphi \). At this point it is important to mention that the result of adding \( g_5 \varphi^5 \) to \( V(\varphi) \) can be quite drastic at the microscopic level already – this term can simply eliminate the transition before scaling behavior develops. We are not considering this option, and focus on the situation where \( Q_5 \) term is small at the microlevel. Then, if it is relevant in the sense of renormalization, it will take the system away from the Ising fixed point to a new (non-Ising) one.

At this point it is important to realize that the paradigm of universality implies that the microscopic form of the action \( V(\varphi) \) does not affect the scaling behavior occurring around \( \varphi = 0 \). The only requirement is that this action should have not more than two equilibrium solutions in the vicinity of \( \varphi = 0 \) away from the critical point. Traditionally, the action is taken as a truncated polynomial \( V(\varphi) = \sum_{n=1}^{n^*} g_{2n} \varphi^{2n} \) with \( n^* \) being as small as possible to insure overall stability. In the presence of the \( \varphi^5 \) term, \( n^* = 3 \) is sufficient. Thus, a natural choice of the model corresponds to the uniform part of the action \( H_u = \int d^d x [V(\varphi) - g_5 \varphi^5] \)
CHAPTER 4. CRITICALITY OF THE $\phi^4$ FIELD MODEL WITH $\phi^5$ TERM

with

$$V(\varphi) = g_2\varphi^2 + g_4\varphi^4 + g_6\varphi^6, \quad (4.1)$$

where $g_2, g_4 > 0$, $g_6 > 0$, $g_5$ are parameters. Without loss of generality we will be using $g_4 = g_6 = 1$, $g_5 > 0$. The range of values of $g_5$ is chosen in such a way as to avoid creating extrema additional to $\varphi = 0$ – at least at the mean field level. This corresponds to the condition

$$|g_5| < g^* = \frac{16}{5\sqrt{3}}\sqrt{g_4g_6} \approx 1.848 \quad (4.2)$$

implying that the $Q_5$ term does not disturb the system strongly at the microscopic scale. Fluctuations may change this situation. Thus, in simulations we will consider the range $0 < g_5 < g^*$. According to the standard practice [1], the action (4.1) must be supplemented by the gradient term $\sim \int d^d x (\vec{\nabla} \varphi)^2 > 0$.

Simulations have been conducted in 2D for the discretized version of the model – placed on a square lattice with periodic boundary conditions. Then, the partition function becomes

$$Z = \int D\varphi \exp(-H), \quad (4.3)$$

with

$$H = -t \sum_{\langle ij \rangle} \varphi_i \varphi_j + \sum_i [V(\varphi_i) - g_5\varphi_i^5], \quad (4.4)$$

where the field $\varphi_i$ is defined at a site $i$ of the square lattice with $L$ sites along each
direction, and the summation $\sum_{(ij)}$ runs over nearest neighbor sites separated by $\Delta L = 1$ distance and coupled by the parameter $t > 0$. This parameter together with $g_5$ will be used to tune the system into the critical point. Thus, in addition to $g_4 = g_6 = 1$ we set $g_2 = 1$.

The measure in (4.3) is defined as $\int D\varphi = \prod_{i=1}^{L^2} \int_{-\infty}^{\infty} d\varphi_i$.

It is also useful to use a simplified (for numerical purposes) version of the model

$$Z = \int D\varphi \exp(-H_1) \prod_i (1 + g_5 \varphi_i^5), \quad (4.5)$$

where

$$H_1 = -t \sum_{(ij)} \varphi_i \varphi_j + \sum_i \left[ a \varphi_i^2 + g_4 \varphi_i^4 + g_6 \varphi_i^6 \right]. \quad (4.6)$$

Following the standard approach [1] that only the first most relevant terms of the Landau expansion matter, the integrand in Eq.(4.5) can be rewritten as $\exp(-H_1 + \ln(1 + g_5 \varphi^5)) \rightarrow \exp(-H_1 + g_5 \varphi^5 - g_5^2 \varphi^{10}/2)$, with the higher order terms dropped. As it is obvious, the truncated model does not need to have the $\sim g_6$ term because there is no instability anymore – due to the term $\sim \varphi^{10}$. Thus, $g_6$ can be set to zero in Eq.(4.6).

The paradigm of Universality predicts that both models should have the same critical behavior. We will present results of the simulations for the truncated as well the full model. Jumping ahead, it will be shown that, while the position of the critical point, $t = t_c$, is different for two models, the critical behaviors are identical within the statistical error (of about 1-2%).

It is important to report that we have found no fixed point at any finite value of $g_5$ within the interval $0 < g_5 \leq 1$ (where the correlation length is diverging). Thus, we conclude that there is only one fixed point – corresponding $g_5 = g_c = 0$. Then the question should be
answered about the scaling dimension $\Delta_5$ of the $g_5$-term. This can be achieved by observing the divergence of the correlation length $\xi \sim g_5^{-\mu_5}$ with some exponent $\mu_5 > 0$ as $g_5 \to 0$ as long as $t = t_c$. Such a divergence has been observed and it is found that $\mu_5$ coincides with the Onsager value $\mu = 8/15$ of the field exponent (within 1-2% of the total error). This implies that $\Delta_5 = 2 - 1/\mu = 1/8$ is the same as the critical dimension $\Delta_1$ of the field $\varphi$.

### 4.3 Duality Transformation

We will be using the dual formulation of the models (4.3,4.5) and will utilize the Worm Algorithm for Monte Carlo simulation[48]. In the dual formulation, the continuous variables \{\varphi_i\} that sit on the sites of the lattice are exchanged for integer valued variables that live on the bonds and sites of the lattice. More specifically, the factor $\exp(t\varphi_i\varphi_j)$ at each bond as well as $\exp(g_5\varphi_i^5)$ at each site are expanded in Taylor series and, then, each term is integrated out with respect to the field $\varphi_i$. The resulting partition function (4.3) is represented in terms of the powers and coefficients of the expansion.

To begin the duality transformation, plug the action 4.4 into the partition function 4.3 to get

$$Z = \int D\varphi \left( \prod_{<ij>} e^{t\varphi_i\varphi_j} \right) \left( \prod_i e^{-a\varphi_i^2 - g_4\varphi_i^4 + g_5\varphi_i^5 - g_6\varphi_i^6} \right). \quad (4.7)$$

Next we expand the exponential $e^{t\varphi_i\varphi_j}$ for each bond and $e^{g_5\varphi_i^5}$ at each site and keep in mind that only even powers of $\varphi_i$ survive the integration. Finally, after selecting all factors contributing to a given power of $\varphi_i$, the partition function can be represented as

$$Z = \sum_{\{N_{ij}\},\{n_i\}} \prod_{<ij>} \left( t^{N_{ij}} \right) \prod_i \left( S(C_i) \frac{g_5^n}{n_i!} \right), \quad (4.8)$$

where $n_i = 0, 1, 2, \ldots, \infty$ is an integer defined at site $i$; $N_{ij} = 0, 1, 2, \ldots$ is an integer defined
on a bond $ij$ connecting sites $i$ and $j$; and

$$S(C_i) = \int_{-\infty}^{\infty} d\varphi \varphi^{C_i} \exp(-a\varphi^2 - g_4\varphi^4 - g_6\varphi^6), \quad (4.9)$$

with the site charge

$$C_i = \sum_{j=\langle i \rangle} N_{ij} + 5n_i \quad (4.10)$$

being even, and where $\sum_{j=\langle i \rangle}$ denotes summation over bonds connected to the site $i$. Thus, the configurational space is fully defined by the bond and the site integers $N_{ij}, n_i$, respectively, with the continuous field $\varphi_i$ integrated out. The numerical value of the integral $S(C_i)$ at each site depends on the total bond and site charges.

The inspection of Eq.(4.8) indicates that the partition function can be represented as a series in even powers of $g_5$:

$$Z = \sum_{N_5=0,2,4,...} B_{N_5} g_5^{N_5}, \quad N_5 = \sum_i n_i, \quad (4.11)$$

where

$$B_{N_5} = \sum\{N_{ij}\} \sum\{\sum_i n_i=N_5\} \prod_{\langle ij \rangle} \frac{i^{N_{ij}}}{N_{ij}!} \prod_i \left(\frac{S(C_i)}{n_i!}\right) \quad (4.12)$$

are positive coefficients independent of $g_5$. This is consistent with the symmetry of the model with respect to simultaneous change $\varphi \rightarrow -\varphi, g_5 ightarrow -g_5$. Thus, the dual representation (4.8-4.10) is free from the sign problem.

It is possible to see that the truncated model (4.5) corresponds, in the dual representation, to limiting the onsite values of $n_i$ in Eqs. (4.8,4.11) to $n_i = 0,1$ only. In other words, in the expansion of $\exp(g_5\varphi_i^5)$ in Eq.(4.3,4.4) only two first terms are kept. According to the
paradigm of universality such a truncation should not affect the scaling properties of the model – that is, in the limit when the correlation length exceeds considerably the lattice constant.

In principle, one can generate arbitrary number of the truncated models which are free from the sign problem – by limiting the onsite factors \( n_i \) up to some maximum value greater than 1. This limitation, obviously, should have no impact on the scaling behavior.

The dual representation (4.8-4.10,4.11,4.12)) is especially convenient in calculating the mean thermodynamical values \( \langle \ldots \rangle \) of \( \sum_i \phi_i^5 \). Evaluation of \( d\ln Z/dg_5 \) in the representations (4.11) and (4.3) gives

\[
\langle \psi \rangle = g_5^{-1} \langle N_5 \rangle, \quad \psi = \sum_i \phi_i^5.
\] (4.13)

Similarly, higher order means \( \langle \psi^m \rangle, \quad m = 2, 3, \ldots \) can be expressed in terms of the means of the higher powers of \( N_5 \).

For the truncated model, the derivative \( d\ln Z/dg_5 \) applied to the representation (4.5) and compared with (4.11) gives the relation similar to Eq.(4.13):

\[
\langle \psi_1 \rangle = g_5^{-1} \langle N_5 \rangle, \quad \psi_1 = \sum_i \frac{\phi_i^5}{1 + g_5 \phi_i^5} \rightarrow \psi,
\] (4.14)

where the last relation is written with respect to the limiting scaling behavior. This aspect will be explicitly addressed below.

## 4.4 Worm Algorithm and Acceptance Ratios

During Metropolis Monte Carlo with the Worm Algorithm, the configuration space is explored by inserting two extra walkers into the theory. We will characterize the configurational space by charges 0, 1 of each walker (historically called by names Masha and Ira).
That is, there are three subspaces: \((0, 0), (0, 1)\) or \((1, 0)\), and \((1, 1)\). The first one corresponds to contributions to the partition function \(Z\) (called as Z-space), the second – to the mean \(\langle \phi \rangle\) (we will call it as \(\varphi\)-space), and the third – to \(\langle \varphi_i \varphi_j \rangle\) (we will call it as G-space). If the walker carries a charge equal to one then we allow it to perform type of update called SHIFT where it proposes to hop to a nearest neighbor site on the lattice at random and simultaneously increment or decrement the bond variable \(N_{ij}\) on each link as it travels.

The acceptance ratios, \(R\), for the SHIFT update are determined from the relative configuration weights – the proposed one over the old one. Suppose a masha is located at site \(i\) and we propose to hop to target site \(j\), then

\[
R = \begin{cases} 
\frac{1}{N_{ij}+1} \frac{S(C_j+2)}{S(C_j)} & \text{for bond number increase } +1 \\
N_{ij} \frac{S(C_i-2)}{S(C_i)} & \text{for bond number decrease } -1.
\end{cases}
\] (4.15)

At finite \(g_5\) the structure of the configurational space changes – there are loops which are not closed. The general condition (4.10) indicates that whenever \(n_i = 1, 3, 5, ...\) at a site \(i\), then there is an odd total number of the integers \(N_{ij}\) at the bonds connecting this site with its neighbors \(j\). Thus, a separate pair of updates are designed to explore this new feature of the configuration space. This is implemented by incrementing or decrementing the \(g_5\) charge \(n_i\) at one of the sites where the masha is located. This procedure, called RECHARGE, changes \(n_i\) by \(\pm 1\) while simultaneously toggling the value of the masha charge at the site between 1 and 0. Accordingly, the system will alternate between the \((0, 0)\) Z-space to the \((1, 1)\) G-space as well as to the \((0, 1)\) or \((1, 0)\) \(\varphi\)-spaces. In the RECHARGE update, the net charge, \(C_i\) at the site will be unaffected if the proposal is accepted. This update can be viewed as flipping a charge of either walker to the "opposite", that is, 1 to 0 or 0 to 1. It can be summarized as:

1. randomly choose a masha currently located at site \(j\)
CHAPTER 4. CRITICALITY OF THE $\phi^4$ FIELD MODEL WITH $\phi^5$ TERM

2. if the masha charge = 1 then propose to make it zero and also increase or decrease the value of $n_j$ at site $j$ by one with probability

$$R = \begin{cases} \frac{g_5}{n_j+1} \frac{S(C_j+4)}{S(C_j)} & \text{to propose increasing } n_j \text{ by one} \\ \frac{n_j}{g_5} \frac{S(C_j-6)}{S(C_j)} & \text{to propose decreasing } n_j \text{ by one} \end{cases}$$

(4.16)

3. alternatively, if the masha charge = 0 then propose to make it one and also increase or decrease the $n_j$ value by one, with ratios

$$R = \begin{cases} \frac{g_5}{n_j+1} \frac{S(C_j+6)}{S(C_j)} & \text{to propose increasing } n_j \text{ by one} \\ \frac{n_j}{g_5} \frac{S(C_j-4)}{S(C_j)} & \text{to propose decreasing } n_j \text{ by one} \end{cases}$$

(4.17)

In the third type of update, the $n_i$ value at the site is changed by $\pm 2$ and there is no change to the masha charge or to the measurement space. It is important to remember that for the purpose of collecting estimators of statistical quantities, we must be consistent in terms of what space we choose for measurement. In our simulations, we only measure in the $Z$-space, that is the space of the partition function, where both walkers carry a charge of zero, however the system may sample other spaces as it evolves (the correlator is always sampled in $G$-space by definition). It can be implemented as:

1. randomly choose a masha currently located at site $j$

2. propose to increase or decrease the $n_j$ value by 2, we do not change the masha charge values at all, the acc. ratios for this update are

$$R = \begin{cases} \frac{g_5^2}{(n_j+2)(n_j+1)} \frac{S(C_j+10)}{S(C_j)} & \text{to propose increasing } n_j \text{ by two} \\ \frac{n_j(n_j-1)}{g_5^2} \frac{S(C_j-10)}{S(C_j)} & \text{to propose decreasing } n_j \text{ by two} \end{cases}$$

(4.18)
CHAPTER 4. CRITICALITY OF THE $\phi^4$ FIELD MODEL WITH $\phi^5$ TERM

We notice that this last update is $\sim g_5^2$ so that for small $g_5$ this second update is accepted with very low probability. In fact, the universality of the model is unaffected by dropping this update entirely as is seen from the results of the truncated model.

4.5 Critical behavior at $g_5 = 0$ by the flowgram method

Before we study the effect of $g_5$ we first examine the pure $\varphi^4$ theory with $g_5 = 0$, which is well known to belong to the Ising universality class. To check this, we measure the critical exponents $\eta$ and $\nu$. In order to determine the $\nu$ exponent we have chosen the following Binder cumulant

$$U_r(t, L) = \frac{\langle r^2 \rangle_G}{r_L^2}, \quad r_L^2 = \sum_{\vec{r}} \vec{r}^2/L^d \propto L^2, \quad (4.19)$$

where $\langle r^2 \rangle_G = \sum_{\vec{r}} G(\vec{r}) \vec{r}^2/\sum_{\vec{r}} G(\vec{r})$, with $G(\vec{r})$ denoting the correlator $\langle \varphi(\vec{r})\varphi(0) \rangle$ taken at two points in 2D space separated by the vector $\vec{r}$; and $\langle ... \rangle$ defines the averaging with respect to the partition function (4.8). To demonstrate that $U_r$ is a scale invariant quantity at the critical point, we have analyzed its behavior vs $t$ for various sizes. Fig. 4.1 shows the crossing point of $U_r$ at $t = t_c \approx 1.3173$ for the parameters $g_2 = g_4 = 1, g_6 = 0, g_5 = 0$. The value of $t_c$ depends on $g_6$. For the case $g_2 = g_4 = g_6 = a = 1, g_5 = 0$ it is $t_c \approx 1.6975$. [The accuracy of $t_c$ is controlled by the maximum system size $L$ simulated]. By the definition, Eq.(4.19), $U_r \to 0$ (as $L \to \infty$) in the disordered phase (where the correlation length is $\sim O(1)$) and $U_r = 1$ in the ordered phase where the coherence length reaches the system size $L$. Thus, formally speaking, any value in the interval $0 < U_r < 1$ belongs to the critical range of $U_r$. In reality, for practical purposes of achieving better accuracy of the critical exponent we have found that it is reasonable to tune $U_r$ into the region where $dU_r/dt$ vs $U_r$ reaches its maximum. Fig. 4.2 shows that this corresponds to $0.5 < U_r < 0.8$. 
Figure 4.1: $U_r$ vs $t$ for various $L$. This crossing point corresponds to $U_B = 0.965$ and it determines $t_c = 1.3173 \pm 0.0003$ (for $g_4 = 1$, $g_6 = 0$, $g_2 = 1$, $g_5 = 0$ in Eqs.(4.8,4.4)).

At $g_5 = 0$ the integers $N_{ij}$ form closed non-oriented loops. Within the Worm Algorithm [48] the evaluation of the correlator corresponds to having one loop with two open ends. In this space, $U_r$ can be constructed as the histogram of the square of the distance $\bar{r}^2$ between two open ends which represent two random walkers. Accordingly $dU_r/dt$ can be found as

$$tdU_r/dt = \sum_{\langle ij \rangle} [(N_{ij}\bar{r}^2)_G - \langle N_{ij} \rangle_G \langle \bar{r}^2 \rangle_G]$$

following direct differentiation vs $t$ in the dual representation (4.8,4.9,4.10).

The result of this procedure – the family of graphs $dU_r/dt$ vs $U_r$ for various $L$ is shown in Fig. 4.2 for $g_4 = a = 1$, $g_6 = 0$. The master curve obtained by the vertical rescaling of the data with the exponent $\nu = 1$ is shown in Fig. 4.3. The lines connecting the data points for
L = 40, 80 are shown in order to emphasize that at these sizes the sub dominant term is still visibly significant so that these data points do not collapse into the master curve. The line for L = 400 is also shown to indicate that all higher sizes L = 120, 160, 200, 320, 400 belong to the master curve within the error 1-2%.

Figure 4.2: Monte Carlo results for dU_r/dt vs U_r as defined in Eq.(4.20) for several system sizes L shown close to each curve. Lines are guides to eye.

Because our system is translationally invariant (we assume periodic boundary condition), the sum over the lattice of the correlator denoted Z' is

\[ Z' = \sum_{ij} G_{ij} = L^2 \sum_{\vec{r}} G(\vec{r}) \]  

(4.21)

Critical correlators are not integrable but in the finite system the divergent correlation length \( \xi \) is cut off by \( L \), which gives access to the anomalous dimension \( \eta \) by
Figure 4.3: Rescaled data shown in Fig. 4.2 with $\lambda(L) = (200/L)^{1/\nu}$, $\nu = 1$. The overall statistical error of the data is $\sim 1 - 2\%$.

\[
\sum_{i,j} \langle \varphi_i \varphi_j \rangle = \frac{1}{Z} \sum_{i,j} G_{ij} = \frac{L^2}{Z} \sum_r G(\vec{r}) \sim L^2 \int_0^\xi r^{1-\eta} dr \sim L^2 L^{2-\eta} \quad (4.22)
\]

Since at $g_5 = 0$ the simulation always stays in the $(1, 1)$ G-space, the estimator for $Z'$ is just 1 on each step. The estimator for $Z$ can be found by noticing that the weight of the configuration $(0,0)$ can be calculated from the weight in the G-space $(1,1)$ when both walkers are located at the same site, say, $j$. Then, it is $\frac{S(C_j^-)}{S(C_j)}$, and, essentially, $Z \sim G(0)$. In other words, the scaling properties of the correlator $\langle \varphi_i \varphi_j \rangle$ and $G(r)/G(0)$ are the same.

Similarly, to how we determined $\nu$, the family of the curves $f(L) = Z'/[L^2 L^2 Z] \sim L^{-\eta}$ if plotted versus $U_r$ for various $L$ can be collapsed to a single master curve by simple rescaling along the vertical axis. The rescaling factor is $\sim L^{-\eta}$. 
Thus to determine critical exponent $\eta$, we measured $f$ and $U_r$ for sizes $L = 16,\ldots,128$ and, then, plotted $f$ vs $U_r$. The family of curves were self-similar with negligible deviations from leading order for $L > 48$, and these curves were amenable to single-parameter rescaling by a factor $\lambda(L)$. The rescaling onto the master curve are shown in Fig. 4.4 with the original curves as an inset. The master curve was chosen as $L_0 = 128$. A log-log plot of the rescaling parameter $\lambda(L)$ vs $L$ yielded $\eta = 0.248 \pm 0.005$ in good agreement with the well known result $\eta = 1/4$ from the Onsager solution of the 2d Ising model. This result is shown in Fig. 4.5.
Figure 4.5: Rescaling factor $\lambda(L)$ versus $L$ plotted on logarithmic axes. The slope gives an estimate for the critical exponent $\eta = 0.248 \pm 0.005$
4.6 Critical behavior at finite $g_5$

Ising critical behavior is characterized by two primary fields $\sim \varphi^2$ and $\sim \varphi$ with the corresponding “charges” $\tau \sim t - t_c$ and $h$. In the space $(\tau, h)$ the divergence of the correlation length occurs with the Onsager exponents $\nu = 1, \mu = 8/15$. In the previous section we have explored the first property and have shown that the $\nu$ exponent is consistent with the Onsager solution. In order to observe the divergence along the second line one should select $t = t_c$ as determined from the previous procedure for largest sizes and to apply the NF method – now at finite $h$. In this case plotting $dU_B/dh$ vs $U_B$ for various $L$ and constructing the master curve by rescaling $dU_B/dh$ into a single master curve by some factor $\lambda(L)$ for each $L$ will give the $\mu$ exponent.

The above logic can be followed in order to determine scaling dimensions of any higher odd terms. Here we will be concerned with the term $\sim \varphi^5$ as the most possibly relevant one – as suggested in Ref.[5]. We have determined the corresponding critical exponent $\mu_5$ from the rescaling procedure of the graphs $dU_B/dg_5$ versus $U_B$ for various $L$.

At this juncture we have to change the type of the Binder cumulant $U_B$. At finite $g_5$ (or in the presence of any other odd term) using the cumulant $U_B = U_r$, Eq.(4.19), is not convenient because the number of open loops is now a dynamical variable. Thus, we choose $U_B = U_2 = \langle \sum_i \varphi^5_i \rangle^2 / \langle (\sum_i \varphi^5_i)^2 \rangle$ built on the $\varphi^5$ term. In the dual representation (4.8) it is

$$U_2 = \frac{(d \ Z/dg_5)^2}{Z \ d^2 \ \ln Z/dg_5^2} = \frac{\langle N_5 \rangle^2}{\langle N_5(N_5 - 1) \rangle}. \quad (4.23)$$

For the full model (4.3,4.4) $U_2 = \langle \psi \rangle^2 / \langle \psi^2 \rangle$, where $\psi$ is defined in Eq.(4.13). Clearly, $U_2 = 0$ at $g_5 = 0$ simply because $\langle \psi \rangle = 0$ and $\langle \psi^2 \rangle$ is finite; and $U_2 = 1$ far away from the critical point – where $g_5 \neq 0$ and fluctuations are suppressed.

For the truncated model the role of $\psi$ is played by $\psi_1$, Eq.(4.14). In the limit $g_5 << 1$ the denominator in $\psi_1$ plays no practical role. More specifically for the truncated model
\[ \langle N_5(N_5 - 1) \rangle = g_5^2[\langle \psi^2 \rangle - \sum_i \langle \varphi_{i0}^2/(1 + g_5 \varphi_i^5) \rangle] \rightarrow g_5^2 \langle \psi^2 \rangle \] because the term \( \sim \langle \psi^2 \rangle \) has the extra factor \( L^2 \) with respect to \( \sim \sum_i \langle \varphi_{i0}^2 \rangle \). We will be evaluating \( U_2 \) in terms of its representation by the dual variable \( N_5 \), Eq. (4.23), for both models.

\[ \text{Figure 4.6: } U_2^{-1} \text{ vs } g_5 \text{ in the truncated model (4.5) for sizes } L \text{ shown close to each curve.} \]

The variation of \( U_2 \) versus \( g_5 \) from 0 to 1, see Fig. 4.6, occurs over the domain shrinking with \( L \rightarrow \infty \) as the power \( \sim L^{-1/\mu_5} \) where \( \mu_5 > 0 \) determines the scaling dimension \( \Delta_5 = 2 - 1/\mu_5 \) of the \( \varphi^5 \) term. [If \( \Delta_5 < d = 2 \), this term is relevant and irrelevant otherwise]. Thus, \( dU_2/dg_5 \propto L^{1/\mu_5} \rightarrow \infty \). This derivative can be expressed in terms of averages of powers of \( N_5 \) with the help of the general relation for the derivative \( d\langle Q \rangle/dg_5 = g_5^{-1}[\langle Q N_5 \rangle - \langle Q \rangle \langle N_5 \rangle] \) of any quantity \( Q \). This relation follows immediately from the representation (4.11) for both models. The result of the simulations for the truncated model are presented in Fig. 4.7.

The family of the curves, Fig. 4.7, can be collapsed to a single master curve, Fig. 4.8, by the scale factor \( \lambda(L) \sim L^{-1/\mu_5} \) with the exponent \( \mu_5 = 0.534 \pm 0.008 \). This exponent
CHAPTER 4. CRITICALITY OF THE $\phi^4$ FIELD MODEL WITH $\phi^5$ TERM

Figure 4.7: $dU_2^{-1}/dg_5$ vs $U_2^{-1}$ in the truncated model (4.5) for sizes $L$ shown close to each curve.

turns out to be consistent with the $\mu$-exponent of the 2D Ising model, $\mu = 8/15$, within 1-2% of the combined error – systematic and statistical. It is important to note that the range of $\lambda$ extends over almost 3 orders of magnitude. In order to emphasize the quality of the collapse, we have included the plot Fig. 4.9 showing two sizes $L = 10, 350$ rescaled to each other within a narrow range of $U_2^{-1} - 1$. A visible deviation from scaling starts for $U_2^{-1} - 1 < 1$. Similar behavior is demonstrated by the full model with $g_6 = 1$. Its master curve is also shown in Fig. 4.8, with the rescaling factor characterized by the same exponent $\mu_5$.

This concludes our analysis of the role of the symmetry breaking term $\varphi^5$ in 2D. Within the accuracy of 1-2% and up to the simulated sizes of $L = 350$ this term has the same scaling dimension as the linear one $\varphi$ in the Ising class. Using similar approach, higher odd terms can be considered too. In response to the question [39] about the role of the odd terms in
Figure 4.8: The master curve obtained by “vertical” rescaling of the plots $dU^{-1}/dg_5$ vs $U_2^{-1}$. The upper curve is from Fig. 4.7 obtained by the rescaling by the factor $\lambda(L)$ to match the data for $L = 350$, that is, $\lambda(350) = 1$. The lower curve is obtained by the same procedure for the data obtained from the full model, $g_6 = 1$, for $L = 10, 20, 40, 80, 160, 200, 250, 320$, with the choice $\lambda(200) = 1$. Inset: The log-log plots of $\lambda$ versus $L$ for the full (the lower data and the line) and truncated (the upper data and the line) models. Solid lines are the linear fits with the slopes $1/\mu_5$ giving $\mu_5 = 0.534 \pm 0.008$. The error includes statistical and systematic contributions. This value is consistent with the Onsager exponent $\mu = 8/15 \approx 0.533$.

The formal mapping [6] of the LG critical point to the field theory, we conjecture that all odd terms have the same critical dimension of the field primary operator – consistent with the Ising criticality.
Figure 4.9: Deviation from the scaling. Two curves, $L = 10, 350$, from Fig. 4.8 are shown in the domain where deviations from scaling are significantly higher than the statistical error of 1% (about 15%). Inset: More detailed view on the linear scale.
Chapter 5

Criticality of the square well fluid

5.1 Introduction

In the previous chapter we approached the problem of the LG criticality from the perspective of the lattice field theory. In this chapter, we take a more direct approach and simulate the fluid directly on the continuum in two dimensions. So far we have discussed the role of higher odd terms in the field theory along the line of the universality paradigm – when a particular form of the action is not important as long as a system is close to the fixed point. The relation of this study to the actual LG criticality stems from the formal mapping of the classical gas to a field theory [6].

The LG critical point has been addressed by direct Monte Carlo simulations by many groups. In Ref.[33] the analysis of 2D Lennard-Jones fluid has been carried out within the hypothesis of the mixing [31, 32, 4], and it has been concluded that the universality of the transition is consistent with the Ising class. However, the maximum size simulated in this work allowed to include only about 400 particles on average, with two relatively small sizes of the simulation box used. Under this condition the applicability of the finite-size scaling (FSS) analysis becomes questionable. The same approach has been used in 3D [34] with the
conclusion that the 3D LG critical point belongs to the $Z_2$ class. The role of corrections to scaling turns out to be much more important in 3D. This, in particular, lead to inconsistent values of the $\nu$ exponent deduced from different quantities.

Monte Carlo simulations have been also conducted for the model interaction potential – the square well in 3D in Ref.[49] (see also references there). The analysis was carried out for a set of box sizes from 6 to 18 hard core radii, and the conclusion was reached that the universality of the critical point is consistent with the Ising class. Later, however, a different result has been obtained for Lennard-Jones potential [50] – the critical exponent $\nu$ was not consistent with the Ising class. The LG criticality has been also addressed in a series of papers [36, 37, 38], where both the critical exponent $\nu$ and the critical histogram were found to be consistent with those of the 3D Ising. [At this point, however, we should notice that the accuracy in the $\nu$-exponent value does not allow to exclude the non-Ising universality [41]]. The approach based on molecular dynamics has been utilized in Ref.[51] and significantly larger sizes have been simulated with the conclusion that the LG criticality in 3D is of Ising type.

It is important to note that the methods used to evaluate the critical exponents in Refs. [33, 34, 49, 50, 51] are strongly dependent on the choice of the values of the critical temperature $T_c$ and pressure $P_c$ (or density). This introduces significant uncertainties in the exponents. In 3D the corrections to scaling must also be included. Thus, the fits become multi-parametric which introduces even larger errors. Furthermore, as pointed out in Ref.[35], the Yang-Yang singularity implies non-analytical corrections to the position of the liquid-vapor coexistence line which makes questionable the extrapolation procedures for the purpose of recovering the $\beta$ exponent.

Overall, it is fare to say that the majority in the scientific community does accept the conjecture that the LG criticality belongs to the Ising class despite that the experimental and numerical evidence may leave some room for doubts – because of quite high uncertainties
in measured indices. Thus, our main motivation is to significantly improve the accuracy in determining the indices.

We apply the NF method to the LG critical point in 2D by measuring directly the critical index $\mu$ (and, independently, $\gamma/\nu$ and $\beta$ as a crosscheck). We also developed a novel method for obtaining the $\nu$ exponent directly. The outcome of our large scale simulations allows to conclude with high certainty that the 2D LG criticality does belong to the Ising class. It is important to note that our analysis is not affected by the mixing effect.

5.2 The mixing effect in the LG criticality

Early approaches to the LG criticality [31, 32, 4, 33, 34] were based on the assumption that its universality belongs to the Ising class, with the primary scaling parameters $\tau$, of the thermal operator, and $h$, of the field operator, being linearly mixed with the physical parameters $t \sim T - T_c$ and $\bar{\mu}$ representing deviations of temperature $T$ and chemical potential $\bar{\mu}$ from their critical values $T_c, \bar{\mu}_c$, respectively. The main consequence of such a mixing is the asymmetry of the diameter $\rho_d = \frac{1}{2}(\rho_l + \rho_g)$, where $\rho_l$, $\rho_g$ are the densities of the liquid and gas phases, which acquires the non-analytical contribution $\sim (-t)^{1-\alpha}$, $t < 0$, where $\alpha$ stands for the scaling exponent of heat capacity. As explained in Ref.[32] (see also in Ref.[1]), this contribution is generic as long as there is asymmetry in the system – following from the admixing of the term $\sim h\varphi^2$ to the standard one $\sim h\varphi$ close to the fixed point, where $\varphi$ is the (real scalar) order parameter of the $\varphi^4$ theory. It is important that the contribution $\sim (-t)^{1-\alpha}$ is subdominant with respect to the main term $\rho_l - \rho_g \sim (-t)^{\beta}$ determined by the exponent of the order parameter $\beta$ – by the token that $\beta + \alpha < 1$. Thus, the dominant scaling behavior controlled by the divergencies of the correlation length $\xi \sim \tau^{-\nu} \to \infty$ at $|h| < h^* = |\tau|^\nu/\mu$ (in the weak field region) [1] and $\xi \sim |h|^{-\mu} \to \infty$ at $|h| > h^*$ (in the strong field region) are still characterized by the Ising exponents $\nu$ and $\mu$. 
The idea of the mixing of three operators $\tau, h$ and the grand potential $\Phi$ with $t, \tilde{\mu}$ and pressure $\tilde{p}$ has been suggested in Ref.[31] and it was noticed that such a mixing should generate an additional contribution $\sim (-t)^{2\beta}$ to $\rho_d$ at $t < 0$. This term turns out to be dominating the one $\sim (-t)^{1-\alpha}$ as $t \to -0$ (but still it is subdominant to the leading scaling). This approach has been further developed in Refs.[35, 36, 37, 52] in connection with the so called Yang-Yang anomaly [53, 35] suggesting that the coexistence line in the space $(t, \tilde{\mu})$ acquires the non-analytical term $\tilde{\mu} \sim (-t)^{2-\alpha}$ in addition to the analytical one $\sim t$. Accordingly, the heat capacity divergence $C_V \sim t^{-\alpha}$ along the coexistence line is shared between $d^2\tilde{p}/dt^2 \sim t^{-\alpha}$ and $d^2\tilde{\mu}/dt^2 \sim (-t)^{-\alpha}$. This anomaly $\sim (-t)^{2\beta}$ has been observed in simulations [36] of 3D square well liquid with, however, a relatively small coefficient and the error bar larger than the value itself. More recently, significantly larger values of the contribution have been claimed in simulations [54, 55]. However, these methods rely on fitting the coexistence histogram and then extrapolating to obtain estimates for the critical parameters and $\rho_d$. This procedure introduces uncontrolled errors – especially at large sizes. Within the flowgram method, which does not rely on either the values of the critical parameters or extrapolation, the error is determined by statistical error of simulations of the Binder cumulants and the scaling quantities. Thus, we can control the error and eventually get desired accuracy for each simulated size for long enough simulations.

It is interesting to note that, along the line of the approach [32], the mixing of pressure with $h$ corresponds to the term $\sim \tilde{p}\varphi$ (in addition to the standard one $\sim h\varphi$) in the Hamiltonian of the $\varphi^4$ theory. It is important that, while the origin of the term $\sim (-t)^{1-\alpha}$ can be simply traced back to a linear (non-singular) combination of the Hamiltonian parameters $\tau, h$ replacing $\tau$ as a coefficient in front of $\sim \varphi^2$, Ref.[32], there is no such an explicit explanation for the term $\tilde{p}\varphi \sim (-t)^{2-\alpha}\varphi$. This raises a question if such a term can emerge from any local combination of powers of $\varphi$ or its derivatives in the Hamiltonian. Such a question is especially important in view of the mapping of the LG system to the field theory [6].
Here we focus on the 2D case. The main part of our results is concerned with determining the leading scaling behavior of the correlation length in the strong and weak field domains. For this purpose, as we will discuss below, the mixing with the pressure can be ignored. However, the corrections to scaling produced by the pressure mixing turn out to be stronger than the corrections produced by the irrelevant terms in the $\varphi^4$ model with exact $Z_2$ symmetry. We will also outline how the singularities of the diameter can be detected by the numerical flowgram method [10] – without relying on the standard approach.

5.3 Strong and weak field domains for LG transition in free space

It has been argued [12] that a generic linear path $t = t(l) \propto l$, $\bar{\mu} = \bar{\mu}(l) \propto l$, where $l \to 0$ is some parameter, toward the critical point lies in the strong field domain as long as the critical exponent $\mu$ is less than $\nu$.

This argument goes as follows: the critical range can be divided into two parts – of strong and weak field [1]. The separation between the two regions are determined by the relation $h^* \sim \tau^{\mu/\nu}$ so that at $|h| > h^*$ the critical singularities are determined by $h$ rather than by $\tau \to 0$. Thus, if $\mu < \nu$, a generic path $\bar{\mu} - \mu_c \sim h - r\tau$ toward the critical point $\tau = 0, h = 0$ with non-zero mixing coefficient $r$ will belong to the region of strong field close enough to the critical point – as sketched in Fig. 5.1. This argument does not take into account the pressure mixing in the complete scaling theory however it is important to note that the weak field and the coexistence lines differ from each other by the Yang-Yang anomaly term $\sim (-t)^{2-\alpha} \to 0$, that is, $\sim L^{(\alpha-2)/\nu} \to 0$ within FSS. This difference is subdominant with respect to the proximity $\sim t \sim L^{-1/\nu} \to 0$ to the critical point (because $\alpha < 1$). This guarantees that the leading divergencies are the same along both lines.

Thus, applying the NF method along an arbitrary linear path toward the critical point
allows measuring the strong field exponent $\mu$ only. This analysis has been conducted in Ref.[12] and the value found is consistent with the Onsager result $\mu = 8/15$ within 1% of combined error.

In order to fully characterize the criticality, the system should also be tuned into its weak field domain, where the $\nu$ exponent can be measured. In this domain the correlation length diverges, $\xi \sim \tau^{-\nu}$, and so does the heat capacity $C_V \sim \tau^{-\alpha}$ (see in Ref.[1]). The divergence of the heat capacity $C$ along a path in the strong field domain is characterized by a much stronger divergence – by the index $\gamma$ (see in Ref.[1]). [In 2D the Onsager solution gives $\alpha = 0$ and $\gamma = 7/4$]. Within FSS [27] approach the corresponding divergencies are $\sim L^{\alpha/\nu}$ and $\sim L^{\gamma/\nu}$. In Ref.[12] it has been suggested to use these two drastically different behaviors
in order to identify the weak field domain without observing directly the coexistence line.

Here we will consider a more general situation – when $t$ and $\bar{\mu}$ are parametrized by two parameters $l, l_1$ as

$$t = t_1 l + t_{11} l_1, \quad \bar{\mu} = \mu_1 l + \mu_{11} l_1,$$

(5.1)

where $l, l_1 \to 0$, and $t_1, t_{11}, \mu_1, \mu_{11}$ are some free parameters. Let’s consider the second derivative $C = d^2\Phi/dl_1^2$ evaluated at $l_1 \to 0$, that is, defined at the path $t = t_1 l, \bar{\mu} = \mu_1 l$, or $C = d^2\Phi/dl^2$ (at $l_1 = 0$) of the grand potential $\Phi$

$$\Phi = L^{-d} F(L^{1/\nu} \tau, L^{1/\mu} h),$$

(5.2)

written in the scaling form in the critical region (where the correlation length exceeds the system size $L$) [27]. Here $F(X, Y)$ is some analytical function, and we have ignored the irrelevant terms $\sim L^{-\theta/\nu}$. According to the complete scaling approach [35, 36, 37, 52], the parameters $\tau, h$ are linear combinations of the system parameters $t, \bar{\mu}$ and pressure deviations $\bar{p}$ from its critical value. Similarly, the potential $\Phi$ is also a linear combination of all three quantities:

$$\Phi = \bar{p} + a_1 \bar{\mu} + a_2 t$$

(5.3)

$$\tau = t + b_1 \bar{\mu} + b_2 \bar{p}$$

(5.4)

$$h = \bar{\mu} + c_1 t + c_2 \bar{p}$$

(5.5)

with some coefficients $a_{1,2}, b_{1,2}, c_{1,2}$.

It is convenient to introduce a response function $C$ as $C = d^2\Phi/dl^2$. At $t_1 = t_{11} = 0$ it is proportional to the compressibility along the critical isotherm $t = 0$, $\bar{\mu} = \mu_1 l$. The quantity $d^2\Phi/dl^2$ evaluated at $\mu_{11} = 0$ is proportional to heat capacity along the path $t = t_1 l, \bar{\mu} = \mu_1 l$. 
CHAPTER 5. CRITICALITY OF THE SQUARE WELL FLUID

It is convenient to eliminate \( \hat{p} \) from Eqs.(5.3,5.4,5.5). Then,

\[
\tau = (1 - b_2 a_2) t + (b_1 - b_2 a_1) \hat{\mu} + b_2 \Phi,  \quad (5.6) \\
h = (1 - c_2 a_1) \hat{\mu} + (c_1 - c_2 a_2) t + c_2 \Phi  \quad (5.7)
\]

Differentiating Eqs.(5.6,5.7) along \( l_1 \) (independently from \( l \)), we find

\[
\tau' = \tau_1 + b_2 \Phi'  \quad (5.8) \\
h' = h_1 + c_2 \Phi'  \quad (5.9)
\]

where \( \tau_1 \equiv (1 - b_2 a_2) t_{11} + (b_1 - b_2 a_1) \mu_{11} \) and \( h_1 \equiv (1 - c_2 a_1) \mu_{11} + (c_1 - c_2 a_2) t_{11} \) and the prime \( \cdot' \) refers to the derivative \( d\cdot/dl_1 \). Then, using Eq.(5.2),

\[
\Phi' = \frac{L^{-d}[L^{1/\nu} F'_{X} \tau_1 + L^{1/\mu} F'_{Y} h_1]}{1 - L^{-d}[L^{1/\nu} F'_{X} b_2 + L^{1/\mu} F'_{Y} c_2]}  \quad (5.10)
\]

where we used the notations \( F'_{X} \equiv \partial F/\partial X, \ F'_{Y} \equiv \partial F/\partial Y \). Similarly, \( C = \Phi'' \) takes the form

\[
C = \frac{L^{-d} [L^{2/\nu} F''_{XX}(\tau_1 + b_2 \Phi')^2 + L^{2/\mu} F''_{YY}(h_1 + c_2 \Phi')^2 + 2F''_{XY}L^{1/\nu+1/\mu}(\tau_1 + b_2 \Phi') (h_1 + c_2 \Phi')]}{1 - L^{-d}[F'_{X} L^{1/\nu} b_2 + F'_{Y} L^{1/\mu} c_2]},  \quad (5.11)
\]

where the notations \( F''_{XX} \equiv \partial^2 F/\partial X^2, \ F''_{YY} \equiv \partial^2 F/\partial Y^2, \ F''_{XY} \equiv \partial^2 F/\partial X \partial Y \) are used.

It is useful to note that, if the differentiation is performed along the path, \( C = d^2 \Phi/dl^2, \ \Phi' = d\Phi/dl \), with respect to \( l \), the expressions (5.10,5.11) remain the same, with the meaning of \( \tau_1, h_1 \) changed. Specifically, \( \tau_1 \equiv (1 - b_2 a_2) t_1 + (b_1 - b_2 a_1) \mu_1 \) and \( h_1 \equiv (1 - c_2 a_1) \mu_1 + (c_1 - c_2 a_2) t_1 \).
5.3.1 Scaling in the strong field domain

Within the early approach to mixing [31, 32, 4, 33, 34] there is no non-analytical terms in \( \tau \), Eq.(5.6), and \( h \), Eq.(5.7), that is, \( b_2 = c_2 = 0 \). This implies that for \( h_1 \neq 0 \) and \( \mu < \nu \), the dominant behavior in Eq(5.11) is \( C \sim L^{-d+2/\mu}[1+KL^{1/\nu-1/\mu}] \), where \( K \equiv 2(\tau_1/h_1)F''_{XY}/F''_{YY} \).

It is important that keeping the system in the critical range implies that either \( X \) or \( Y \) are of the order of unity. In the strong field domain \( Y = L^{1/\mu}h \sim 1 \), that is, \( h \sim L^{-1/\mu} \) and \( X \sim \tau/h^{\mu/\nu} \sim l^{1-\mu/\nu} \rightarrow 0 \) as long as \( \mu < \nu \). Since, in general, \( F \) admits the linear term \( \sim X \), the coefficient \( K \) is \( \sim 1 \). Thus, in 2D the linear mixing approach [31, 32, 4, 33, 34] implies \( C \sim L^{7/4} + KL^{7/8} \). We note that the subdominant term is diverging, that is, it is stronger than the standard correction to scaling \( \sim L^{-\omega} \) which in 2D is characterized by \( \omega = 2 \).

As the analysis of Eqs.(5.11,5.10) indicates, while not changing the dominant scaling divergence \( C \sim L^{-d+2/\mu} = L^{\gamma/\nu} \) (by the token of the scaling identities), the complete scaling approach introduces the dominant correction to scaling \( \sim L^{-2d+3/\mu} \) which in 2D gives \( \sim L^{13/8} \) with the coefficient proportional to the pressure mixing term \( \sim c_2 \). More specifically

\[
C \rightarrow h_1^2F''_{YY}L^{7/\tau}[1 + 3c_2F_Y'L^{\gamma+1/\rho} + KL^{1-\frac{1}{\rho}}]
\sim L^{7/4} + 3c_2F_Y'L^{13/8} + KL^{7/8}. \tag{5.12}
\]

Thus, observing the subdominant diverging term in the strong field domain along a linear path toward the critical point gives a possibility of detecting the pressure mixing term \( \sim c_2 \) in Eq.(5.9) which is responsible for the correction \( \sim (-t)^{2\beta} \) to the diameter [31, 35, 36, 37, 52].

Using Eq.(3.3) the derivative of the Binder cumulant along the linear path in the strong field domain becomes

\[
\frac{dU_B}{dl_1} = L^{1/\mu}U_Y'(h_1 + c_2\Phi') + L^{1/\nu}U_X'(\tau_1 + b_2\Phi'). \tag{5.13}
\]
If $c_2 = 0$, the dominant and subdominant divergencies are $\dot{U} \sim h_1 L^{1/\mu} + \tau_1 L^{1/\nu}$ which in 2D gives $\dot{U} \sim h_1 L^{15/8} + \tau_1 L^1$. If $c_2 \neq 0$, the subdominant divergence is replaced by the stronger one as

$$\frac{dU_B}{dl_1} \rightarrow U_Y' h_1 [L^{1/\mu} + c_2 F_Y' L^{-d + 2/\mu}] \sim L^{15/8} + c_2 F_Y' L^{7/4}. \quad (5.14)$$

We note that the derivatives of $F, U$ are evaluated at $X = 0, Y \sim 1$ so that these become parameters $\sim 1$ if $C, dU_B/dl_1$ are plotted versus $U_B$. At this point we note that we were unable to detect $c_2$ with reliable accuracy – due to the presence of the next subdominant term. More details will be given below in Sec.5.4.2.

5.3.2 Scaling in the weak field domain

As the above analysis indicates, the strong field regime occurs as long as $h_1 \neq 0$ in Eq.(5.9). [$h_1 = (1 - c_2 a_1) \mu_{11} + (c_1 - c_2 a_2) t_{11} \neq 0$ for the derivatives along $l_1$, and $h_1 = (1 - c_2 a_1) \mu_1 + (c_1 - c_2 a_2) t_1$ for the derivatives along $l$].

The weak field linear path corresponds to $h_1 = (1 - c_2 a_1) \mu_1 + (c_1 - c_2 a_2) t_1 = 0$ and

$$\tau_1 = \left[1 - b_2 a_2 - \frac{(b_1 - b_2 a_1)(c_1 - c_2 a_2)}{1 - c_2 a_1}\right] t_1. \quad (5.15)$$

Similarly to the case considered above, the terms $\sim c_2, b_2$ in Eqs.(5.4,5.5) introduce subdominant corrections to scaling in the weak field regime too, and these corrections are stronger than the standard irrelevant terms in $Z_2$ criticality. In order to obtain the leading subdominant terms, we note that $F(X,Y)$ in Eq.(5.2) and $U(X,Y)$ in Eq.(3.3) are analytical functions of $X,Y$ and also are even with respect $Y \rightarrow -Y$. Thus, in the limit $Y \rightarrow 0$ (weak field domain) the derivatives $F_Y' \rightarrow F''_Y Y$ and $U_Y' \rightarrow U''_Y Y$. Furthermore, $Y = L^{1/\mu-d} c_2 F(X,0) \sim L^{1/\mu-d} \rightarrow 0$ (since $h_1 = 0$). Using these relations, the scaling of $C$ up to
the main subdominant term becomes

$$C \rightarrow \tau^2_1 F'_{XX} L^{\frac{\alpha}{\nu}} \left[ 1 + K_C c_2^2 L^{-\frac{2\beta}{\nu}} \right],$$  \hspace{1em} (5.16)

where we used the hyperscaling relation $\alpha = 2 - d \nu$ and the identity $\beta/\nu = d - 1/\mu$; $K_C \equiv \frac{F'_{YY} (F'_{XX})^2}{F''_{XX}} \sim 1$. That is, in 2D $C \sim \ln L[1 + o(c_2^2 L^{-1/4})]$. It is worth mentioning that $C$ evaluated along the actual coexistence line, $h = 0$, does not contain the term $\sim K_C$ and the leading correction becomes $\sim b_2 L^{\frac{2\alpha-1}{\nu}} F'_{X}$. This is discussed below.

Similarly,

$$\frac{dU_B}{dl} \rightarrow U'_X \tau_1 L^{\frac{\alpha}{\nu}} \left[ 1 + b_2 F'_{X} L^{\frac{\alpha-1}{\nu}} + K_U c_2^2 L^{-\frac{2\beta}{\nu}} \right],$$  \hspace{1em} (5.17)

where $K_U \equiv \frac{U''_{YY} F'_{XX}}{F''_{XX}} \sim 1$.

We note that we were not able to determine $b_2$ with any confidence from (5.16,5.17). [The contribution $\sim c_2^2$ in this domain is much weaker than in the strong field domain, and therefore, given the estimate for $c_2$ in Sec.5.4.2, it is virtually undetectable].

### 5.3.3 Scaling along the coexistence line

The coexistence line is determined by $h = 0$ in Eq.(5.7), that is, $\bar{\mu} = -(1 - c_2 a_1)^{-1}[(c_1 - c_2 a_2)t + c_2 \Phi]$ which contains the Yang-Yang anomaly $\bar{\mu} \sim \Phi \sim t^{2-\alpha}$, Ref.[35]. Accordingly, Eq.(5.6) becomes $\tau = \tau_1 l + \bar{b}_2 \Phi(X, 0) = \tau_1 l + \bar{b}_2 L^{-d} F(X, 0)$, $X = L^{1/\nu} \tau$, where $\tau_1$ is given in Eq.(5.15) and $\bar{b}_2 = b_2 - c_2 (b_1 - b_2 a_1)/(1 - c_2 a_1)$. Then, $\Phi' = d\Phi(X, 0)/dl$ and $C_{oo} = \Phi'' = d^2 \Phi(X, 0)/dl^2$ become

$$\Phi' = L^{\frac{\alpha-1}{\nu}} \frac{\tau_1 F'_{X}}{1 - L^{\frac{\alpha-1}{\nu}} \bar{b}_2 F'_{X}},$$  \hspace{1em} (5.18)
\[ C_{co} = L^\frac{\alpha}{\nu} \frac{F''_{XX} \cdot (\tau_1 + \tilde{b}_2 \Phi')^2}{1 - L^{\frac{\alpha-1}{\nu}} \tilde{b}_2 F'_{X}}, \] (5.19)

where \( F'_X = dF(X,0)/dX \) and \( F''_{XX} = d^2F(X,0)/dX^2 \) and \( X \sim 1 \). It is worth mentioning that, up to the "-" sign and some coefficient, \( C_{co} \) coincides with the heat capacity \( C_V \) along the critical isochore.

In the limit \( L \to \infty \), \( C_{co} \sim L^{\frac{\alpha}{\nu}} F''_{XX} \cdot (\tau_1^2 + 3\tilde{b}_2 L^{(\alpha-1)/\nu} F'_X) \). Thus, while the dominant divergence \( \sim F''_{XX} \tau_1^2 L^{\alpha/\nu} \) is the same along the weak field linear path, Eq.(5.16), and along the coexistence line, Eq.(5.19), the dominant correction to scaling are different. In the first case it is \( \sim L^{(\alpha-2\beta)/\nu} c_2^2 \) and in the second \( -\sim \tilde{b}_2 L^{(2\alpha-1)/\nu} \) which in 2D \( \sim L^{-1} \ln^2 L \). It is worth mentioning that in 2D Ising model the subdominant term is weaker \( \sim L^{-\theta/\nu} = L^{-2} \).

The derivative of the Binder cumulant along the coexistence line in the limit \( L \to \infty \) becomes

\[ \frac{dU_B}{dt} \to U'_X L^\frac{1}{\nu} [\tau_1 + \tilde{b}_2 F'_X L^{\frac{\alpha-1}{\nu}}], \] (5.20)

that is, the term \( \sim c_2^2 L^{-2\beta/\nu} \) from Eq.(5.17) is absent (here \( U'_X = dU(X,0)/dX \) and \( X \sim 1 \)).

### 5.3.4 Non-analytical contributions to density

Let’s evaluate density in the critical domain using the definition \( \rho = \partial \hat{p}/\partial \hat{\mu} \) in Eq.(5.3). It gives \( \rho + a_1 = \partial \Phi/\partial \hat{\mu} \). Differentiation \( \partial \rho/\partial \hat{\mu} \) of Eqs.(5.4,5.5) gives \( \partial \tau/\partial \hat{\mu} = b_1 + b_2 \rho \) and \( \partial h/\partial \hat{\mu} = 1 + c_2 \rho \), respectively. Using these last two relations in the first equation and keeping in mind the form (5.2), we get

\[ \rho + a_1 = L^{\frac{1-d}{\nu}} F'_X \cdot (b_1 + b_2 \rho) + L^{\frac{1-d}{\nu}} F'_Y \cdot (1 + c_2 \rho). \] (5.21)
Solving for $\rho$ gives

$$\rho = \rho_c + b_1 F'_X L^{1-d} + L^{1-d} F'_Y \frac{1}{1 - b_2 F'_X L^{1-d} - L^{1-d} F'_Y},$$

\hspace{1cm} (5.22)

where $\rho_c = -a_1$ has the meaning of the critical density. In the strong field domain, $Y \sim 1, X \to 0$, the leading non-analytical term is $\sim L^{-d+1/\mu} = L^{-\beta/\nu}$.

The contribution $\sim L^{-\beta/\nu}$ vanishes in the weak field domain $X \sim 1, Y \to 0$. Considering that, according to Eqs. (5.1, 5.7), $Y = [h_1 l + c_2 \Phi] L^{1/\mu}$ and $h_1 = [(1 - c_2 a_1) \mu_1 + (c_1 - c_2 a_2) t_1] = 0$ (at $l_1 = 0$), the term $F'_Y$ becomes $F'_Y = F''_{YY} c_2 L^{1/\mu} \Phi \sim L^{1/\mu-d}$. Thus, the non-analytical contributions along the weak field path become

$$\rho = \rho_c + c_2 F F''_{YY} L^{-\frac{2\beta}{\nu}} + o(c_2 L^{-\frac{4\beta}{\nu}}) + b_1 F'_X L^{\frac{\alpha-1}{\nu}},$$

\hspace{1cm} (5.23)

where $F, F'_X, F''_{XX}$ are evaluated at $Y = 0$ and $X \sim 1$.

This analysis shows that density along the linear path in the weak field critical domain toward the critical point is characterized by the anomalies $\sim t^{1-\alpha} \sim L^{(\alpha-1)/\nu}$, Refs. [31, 32], and the stronger one $\sim t^{2\beta} \sim L^{-2\beta/\nu}$, Ref. [31], following from the complete scaling approach. It is important that in order to observe these anomalies there is no need to tune the system into the coexistence line – it is enough to approach the critical point within the weak field critical domain, that is characterized by $h_1 = 0$ in Eq. (5.9). As it has been explained above and will be demonstrated below, this condition can be realized by observing the minimum of $C$, Eq. (5.11), as a function of the linear slope in the parameter space $(t, \check{\mu})$.

### 5.4 The Square Well Fluid Model

Here we will analyze the LG transition in 2D gas of classical particles by simulating it directly. We choose the simplest interacting potential – the square well [49]. The NF method
will be used to determine the critical behavior in this case too.

The system of classical particles is described by the grand canonical partition function

$$ Y = \sum_{N=1}^{\infty} \frac{1}{N!} e^{\tilde{\mu}N} \int d\vec{r}_1 ... d\vec{r}_N e^{-V}, \quad (5.24) $$

where $V = (1/2) \sum_{ij} v(\vec{r}_i - \vec{r}_j)$ is the potential energy of binary interaction (normalized by temperature) between $N$ particles located at $\vec{r}_i$, $i = 1, 2, ... N$ within the square area $L^2$ (now $L$ is a continuous length); $\tilde{\mu}$ is the chemical potential (normalized by temperature). The interaction energy $v(\vec{r})$ between two particles separated by a vector $\vec{r}$ is taken as the square well potential. That is, $v = \infty$, if $|\vec{r}| < \sigma$, $v = -\epsilon$, if $\sigma \leq |\vec{r}| \leq \lambda \sigma$, and $v = 0$, if $r > \lambda \sigma$.

Here $\sigma$ and $\lambda \sigma > \sigma$ are the hard and soft core diameter, respectively, and $\epsilon > 0$ characterizes attraction within the soft core shell. Since temperature is absorbed into the definition of $\epsilon$, we will be calling $1/\epsilon$ as ”temperature” $T$ and $\tilde{\mu}$ as “chemical potential”. Simulations have been conducted for $\lambda = 1.5$ and $\sigma = 1.0$.

Metropolis monte carlo is conducted by random insertion or deletion of particles according to the configuration weight. We can propose to either insert a particle to a randomly chosen spot $\vec{r}_j$, or propose to remove an existing particle (at $\vec{r}_j$) with acceptance ratios:

$$ R_{\text{insert}} = \begin{cases} 0 & \text{if overlap occurs} \\ \min(1, \frac{V}{N+1} e^{\beta(n_j \epsilon + \tilde{\mu})}) & \text{otherwise} \end{cases} \quad (5.25) $$

$$ R_{\text{remove}} = \min(1, \frac{N}{V} e^{-\beta(n_j \epsilon + \tilde{\mu})}) \quad (5.26) $$

where $n_j$ is the number of particles within distance $\lambda$ of position $\vec{r}_j$.

Below we will apply the general analysis presented in the previous section, and consider the derivatives $C = d^2 \Phi/dl^2$ and $dU_4/dl$ along a linear path toward the critical point $\epsilon =$
Figure 5.2: Polar representation of the system parameters with $\epsilon_c = 0.5540$ and $\tilde{\mu}_c = -3.701$ as found in Ref.[12].

$\epsilon_c, \tilde{\mu} = \tilde{\mu}_c$ in order to identify the weak field line $h_1 = 0$. Such a path is parametrized as shown in Fig. 5.2:

$$\tilde{\mu} = -l \sin \phi, \quad t = \epsilon - \epsilon_c = l \cos \phi, \quad (5.27)$$

and it corresponds to some angle $\phi = \phi_V$ when only the part linear in $\tilde{\mu}$, $t$ in Eq(5.7) becomes zero, that is,

$$\tan \phi_V = \frac{c_1 - c_2 a_2}{1 - c_2 a_1}. \quad (5.28)$$

The angle $\phi_V$ will be found below by observing a minimum of $C$ as a function of $\phi$ for fixed $l$. 
It is important to note that, as $L$ increases, the critical domain of $T$, $\tilde{\mu}$ shrinks as $\sim L^{-1/\nu} \to 0$ or $\sim L^{-1/\mu} \to 0$ depending on how the critical point is approached. In terms of the representation (5.2), the strong and weak field critical domains correspond to $Y \sim 1, X \to 0$ and $Y \to 0, X \sim 1$, respectively. In other words, if $T, \tilde{\mu}$ are tuned to keep $U_4$ within its critical range for all simulated sizes, it is guaranteed that the system is critical for a given size $L$. This means that any quantity demonstrating scaling behavior will scale as a power of $L$ determined by its scaling dimension – if plotted vs $U_4$.

For the sake of completeness, we will first discuss the generic situation – a path in the strong field domain with respect to the leading scaling only.

### 5.4.1 Determination of critical point

In the plane $(\tilde{\mu}, T)$ there is a line of 1st order phase transitions between low and high density phases. This line ends at the critical point at some $\tilde{\mu} = \mu_c, T = T_c$. One of the significant difficulties in analyzing the LG transition is in finding this point in a controlled manner. Below, we will address this difficulty with the help of the NF method which leads to the critical point automatically – along the same line as discussed in previous sections. For this purpose we consider the following Binder cumulant

$$U_4 = \frac{\langle (N - \langle N \rangle)^2 \rangle^2}{\langle (N - \langle N \rangle)^4 \rangle}.$$  

As discussed in Ref. [7], this cumulant has a specific form: away from the coexistence line it is $U_4 = 1/3$ in the limit $L \to \infty$. At the coexistence line it has two dips corresponding to the densities of liquid and gas, with the peak in between corresponding to $U_4 = 1$. Above the critical point this maximum tends toward the value $U_4 = 1/3$. Thus, at the critical point the dips approach each other, with the peak reaching some intermediate value $1/3 < U_c < 1$. This value is scale invariant [38]. Fig. 5.3 illustrates the functional form of the cumulant.
with respect to chemical potential and the NF flowgram schematic as \( L \to \infty \).

![Sketch of \( U_4(\tilde{\mu}, L) \) dependence](image)

**Figure 5.3:** Sketch for \( U_4(\tilde{\mu}, L) \) dependence. The arrows indicate the evolution of the maximum as \( L \to \infty \) at \( T < T_c \) (upper), \( T > T_c \) (lower) and \( T = T_c \) (horizontal).

In other words, the critical point corresponds to the separatrix of the maximum of \( U_4 \) as a function of \( T, \tilde{\mu} \) with respect to \( L \to \infty \). This suggests a protocol for finding the critical point: 1. choose some \( T \) and find maximum of \( U_4 \) by adjusting \( \tilde{\mu} \) for each size \( L \); 2. If this maximum flows toward 1 (toward 1/3), increase (decrease) \( T \) and repeat the previous step until the flow of \( U_4 \) maximum (versus \( L \)) saturates to a constant value \( U^*_4 \). The result of this procedure is shown in Fig. 5.4 with the black line forming a separatrix of the two regimes. It is important to emphasize that the accuracy of \( T_c = 0.5540 \pm 0.0005 \) and \( \tilde{\mu}_c = -3.700 \pm 0.005 \) is limited only by the maximum system size simulated and the numerical accuracy of \( U_4 \). Obviously, no fitting procedure with respect to \( T_c, \mu_c \) is required. For the universal value of the maximum, we found \( U^*_4 = 0.856 \pm 0.005 \) in agreement with the Ising model exact known
Figure 5.4: $U_4(L)$ maxima versus $L$ for $8 < L < 56$. The black line is the separatrix at $T_c = 0.5540$. 
value for the critical point which is $U_{4,\text{Ising}}^* = 0.85622$ [56].

### 5.4.2 Critical behavior in the strong field

Within the field theory of $Z_2$ criticality the FSS behavior of heat capacity $C = -d^2\Phi/d\tau^2$ is insensitive to the path toward the critical point $\tau = 0$, $h = 0$. In the weak and strong field regions $C \sim L^{\alpha/\nu}$ and $C \sim L^{\varepsilon/\mu}$, respectively. However, the scaling relations guarantee that $\alpha/\nu = \varepsilon/\mu$ (see e.g. in [1]). In 2D Ising model $\alpha = \varepsilon = 0$ which implies log-divergence $C \sim \log L$. The situation is different in the case of the LG critical point due to the mixing effect.

Along a path toward the critical point belonging to the strong field region energy $E$ and particle number $N$ fluctuations are linearly mixed. Thus, the divergence of a second derivative of $\Phi$ either along $t$ or any other direction is controlled by the much stronger divergence of compressibility. Within the FSS this gives for the derivative $\sim d^2\Phi/dh^2 \sim L^{-d+2/\mu} = L^{\gamma/\nu}$. The only requirement is that $Y \sim 1$ in Eq.(5.2). Then, because of the mixing (5.3,5.4,5.5) the dominant term is $\sim F''_{YY} L^{-d+2/\mu} \sim L^{\gamma/\nu}$ (by the token of the scaling identities).

As discussed in Sec. 5.3, such a leading divergence is typical for any generic path – except for some special angle $\phi = \phi_V$ in Eq.(5.27) for which $h_1 = 0$ in Eq.(5.9). The result of measuring $C = d^2\Phi/dl^2$ along the path $\phi = \pi/2$ is shown in Fig. 5.5, that is, along the path $t_1 = 0$, $\mu_1 \neq 0$ and $l \to 0$ using the notations of Sec. 5.3. The value of $\tilde{\mu} = \mu_1 l$ was adjusted in such a way that $U_4$ falls into its critical range for each size $L$.

For large enough $L$ the function $C$ vs $U_4$ is universal up to a scaling factor. The “vertical” rescaling of $C$ for various $L$ by a factor $\lambda(L) \sim L^{-(1-1/8)/\mu}$ allows obtaining the exponent which turns out to be consistent with the Onsager value $7/4$ as indicated in Fig. 5.6. The error $\sim 2\%$ includes the subdominant scaling contribution.

The analysis presented in Sec. 5.3.1 indicates, the complete scaling approach predicts
Figure 5.5: The master curve of the specific heat $C$ vs $U_4$ along the path $t = 0, \bar{\mu} = \mu_1 l$ for various system sizes $L$ obtained by rescaling particular curves along the “vertical” direction until each data set overlaps with the curve corresponding to $L = 36$. Inset: The non-rescaled data of $C$ vs $U_4$ for sizes shown close to each curve.
Figure 5.6: Rescaling factor $\lambda(L)$ versus $L$ for the data shown in Fig. 5.5. The slope of the fit line (solid straight line) gives the exponent $(1 - 1/\delta)/\mu = \gamma/\nu = 1.76 \pm 0.02$ which is consistent with the Onsager value $\gamma/\nu = 7/4 = 1.75$.

Figure 5.7: Data points: The remainder $C_r$ of $C$ from Fig. 5.5, with the dominant term $\sim L^{7/4}$ subtracted. The fit (solid line) is done by the subdominant contribution $\sim L^{7/8}$ from Eqs.(5.11,5.12) where $c_2$ is set to zero.
Figure 5.8: The master curve of $\frac{dU_4}{dl}, \phi = \pi/2$, vs $U_4$, for various system sizes $L$ obtained by the "vertical" rescaling to the curve corresponding to $L = 30$. Inset: the original curves for sizes shown close to each data set.

Figure 5.9: The log-log plot of the rescaling parameter from the data shown in Fig. 5.8. The slope of the fit line (solid straight line) gives the $\mu \approx 0.535 \pm 0.005$ exponent consistent with the Onsager value $8/15$. 
the dominant correction to scaling $\sim c_2 L^{13/8}$, Eq.(5.12), with the next term $\sim L^{7/8}$ existing even if $c_2 = b_2 = 0$ in Eqs.(5.8,5.9). We have performed the analysis of the subdominant contribution and concluded that it can be accounted for solely by the term $\sim L^{7/8}$ within the statistical errors $\leq 0.5\%$ of simulations. [The fit of $C$ with the dominant term $\sim L^{7/4}$ subtracted is shown in Fig. 5.7]. This, of course, does not exclude that the pressure mixing coefficient $c_2$ is finite. Our data allows only to give the upper bound on $|c_2|$ as $|c_2| \leq 0.01K/3F_Y$ form Eq.(5.12).

Similarly, the derivative $dU_4/dl$ along the same path demonstrates the strong field leading scaling $dU_4/dl \sim L^{1/\mu}$ in the critical domain of $U_4$. The result of the flowgram analysis is shown in Fig. 5.8 with the rescaling factor $\lambda$ plotted in Fig. 5.9. The final value of the exponent $\mu = 0.532 \pm 0.005$ is consistent with the Onsager value $\mu = 8/15$. Given the systematic error below the statistical one in Figs. 5.8,5.9, we conclude that the subdominant term $\sim c_2 L^{7/4}$, Eq.(5.14), cannot be reliably resolved from this data as well.

Another derivative was also measured along this path, that is compressibility. The leading power law scaling of isothermal compressibility, $\kappa_T$, with linear system size $L$ in perfectly symmetric systems is

$$\kappa_T \sim L^{\tilde{\nu}}$$

(5.30)

Using scaling relations it is possible to prove that the same divergence dominates in the strong field limit of the asymmetric liquid gas. Specifically,

$$\kappa_T \sim h^{\frac{1}{\tilde{\nu}}-1} \sim L^{(1-\frac{1}{\tilde{\nu}})\frac{1}{\mu}}$$

(5.31)

We measured the second moment of the total system density, $\langle \delta N^2 \rangle = \langle (N - \langle N \rangle)^2 \rangle$ which is the same as $\kappa_T$ up to a constant. We scanned in the vicinity of the critical region for sizes $L = 6,12,...,84$. We applied the flowgram method speculating that the curves
would be related by a power law $L^c$ with exponent $c$ to be determined. These curves were indeed self-similar and were collapsed onto each other by multiplication by a single factor $\lambda(L)$, see Fig. 5.10. Log-log plots of $\lambda(L)$ versus $L$ have slope $1.75 \pm 0.01$ (see Fig. 5.11) which is within 1% of the our prediction $(1 - \frac{1}{\delta})\frac{1}{\mu} = \frac{7}{4}$.

Figure 5.10: $\delta N^2$ versus $U_4$ for sizes $L = 6, 12, \ldots, 84$ rescaled by a factor $\lambda(L)$ which collapses each curve to $L = 36$ ($\lambda(36) = 1$). Inset: $\langle \delta N^2 \rangle$ versus $\langle U_4 \rangle$ for the same sizes.

The error in $\langle \delta N^2 \rangle$ comes from both statistical errors, and systematic errors due to neglecting sub-leading terms in the power law scaling. The systematic error is significant for $L = 6$ and 12 but tends to zero as $L$ increases. For $L > 12$, the total error is less than 1% so we combine the two. Finally, the error in the critical exponent is determined by the range of slopes that can be fitted within the error bars of the log-log plot.
5.4.3 Critical behavior in the Weak field

As mentioned above, there should be a minimum of \( C = d^2 \Phi / dl^2 \) as a function of the angle \( \phi \) at some \( \phi = \phi_V \) in the representation (5.27). This minimum corresponds to the weak field domain which coincides with the coexistence line \( h = 0 \) in the case \( c_2 = 0 \) in Eq.(5.9). It lies in the quadrant \( t > 0, \tilde{\mu} < 0 \) in Fig. 5.2.

The coexistence line is characterized by some angle \( \phi = \phi_V(l) \), which, in general, should be a function of \( l \). However, in our simulations we were unable to detect any such a dependence beyond 0.2\% of the margin of error up to the simulated sizes \( L = 48 \) while measuring \( C(l, \phi_V) \). We have also didn’t find any deviations from the weak field domain while measuring the \( dU_4/dl \) vs \( U_4 \) at \( \phi_V = \text{const} \) up to the simulated sizes \( L = 66 \). This indicates that it is fare to set \( \phi_V = \text{const} \) in the analysis.

We introduce the derivative \( C = -L^{-2} d^2 \ln Z / dl^2 \) at fixed angle \( \phi \). Keeping in mind that
Figure 5.12: $C$, Eq.(5.32), versus $\phi$ for $l = 10^{-6}$ close to minimum at $\phi = \phi_V$ for various sizes $L$ shown near each curve.

$Z \sim \sum \exp(-E\epsilon + \bar{\mu}N)$ and also Eq.(5.27), we find

$$C = \frac{1}{L^2}[\cos^2 \phi\langle \delta E^2 \rangle + \sin^2 \phi\langle \delta N^2 \rangle + \sin(2\phi)\langle \delta N\delta E \rangle]$$  \hspace{1cm} (5.32)

where $\delta E, \delta N$ are fluctuations of $E$ and $N$, respectively. If the simulations were conducted exactly at the coexistence line, this derivative would represent the isochoric specific heat capacity $C_V$. However, as discussed above, the FSS dominant divergence of $C \sim L^{\alpha/\nu}$ along the weak field path is the same as for $C_V$.

In order to find $\phi_V$ measurements of $C = C(l, \phi)$, Eq.(5.32), were conducted for various $\phi$ around the minimum of $C$ vs $\phi$ for several system sizes and at fixed $l$. Fig. 5.12 displays
Figure 5.13: Histograms of density along the straight path toward the critical point, Fig. 5.2, for three angles close to $\phi = \phi_V$.

the results of such measurements giving the angle $\phi_V = 69.5^\circ \pm 0.1^\circ$. Fig. 5.13 shows three histograms of the density collected at $\phi = \phi_V$ and at slightly different angles. The top panel, where $\phi = \phi_V$, features the bimodal distribution corresponding to LG coexistence. The middle and the lower panels represent liquid and gas, respectively. This indicates that within the sizes simulated there is no significant difference between the coexistence line and the linear path in the weak field domain. This is also consistent with the upper estimate on $c_2$ obtained above. The angle $\phi_V$ determines the combination (5.28) of the mixing coefficients from Eqs.(5.3,5.4,5.5).

The derivative of the Binder cumulant $U_4$ along this linear path (at $\phi = \phi_V$) is characterized by the dominant scaling behavior $\sim L^{1/\nu}$, as the comparison with Eq.(5.17) indicates. In terms of the variables $t, \bar{\mu}$

$$
\frac{dU_4}{dt} = \cos \phi_V \left[ \frac{dU_4}{dt} - \tan \phi_V \frac{dU_4}{d\bar{\mu}} \right]
$$

(5.33)
CHAPTER 5. CRITICALITY OF THE SQUARE WELL FLUID

with the help of Eq.(5.27). The family of the curves $dU_4/dl$ vs $U_4$ is shown in Fig. 5.14. The data points have been collected along the continuation of the weak field line beyond the critical point – that is, at $\phi = (69.5 + 180)^\circ$ – in the quadrant $\bar{\mu} > 0$, $\epsilon < \epsilon_c$. [ This path corresponds to $\tau > 0$ in the $\phi^4$ theory]. As can be seen, the curves can be collapsed to a master plot by the “vertical” rescaling for sizes above $L = 18$. The log-log plot of the rescaling parameter vs $L$ gives the critical exponent $\nu = 0.99 \pm 0.02$ as shown in Fig. 5.15. This value is consistent with the Onsager result $\nu = 1$. The error includes statistical and systematic errors. [The minimal statistical error of less than 1% characterizes the data points close to the minimum of the master curve – that is, in the domain $0.55 < U_4 < 0.75$ in Fig. 5.14]. The smallest sizes fall out from the collapse due to the subdominant scaling contributions.

5.4.4 Order Parameter beta exponent

The order parameter which is the difference in density between the liquid and gas phases, $\rho_l - \rho_g$, was estimated by observation of the density distribution function $P(\rho, L)$. In the immediate vicinity of the critical point, it has two peaks corresponding to the characteristic density of each phase for a given $L$. These peaks gravitate inward toward the critical density $\rho_c \approx 0.350 \pm 0.005$ in the limit $L \to \infty$. This FSS approach is governed by eq. (3.2).

$P(\rho, L)$ is plotted for a set of increasing system sizes in Fig. 5.16. Then the values of $\rho_l(L)$ and $\rho_g(L)$ are estimated from the locations of the maxima. The log-log plot of $\rho_l(L) - \rho_g(L)$ vs $L$ is highly linear and has a slope $= 0.125 \pm 0.005$ in agreement with the Ising value $\beta = 1/8$. 
Figure 5.14: The master curve of $\frac{dU_4}{dl}$ vs $U_4$ at $\phi = \phi_V = (69.5 + 180)^\circ$ (that is, along the continuation of the coexistence line beyond the critical point in Fig. 5.2) for various system sizes $L$ obtained by the “vertical” rescaling to the curve corresponding to $L = 30$. The data points for $L = 12, 18$ are connected by lines as an indication that these sizes fall out from the master curve. Inset: the original curves for sizes shown close to each data set.
Figure 5.15: Log-log plot of the rescaling parameter $\lambda_nu(L)$ of $dU_4/dl$ from Fig. 5.14, with the smallest sizes $L = 12, 18$ excluded. The slope of the straight fit line gives $\nu = 0.99 \pm 0.02$.

Figure 5.16: The distribution of the density, $P(\rho, L)$, for different system sizes $L$. 
Figure 5.17: Log-Log plot of the difference in the peaks $\rho_l(L) - \rho_g(L)$ vs $L$. 

$\varphi = 69.5^\circ$

$l = 0.00001$

slope line = $-0.125 \pm 0.001$

$\rho_l - \rho_g \sim L^{-\beta/\nu}$

$\beta/\nu_{ising} = 1/8$
Chapter 6

Luttinger transition in superclimbing dislocation

6.1 Introduction

The concept of LL turns out to be relevant to solid $^4$He as well. As found in ab initio simulations [57], screw dislocation with Burgers vector along the high symmetry axis possesses superfluid core. This 1D topological structural defect is essentially the bosonic LL. There is, however, a significant difference between a dislocation with superfluid core and a conducting wire. The dislocation is a dynamical string able to change its shape and to move within crystal. In quantum crystals the string dynamics must be treated quantum mechanically. This raises a plethora of questions traditionally more relevant to high energy physics. One key question is about how the dislocation dynamics interact with its core superfluidity.

This question is especially relevant in connection with the superflow through solid $^4$He observed first in the UMASS group [15, 58, 59] and then confirmed by other groups [16, 60, 19]. There is one strikingly unexpected feature serendipitously observed by the UMASS group [15]: during the superflow events the solid exhibits a response to external chemical
potential, practically, the same way as liquid does – absorbing or expelling a macroscopic fraction of atoms. This effect, which was called giant isochoric compressibility (or syringe effect) in Ref. [20], represents a mechanism of crystal growth from inside out. Both effects are now at the focus of the experimental and theoretical efforts in the field of superfluidity and quantum crystals.

It is important to realize that a dislocation with superfluid core in a crystal represents a supersolid state of matter – that is, the coexistence of superfluidity with crystalline symmetry both formed by the same atoms (see the discussion about various types of supersolidity in [61]). Indeed, despite breaking the hexagonal close packing symmetry (hcp) of the ideal crystal, the dislocation [57] aligned with the high symmetry axis preserves perfect periodicity of the crystal along this axis. It also retains the $C_6$ symmetry of rotations with respect to the dislocation core. This supersolid, however, is quite different from the supersolid phase of ideal crystal confining a condensate of zero point vacancies contemplated by Andreev and Lifshitz [62]. As has been shown in Ref.[63], vacancies in solid $^4$He attract each other and, therefore, cannot form stable Bose-Einstein condensate at zero temperature ($T$) in ideal crystal – they tend to agglomerate into dislocation loops. The situation is completely different in vicinity of topological defects where local strain is topologically protected and, thus, induces stable low-D superfluidity [64] along some dislocations [57, 20] and some grain boundaries [65].

There is a new property that emerges due to the core superfluidity: such a dislocation can perform non-conservative motion, that is, climb [66]. In Ref.[20] this effect has been called superclimb – climb supported by superflow along the dislocation core. A pure screw dislocation cannot perform superclimb. However, deviations of the core orientation from the direction of the Burgers vector transforms screw dislocation into edge dislocation (see in, e.g., [66, 14]). In this case, the core retaining its superfluidity can perform superclimb. In this case, as discussed in [20], spectrum of excitations is no more linear in the momentum along the core. Thus, a superclimbing dislocation is not expected to be LL and should be
classified as non-LL.

The superclimb has been proposed in Ref.[20] as a possible explanation for the syringe effect. In other words, edge dislocations with superfluid core can supply matter into (from) the solid by building (dissolving) incomplete atomic planes. The syringe effect has also been seen by the Univ. of Alberta group, [16], and very recently confirmed in its most conspicuous form in Ref.[19]. At the moment, however, there is no direct proof that the syringe effect is due to the superclimb of dislocations. Thus, it is important to find features of the dislocation scenario which can be tested experimentally.

The main prediction about superclimb put forward in [20] is about edge dislocation aligned with single Peierls potential (see in [66, 14]) valley. Such a dislocation becomes self-trapped by the potential at $T = 0$. Thus, if all the edge dislocations with superfluid core were self-trapped, the syringe effect should vanish. However, a generic dislocation network in real crystals is mostly disordered. Thus, there should be dislocations which are not aligned with the Peierls valleys. Accordingly, such dislocations are characterized by finite density of jogs (see in [66]) which form a quantum fluid supporting superclimb even at $T = 0$ [67].

Here we revise the conjecture [67] based on the standard analysis of the relevance of Peierls potential. Our main result is that, as temperature decreases, superclimb of a generic edge dislocation (that is, not aligned with one Peierls valley) with superfluid core must be suppressed. This reinstates the linear excitation spectrum and, consequently, the LL character of the superfluidity along the core. Below we will, first, briefly review the superclimb effect. Then, we will discuss the results of large scale simulations of the model of the superclimbing dislocation and will present the evidence for the emergence of the LL behavior as well as its destruction by bias. Finally, we will discuss the features to look for in experiment in order to test the dislocation scenario for the superflow and the syringe effects.
6.2 Luttinger Liquid

The Luttinger Liquid (LL) is the universal description for 1D conducting quantum systems. Both fermionic and bosonic quantum wires are generically described by the harmonic model of collective sound-like excitations [13]. Essentially the same approach applies to spin $S = 1/2$ chains too (see in Ref.[68]). The luttinger liquid is described by the action in imaginary time $\tau$:

$$H_{LL} = \int_0^\beta d\tau \int_0^L dx \left[ \frac{K}{2} (\partial_x \phi)^2 + \frac{K}{2v} (\partial_\tau \phi)^2 \right]$$

(6.1)

where $\phi$ is the quantum phase, $v$ is the speed of sound, $K$ is the luttinger parameter. The product $\rho_s = K v$ stands for the superfluid stiffness and $\kappa = \frac{K}{2v}$ determines the compressibility. In real time, the action (6.1) describes the linear spectrum of excitations. The choice $L = v/\beta$ is the usual way to symmetrize the system with respect to space and time.

If there is a lattice and the filling factor is integer, then there is no difference between the quantum $D = 1 + 1$ system and a classical 2D layer. In both cases, the Berezinskii-Kosterlitz-Thouless (BKT) transitions can occur at $K = K_c$ regardless of $v$. The BKT transition is a phase transition in the two-dimensional XY model. It is a transition from bound vortex-antivortex pairs at low temperatures to unpaired vortices and anti-vortices at some critical temperature [69]. To understand the BKT transition explicitly, rescale space and time so that $v = 1$ so that the hamiltonian can be written

$$H = \int d^2 x' \frac{K}{2} (\nabla \phi)^2$$

(6.2)

Now using the variational principle (or “principle of least action”) $\delta H = 0$ we find that the equation of motion for the single degree of freedom $\phi(r)$ (we assume amplitude of the wave function is constant) is the Laplace equation $\nabla^2 \phi = 0$. This has two solutions $\phi(r) = \text{constant}$ (the ground state) and $\phi(r) = \ln(r - r_0)^n$ corresponding to vortex solutions where
CHAPTER 6. LUTTINGER TRANSITION IN SUPERCLIMBING DISLOCATION

\( n \) is the integer vortex charge obtained from integrating \( \nabla \phi \) over a contour surrounding \( r_0 \) so that \( \nabla \phi = 2 \pi n \). Then the energy of a vortex centered at \( r = 0 \) is \( E_{vor} = Kn^2 \pi \ln \frac{L}{a} \) where \( a \) is the lattice spacing and \( L \) is the system size.

The entropy of a single vortex is \( S = \ln((L/a)^2) \), taking Boltzmann’s constant \( k_B = 1 \), since we can create a vortex center at each of \( L^2 \) plaquettes on the square lattice. Then the Helmholtz free energy of a single vortex is

\[
F = E - TS = (\pi K - 2T) \ln\left(\frac{L}{a}\right),
\]

so that if \( T > \frac{K}{2\pi} \) then the system can lower its free energy by allowing vortex pairs to unbind and proliferate in the system. At \( T = 1 \) the critical coupling condition is \( K_c = \frac{2}{\pi} \).

Note that the energy of vortex pair separated by some distance \( R \) is \( \pi K(n_1 + n_2)^2 \ln(L/a) - 2\pi Kn_1n_2\ln(R/a) \) which means that vortices have a coulomb type interaction. The interaction is repulsive if \( n_1, n_2 \) have the same sign and attractive if they have opposite signs. If the system is charge neutral so that \( \sum_i n_i = 0 \) then only vortex pair states may exist. Both phases above and below \( K_c \) are disordered, however the vortex pairs become unbound below \( K_c \).

6.3 Response to Gauge Fields and Winding Numbers

On the lattice the continuous derivative becomes discrete: \( \partial_x \phi(x, \tau) \rightarrow \nabla_x \phi = \phi(x + 1, \tau) - \phi(x, \tau) \) where we use \( a = 1 \) as the lattice spacing in \( x \). The continuous time derivative transforms as \( \partial_\tau \phi(x, \tau) \rightarrow \nabla_\tau \phi = [\phi(x, \tau + \Delta\tau) - \phi(x, \tau)]/\Delta \tau \), where \( \Delta \tau \) is the unit of the time discretization \( \Delta \tau = \beta/N_\tau \rightarrow 0 \), with \( N_\tau \) being the number of time slices in the time interval \( (0, \beta) \) [recall to impose \( x-t \) symmetry we may choose \( \beta = L/v \)]. Then, the compactness of \( \phi \) is taken into account by using the Villain transformation \( \vec{\nabla} \phi \rightarrow \vec{\nabla} \phi + 2\pi \vec{m} \) \[70, 71\], where the vector sign refers to the space-time directions and \( \vec{m} = (m_\tau, m_x) \) stands...
for integer variables defined on (and oriented along) bonds between neighboring sites of the space-time lattice. This approach allows treating $\phi$ as a non-compact gaussian variable – on the expense of introducing the bond variables $\vec{m}$.

The thermodynamics of the model (6.1) (with the substitution $\nabla\phi \to \nabla\phi + 2\pi \vec{m}$) can be accounted for within the partition function

$$Z = \sum_{\{\vec{m}\}} \int D\phi \exp(-S), \quad (6.4)$$

$$S = \sum_{(\tau,x)} \left[ \frac{K}{2v\Delta\tau} (\nabla_{\tau}\phi + 2\pi m_{\tau} + \frac{\delta \phi_{\tau}}{L})^2 + \frac{K v \Delta\tau}{2} (\nabla_{x}\phi + 2\pi m_{x} + \frac{\Delta\tau \delta \phi_{\tau}}{\beta})^2 \right] \quad (6.5)$$

The quantities $\frac{\delta \phi_{\tau}}{L}$ and $\frac{\Delta\tau \delta \phi_{\tau}}{\beta}$ are gauge fields or “Thouless twists” imposed on the links that violate the periodic boundary conditions because the degrees of freedom are single valued. Physically, we might think of this as imposing a sudden discontinuous change in the phase by some amount $\Phi$. $\Phi$ may be spread out over the system so that as $L \to \infty$, $\delta \phi = \Phi/L \to 0$. The question is how the system responds to this. If the system is completely disordered, there would be no response. We shall also see that the system may possess a quasi-long-range order or a “spin rigidity”.

It is convenient to use the Poisson identity $\sum_{m} f(m) \equiv \sum_{n} \int dm f(m) \exp(2\pi i mn)$ at each bond along the line of the derivation of the J-current model [72]. Then, the integrations over $\vec{m}$, $\phi$ can be carried over exactly. This transforms Eq.(6.4) into

$$Z = \sum_{\{\vec{J}=(J_{x},J_{\tau})\}} \exp(-S_{J}), \quad (6.6)$$

where
The integer bond oriented currents \( \vec{J} \) (that is, \(|\vec{J}| = 0, 1, 2, \ldots \)) between neighboring sites satisfy the Kirchhoff’s conservation rule, and the summation is performed over all bonds \( b_{ij} \) between all pairs of neighboring sites \( i \) and \( j \). It should be kept in mind that \( \vec{J} = (J_x, J_\tau) \) is oriented either along a spatial or a temporal bond. In other words if \( b_{ij} \) is a bond along \( X \)-direction, the current along this bond has zero temporal component, \( J_\tau = 0 \). Similarly, \( J_x = 0 \) on a bond oriented along the imaginary time axis.

In the limit \( \delta \phi_x \to 0 \), the leading dependence of \( Z \) becomes

\[
Z \propto e^{-\langle W_x^2 \rangle \delta \phi_x^2 - \langle W_\tau^2 \rangle \delta \phi_\tau^2}
\]

where \( W_x = \frac{1}{L} \sum_{b_{ij}} J_x \) and \( W_\tau = N^{-1} \sum_{b_{ij}} J_\tau \) are the topological winding numbers. These numbers capture topological properties of the system that are not reducible by local deformations of the \( J \)-current. Comparing with Eq. (6.1) we see that the renormalized topological coupling constants are defined by

\[
K_R v_R = \frac{L}{\beta} \langle W_x^2 \rangle, \quad \frac{K_R}{v_R} = \frac{\beta}{L} \langle W_\tau^2 \rangle,
\]

so that

\[
K_R = \sqrt{\langle W_x^2 \rangle \langle W_\tau^2 \rangle}, \quad v_R = \frac{L}{\beta} \sqrt{\langle W_x^2 \rangle \langle W_\tau^2 \rangle},
\]

where \( K_R \) is the renormalized luttinger parameter and \( v_R \) is the renormalized speed of sound.

For \( K > K_c \), and as long as we are at integer filling factor, \( K_R \approx K \) and \( \Delta \tau v_R \approx \Delta \tau v = 1 \). Physically, we will be interested in Section 6 in the renormalized superfluid stiffness \( \rho_s \) and renormalized compressibility \( \kappa \) defined by
\[ \rho_s = \frac{L}{N_\tau} \langle W_x^2 \rangle, \]  
\( \text{(6.11)} \)

and

\[ \kappa = -\frac{N_\tau}{L} \frac{\partial^2 \ln Z}{\partial \mu^2} = \frac{N_\tau}{L} [\langle W_x^2 \rangle - \langle W_x \rangle^2], \]  
\( \text{(6.12)} \)

where \( N_\tau = \beta / \Delta \tau \).

### 6.4 Superclimb and the giant isochoric compressibility

Dislocations are most typical 1D structural topological defects in crystals (see in Refs.[66, 14]). These are characterized by position and shape of its core as well as by the Burgers vector which is determined by the crystalline symmetry. Symmetry relevant to solid \(^4\)He is the hexagonal close packed (hcp) structure (see in Ref.[66]). Its highest symmetry axis is called C-axis and it has \( C_6 \) symmetry. It is perpendicular to the basal planes which are triangular 2D lattices. The hcp structure has two basic types of dislocations – with Burgers vector belonging to the basal plane and along the C-axis.

*Ab initio* simulations of dislocations with the Burgers vector along the C-axis have found that these dislocations in solid \(^4\)He have superfluid core. Superfluidity of the screw dislocation (with the core and the Burgers vector being along the C-axis) has been reported in Ref.[57]. Similarly, the superfluid core has been found in the edge dislocation with the Burgers along C-axis, and it has been reported in Ref.[20].

There is a significant difference between the two dislocations – while the edge dislocation can perform superclimb [20] as a linear response on chemical potential \( \mu \), the screw one cannot. Thus, a dislocation with superfluid core meandering through solid should consist
of edge and screw segments. A possible resulting network of such dislocations is shown in Fig. 6.1. One superclimbing segment of length $L$ of the network is schematically shown in Fig. 6.2. The matter can be fed into the dislocation from its ends contacting other dislocations with superfluid core or a reservoir with superfluid. As a result, extra matter is supplied to or taken away from an incomplete basal plane of atoms. Accordingly, the dislocation core (depicted by the ragged solid line in Fig. 6.2) can shift (up or down).

It is important to discuss the role of external bias by chemical potential $\mu$. A small changes of chemical potential imposed on a liquid results in a small change of the liquid density $\rho$. The corresponding dependence $\rho$ versus $\mu$ is smooth with the finite slope $d\rho/d\mu$ which is the isochoric compressibility. In a standard $LL$ liquid this quantity is independent of the length $L$. The situation is very different in the case of the superclimbing dislocation:
imposing a finite bias by $\mu$ does not produce any significant change of the superfluid density inside the core. Instead, the core shifts (up or down as sketched in Fig. 6.2) by the amount exactly determined by the number of atoms $N$ traveled along the core to build an incomplete atomic plane (shown by dashed lines in Fig. 6.2). In this case the isochoric compressibility $\kappa = L^{-1}dN/d\mu$ becomes ”giant” [20] – that is, $\kappa \propto L^2$. For consistency this feature reported in Ref.[20] will be explained in detail below.

A superclimbing dislocation [20] is modeled as an elastic string of length $L$. In the absence of the Peierls potential it is represented by the action in imaginary time $\tau$:

$$S = \int_0^\beta d\tau \int_0^L dx [-i(y + n_0)\partial_t \phi + \frac{\rho_0}{2}(\partial_x \phi)^2 + \frac{\kappa_0}{2}(\partial_x^2 \phi)^2 + \frac{G}{2}(\partial_x y)^2 - \mu y],$$

(6.13)

(in units $\hbar = 1, K_B = 1$), where all distances (here and below) are measured in terms of a typical interatomic distance. This action describes the displacement $y = y(x, \tau)$ of the dislocation, depicted in Fig. 6.2, from its equilibrium position, $y = 0$. As mentioned above,
$y(x, \tau)$ determines the total amount of atoms $\Delta N$ entered (exited) through the dislocation ends. This implies

$$\Delta N(\tau) = \int_0^L dxy(x, \tau).$$

(6.14)

The quantity $\phi = \phi(x, \tau)$ represents the superfluid phase defined along the superfluid core. Here $\beta = 1/T$, $\rho_0$ and $\kappa_0$ are bare superfluid stiffness and superfluid compressibility, respectively; $G$ stands for the effective tension of the dislocation ($\sim$ shear modulus); and the last term accounts for the bias by chemical potential $\mu$. The quantity $n_0$ describes average (linear) density of bosons. We consider the limit $\omega \to 0$, $q \to 0$. Thus, $\sim (\partial_\tau y)^2$ representing kinetic energy of the dislocation is omitted from Eq. (6.13). To exclude the zero mode where the uniform shift of the dislocation as a whole costs no energy, the boundary condition $y(x = 0, \tau) = y(x = L, \tau) = 0$ is used. This condition is, in particular, relevant to the type of a network shown in Fig. 6.1, where the meeting region of the screw and edge segments plays the role of the pinning point for superclimb – because the screw segment cannot perform superclimb for arbitrary small bias $\mu$.

If there were no climb (that is, $y = 0$), the model (6.13) would represent the standard LL characterized by the linear excitation spectrum $\omega = \sqrt{\rho_0/\kappa_0} \cdot q$ with respect to the wavevector $q$ along the dislocation [13]. The situation changes dramatically in the presence of the climb. The imaginary term in Eq. (6.13) (the Berry term) counts how many particles passed through the dislocation core and ended up in an extra row of atoms advancing dislocation by $y$. This effect changes the spectrum from linear to parabolic. Indeed, variational equations $\delta S/\delta \phi = 0$, $\delta S/\delta y = 0$ following from the action (6.13) give $\partial_\tau^2 y - G\rho_0 \partial_x^4 y = 0$ in the long wave limit. In real time $t = i\tau$ this corresponds to the parabolic spectrum $\omega = \sqrt{G\rho_0} \cdot q^2$ as $q \to 0$. Thus, the action (6.13) describes a non-LL.
CHAPTER 6. LUTTINGER TRANSITION IN SUPERCLIMBING DISLOCATION

Figure 6.3: One block of the dislocation network built by dislocations with superfluid core. Superclimbing dislocations – the edges along X and Z directions – bend in response to the bias by chemical potential $\mu$, as shown by the bulging line. The added matter is depicted by dashed lines (only one edge is shown to bulge).

6.4.1 Giant isochoric compressibility

If the superfluid stiffness $\rho_0$ in Eq.(6.13) is finite and the dislocation ends are connected to a superfluid reservoir, biasing by finite $\mu$ will result in the dislocation bowing by $y \sim L^2 \mu/G$. More accurately, the solution minimizing the action (6.13) is $y(x) = x(L - x)\mu/2G$ which corresponds to $DN = \int dxy = \mu L^3/12G$. Accordingly, the compressibility

$$\kappa = \frac{d\Delta N}{Ld\mu} \to \kappa_g = \frac{L^2}{12G} \propto L^2$$

(6.15)

becomes giant as opposed to $\kappa = \kappa_0 \propto L^0$ in the absence of the variable $y$ in Eq.(6.13).

It is important to realize that a sample of bulk solid $^4$He permeated by a uniform network of such dislocations must show a finite 3D compressibility $\kappa_{3D}$ – very similar to that of a
3D liquid. In other words, $\kappa_{3D}$ is independent of the dislocation density (as long as this density is small in units of interatomic distance). Let’s demonstrate this using a simplistic example of a network consisting of rectangular parallelepipeds with edges of typical lengths $L_x, L_y, L_z$. One element of such a network is sketched in Fig.6.3. Let’s presume that the edges of length $L_x$ along X direction represent edge (superclimbing) segments of dislocations with superfluid core. The distance $L_y$ characterizes a typical separation between such segments. The distance $L_z$ characterizes a typical length of the screw (non-superclimbing) segments (as sketched in Fig. 6.1).

Biasing the network by $\mu$ results in bowing the edge segments by $y \sim \mu L_x^2/G$. This implies an additional amount of atoms $\Delta N \sim yL_x \sim \mu L_x^2/G$ per each element. Consequently, the bulk density $\delta n$ changes as

$$\delta n \approx \frac{\Delta N}{L_xL_yL_z} \sim \frac{L_x^2}{L_yL_z}\frac{\mu}{G}.$$  

Thus, $\kappa_{3D} = \frac{\delta n}{\delta \mu}$ depends only on the ratio of the free segment lengths. In other words, uniformly increasing all lengths $L_x, L_y, L_z$ by the same factor, say, 2 does not change the above result (6.16), while decreasing the dislocation density by the factor of 4.

It is important to note that it is enough to apply $\mu$ just at a point contact with the network to introduce the density change (6.16). This is the same outcome as if $\mu$ were applied to a fluid. In contrast, applying $\mu$ (at any point) to an ideal solid (without dislocations) does not cause any detectable change of its overall density. In this sense the response (6.16) of the real solid should be viewed as giant. Clearly, if the superclimbing segments are to evolve into LLs and, thus, to lose their giant compressibility (6.15), the response (6.16) of the solid (the syringe effect) will vanish, that is $\kappa_{3D} = 0$.

As a matter of fact, the response on $\mu$ is not completely that of a liquid, where in equilibrium pressure variation distributes uniformly over the whole liquid – in accordance with the Pascal law. Viewing this property from the perspective of chemical potential, a
pressure change $\Delta P$ in a liquid in response on applying a change $\mu$ of chemical potential must be exactly equal to $\mu$. This constitutes a maximum possible syringe effect. In a solid permeated by the dislocation network, while the compressibility $\kappa_{3D}$ is finite as described above, the resulting pressure change is only $\Delta P$ is only proportional to $\mu$, with the coefficient proportionality less than unity.

6.4.2 Collective effects

As described in Ref.[73], presence of an ensemble of dislocations modifies the isochoric compressibility. The main effect comes from the overall compression of the solid as extra matter $\Delta N$ enters (exits) it. Referring to one element of the network, Fig. 6.2, the energy of the bowing with account for the compression energy $\sim K_{el} L_x L_y L_z \Delta N^2 / 2N^2$, where $N \sim L_x L_y L_z$ stands for the total number of atoms in the volume of one cell and $K_{el}$ stands for the compression modulus, can be written as

$$E \sim G y^2 \frac{2}{2L_x} + \frac{K_{el} \Delta N^2}{2L_x L_y L_z} - \mu y L_x, \quad \Delta N \sim y L_x. \quad (6.17)$$

The equilibrium value for $y$ follows from the minimization of $E$. This gives the fractional density change $\Delta N/N$ and the corresponding pressure change in the solid as $\Delta P \sim K_{el} \Delta N/N$:

$$\Delta P \approx \frac{K_{el}}{GL_y L_z L_x^2 + K_{el}} \cdot \mu. \quad (6.18)$$

If the shear modulus were zero, that is, $G = 0$, the pressure change would be exactly that of a liquid. This limit can also be reached in the case of a highly asymmetric network with $L_x >> \sqrt{L_y L_z}$. 
6.4.3 Compressibility and dislocation excitation spectrum

Concluding this section, we emphasize that the renormalized compressibility $\kappa$ and the superfluid stiffness $\rho_s$ both determine the spectrum of excitations of the dislocation as $\omega = \sqrt{\rho_s/\kappa q}$, with $q$ being a wavevector along the dislocation. In the case of the screw dislocation both $\kappa$ and $\rho_s$ are finite (that is independent of $q$) and, thus, the spectrum is sound-like. This implies the LL behavior. In the case of the superclimbing edge dislocation $\kappa$ depends on the wavelength as $\kappa \sim 1/q^2$ (up to the dislocation length $\kappa \sim L^2$), and this leads to the parabolic spectrum $\omega \propto q^2$ as mentioned previously. This why superclimbing dislocation represents non-LL. If superclimb is suppressed by, say, Peierls potential or impurities, $\kappa$ becomes finite and the linear spectrum is recovered – that is, the LL is restored. Below we will discuss that the suppression of superclimb can also occur without any impurities and potential – as $T \to 0$. This constitutes the emergence of the LL.

6.5 Superclimb beyond the gaussian approximation

The discussion in the previous section was based on the gaussian approximation, that is, it ignored the compact nature of the phase $\phi$ in the action (6.13). In other words, the possibility of instantons in the $D = 1+1$ space-time was not taken into account. Furthermore, there is no term corresponding to the Peierls potential in the action (6.13). In its simplest form $\sim \int d\tau \int dx \cos(2\pi y)$ this term takes into account the periodic potential imposed by the lattice and seen by the dislocation during its climbs. As discussed in [20] this term suppresses the superclimb at $T = 0$, if the equilibrium configuration corresponds to $y(x) = 0$ (or any other minimum $y = n$, $n = \pm 1, \pm 2, ...$). Then, the compressibility becomes finite (with respect to $L \to \infty$), and the spectrum of excitations becomes sound-like. In other words, the LL behavior of the dislocation core superflow is restored as long as the dislocation is aligned with one of the Peierls valleys.
CHAPTER 6. LUTTINGER TRANSITION IN SUPERCLIMBING DISLOCATION 89

Generically, however, dislocations form a network containing dislocations not aligned with Peierls valleys. More specifically, the dislocation end at $x = 0$ may be pinned at, say, $y(x = 0, \tau) = 0$ and the other one at $y(x = L, \tau) = n$ with $n \neq 0$. This dislocation is said to be tilted in the Peierls potential. Accordingly, it has $n$ jogs even at $T = 0$. Such geometrical jogs can be taken into account by shifting $y \to y + n \cdot x/L$ in the action and accordingly in the Peierls energy $\int dx \cos(2\pi y/a) \to \int dx \cos(2\pi y + 2\pi nx/L)$, where now the boundary condition becomes $y(0, \tau) = y(L, \tau) = 0$.

The standard approach to treating the $\cos(...)$ potential (see, e.g., in Ref.[14]) is based on the assumption that the term $2\pi nx/L$ washes out the potential. As suggested in [67] this implies that the geometrical jogs form quantum fluid of jogs which protect the superclimb from suppression at $T = 0$. In other words, the compressibility $\kappa$ should remain giant as given by Eq.(6.15) at $T = 0$. Accordingly the excitation spectrum remains quadratic in $q$, that is, the superfluidity along the core is of the non-LL type. This argument, however, has not been verified numerically.

Here we analyze a tilted superclimbing dislocation beyond the gaussian approximation by Monte Carlo simulations of the model [20] with no Peierls potential. The main purpose of this is to understand the role of compactness of the phase $\phi$ in the action (6.13). As will be shown below, this property turns out to be crucial as $T \to 0$ leading to the restoration of the LL character of the core superfluidity by suppressing the superclimb. At this point we also mention that the external bias $\mu$ in the action (6.13) can destroy the LL and restore the superclimb as long as $\mu$ exceeds a threshold which is macroscopically small with respect to $L$. This effect will be discussed later – in the section 6.6.

6.5.1 Dual representation

Here we will go beyond the gaussian approximation in (6.13) and take into account the compact nature of the phase $\phi$ by allowing vortices (instantons) to exist in the space-time...
(x, τ). This, in particular, can be achieved by discretizing the space-time so that \( \int d\tau \int dx \ldots \) transforms into a sum over the space-time lattice. The discretization of space is justified by the presence of the crystalline 3D lattice introducing the natural increment \( \Delta x \approx a \) determined by a typical interatomic distance \( a \) along the dislocation core.

Discretizing and transforming the action (6.13) following the same methods as in Sec. 6.3 and after integrating out the variable \( y \), we get that the dual action \( S_J \) in the long-wave limit as

\[
S_J = \sum_{b_{ij}} \left[ \frac{J_x^2}{2\tilde{\rho}_0} + \frac{\tilde{G}}{2}(\nabla_x J_\tau)^2 - \tilde{\mu} J_\tau \right],
\]

with \( \tilde{G} = G\Delta\tau, \tilde{\mu} = \mu\Delta\tau \) and \( \tilde{\rho}_0 = 1/[2\ln(2/\rho_0\Delta\tau)] \) (in the limit \( \Delta\tau \to 0 \) [70]) and the same divergence free constraint applies. The boundary condition for \( y \) is transformed into \( J_\tau(x = 0, \tau) = J_\tau(x = L, \tau) = 0 \) in addition to the periodic boundary condition along time: \( \vec{J}(x, \tau + \beta) = \vec{J}(x, \tau), \vec{J}(x + L, \tau) = \vec{J}(x, \tau) \).

The striking difference between the action (6.19) and the standard one (6.7) of the J-current model [72] describing LL is the absence of the term \( \sim J_\tau^2 \). As we will show below, such a term will be emerging as \( T \to 0 \) and \( \mu \to 0 \). Additionally, the filling factor \( n_0 \) has been “gauged away”, or integrated out by \( y \). [In the standard luttinger theory \( n_0 \) plays a crucial role in the BKT transition].

In addition to measuring \( \rho_s \) and \( \kappa \) as defined in terms of the windings (6.11, 6.12), we also calculated

\[
\kappa_1 = \frac{\langle N \rangle}{L\mu} = \frac{\langle W_\tau \rangle}{L\mu}
\]

characterizing the total number of atoms \( \langle N \rangle = \langle W_\tau \rangle/N_\tau \) injected into the solid due to the
superclimb. Both quantities $\kappa$ and $\kappa_1$ coincide with each other as $\mu \to 0$. In general, these are related by the exact formula $\kappa = d(\mu \kappa_1)/d\mu$. Simulations were performed by the Worm Algorithm [48].

### 6.5.2 Emergence of the LL behavior

Here we will present the evidence that, as the dislocation length $L$ and the inverse temperature $\beta$ both increase as $\beta \propto L \to \infty$, the compressibility $\kappa$ crosses over from being “giant” (6.15) to $\kappa = \kappa_{\text{eff}}$ saturating to a finite value in this limit. This implies the reconstruction of the excitation spectrum from parabolic to linear. In other words, the superclimb is being suppressed and the LL behavior emerges. We will also show that the phase diagram of the system (6.6,6.19) in the plane $(\rho_0, G)$, $\mu = 0$, features two phases – LL and insulator (where both $\rho_s$ and $\kappa$ vanish).

Strictly speaking, all results of simulations of the model (6.6,6.19) should be considered in the limit $N_\tau \to \infty$ in order to achieve the continuous time result. Practically, $N_\tau$ should be taken as large as needed to stop simulated quantities being dependent on $N_\tau$ for a given value of $\beta$. The result of this procedure is shown in Fig. 6.4. The compressibility deviates from its giant value, Eq.(6.15), as temperature decreases and asymptotically approaches some value which is more than one order of magnitude smaller than $\kappa_g$, Eq.(6.15), for a given size $L$. The question is how the asymptotic value of $\kappa$ depends on $L$. The result of simulations for several sizes $L$ are presented in Fig. 6.5. As can be seen, the asymptotic values of $\kappa$ (in the limit $T \to 0$) are independent of $L$ for large enough $L$. The asymptotic independence of $\kappa$ on $L$ is seen much more clearly in Fig. 6.6 where $T^{-1} = \beta$ is scaled as $\sim L \to \infty$.

A comment is in order about the procedure used to collect the data in Figs. 6.5,6.6 and from now on. We have checked that, while changing specific values, the qualitative behavior of $\kappa$ remains the same for a fixed value of $N_\tau$ for given $L$ without formally achieving the quantum limit of continuous time. Thus, the data in Fig. 6.5 and below are presented for
Figure 6.4: $\kappa$, Eq.(6.12), vs $\beta = T^{-1}$ for $L = 60, G = 2.3, \rho_0 = 4, \mu = 0$. Inset: $\kappa$ vs the number of time slices $N_t$ for two temperatures (shown close to each curve). The horizontal dashed line corresponds to the value of the "giant" compressibility, Eq.(6.15).

$T = 1/N_\tau$, that is, for the choice $\Delta \tau = 1$ (and $\tilde{C} = G, \tilde{\rho}_0 = \rho_0, \tilde{\mu} = \mu$).

The dependence $\kappa$ vs $T$ is characterized by some typical temperature $T = T_L$ and the range $\Delta_L$ below which $\kappa$ becomes significantly suppressed. In order to evaluate $T_L$ and the width $\Delta_L$ we have found the best fit of $\kappa$ vs $1/T$ using $T_L$ and $\Delta_L$ as the fit parameter in the fit function taken as $\ln(\kappa) = A - B \cdot \tanh(\Delta_L \cdot (T^{-1} - T_L^{-1}))$, with $A$ and $B$ chosen from the limiting values of $\kappa$ at the highest and lowest $T$ for each $L$. This function has produced fits which are acceptable within the statistical errors of the data for all curves. We have found that the crossover temperature $T_L \sim 1/\ln L$ and its width $\Delta_L \sim 1/\ln L$. More specifically, for $G = 2.3, \rho_0 = 4, \mu = 0$, the dependencies on $L$ are $T_L^{-1} = a \ln L + b$, with $a = 5.02, b = -6.27$ and $\Delta_L^{-1} = a' \ln L + b'$ with $a' = 1.53, b' = 0.09$. This dependencies are shown in Fig. 6.7.
Figure 6.5: $\kappa$ vs $\beta = T^{-1}$ for the lengths $L = 40, 80, 140$ (shown close to each curve). The horizontal dashed lines are the corresponding values of the “giant” compressibility, Eq.(6.15). Inset: superfluid stiffness vs $T^{-1}$ for the same sizes. The model parameters are $\rho_0 = 4, G = 2.3, \mu = 0$ in Eq.(6.19).

The question is how the emerged compressibility in the limit $L = \infty$ depends on the parameters of the model (6.19). Fig. 6.6 presents results of simulations for various values of $G$. The limiting value of $\kappa_{eff} = \kappa$ taken from the saturated behavior at large $L$ from Fig. 6.6 turns out to be $\kappa_{eff} \sim 1/G^b$, $b = 7.8 \pm 0.1$ for $G < 2.6$. This dependence is shown in Fig. 6.8. We have tested several values of $\rho_0$ and didn’t find any dependence of the power $b$ on it.

The effect of emergence of finite $\kappa$ occurs above some length $L^*$ (as long as $T \sim L^{-1}$). For $L < L^*$ the compressibility behaves as $\sim L^2/G$, Eq. (6.15). For $L > L^*$ it levels off at $\sim 1/G^b$. Thus, the relation $L^2/G \sim G^{-b}$ determines the crossover scale $L^* \sim G^{(1-b)/2}$ diverging in the limit $G \to 0$. Below we will discuss the deviations from the power law seen
in Fig. 6.8 for $G \geq 2.6$.

### 6.5.3 Quantum phase transition (QPT).

If the parameter $G$ exceeds a certain threshold $G_c$ for a given $\rho_0$, there is no more saturation of $\kappa$, Eq.(6.12), to a finite value in the limit $\beta \propto L \rightarrow \infty$. Instead it flows to zero. This behavior is clearly exhibited by three lower curves in Fig. 6.6 – corresponding to $G > 2.7$. The same tendency is seen in Fig. 6.8 where the linear log-log dependence is violated for the same values of $G$ (read off from Fig. 6.6 at the maximum $L$ simulated). In fact, both $\kappa$ and $\rho_s$,Eq.(6.11), flow to zero for these values of $G$. This behavior implies insulating state of the dislocation – when both superclimb and superflow along the core seize to exist.
Phase diagram mapping the two ground state phases of the dislocation is shown in Fig. 6.9. In the LL region $\kappa$, Eq.(6.12), and the superfluid stiffness, Eq.(6.11), both saturate to finite values in the limit $T^{-1} \sim L \to \infty$. In the region "insulator" both quantities approach zero values as $T^{-1} \sim L \to \infty$.

A presence of the transition in the model (6.6), (6.19) is unexpected because the Kosterlitz-Thouless (KT) argument (see in Ref.[14]) indicates that there should be no proliferation of the vortex pairs. Let’s demonstrate this by performing duality transformation on the model (6.19). The Kirchhoff’s constraint on the currents $\vec{\nabla} J = 0$, where $\vec{\nabla}$ stands for discrete gradient, can be satisfied by the substitute $J_x = \nabla_y \Phi$, $J_y = -\nabla_x \Phi$, where $\Phi$ are integers defined at sites of the dual lattice [74]. Using this in Eq.(6.19) and utilizing the Poisson summation identity (along the same line how the action (6.19) was derived from the original one (6.13)), we obtain the lattice gas model $Z = \sum_{\{n_i\}} e^{-S_g}$, $S_g = \frac{1}{2} \sum_{\vec{r}, \vec{r}'} U(\vec{r} - \vec{r}') n(\vec{r}) n(\vec{r}')$,
where \( n(\vec{r}) \) are integers defined on the sites of the dual lattice and \( U \) is the interaction potential with Fourier components \( \tilde{U} = (2\pi)^2/[\rho_0^{-1}\omega^2 + Gq^4] \) in the limit \( \omega \to 0 \) and \( q \to 0 \). The integers \( n \) describe vortices. In contrast with the standard superfluid, where vortices interact by logarithmic potential (see in Ref.[14]), here the potential is much stronger than logarithm. It is also strongly asymmetric: along space it is increasing with separation between two points \( (x, \tau) \) and \( (x', \tau') \) as \( \sim |x - x'| \) and along time as \( \sim \sqrt{|\tau - \tau'|} \). Thus, according to the KT argument a vortex-antivortex pair cannot proliferate to destroy the algebraic order along the dislocation. However, in spite of this criterion, our simulations of the model (6.19) show that there is a transition into insulating state.

As more detailed analysis presented in the Appendix A shows that the transition corresponds to the BKT transition[69, 14] with the universal jump \( 2/\pi \) in the effective Luttinger parameter \( K = \sqrt{\rho_s \kappa} \). It is also important to notice that the transition is insensitive to the
6.6 Roughening induced by chemical potential

The above results indicate that, in the absence of the bias by chemical potential $\mu$, the model (6.6,6.19) has only two ground states – either insulator or Luttinger Liquid marked by "insulator" and "LL" in Fig. 6.9, respectively. As temperature increases the compressibility crosses over to the "giant" value (6.15).

The LL state corresponds to smooth dislocation (with $\kappa = \kappa_{eff}$) because fluctuations of the dislocation shape $y(x,\tau)$ are strongly suppressed. This situation changes quite dramatically in the presence of finite $\mu$ in the action (6.19). Namely, the smooth state of the
dislocation can be destroyed by the bias $\mu \neq 0$. As a result, the giant compressibility is restored. This implies the roughening transition of the dislocation — fluctuations of the dislocation shape become diverging as $\sim \ln L$ in the rough phase, where $\kappa = \kappa_g$, Eq.6.15.

Simulations of the model (6.6,6.19) at finite $\mu$ have revealed two regimes: i) a crossover from smooth to rough dislocation at $T > T_H$; ii) A jump-like behavior characterized by strong hysteresis at $T < T_H$ featuring a coexistence of the smooth and rough phases of the dislocation.

6.6.1 The smooth-rough crossover

The crossover behavior at $T > T_H$ is shown in Fig. 6.10. As can be seen, the width of the crossover becomes smaller for larger $L$. To characterize this dependence, we have measured the value $\mu_{0.5}$ of $\mu$ where $\kappa_1$ reaches 1/2 of its ”giant” value (6.15) for a given size $L$. This dependence turns out to be $\mu_{0.5} \sim L^{-c}$, $c = 1.21 \pm 0.05$, and it is shown in Fig. 6.11.
Figure 6.10: $\kappa_1$ vs $\mu$ for sizes $L$ shown close to the corresponding plot, $G = 2.3, \rho_0 = 4, T = 0.0556, T_H \approx 0.0435$. Dashed lines show the “giant” values (6.15) for the corresponding size $L$. 
Figure 6.11: The log-log plot of the crossover value of $\mu_{0.5}$ vs $L$ taken from the data in Fig. 6.10.

Figure 6.12: Hysteretic behavior of the compressibility $\kappa_1$, Eq. (6.20), vs $\mu$. The dashed line shows the "giant" value, Eq.(6.15), for $L = 100$, $T = 0.025$, $\rho_0 = 4$, $G = 2.3$. The arrows show the direction of the hysteretic loop: each point corresponds to simulations for $2 \cdot 10^{10}$ MC steps for a given value of $\mu$. 
Figure 6.13: Width $\Delta \mu$ of the hysteretic loop vs $1/T$ for $L = 100, G = 2.3, \rho_0 = 4$. Solid line is the fit by $\Delta \mu = \mu_0 \ln(T_H/T)$, $\mu_0 = 0.0346$, $T_H = 0.0436$. 
6.6.2 Hysteretic behavior of the smooth-rough dislocation

At temperatures $T < T_H$ the roughening transformation behaves alike 1st order phase transition because it shows strong hysteresis, Fig. 6.12. The width $\Delta \mu$ of the hysteresis, Fig. 6.13, saturates to a finite value as $T \to 0$ (determined by purely quantum fluctuations). Hysteresis vanishes at $T = T_H \approx 0.0435$ (for the chosen parameters).

We should emphasize that the existence of a phase transition in 1D system characterized by a local order parameter is forbidden at finite $T$ [1]. In particular, 1st order transition should be a crossover characterized by activation with a typical finite energy given by the width of the domain wall between two phases. Thus, the interpretation of the strong hysteresis at finite $T$ requires caution. In this respect we note that, similarly to the dislocation roughening in the presence of the Peierls potential [75], there is no local description of the rough state because it is a global property of the whole dislocation. Thus, the ”no-go theorem” [1] does not actually apply. Further studies are required in order to see if the observed hysteresis features a true finite-$T$ transition characterized by extensive energy barrier (rather than an intensive one in the case of the crossover).

6.6.3 Emergent LL in Solid He

The effect of emergence of LL behavior in a model which should be a non-LL according to the standard analysis can be viewed from another perspective. The original model (6.13) features a strong asymmetry between space and time because its excitation spectrum is parabolic – changing unit of space by a factor of two requires changing the unit of time by the factor of four in order to keep the spectrum unchanged. In the LL phase (smooth phase) the spectrum becomes linear which implies restoration of the space-time symmetry. Furthermore, the nature of the QPT is also consistent with the space-time symmetry. Thus, the edge dislocation with superfluid core features the emergence of the symmetry between
space and time (in \(D = 1 + 1\)) in its ground state in thermodynamic limit.

The question to answer is why the emergence of the LL is not "seen" by the elementary dimensional analysis, and also why there is the BKT transition despite that the KT argument predicts none. The qualitative explanation [76] comes naturally in terms of the loops in Eq.(6.19). As the weight of each element \(\vec{J}\) becomes larger, its discreteness becomes more and more important so that more configurations will have currents \(J_\tau\) with no neighbors. In such a situation the discrete gradient \((\nabla_x J_\tau)^2\) becomes essentially \(J_\tau^2\). This transforms the action (6.19) effectively into the form typical for the standard J-current model [72] describing LL as well as the BKT transition at integer filling.

It would be useful to find an argument for the effect in terms of the fields. One insight can be gained from the following consideration: one jog passing along the length \(L_x\) of the dislocation carries a string of atoms \(\Delta N = L_x\) (which advances an incomplete basal plane by one interatomic distance). This means that each jog is essentially a macroscopically heavy particle which as long as \(L_x \gg 1\). Thus, such a particle can be localized easily at low \(T\) which automatically implies suppression of the superclimb.

6.7 Dynamics

A rough superclimbing dislocation is unstable with respect to chemical potential bias, \(\mu\), determined by the typical length of dislocations with superfluid core [73]. In particular, a rough dislocation is unstable with respect to unlimited growth if \(\mu > \mu_c \sim \frac{1}{L}\). While there are several possible channels for the dynamics [73], here we will concentrate on Bardeen-Herring loop generation in the bulk. This allows a possible explanation of the syringe effect as well as superflow through the solid.

The bias \(\mu\) is an increase of the chemical potential liquid \(\mu_l\) with respect to the solid by applying pressure or by the fountain effect, that is \(\mu = \mu_s - \mu_l < 0\), so that atoms favor
solidity over the liquid phase. There is an energy gain due to bowing $\delta E_b \sim |\mu \delta N|$ that is proportional to the area swept out. This energy competes with the energy cost due to the core length increase $\delta E \sim L - L_0$. For large enough $L$, the energy due to gain by bowing always dominates the elastic energy cost. In the limit $\mu \to 0$ (meta) stability is protected by a macroscopic energy barrier which vanishes for $|\mu| > \frac{1}{L_0}$. The dislocation becomes unstable towards inflation.

Single loop dynamics is characterized by a ballistic regime and the dissipative regime where phase slips occur. On the timescale of minutes, the dynamics is dominated by dissipative processes. The ballistic stage is too short to account for the syringe effect. Here we study the dynamical equations of motion of a single dislocation in the ballistic regime.

To study the dynamics of the action in Eq. 6.13 it is important to parametrize the action so that all types of string configurations, such as complex bowed shapes, may appear in the solutions to the equations of motion. Consider a string in the plane defined by $\vec{r}_\gamma = (x(\xi), y(\xi))$ where the endpoints are fixed so that $x(\xi_0, t) = x_0, y(\xi_0, t) = 0, x(\xi_N, t) = L, y(\xi_N, t) = 0$ for $\xi \in [\xi_0, \xi_N]$ where $L$ is the length of the straight dislocation oriented along the $x$ axis at $t = 0$. Typically, we choose $x_0 = 0$ or $x_0 = -L$ for full symmetry. A schematic illustration is shown in Fig. 6.14.

![Figure 6.14: Schematic of the geometry and boundary conditions for the dynamical superclimbing dislocation with fixed ends.](image)
Then we will consider the action 6.13 in real time in the form

\[ S = \int_{t_0}^{t} \int_{\xi_0}^{\xi_N} dt \, d\xi \left[ -\phi (x_\xi y_t - y_\xi x_t) + \frac{\rho_0}{2} \frac{\phi_\xi^2}{(x_\xi^2 + y_\xi^2)} + G \sqrt{x_\xi^2 + y_\xi^2} \right], \quad (6.21) \]

where the subscript notations \( x_\xi = \frac{\partial x}{\partial \xi} \) and \( x_t = \frac{\partial x}{\partial t} \) are used for space and time derivatives, respectively. Here it is important to note that in the first term, which is the berry phase term, we restrict the evolution of the dislocation line to the direction orthogonal to the string tangent vector. Thus, the local velocity of the core becomes \( v_\perp = -\frac{x_t y_\xi}{\sqrt{x_\xi^2 + y_\xi^2}} + \frac{y_t x_\xi}{\sqrt{x_\xi^2 + y_\xi^2}} \).

We do this because the longitudinal evolution along the core is already accounted for by the superfluid term. The second term is just the energy due to the current. Finally, the last term proportional to \( G \) is the energy due to the length of the string which changes due to bowing. Note that this term, reduces to the same term in 6.13 in the limit of small displacements from equilibrium (nearly straight line dislocations).

The variation of the action gives the equations of motion

\[ x_t = \frac{y_\xi}{(x_\xi^2 + y_\xi^2)} \partial_\xi F_\phi, \quad y_t = -\frac{x_\xi}{(x_\xi^2 + y_\xi^2)} \partial_\xi F_\phi, \quad (6.22) \]

\[ \phi_t = \frac{y_\xi \phi_\xi}{x_\xi (x_\xi^2 + y_\xi^2)} \partial_\xi F_\phi + \frac{1}{x_\xi} \partial_\xi F_y, \quad (6.23) \]

\[ F_\phi = \frac{\partial S}{\partial \phi_\xi} = \frac{\rho_0 \phi_\xi}{\sqrt{(x_\xi^2 + y_\xi^2)}}, \quad F_y = y_\xi \left( \frac{G}{\sqrt{(x_\xi^2 + y_\xi^2)}} - \frac{\rho_0 \phi_\xi^2}{2(x_\xi^2 + y_\xi^2)^{3/2}} \right). \quad (6.24) \]

Simulations of Eq.(6.22,6.23,6.24) have been conducted by Mathematica. The initial evolution was characterized by low numerical errors. However, the error accumulation became uncontrolled at times qualitatively corresponding to the condition Eq. (6.26) for the instability. Thus, we cannot make any claim about the behavior of the system beyond the time of the numerical instability.
6.7.1 Metastability of the biased dislocation

In order to test for stability we fixed the initial segment length $L$, and fixed $G = \rho_0 \equiv \rho_s = 1$ and observed the numerical solutions to the equations of motion. The discretization $\xi_N = 10000$ was chosen. For $\mu < \mu_c$ we observed solutions that bowed like a plucked guitar string but did not continue to inflate beyond a radius obtained within the gaussian approximation. At $\mu = \mu_c$ the values shown in Fig. 6.15, the inflation continues unbounded and overhangs develop. Indeed, as shown in Fig. 6.15 the threshold is clearly in agreement with $\mu_c \sim \frac{1}{L}$ obtained analytically in Ref. [73].

![Figure 6.15: Threshold for instability $\mu_c$ versus linear system size $L$ for $G = \rho_s \equiv \rho_0 = 1$ plotted on logarithmic axes. The slope is $-1.01 \pm 0.005$ in agreement with the theoretical prediction.](image)

6.7.2 Linear approximation for the superfluid phase

Here we consider smooth growing linear solutions to the imposition of a chemical potential, $\phi = \frac{x}{t} \mu t$. Then $\phi_t = \mu$ and the current $J = \nabla_x \phi = \frac{\mu t}{L}$, where the parametrization $x = \xi$ is chosen. If this solution is plugged into the action in Eq. 6.21 and the action is linearized with respect to $y_\xi^2$, the coefficient in front of this term becomes negative. This results in the
instability at times given by

$$t_{\text{inst}} \approx \frac{L}{\mu} \sqrt{\frac{2G}{\rho_0}}. \quad (6.25)$$

For the case of asymmetric boundary conditions, the time to instability was measured by observing the numerical solutions of the PDE's in equations 6.22, 6.23 where the phase was held fixed at one endpoint of the dislocation $\phi(x = 0, t) = 0$ and the phase at the other end was allowed to grow linearly with time $\phi(x = L, t) = \mu t$.

![Graph showing the relationship between numerical instability time and system size L](image)

Figure 6.16: Numerical instability time versus system size $L$ for the case of asymmetric boundary conditions and $G = \rho_s \equiv \rho_0 = 1$. The slope of the fit line on the log-log axes is in agreement with the theoretical prediction for a physical instability in the linearized action.

We observed instabilities in the numerical solutions to be in close agreement with the functional dependence predicted by the linearized action in 6.26 as shown in Figs. 6.16, 6.17, 6.18.

### 6.7.3 Bardeen-Herring loop generation

The Bardeen-Herring mechanism for climbing edge dislocations is the analog of the Frank-Reed instability for gliding dislocations [77], which is a process wherein an initially straight
Figure 6.17: Numerical instability time versus system size $\mu$ for the case of asymmetric boundary conditions and $G = \rho_s \equiv \rho_0 = 1$. The slope of the fit line on the log-log axes is in agreement with the theoretical prediction for a physical instability in the linearized action.

Figure 6.18: Numerical instability time versus system size $G/\rho_0$ for the case of asymmetric boundary conditions and $\mu$ slightly more than $\mu_c(L)$. The slope of the fit line on the log-log axes is in agreement with the theoretical prediction for a physical instability in the linearized action.
segment bows and develops overhangs due to the bias. Eventually, these overhangs touch and a loop separates from the main dislocation. This process constitutes the phase slip effect. It is cyclic and is characterized by a time $t_{FR}$ needed for the loop to grow until the overhangs merge\[73]. The estimate of such a time is given by

$$t_{FR} \sim L^{3/2} \frac{1}{\sqrt{\rho_0|\mu|}},$$

(6.26)

where we have assumed symmetric boundary conditions $\phi(x = 0, t) = \mu t = \phi(x = L, t)$. Such boundary conditions relate to the syringe effect, that is matter accumulation in the bulk. The numerical solutions to the equations of motion were obtained for $G = \rho_0 = 1$ fixed and varying the length for $\mu \approx \mu_c(L)$. We measured the time to fully develop overhangs. Generally, the solutions display numerical instabilities approximately around the time at which the overhangs touch, or slightly before or after it. The dependence of the measured $\mu^{1/2} t_{FR}$ versus $L$ is shown on the log-log scale in Fig. 6.19. The slope $\approx 1.43$ is in rough agreement with the theoretical prediction $3/2$ [73].

Figure 6.19: Bardeen-Herring overhang generation time $t_{FR}\mu^{1/2}$ versus $L$. The slope of the fit line on the log-log axes is 1.42 in rough agreement with the theoretical prediction of $3/2$. 

\[slopes\]
Chapter 7

Summary and Future Work

7.1 Conclusions

Summarizing, the numerical flowgram method has been applied to the problem of LG criticality in 2D. The critical correlation length exponents in strong and weak fields $\mu$, $\nu$ have been determined to be consistent with 2D Ising class within the combined error of 1-2%. The main advantage of the method is that it does not require the accurate knowledge of the position of neither the critical point nor the coexistence line. Instead, these quantities follow as a byproduct of the method.

The role of the odd terms in the real scalar field theory near the critical point has been addressed in the context of the general mapping of the LG transition to the field theory. The analysis of the $\phi^5$ term revealed that its critical dimension is the same as that of the linear term $\phi$. We have put forward a conjecture that all odd terms have the same critical dimension at the symmetric critical point of Ising type. This excludes the possibility of non-Ising LG criticality.

We have introduced the J-current type model (6.19) describing tilted superclimbing dislocation. According to the elementary scaling analysis such a dislocation should exhibit
non-LL behavior. In contrast, Monte Carlo simulations reveal the emergence of the LL as temperature is lowered and the system size exceeds certain scale determined by the line tension $G$ (bare shear modulus). This scale is characterized by high power independent of the bare superfluid stiffness. The emerging LL can also undergo the BKT transition into insulating state. The LL behavior can be destroyed by macroscopically small external bias by chemical potential. As a result, the giant isochoric compressibility can be reinstated even at $T = 0$. Our model provides predictions for the corresponding bias and temperature dependencies which can be tested experimentally. Our numerical simulations for the dynamics of the dislocation in the ballistic regime support analytical predictions for the instability threshold. We also observed the Bardeen-Herring loops generation in the strongly non-linear regime (beyond the threshold) and determined the time of their development and separation from the main dislocation. This also agrees with the analytical prediction.

In the next section we will outline proposals for experiments aimed at testing the most important features of the model. If observed these would be a proof for the dislocation scenario for the superflow-through-solid and the syringe effects.

7.2 Future Work

7.2.1 Scaling of the LG diameter

As noted in Chapter 5, one of the outstanding problems is to determine the leading corrections to scaling of the rectilinear diameter. We note that the strongest evidence for the term $\sim t^{23}$ may be obtained from the direct evaluation of $d\rho/dl = L^{-d}d\langle N\rangle/dl$ (by keeping $l_1 = 0$ in Eq.(5.1)) using the cumulants $\langle N \rangle$, $\langle E \rangle$, $\langle N^2 \rangle$, $\langle E^2 \rangle$, $\langle EN \rangle$, where $N$, $E$ stand for the number of particles and the total energy, respectively, and $\langle \ldots \rangle$ denotes the statistical mean evaluated with the Boltzmann factor $\sim \exp(-H_c - t_1 lE + \mu_1 lN)$, where
$H_c \equiv E/T_c - N\tilde{\mu}_c$ stands for the action at the critical point. Then

$$\frac{d\rho}{dl} = L^{-d} \left[ (\langle N^2 \rangle - \langle N \rangle^2)\mu_1 - (\langle EN \rangle - \langle E \rangle \langle N \rangle) t_1 \right], \quad (7.1)$$

where $\mu_1$ and $t_1$ obey the condition $h_1 = (1 - c_2 a_1)\mu_1 + (c_1 - c_2 a_2) t_1 = 0$. Since $X = L^{1/\nu} l + o(b_2 L^{-d+1/\nu}) \sim 1$, we find $l \sim L^{-1/\nu}$ and, consequently, $d.../dl \sim L^{1/\nu}$ which implies $d\rho/dl \rightarrow 4(\beta/\nu)c_2 F'_Y Y L^{(1-2\beta)/\nu} \rightarrow \infty$ as $L \rightarrow \infty$ from Eq. (5.23). In 2D this divergence becomes $d\rho/dl \sim L^{3/4}$. If $|c_2| << 1$ the term $\sim b_1$ in Eq.(5.23) (giving $d\rho/dl \sim b_1 F'_X L^{\alpha/\nu} \sim \ln L$) may dominate at not very large $L$. Thus, this becomes a candidate project for future numerical work.

### 7.2.2 Stress anisotropy induced by superclimb.

The superclimb effect results in injecting (removing) basal atomic planes. For a single hcp crystal confined in a rigid box this implies additional average deformation along the C-axis. If $DN$ atoms were injected to form $DM$ basal layers in a $^4$He crystal made of $M$ basal layers, the created average strain can be estimated as $u_{zz} \approx DM/M$. This will produce an average stress $\sigma_{zz} \approx C_{zzzz} DM/M$ and $\sigma_{xx} = \sigma_{yy} \approx C_{xxxx} DM/M$, where $z$-axis is along the hcp axis and $x, y$ are orthogonal coordinates along the basal plane. Here $\sigma_{ij}$ is the stress tensor [78] and $C_{ijkl}$ are elastic constants of hcp solid $^4$He. Thus the asymmetry of the stress becomes $\alpha_\sigma = \sigma_{zz}/\sigma_{xx} \approx C_{zzzz}/C_{xxxx}$. Measuring the asymmetry and comparing with the known elastic moduli will provide a crucial information on the mechanism of the syringe effect. In polycrystals there could also be some asymmetry if the C-axis of the crystallites is not fully randomly oriented.
CHAPTER 7. SUMMARY AND FUTURE WORK

7.2.3 Threshold for superclimb

Important aspect of our discussion is the existence of the threshold for superclimb: The syringe effect should vanish in the limit $T \to 0$ and $\mu \to 0$ even in samples free from $^3$He impurities. $[^3\text{He suppresses superflow and the syringe}[15, 16, 19]$]. At this juncture it is important to emphasize that stopping the syringe effect does not imply stopping the superflow along the core. Thus, observing a suppression of the syringe effect without suppressing superflow would be a ”smoking gun” for the superclimb mechanism [20] and for the emergence of LL. Accordingly, studying the syringe and the superflow effects in extremely clean samples of solid $^4$He at very low temperatures and biases becomes of crucial importance.

There is, however, a significant obstacle. As mentioned in Ref.[73], the current experiments [15, 16] and also [19] are likely to be in the regime of large $\mu$, that is, in the dislocation rough state induced by the bias where $\kappa = \kappa_1 = \kappa_g$, Eq.(6.15), even at $T = 0$. The analysis [73] focuses on the geometrical instability of dislocations with superfluid core: once chemical potential bias exceeds the threshold $\mu_c \sim GL^{-1}$, such dislocations become unstable with respect the inflation which constitutes a mechanism of the crystal growth from inside out. In this case a single inflating dislocation builds one whole atomic extra plane. As described in Sec. 6.6.1, there is even stronger condition for the destruction of the LL behavior – characterized by the threshold $\mu_c \sim L^{-1.2} << L^{-1}$ in the limit $L \to \infty$. Practically, for dislocations with a typical length $L \sim 1\mu m$ and larger the threshold becomes smaller than $\sim 10$ mbar. Translating the temperature scale from Fig. 6.5, to the temperatures in the units $\sim 1$ K, relevant to superfluidity of the dislocations in solid $^4$He, gives the range $T \leq 1 - 10$mK where the suppression of the syringe effect should be looked for. Furthermore, as described in Sec.6.6.2, there should be strongly hysteretic behavior at low $T$. Searching for the hysteresis may also provide a crucial information. To what extent such measurements at low $T$ and $\mu$ are feasible remains to be seen.
CHAPTER 7. SUMMARY AND FUTURE WORK

7.2.4 Sudden stopping of the pressure evolution in the supersolid

A remarkable feature presented in Fig.2a of Ref.[19] reveals a sudden stopping of the pressure evolution. Clearly this feature is inconsistent with any type of activation behavior usually resulting in exponential relaxation. We propose a scenario for this effect: initially long superclimbing dislocations evolve into a structure characterized by small lengths \( L_x \) of the free segments. Accordingly, once the resulting chemical potential equilibrates over the whole sample these segments may enter the LL regime – where the superclimb is suppressed because both \( \mu \) and \( T \) are below the threshold determined by \( L_x \). This should result in the sudden stopping of the pressure variation. More studies of the time evolution can provide crucial information about the nature of this feature.

7.2.5 Equilibrium syringe fraction.

As mentioned above, syringe effect implies a liquid-like response of solid on chemical potential. The question is if anything specific can be said about the nature of the conducting network of dislocations. In this respect an important insight can be gained from Ref.[19]. In this experiment the upper part of solid \(^4\)He (see Fig.1 of Ref.[19]), which is about 0.3 mm thick, was deformed by about 1 \( \mu \)m. This resulted in an immediate elastic response \( \sim 10 \) mbar at the other end of the sample (about 10 mm away) followed by much slower and stronger pressure increase reaching (equilibrium) values about 0.2 bar (see Fig.2a in Ref.[19]). It is instructive to compare this number with the pressure imposed in the upper chamber \( \sim 0.3 – 1 \) bar which resulted from strain \( \sim 3 \cdot 10^{-3} \). Since these values are only a factor of 2-5 different, some information can be drawn about the asymmetry between the lengths of the dislocation network with the help of the relation (6.18). More consistent studies of the dependence of \( \Delta P \) vs imposed strain and in situ measurements of the compression modulus may shed more light on the nature of the syringe effect.
We also suggest focusing on interaction between glide (see in Refs. [78, 66]) and superclimb of dislocations as a test for the dislocation scenario. The question is to what extent the giant plasticity of solid $^{4}$He [79] may affect the superflow and/or superclimb. The effect [79] consists of softening of the shear modulus $G_{el}$ as temperature increases above $\sim 20 - 100$ mK. While in polycrystalline samples the softening is about 10-20% of the zero temperature value, in a monocrystal it can reach 80-90%. The main reason for this effect is glide of basal plane dislocations. It is important to note that these dislocations are not superfluid, and, therefore, they cannot contribute directly to the superclimb. They, however, can affect the syringe response through modifying the shear modulus. We see the main channel for this through contributing to the effective compression modulus $K_{el}$ of the polycrystalline medium as $K_{el} = K_0 + \gamma G_{el}(T)$, with $\gamma > 0$ being a geometrical coefficient determining how averaging of the crystallites orientation contributes to the average $K_{el}$. Obviously, as $G_{el}$ softens with increasing $T$, the compression modulus should soften too. In accordance with Eq.(6.18) this implies a decreasing $\Delta P$ with temperature. In this regard we note that, as Fig.2a of Ref.[19] indicates, the equilibrium pressure change is indeed a decreasing function of temperature. More comparative studies of this dependence with the shear softening data [79] will be very useful. [At this point we note that the core tension $G$ of a particular superclimbing segment (see in Eqs.(6.13,6.19)) should not be significantly affected by the plasticity effect in the case of low density of basal dislocations because core of a particular superclimbing edge segment "sees" the ideal crystal in its close vicinity].
Appendix A

Universality of transition to insulating state

Here we support our statement that the quantum transition to the insulating state of the model (6.6,6.19) is of the BKT type. The analysis is conducted for two points at the phase diagram line, Fig. 6.9, – corresponding to $\rho_0 = 0.8, 1$.

The model (6.6.6.19) appears to be very different from the standard J-current model \[72\]

\[ H_{XY} = \int d^2 x K (\nabla \phi)^2 / 2, \]

which describes the compact U(1) phase $\phi$ in 2D and features the BKT transition at the critical value $K_c = 2/\pi$ of the Luttinger parameter $K$ \[14\].

If the model (6.6.6.19) undergoes the same type of the transition (at $\mu = 0$), for each value of $\rho_0$ there should be such a critical value $G = G_c$ that the evolution of the renormalized Luttinger parameter $K = \sqrt{\rho_s K}$ (defined in terms of the windings, Eqs.(6.11,6.12), should follow the solution of the renormalization group (RG) equations with the critical value $K_c$. Such an analysis has been pioneered in Ref.[80].

The RG equations have a form (see in Ref.[14])

\[ \frac{du}{d \ln l} = 2(1 - g)u, \quad \frac{dg}{d \ln l} = gu^2 , \]  

(A.1)
Figure A.1: The parameter $\sqrt{-C}$ versus $G$ for $\rho_0 = 1$. The solid line is the fit by $\sqrt{-C} = A \cdot (G - G_c)^{0.5}$, $G_c = 1.299$, $A = 2.886$.

where $u$ stands for the vortex fugacity and $g = K/K_c$. The parameter $l$ determines typical scale of the renormalization. Numerically, $l$ can be associated with the system size as $l = L/L_0$ up to an arbitrary constant factor $L_0$.

A general solution of the system (A.1) can be expressed in terms of two constants of integration, $C$, $l_0 > 0$, determined by the initial values of $u$ and $g$, which in their turn are
APPENDIX A. UNIVERSALITY OF TRANSITION TO INSULATING STATE

set by the microscopic model (6.6.6.19). The solution has a form \( u^2 = 2[\xi^2 + C] \),

\[
F(\xi) = 4 \ln \left( \frac{l}{l_0} \right), \quad \xi = \frac{1}{g} - 1 = \frac{K_c}{K} - 1,
\]

where for \( C > 0 \)

\[
F(\xi) = \ln(\xi^2(l) + C) - \frac{2}{\sqrt{C}} \tan^{-1} \left( \frac{\sqrt{C}}{\xi} \right),
\]

and

\[
F(\xi) = \ln(\xi^2(l) - C^2) + \frac{1}{\sqrt{-C}} \ln \left( \frac{\xi(l) - \sqrt{-C}}{\xi(l) + \sqrt{-C}} \right).
\]

for \( C < 0 \). The case \( C = 0 \) describes the separatrix \( u = \sqrt{2}\xi \) given by

\[
F(\xi) = 2 \ln |\xi| - \frac{2}{\xi}.
\]

In order to check if the flow of the renormalized Luttinger parameter \( K(l) \), obtained from simulations of the model (6.6.6.19) can be described by the RG equations (A.1), we tried to fit our Monte Carlo data for \( K \) at large \( L \) by either solution, Eqs.(A.2,A.4), with the properly chosen \( C \)-constant for each \( G \). We have analyzed the values \( \rho_0 = 0.8, 1.0 \) for which the large \( L \) behavior is almost symmetric between space and time. Our finding is that the data can be fit by \( C < 0 \), Eq.(A.4), and \( \xi > 0 \) with \( K_c = 2/\pi \) for each value of \( G \).

It is important to note that \( C \to 0 \) determines a diverging correlation length \( L_c \sim \exp(1/4\sqrt{-C}) \to \infty \) with \( C \) depending on the deviations from the critical parameter (see in Ref.[14]). In our case for fixed \( \rho_0 \) we expect \(-C \sim G - G_c > 0 \) (if the data fits the RG prediction). Practically, the data were substituted into the function \( F \), Eqs.(A.2, A.4), and plotted vs \( 4 \ln L \). The value of \( C \) for a given \( G \) has been adjusted so that the slope of \( F \)
vs $4 \ln L$ is unity. A good fit could only be achieved for the solution (A.4). The result of this procedure for 10 values of $G$ is presented in Fig. A.1. As can bee seen, the data points are consistent with the RG prediction $(-C)^{0.5} \sim (G - G_c)^{0.5}$ with $G_c \approx 1.30$. Thus, the transition is of the BKT type.

The above analysis has been conducted for values $\rho_0$ and $G$ guaranteeing that the renormalized $\rho_s$ and $\kappa$ at large $T^{-1} = L$ are approximately equal to each other. This choice was dictated by simplicity of the analysis and also faster convergence of the simulations. It is natural to assume that the universality does not change when $\rho_s$ and $\kappa$ become significantly asymmetric. Thus, we conclude that the whole line of the transitions $G = G_c(\rho_0)$ in the space $\rho_0, G$, Fig. 6.9 belongs to the BKT universality.
References

REFERENCES

42. V. N. Bondarev, private communication, 2016.


60. A. Haziot, D. Y. Kim, M. Chan, presented at the APS Meeting Abstracts.


REFERENCES

76. B. Svistunov, private communication.


