

การแก้ไขสเกลลิงในพลศาสตร์การจัดระเบียบเฟสของระบบ XY สองมิติ



นายเพชร ชุนเพชร

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

วิทยานิพนธ์นี้เป็นส่วนหนึ่งของการศึกษาตามหลักสูตรปริญญาวิทยาศาสตรมหาบัณฑิต

สาขาวิชาฟิสิกส์ ภาควิชาฟิสิกส์

คณะวิทยาศาสตร์ จุฬาลงกรณ์มหาวิทยาลัย

ปีการศึกษา 2552

ลิขสิทธิ์ของจุฬาลงกรณ์มหาวิทยาลัย

CORRECTIONS TO SCALING IN PHASE-ORDERING DYNAMICS OF TWO-
DIMENSIONAL XY SYSTEM



Mr. Petch Khunpetch

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

A Thesis Submitted in Partial Fulfillment of the Requirements
for the Degree of Master of Science Program in Physics

Department of Physics

Faculty of Science


Chulalongkorn University

Academic Year 2009

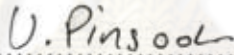
Copyright of Chulalongkorn University

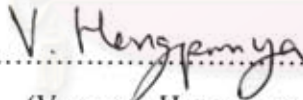
Thesis Title CORRECTIONS TO SCALING IN PHASE-ORDERING DYNAMICS
 OF TWO-DIMENSIONAL XY SYSTEM
By Mr. Petch Khunpetch
Field of Study Physics
Thesis Advisor Varagorn Hengpunya, Ph.D.


Accepted by the Faculty of Science, Chulalongkorn University in Partial
Fulfillment of the Requirements for the Master's Degree


..... Dean of the Faculty of Science
(Professor Supot Hannongbua, Dr.rer.nat.)

THESIS COMMITTEE


..... Chairman
(Associate Professor Udomsilp Pinsook, Ph.D.)


..... Thesis Advisor
(Varagorn Hengpunya, Ph.D.)


..... Examiner
(Jessada Sukpitak, Ph.D.)


..... External Examiner
(Assistant Professor Tanakorn Osotchan, Ph.D.)

4972425923 : MAJOR PHYSICS

KEYWORDS : SCALING PHENOMENA / PHASE-ORDERING DYNAMICS/
TWO-DIMENSIONAL XY SYSTEM / THE KOSTERLITZ-THOULESS
TRANSITION

PETCH KHUNPETCH : CORRECTIONS TO SCALING IN PHASE-
ORDERING DYNAMICS OF TWO-DIMENSIONAL XY SYSTEM.

THESIS ADVISOR : VARAGORN HENGPUNYA, Ph.D., 53 pp.

Scaling phenomena in nonequilibrium dynamics are very important and challenging problem in condensed matter physics. In this thesis, we investigated the scaling phenomena in phase-ordering dynamics. The purpose of the thesis is to determine dynamical scaling properties and its correction forms in phase-ordering dynamics of two-dimensional XY system.

We consider quenches in nonconserved two-dimensional XY system between any two temperatures below the Kosterlitz-Thouless transition temperature. The first-order correction to correlations associated with the amplitude fluctuations is investigated. In order to solve this problem, we treat the small amplitude fluctuations comparing to the phase fluctuations. Then, the dynamics of phase and amplitude fields become uncoupled. The dynamics of the phase field is referred as the zeroth-order theory while for the amplitude field is referred as the first-order correction. We find that, at late times, the nonequilibrium parts of both zeroth- and first-order correlations exhibit scaling.

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Department : Physics
Field of Study : Physics
Academic Year : 2009

Student's Signature Petch Khanpetch.....
Advisor's Signature V. Hengpunya.....


เพชร ขุนเพชร : การแก้ไขสเกลลิงในพลศาสตร์การจัดระเบียบเฟสของระบบ XY สองมิติ. (CORRECTIONS TO SCALING IN PHASE-ORDERING DYNAMICS OF TWO-DIMENSIONAL XY SYSTEM) อ.ที่ปรึกษา
วิทยานิพนธ์หลัก : ดร. วรากร เอ็งปัญญา, 53 หน้า.

ปรากฏการณ์สเกลลิงในพลศาสตร์นอกสมดุลเป็นปัญหาที่มีความสำคัญและท้าทายในฟิสิกส์ของสสารควบแน่น ในวิทยานิพนธ์นี้เราสืบสวนปรากฏการณ์สเกลลิงในพลศาสตร์การจัดระเบียบเฟส จุดประสงค์ของวิทยานิพนธ์นี้คือคำนวณหาคุณสมบัติสเกลลิงเชิงพลวัตและรูปแบบการแก้ไขในพลศาสตร์การจัดระเบียบเฟสของระบบ XY สองมิติ

เราพิจารณาการลดอุณหภูมิในระบบ XY สองมิติแบบไม่อนุรักษ์ระหว่างสองอุณหภูมิใดๆที่ต่ำกว่าอุณหภูมิการเปลี่ยนแบบคอสมอโรลิตซ์-เทาลอสต์ การแก้ไขสหสัมพันธ์อันดับที่หนึ่งเนื่องจากการกระเพื่อมของอำนาจก่อกวน ในการแก้ปัญหานี้เราให้การกระเพื่อมของอำนาจมีค่าน้อยเมื่อเทียบกับการกระเพื่อมของเฟส ดังนั้นพลวัตของสนามเฟสและสนามอำนาจจึงไม่ขึ้นต่อกัน โดยเราพิจารณาการพลวัตของสนามเฟสเป็นทฤษฎีอันดับที่ศูนย์ในขณะที่การพลวัตของสนามอำนาจเป็นการแก้ไขอันดับที่หนึ่ง เราพบว่าเมื่อเวลาล่วงเลยไปนานส่วนนอกสมดุลของสหสัมพันธ์ทั้งในทฤษฎีอันดับที่ศูนย์และการแก้ไขอันดับที่หนึ่งแสดงสเกลลิง

ศูนย์วิทยทรัพยากร จุฬาลงกรณ์มหาวิทยาลัย

ภาควิชา ฟิสิกส์
สาขาวิชา ฟิสิกส์
ปีการศึกษา 2552

ลายมือชื่อนิสิตเพชร ขุนเพชร.....
ลายมือชื่ออ.ที่ปรึกษาวิทยานิพนธ์หลัก.....

Acknowledgements

I would like to thank Dr. Varagorn Hengpunya, from whom I have got a chance to work in this field. I really appreciate all his suggestions and encouragement during this study. I would also like to thank all people in forum for theoretical science (FTS).

I would like to thank Assoc. Prof. Dr. Udomsilp Pinsook, Dr. Jessada Sukpitak and Asst. Prof. Dr. Tanakorn Osotchan who are on this thesis committee. I really appreciate their suggestions and comments.

A lot of thanks go to all my friends. I have had enjoyable time with them.

Last but not least, I would like to thank my parents who always support, understand and stand by me.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Contents

Abstract (Thai)	iv
Abstract (English).....	v
Acknowledgements	vi
Contents	vii
List of Figures.....	ix
CHAPTER	
I Introduction.....	1
II Theories of Phase-ordering and Nonequilibrium Critical Dynamics.....	5
2.1 Phase-ordering Dynamics	6
2.1.1 Dynamical Models	6
2.1.2 Correlation Functions and the Scaling Hypothesis	9
2.1.3 Growth Laws	11
2.2 Nonequilibrium Critical Dynamics	12
2.2.1 Dynamical Models and the Scaling Hypothesis	12
2.3 Some Remarks on Hamiltonians	14
2.3.1 Lattice Models	15
2.3.2 Continuum Models	15

III The Model and Dynamics	17
3.1 The Coarse-grained 2D XY Model	19
3.1.1 The Zeroth-order Theory	20
3.1.2 The First-order Approximation	20
3.2 Dynamics	21
3.3 Correlation Functions	23
IV The Zeroth-order Theory	25
4.1 Dynamics	26
4.2 Correlation Functions	27
4.3 Analytic Results	29
4.4 Discussion	30
V The First-order Correction	32
5.1 Dynamics	33
5.2 Correlation Functions	37
5.3 Analytic Results	37
5.4 Discussion	38
VI Conclusions	40
References	42
Appendices	47
Appendix A: Determination of $C^\theta(r, t, t')$	47
Appendix B: Evaluation of $C^\rho(r, t, t')$	51
Vitae	53

List of Figures

2.1 Schematic phase diagram of the Ising model. 7



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

CHAPTER I

Introduction

The physics phenomena which we shall be concerned involve not one or two but of order 10^{23} particles. It is not possible to observe the motion of each of 10^{23} particles. However, they exhibit scaling. The scaling phenomena provide us with something simple out of very complicated things, not depending on such details as types of particles, interactions, dynamics, etc. The scaling phenomena in phase transitions and, in particular, critical phenomena have been already known for a long while. The first notion of scaling theory of equilibrium phase transitions was formulated in the 1960s [9] and, later, it has been successfully applied to many different systems. Now, the scaling theory of equilibrium phase transitions are well understood. Nonetheless, the scaling theory of nonequilibrium phase transitions is not fully appreciated because the theory of nonequilibrium phase transitions is not completed. The study of nonequilibrium phase transitions will need many explanations. The scaling phenomenon in nonequilibrium phase transitions is the subject matter of this thesis. Before going into details, we will state the problems.

A system quenched from a high-temperature disordered phase into a low-temperature ordered phase does not order instantaneously. Instead, the length scale of ordered regions grows with time as the different broken-symmetry phases compete to select the equilibrium state. The dynamical evolution of the system is known as phase-ordering dynamics [2]. It is worth noticing that, from the computer simulations and the experimental results, most phase-ordering systems show a scaling phenomenon when they approach to an equilibrium state. Such ordering processes are observed in many systems such as spin systems, solids and

fluids. These stochastic and nonequilibrium processes have been very challenging problems in condensed matter physics [5].

Next, we address the other ordering process. Consider a system quenched from either a high-temperature disordered or low-temperature ordered state into the critical state (i.e. the state of the system at or near the critical point). Following the quench, the system tries to equilibrate itself from the initially nonequilibrium critical state to the equilibrium critical state. The study of this kind of dynamics known as nonequilibrium critical dynamics [40]. Same as phase-ordering systems, most nonequilibrium critical dynamics systems exhibit scaling.

How important is the study of the theories of phase-ordering and nonequilibrium critical dynamics? As mentioned above, we are, now, lacking of the general theory of nonequilibrium statistical mechanics. The study of these theories partially answer the problem.

There are various kinds of models in statistical mechanics. The case where the dimensionality $d = 2$ is very interesting and weird. In this case, the behaviour of a spin system depends crucially on the numbers of component n of the order-parameter [39]. There is a phase transition with spontaneous magnetisation for the case $n = 1$ (Ising model). While, in the case $n \geq 2$, there is no spontaneous magnetisation. However, the case $n = 2$ (XY model) is the special case. One can prove that there is a phase transition with no spontaneous magnetisation concerned. The two-dimensional (2D) XY model, in addition, is not only an interesting model on its own, but is also as a prototype of various models in condensed matter physics such as superfluids and superconductors [19]. The 2D XY model is the model which we used in our study.

In this work, we will investigate the scaling property of the 2D XY model in theory of phase-ordering dynamics. We consider first-order correction to correlations associated with the amplitude fluctuations for quench the system to the critical state. In order to solve this problem, we treat the amplitude fluctuations small compared to the phase fluctuations. Then, the dynamics of phase and am-

plitude fields become uncoupled. The dynamics of the phase variable is referred as the zeroth-order theory while for the amplitude variable is referred as the first-order correction. We find that the nonequilibrium part of the correlations both zeroth-order and first-order exhibit scaling. The scaling form of the amplitude-amplitude correlations is referred as the corrections to scaling in phase-ordering dynamics of the 2D XY model. The study of the form of corrections to scaling is very important since the form of corrections to scaling can be used to determine the correct asymptotic scaling exponents and scaling functions which characterise the systems [37]. A brief content of the thesis is as follows.

In Chapter 2, we give a brief review of theories of phase-ordering and non-equilibrium critical dynamics. We will introduce the dynamical quantities of a system such as the equal-time and two-time pair correlation functions and auto-correlation functions as well as its scaling forms. We end the chapter with some remarks on modelled Hamiltonians.

In Chapter 3, 4 and 5, we will examine the phase-ordering dynamics of the 2D XY model. In Chapter 3, we will introduce the 2D XY model used in our study. The spin-wave approximation which we referred as the zeroth-order theory, allows us to solve the problem exactly. The first-order approximation which is the key technical point in the thesis will be discussed. In this study, we assume that the dynamics of the system is of purely relaxational and nonconserved type, i.e. the dynamics is governed by the time-dependent Ginzburg-Landau (TDGL) model or model A. We also calculated the approximated correlation functions.

In Chapter 4 and 5, the scaling properties of the 2D XY model in the theory of phase-ordering dynamics will be studied. In Chapter 4, we solve the zeroth-order theory analytically. We give an explicit formulation for the two-time pair correlation function and show that, at late times, the equal-time pair correlation function is scaled with a single characteristic length $L(t) \sim t^{1/2}$. These results confirm the prediction by Rutenberg and Bray [20].

In Chapter 5, we will present a detailed calculation of the first-order cor-

rection. We find scaling solution for equal-time correlations characterised by a time-dependent length $L(t) \sim t^{1/2}$ associated with states with vortex pairs.

Finally, we end this thesis with Chapter 6. This chapter will give a brief summary and conclusion of all results obtained under the investigation pursued in this study.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

CHAPTER II

Theories of Phase-ordering and Nonequilibrium Critical Dynamics

The theory of phase-ordering dynamics has a story going back more than four decades to the pioneering work of Lifshitz [10], Lifshitz and Slyozov [11] and Wagner [12], including many excellent reviews by Gunton *et al* [13], Binder [14], Furukawa [15] and Langer [16]. The scaling approach to phase-ordering dynamics began about two decades ago and the study has been concentrated mostly on simple scalar order parameters, such as binary alloys and Ising models [2, 15, 21, 22]. The recent interest focuses on system with complicated order parameters, for example vector and tensor fields.

While, in the theory of nonequilibrium critical dynamics, a lot of progress has been made since the introduction of the idea of dynamical scaling hypothesis [40]. As one knows, scaling concepts are very important in the study of equilibrium critical phenomena. Janssen and colleagues has opened up the way for a scaling treatment in nonequilibrium critical dynamics [17]. Moreover, Zheng and colleagues have successfully applied the scaling hypothesis to determine all static critical exponents [40].

In this chapter, we review the theory of phase-ordering dynamics in Section 2.1 and theory of nonequilibrium critical dynamics in Section 2.2. Some remarks on the Hamiltonian are briefly discussed in Section 2.3.

2.1 Phase-ordering Dynamics

A system tries to equilibrate itself from the initially nonequilibrium state when it is quenched from the homogeneous phase into a broken-symmetry phase, called phase-ordering dynamics. The theory remains a challenge more than four decades after the first theoretical papers appeared. Here, we will give an example: the ferromagnetic Ising model in zero magnetic field. The ferromagnetic Ising model is one of the simplest and most fundamental models of statistical mechanics. Each such system can be described by classical spin variables \vec{S}_i with two possible values $S_i = \pm 1$. The two values stand for an elementary magnet pointing up or down. The schematic phase diagram of the Ising model is shown in Figure 2.1. The system is in a disordered (paramagnetic) phase and the spontaneous magnetisation is zero at high temperatures, while at low temperatures, below the critical temperature T_c , the system is in an ordered (ferromagnetic) phase. For $0 < T < T_c$, the system exhibits a net magnetisation, which can be either positive or negative. Suppose that the system is suddenly quenched from an initially disordered equilibrium phase at high temperature, T_i , into an ordered nonequilibrium phase at low temperature, T_f . Following the quench, the system tries to equilibrate itself from the initially nonequilibrium state. During the evolution, different two equilibrium phases compete to grow or coarsen with time.

2.1.1 Dynamical Models

First of all, we need to set up a model for describing the system that we want to study. In principle, the model may be a lattice or continuum model depending on the nature of the system. However, in practice, it is more convenient to work with the continuum model and, even though the true microscopic nature of the system is not continuous, this kind of model can always be set up as an effective model (see Section 2.3).

Let the system be described by a scalar order-parameter field $\phi(\mathbf{x}, t)$ as a

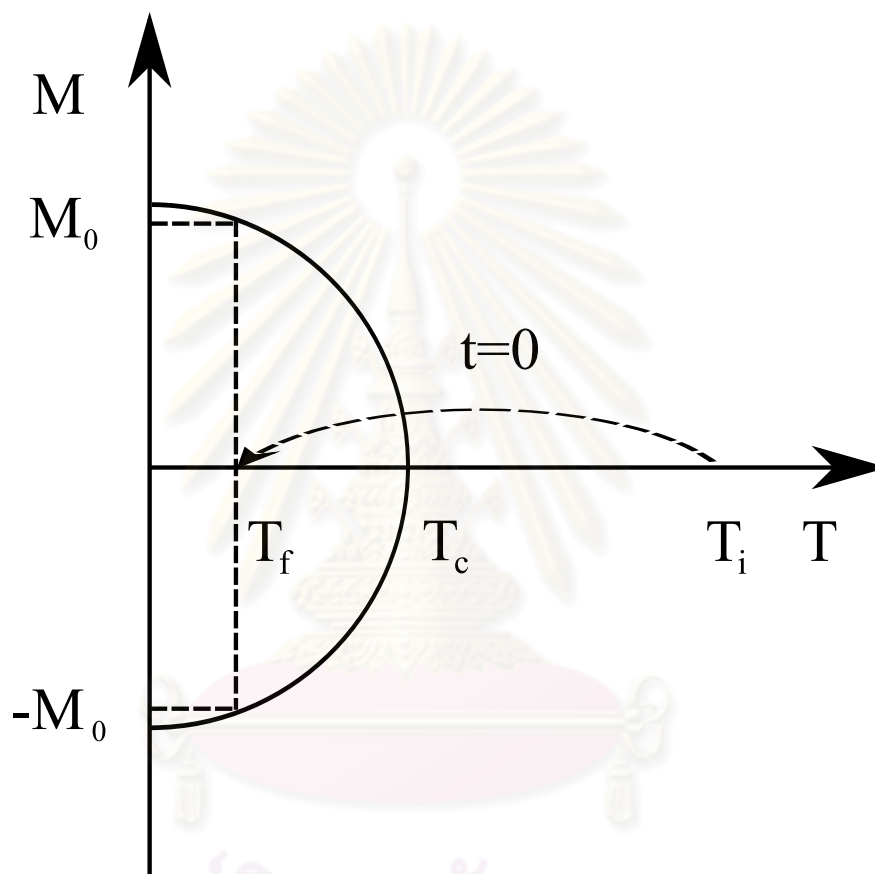


Figure 2.1: Schematic phase diagram of the Ising model.

ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

function of position $\mathbf{x} = (x_1, \dots, x_d)$ and time t . A suitable Hamiltonian functional describing the ordered phase is

$$H[\phi(\mathbf{x}, t)] = \int d^d x \left\{ \frac{1}{2} [\nabla \phi(\mathbf{x}, t)]^2 + V[\phi(\mathbf{x}, t)] \right\}, \quad (2.1)$$

where $V[\phi(\mathbf{x}, t)]$ is the potential function. The Hamiltonian functional is usually taken to be of Ginzburg-Landau form,

$$H[\phi(\mathbf{x}, t)] = \int d^d x \left\{ \frac{1}{2} [\nabla \phi(\mathbf{x}, t)]^2 + \frac{1}{2} r_o \phi^2(\mathbf{x}, t) + \frac{1}{4} u_o \phi^4(\mathbf{x}, t) \right\}, \quad (2.2)$$

all of coefficients r_o and u_o , in principle, depend on temperature. The Hamiltonian, Eq. (2.2), provides a good description associated with long-wavelength, slow spatial variations of $\phi(\mathbf{x}, t)$. In general, $V[\phi(\mathbf{x}, t)]$ need only have a double-well structure in the ordered phase such that the two minima correspond to the two equilibrium states, while the gradient-squared term in Eq. (2.1) associates an energy cost with an interface between the phases.

Now, to describe the dynamical process, an equation of motion for the order-parameter field is needed. The simplest stochastic dynamical model is one in which there is a single nonconserved field in contact with a constant temperature heat bath. This model is variously called the Glauber model and the time-dependent Ginzburg-Landau (TDGL) model. The only ‘‘slow’’ variable is $\phi(\mathbf{x}, t)$, whose equation of motion is

$$\begin{aligned} \frac{\partial \phi(\mathbf{x}, t)}{\partial t} &= -\Gamma \frac{\delta H[\phi(\mathbf{x}, t)]}{\delta \phi(\mathbf{x}, t)} + \xi(\mathbf{x}, t) \\ &= \Gamma \left\{ \nabla^2 \phi(\mathbf{x}, t) - V'[\phi(\mathbf{x}, t)] \right\} + \xi(\mathbf{x}, t), \end{aligned} \quad (2.3)$$

where Γ is a kinetic coefficient, $V'[\phi(\mathbf{x}, t)] \equiv dV[\phi(\mathbf{x}, t)]/d\phi(\mathbf{x}, t)$ and $\xi(\mathbf{x}, t)$ is the noise from thermal fluctuation. We assume that $\xi(\mathbf{x}, t)$ is a Gaussian white noise with zero average and satisfies the fluctuation-dissipation theorem

$$\langle \xi(\mathbf{x}, t) \xi(\mathbf{x}', t') \rangle_\xi = 2\Gamma k_B T \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'), \quad (2.4)$$

where $\langle \dots \rangle_\xi$ means the statistical average over the ensemble of noises. This equation is simply the generalisation to continuous fields of the Langevin equation

for a velocity. It provides a good description for dynamics of the Ising model as well as an order-disorder transition in binary alloys and the equation of motion of this type represents purely relaxational dynamics. The equation of motion seems to have been first employed by Landau and Khalatnikov in order to explain the anomalous attenuation of sound in helium near the λ -point [3].

A simple modification of the nonconserved dynamics gives us a conserved dynamics. This model, which is called the Cahn-Hilliard model, can be obtained by replacing Γ by $-\lambda\nabla^2$:

$$\begin{aligned}\frac{\partial\phi(\mathbf{x},t)}{\partial t} &= \lambda\nabla^2\frac{\delta H[\phi(\mathbf{x},t)]}{\delta\phi(\mathbf{x},t)} + \xi(\mathbf{x},t) \\ &= -\lambda\nabla^2\left\{\nabla^2\phi(\mathbf{x},t) - V'[\phi(\mathbf{x},t)]\right\} + \xi(\mathbf{x},t).\end{aligned}\quad (2.5)$$

Similarly, the thermal noise is a Gaussian distributed with zero mean and must satisfy

$$\langle\xi(\mathbf{x},t)\xi(\mathbf{x}',t')\rangle_\xi = -2\lambda k_B T \nabla^2\delta(\mathbf{x} - \mathbf{x}')\delta(t - t')\quad (2.6)$$

to ensure that the fluctuation-dissipation theorem is obeyed. As in nonconserved case, the conserved case is a purely relaxational dynamics. It describes, for example, the phase separation of the binary alloys. In the language of Halperin and Hohenberg classification scheme [3], these dynamical equations are called model A and B, respectively. As the system was quenched from a high-temperature disordered phase, we shall take the initial conditions to represent a completely disordered state, given by

$$\langle\phi(\mathbf{x},0)\phi(\mathbf{x}',0)\rangle_o = \Delta\delta(\mathbf{x} - \mathbf{x}'),\quad (2.7)$$

where $\langle\dots\rangle_o$ represents the statistical average over the ensemble of initial conditions and Δ controls the size of the initial fluctuations in ϕ .

2.1.2 Correlation Functions and the Scaling Hypothesis

Now, we will define dynamical quantities of the system, i.e. correlation functions. The first two correlation functions to be introduced are the equal-time pair

correlation function

$$C(r, t) \equiv \langle \phi(\mathbf{x}, t) \phi(\mathbf{x} + \mathbf{r}, t) \rangle, \quad (2.8)$$

and its Fourier transform, the equal-time structure factor,

$$S(k, t) \equiv \langle \phi_{\mathbf{k}}(t) \phi_{-\mathbf{k}}(t) \rangle, \quad (2.9)$$

where $\langle \dots \rangle$ indicates an average over the ensembles of thermal noises and initial conditions. The structure factor can be directly measured in experiments such as neutron scattering experiments [2].

From the computer simulation and the experimental results [2], we found that, at late times, phase-ordering systems will grow in a special manner such that the domain patterns look statistically the same, if rescaled. The dynamical scaling hypothesis states that, at late times, there would be only one characteristic length scale which is solely responsible for the evolution of the system. This means that if we rescale all the length scales of the system by the characteristic length scale we will essentially end up with the same system at any time. It should be emphasised that the dynamical scaling has not been proved directly but arises out of the computer simulation and the experimental results, except in some simple models such as the one-dimensional Glauber model [23] and the n -vector model with $n \rightarrow \infty$ [24]. The existence of a single characteristic length scale, according to the scaling hypothesis, implies that the pair correlation function has the scaling form

$$C(r, t) = f[r/L(t)], \quad (2.10)$$

where $L(t)$ is the single characteristic length scale. The function $f(x)$ is called the scaling function for the equal-time pair correlation function. The corresponding scaling form for the equal-time structure factor is given by

$$S(k, t) = L(t)^d g[kL(t)], \quad (2.11)$$

where d is the spatial dimensionality and $g(y)$ is the Fourier transform of $f(x)$. The scaling forms, Eq. (2.10) and Eq. (2.11), are well supported by simulation data and experiment [2].

The other correlation functions, the two-time pair correlation function, defined by

$$C(r, t, t') \equiv \langle \phi(\mathbf{x}, t) \phi(\mathbf{x} + \mathbf{r}, t') \rangle, \quad (2.12)$$

and, in particular, the autocorrelation function, defined by

$$A(t) \equiv \langle \phi(\mathbf{x}, t) \phi(\mathbf{x}, 0) \rangle, \quad (2.13)$$

are also of interest. If the dynamical scaling hypothesis holds, the two-time pair correlation function, $C(r, t, t')$, and the autocorrelation function, $A(t)$, can be written in the scaling form as

$$C(r, t, t') = h \left[\frac{r}{L(t)}, \frac{r}{L(t')} \right] \quad (2.14)$$

and

$$A(t) \sim L(t)^{-\lambda}, \quad (2.15)$$

where λ is a non-trivial scaling exponent and $h(x, y)$ is the scaling function for the two-time pair correlation function.

2.1.3 Growth Laws

We have seen that as time proceeds this domain structure coarsens and the average radius of the domain grows. It is found that, in the scaling regime, the dynamics are governed by a single characteristic length scale, the domain size $L(t)$, which increases with a power law in time. Most systems usually have a power growth law, characterised by a dynamical exponent, z , as

$$L(t) \sim t^{1/z}. \quad (2.16)$$

The exponent, $1/z$, is often called the growth exponent. The exponent z depends on the symmetry of the order-parameter field but not on the microscopic details of the system [2].

However, there still be no general method to find the exponent z for all systems but some models are well understood. For example, It is well established that $z = 2$ for nonconserved scalar and vector fields, $z = 3$ for conserved scalar fields and $z = 4$ for conserved vector fields [2].

2.2 Nonequilibrium Critical Dynamics

Critical phenomena are one of the old subjects of statistical mechanics. Many of the basic facts of critical phenomena were observed. However, the completed theory of equilibrium critical phenomena was formulated nearly 40 years ago. In contrast to the equilibrium theory, the theory of nonequilibrium critical dynamics is not yet fully completed because we are lack of the general theory of nonequilibrium statistical mechanics. Nonetheless, a lot of progress has been made since the introduction of the dynamical scaling hypothesis [40]. Janssen, Schaub and Schmittmann has opened up the way for a scaling treatment in nonequilibrium critical dynamics [17]. Many authors attempted to extend the dynamical scaling hypothesis to a variety of model systems [25, 26].

In this thesis, we will be looking at the nonequilibrium critical dynamics of the two-dimensional (2D) XY model. We may say that theory of phase-ordering dynamics of the 2D XY model is the subject matter of this thesis in the sense that the model tries to equilibrate itself when it is quenched from the homogeneous phase into a broken-symmetry phase (i.e. critical phase). In the following subsection, we will give an introduction to the scaling theory of nonequilibrium critical dynamics. We will introduce dynamical models and the dynamical scaling hypothesis. However, the definition of the 2D XY model and its approximation are not given here, but in Chapter 3.

2.2.1 Dynamical Models and the Scaling Hypothesis

As in the theory of phase-ordering dynamics, we first need to define a dynamical model for describing the system in order to be able to explain the phenomena being studied. Since, we have already done this in a rather general way in Section 2.1, we will not repeat it again here. However, in addition to quenches from the high-temperature disordered phase, quenches from the low-temperature ordered phase to the critical state can also be considered. In this case, the initial condition

is given by

$$\langle \phi(\mathbf{x}, 0)\phi(\mathbf{x}', 0) \rangle_o = C_{eq}(r, T_i), \quad (2.17)$$

where $r = |\mathbf{x} - \mathbf{x}'|$, T_i is the temperature of the system before the quench and $C_{eq}(r, T)$ is the equilibrium correlation function at temperature T .

According to the conventional theory of nonequilibrium critical dynamics [17], the system will relax to the new equilibrium critical state through a nonequilibrium scaling state characterised by a single characteristic length scale, $\xi(t)$, after it is quenched from the initial state. In this nonequilibrium scaling state, the equal-time pair correlation function and the structure factor have the form

$$C(r, t) = \frac{c}{r^{d-2+\eta}} f[r/\xi(t)], \quad (2.18)$$

and

$$S(k, t) = k^{-2+\eta} g[\xi(t)k], \quad (2.19)$$

where d is the dimension of the space, c is a constant and η is the usual equilibrium critical exponent. The first factor in Eq. (2.18) is just the equilibrium critical correlation function, $C_{eq}(r)$. It is thus necessary that the scaling function, $f(x)$ at $x = 0$ must be unity, i.e. as $t \rightarrow \infty$, the system should be in equilibrium. The single characteristic length scale, $\xi(t)$, can, in fact, be interpreted as the length scale up to which the equilibrium critical correlation has been established at time t . Hence, it may be called the “nonequilibrium correlation length”.

Janssen *et al* showed that the nonequilibrium correlation length increases in time with a power law

$$\xi(t) \sim t^{1/z}, \quad (2.20)$$

where z is the so-called dynamic exponent in (near) equilibrium critical dynamics. This results implies that both nonequilibrium and (near) equilibrium critical dynamics are governed by the same exponent. Furthermore, it was also showed that the relation $\xi(t) \sim t^{1/z}$ does not depend on the nonequilibrium initial states.

Next, the other dynamical quantity of interest is the two-time pair correlation function. For $t \gg t'$, the correlation is given by

$$C(r, t, t') = \left[\frac{\xi(t')}{\xi(t)} \right]^\lambda h \left[\frac{r}{\xi(t)} \right], \quad (2.21)$$

where the exponent λ is a new non-trivial critical exponent [18, 27]. The exponent λ can be obtained from the decay of the autocorrelation function, which satisfies the power law

$$A(t) \sim \xi^{-\lambda} \sim t^{-\lambda/z}. \quad (2.22)$$

Note that the similarities of the scaling forms for correlations in both theories do not, in any sense, imply that the physics of both dynamics are the same. In particular, the scaling exponents z and λ which have been used in both theories are totally different exponents and do not have any obvious relationship between them. If there exists any relationship, it has yet been proved.

2.3 Some Remarks on Hamiltonians

In the study of the phase transition in modern statistical mechanics, there has been considerable interest in model Hamiltonian such as the Ising model, the Potts model, the Heisenberg model, the XY model, the Baxter model, and even the non-linear sigma model [9]. Nevertheless, there have been only a handful of exactly solvable model. For example, the two-dimensional Ising model in zero magnetic field was solved by Lars Onsager in 1944 but it still has not been solved in an external magnetic field [9]. Much effort has been extended to solve it in three dimensions in zero field but it remain unsolved. However, these models have been of very importance in modern statistical mechanics [9].

All model Hamiltonians may be broadly divided into two categorises, i.e. lattice and continuum models. In this section, we will give a briefly discuss about these models.

2.3.1 Lattice Models

The Ising, Potts, Heisenberg and XY models are examples of microscopic or lattice models. These models are defined on a lattice which a variable is allowed to take a definite value at each site. For example, to define the Ising model a spin variable, \vec{S}_i , $i = 1, 2, 3, \dots, N$ which is allowed to take the value ± 1 , is placed on each lattice site. These kinds of models are usually aimed to be models at the microscopic level and the Hamiltonian is called the microscopic Hamiltonian. For an equilibrium state, physical informations are kept in the partition function. The canonical partition function is given by

$$Z = \sum_r e^{-\beta E_r}, \quad (2.23)$$

where the sum is over all the state r with energy E_r and $\beta = 1/k_B T$ with k_B Boltzmann's constant and T the temperature. In the study of statistical mechanics, we begin with the microscopic Hamiltonian and try to evaluate the partition function directly. However, it is often very difficult to work out in the critical states where correlation lengths diverge. To study critical phenomena, it is more useful to introduce semi-phenomenological field theories, where the order-parameter is treated as a continuous classical field. The continuum limit of the lattice model will be described below.

2.3.2 Continuum Models

In contrast to lattice models, continuum models are generally meant to be models at an intermediate level between the microscopic and macroscopic level called mesoscopic or coarse-grained models. Furthermore, these models may also be considered as the continuum limit of a lattice model providing what is called an effective field theory. Examples of continuum models are the Gaussian model and Ginzburg-Landau model.

In this thesis, our problem is treated as a coarse-grained model. So, we will introduce the idea of coarse graining and its partition function. The system is

divided up into blocks with dimensions large compared to any microscopic length such as the interparticle spacing. There are a large number of particles and approximately uniform in each block. The average of the order-parameter field, $\phi(\mathbf{x})$, over the particles in a block centered at \mathbf{x} is $\tilde{\phi}(\mathbf{x})$. This process of averaging over many particles in some volume of space is called *coarse graining* and $\tilde{\phi}(\mathbf{x})$ is often called the *coarse-grained order-parameter field* [19]. The partition function is a functional integration:

$$Z = \int D\tilde{\phi}(\mathbf{x}) e^{-[\tilde{H} - \int d^d x h(\mathbf{x})\tilde{\phi}(\mathbf{x})]/k_B T}. \quad (2.24)$$

\tilde{H} is called the coarse-grained Hamiltonian or the free energy and $h(\mathbf{x})$ is an external field.

Note that, in this work, we denote $\tilde{\phi}(\mathbf{x})$ by $\phi(\mathbf{x})$.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

CHAPTER III

The Model and Dynamics

The rotations in a two-dimensional plane is the simplest continuous symmetry ($U(1)$ or $O(2)$). In the language of group theory, the symmetry associated with these groups is often called XY-symmetry because rotations are usually done in the XY-plane. The order-parameter that breaks this symmetry can be either a two-dimensional vector or a complex number. The XY model is used for the systems such as superfluid helium, superconductors and hexatic liquid crystals with a complex or two-dimensional vector order-parameter [19]. According to the theorem of Mermin and Wagner, the two-dimensional (2D) XY model has no long-range order at any finite temperature [28]. However, the system has a phase transition, but it cannot be of the usual type with finite order-parameter below T_c . Kosterlitz and Thouless [6, 7] first predicted that the system undergoes a rather special kind of phase transitions, known as the Kosterlitz-Thouless transition. They predicted a phase transition from a short-range disordered phase to a quasi-long-range ordered phase, called the Kosterlitz-Thouless phase, where the order-parameter is everywhere zero. The transition temperature is called the Kosterlitz-Thouless transition temperature, T_{KT} . Above the transition temperature T_{KT} , the order-parameter pair correlation function decays exponentially as usual, with some correlation length ξ . Below the transition temperature, it decays like a power law of distance. In the conventional phase transition, critical state is characterised by a power-law decay of the order-parameter pair correlation function. Then, the Kosterlitz-Thouless phase is critical.

The Kosterlitz-Thouless transition may also be interpreted as a topological

phase transition because a simple heuristic argument due to the paper of Kosterlitz and Thouless [7] indicates how vortices can lead to a second-order phase transition in the XY model. Vortices are topological defects. Apart from the spin-wave excitations, there exists vortices which are closely bound in pairs, i.e. the vortex-antivortex pairs, below the Kosterlitz-Thouless transition temperature, T_{KT} . The size of defect pairs increases when the temperature is increased. They become free vortices at $T = T_{KT}$. We can see that the spin-wave excitations are responsible for destroying any long-range order in the system while the interaction energy of the vortices causes the phase transition. The simplest form of topological defect is the domain walls which occur in systems described by scalar fields. They are walls which separate domains of the two equilibrium phases. The local changes in the order-parameter can move the wall but cannot destroy it. The existence of such defects requires that $n \leq d$, where n is the number of components of the order-parameter and d is the dimension of the system. For $n = 2$ these defects are points (“vortices”) for $d = 2$ or lines (“strings” or “vortex lines”) for $d = 3$. For $n = 3$, $d = 3$, they are points (“hedgehogs” or “monopoles”) [2]. The roles played by vortices have already been studied intensively [2]. However, their roles in nonequilibrium systems are still not completely understood. In this and the rest of the thesis, we will investigate the roles of the vortices in nonequilibrium dynamics of the 2D XY model. Quenching from at or below the Kosterlitz-Thouless transition temperature, T_{KT} , to low-temperature phase will be studied here.

This chapter is organised as follows. In Section 3.1, we will introduce the coarse-grained two-dimensional XY model used in our study. We will propose some approximation scheme. First, the concept of the spin-wave approximation are presented. This analysis is referred as the zeroth-order theory. Next, we will introduce the first-order approximation to obtain the approximated Hamiltonian. In Section 3.2, the dynamics of the system is given. Finally, the approximated correlation functions are calculated within the first-order approximation.

3.1 The Coarse-grained 2D XY Model

The microscopic two-dimensional (2D) XY model consists of N two-component spins, denoted by \vec{S}_i lying on a two-dimensional square lattice of size $L \times L = N$. The magnitude of the spins are constant which usually is set to unity. The Hamiltonian of the microscopic 2D XY model is given by

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j, \quad (3.1)$$

where J is the exchange coupling constant and $\langle ij \rangle$ denotes a sum over nearest neighbour spins. Nonetheless, it is convenient to study the continuum limit of a lattice model in terms of a coarse-grained order-parameter field (as discussed in Sec. 2.3). The coarse-grained 2D XY model is a system of a two-component order-parameter field, $\vec{\phi}(\mathbf{x}, t)$, constrained to rotate in the XY-plane. The Hamiltonian of the 2D XY model is given by

$$H[\vec{\phi}] = \int d^2\mathbf{x} \left[\frac{1}{2} |\nabla \vec{\phi}|^2 + V(|\vec{\phi}|) \right], \quad (3.2)$$

where $V(|\vec{\phi}|)$ need only have a wine bottle structure in the ordered phase such that the global minima correspond to the infinite ground states. In this work, the potential $V(|\vec{\phi}|) = V_0(1 - |\vec{\phi}|^2)^2$ is used. In the ground states, the field has unit magnitude.

According to the Kosterlitz-Thouless theory [7, 8], the equilibrium correlation function, $C_{eq}(r) \equiv \langle \vec{\phi}(\mathbf{x}, t) \cdot \vec{\phi}(\mathbf{x} + \mathbf{r}, t) \rangle_{eq}$, of the Kosterlitz-Thouless phase has the asymptotic equilibrium correlations through

$$C_{eq}(r) \sim r^{-\eta}, \quad (3.3)$$

where η is the equilibrium critical exponent. The exponent η depends on temperature, with $\eta(T) = k_B T / 2\pi \rho_s(T)$. They are directly measured in experiments. The quantity ρ_s is the coarse-grained spin-wave stiffness of the system which we will describe in the following subsection.

3.1.1 The Zeroth-order Theory

Above zero temperature, the system deviates from the completely ordered or ground state, where all the spins align in the same direction. However, at very low temperature, only low-lying excited states dominate in equilibrium. Low-lying excited states of the system are states in which neighbouring spins almost aligns in the same direction. In this chapter, we use the limit $V_0 \rightarrow \infty$, i.e. neglecting the fluctuation of the amplitude of the field altogether. Then, the field has constant unit magnitude and the potential V becomes zero. The dynamics have only phase fluctuations. Then, the order-parameter field is written in terms of the phase variable as

$$\vec{\phi} = \cos \theta \mathbf{i} + \sin \theta \mathbf{j}, \quad (3.4)$$

where \mathbf{i} and \mathbf{j} are Cartesian unit vectors, and the Hamiltonian functional takes the form

$$H = \frac{\rho_s}{2} \int d^2\mathbf{x} (\nabla\theta)^2. \quad (3.5)$$

This approximation is the so-called spin-wave approximation and the resultant Hamiltonian is called the spin-wave Hamiltonian. The coefficient ρ_s is called the *spin-wave stiffness* or *helicity modulus* in magnetic systems, the *superfluid density* in superfluids, and is often referred to simply as a *rigidity*. In d dimensions, ρ_s has units of energy/(length) $^{d-2}$ or force/(length) $^{d-3}$.

3.1.2 The First-order Approximation

According to the zeroth-order theory, the phase of the field fluctuates only but, with the nature at the coarse-grained level, the field fluctuates both in its amplitude and phase. So, we may write the order-parameter field in terms of these two variables as

$$\vec{\phi} = \phi \cos \theta \mathbf{i} + \phi \sin \theta \mathbf{j}. \quad (3.6)$$

Inserting Eq. (3.6) in Eq. (3.2) one has

$$H = \int d^2\mathbf{x} \left\{ \frac{1}{2} [\phi^2 (\nabla\theta)^2 + (\nabla\phi)^2] + V(\phi) \right\}. \quad (3.7)$$

At this stage no approximations has been done. The key step in this work is the introduction of some approximation scheme. Investigation of the Hamiltonian Eq. (3.7) shows that the fields ϕ and θ are coupled through the term $\int d^2\mathbf{x} \frac{1}{2} \phi^2 (\nabla\theta)^2$. The first step is to introduce, in addition to the order-parameter fields $\phi(\mathbf{x}, t)$ and $\theta(\mathbf{x}, t)$, the fluctuating field $\rho(\mathbf{x}, t)$ defined by

$$\phi = 1 - \rho. \quad (3.8)$$

The field $\rho(\mathbf{x}, t)$ is to describe the fluctuations of amplitude about the ordered state, which goes to zero at late times. It is interesting to contrast that the field ρ is referred as the “fast” variable while the field θ is the “slow” variable of the system.

According to the physical picture described above, we treat the amplitude fluctuations small compared to the phase fluctuations. Then, we obtain the approximated Hamiltonian in terms of ρ , $\nabla\rho$ and $\nabla\theta$ as

$$H \approx \int d^2\mathbf{x} \frac{\rho_s}{2} (\nabla\theta)^2 + \int d^2\mathbf{x} \left[\frac{1}{2} (\nabla\rho)^2 + 4V_0\rho^2 \right]. \quad (3.9)$$

The first term is the energy due to phase fluctuations, called spin-wave Hamiltonian and the last term is the energy due to amplitude fluctuations. It is worth noticing that the approximated Hamiltonian, Eq. (3.9), reduces to the spin-wave Hamiltonian, Eq. (3.5), in the limit $V_0 \rightarrow \infty$.

3.2 Dynamics

In this work, we consider quenches in the nonconserved coarse-grained 2D XY model between any two temperatures at or below the Kosterlitz-Thouless transition temperature, T_{KT} ¹. Now, to describe the dynamical process, an equation of motion for the order parameter field is needed. Since, in this approximation, the system has two degree of freedom (i.e. the phase and amplitude variables) which

¹The Kosterlitz-Thouless temperature of the 2D XY model on a square lattice is estimated to be 0.90 [29, 30].

are independent each other. The dynamics of each of the fields is treated as the time-dependent Ginzburg-Landau (TDGL) model or model A in the presence of Gaussian noise. The equations of motion satisfied by the order-parameter fields $\theta(\mathbf{x}, t)$ and $\rho(\mathbf{x}, t)$ are

$$\frac{\partial\theta(\mathbf{x}, t)}{\partial t} = -\Gamma_\theta \frac{\delta H}{\delta\theta(\mathbf{x}, t)} + \xi(\mathbf{x}, t), \quad (3.10)$$

and

$$\frac{\partial\rho(\mathbf{x}, t)}{\partial t} = -\Gamma_\rho \frac{\delta H}{\delta\rho(\mathbf{x}, t)} + \zeta(\mathbf{x}, t). \quad (3.11)$$

The thermal noises $\xi(\mathbf{x}, t)$ and $\zeta(\mathbf{x}, t)$ can be assumed to be Gaussian white-noise with zero mean, with correlations satisfy the fluctuation-dissipation theorem

$$\langle \xi(\mathbf{x}, t)\xi(\mathbf{x}', t') \rangle_\xi = 2\Gamma_\theta k_B T \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'), \quad (3.12)$$

and

$$\langle \zeta(\mathbf{x}, t)\zeta(\mathbf{x}', t') \rangle_\zeta = 2\Gamma_\rho k_B T \delta(\mathbf{x} - \mathbf{x}') \delta(t - t'), \quad (3.13)$$

where $\langle \dots \rangle_\xi$ and $\langle \dots \rangle_\zeta$ denotes the statistical average over the noise ensembles. Γ_θ and Γ_ρ are the kinetic coefficient for phase and amplitude variables, respectively.

Using the approximated Hamiltonian, Eq. (3.9), one easily finds that

$$\frac{\partial\theta(\mathbf{x}, t)}{\partial t} = \Gamma_\theta \rho_s \nabla^2 \theta(\mathbf{x}, t) + \xi(\mathbf{x}, t). \quad (3.14)$$

and

$$\frac{\partial\rho(\mathbf{x}, t)}{\partial t} = \Gamma_\rho [\nabla^2 \rho(\mathbf{x}, t) - 8V_0 \rho(\mathbf{x}, t)] + \zeta(\mathbf{x}, t). \quad (3.15)$$

As mentioned above, the approximated Hamiltonian, Eq. (3.9) reduces to the spin-wave Hamiltonian, Eq. (3.5) in the zeroth-order theory (i.e. in the limit $V_0 \rightarrow \infty$). Then, the equations of motion reduce to the equation of motion of phase variable only, Eq. (3.14). While at first-order approximation, we extend to include the dynamics with amplitude fluctuation corresponding to the equation of motion Eq. (3.15).

The system was initially in equilibrium at the temperature T_i (at or below T_{KT}) and was then quenched to the temperature T_f below T_{KT} . The Hamiltonian

of the system is the approximated Hamiltonian, Eq. (3.9) and, then, the Fourier transform of the initial phase-phase and amplitude-amplitude correlation function are denoted by $\langle \theta_{\mathbf{k}}(0)\theta_{-\mathbf{k}}(0) \rangle_o$ and $\langle \rho_{\mathbf{k}}(0)\rho_{-\mathbf{k}}(0) \rangle_o$, respectively. $\langle \dots \rangle_o$ denotes the average over all initial configurations, i.e. with respect to the canonical distribution at T_i and $e^{-H/k_B T_i}$.

3.3 Correlation Functions

It is now time to discuss the dynamical quantities of interest. We start with the definition of the two-time pair correlation

$$\begin{aligned} C(r, t, t') &\equiv \langle \vec{\phi}(\mathbf{x}, t) \cdot \vec{\phi}(\mathbf{x} + \mathbf{r}, t') \rangle \\ &= \langle \phi(\mathbf{x}, t)\phi(\mathbf{x} + \mathbf{r}, t') \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle, \end{aligned} \quad (3.16)$$

where $\langle \dots \rangle$ represents the average over initial conditions and over the thermal noises. By using Eq. (3.8), the correlations are written in the form

$$C(r, t, t') = \langle [1 - \rho(\mathbf{x}, t) - \rho(\mathbf{x} + \mathbf{r}, t') + \rho(\mathbf{x}, t)\rho(\mathbf{x} + \mathbf{r}, t')] \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle. \quad (3.17)$$

At first-order the cross terms $\langle \rho(\mathbf{x}, t) \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle$ and $\langle \rho(\mathbf{x} + \mathbf{r}, t') \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle$ vanish and the correlation becomes

$$C(r, t, t') \approx C^\theta(r, t, t') + C^\rho(r, t, t')C^\theta(r, t, t'), \quad (3.18)$$

where $C^\theta(r, t, t') \equiv \langle \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle$ and $C^\rho(r, t, t') \equiv \langle \rho(\mathbf{x}, t)\rho(\mathbf{x} + \mathbf{r}, t') \rangle$.

Similarly, the autocorrelation function is given by

$$\begin{aligned} A(t) &\equiv \langle \vec{\phi}(\mathbf{x}, t) \cdot \vec{\phi}(\mathbf{x}, 0) \rangle \\ &= \langle \phi(\mathbf{x}, t)\phi(\mathbf{x}, 0) \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x}, 0)] \rangle. \end{aligned} \quad (3.19)$$

In the first-order approximation, the autocorrelation becomes

$$\begin{aligned} A(t) &= \langle [1 - \rho(\mathbf{x}, t) - \rho(\mathbf{x}, 0) + \rho(\mathbf{x}, t)\rho(\mathbf{x}, 0)] \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x}, 0)] \rangle \\ &\approx A^\theta(t) + A^\rho(t)A^\theta(t), \end{aligned} \quad (3.20)$$

where $A^\theta(t) \equiv \langle \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x}, 0)] \rangle$ and $A^\rho(t) \equiv \langle \rho(\mathbf{x}, t)\rho(\mathbf{x}, 0) \rangle$. Note that $A(t) \equiv C(0, t, 0)$. So, $A^\theta(t) = C^\theta(0, t, 0)$ and $A^\rho(t) = C^\rho(0, t, 0)$.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

CHAPTER IV

The Zeroth-order Theory

There are few exactly solvable models in theory of phase-ordering dynamics but these models are quite far from describing the physical systems of interest. However, the models are interesting because they showed the scaling property at late times [2]. Here, we will give a few examples of exactly solvable models. First is the n -component vector model in the limit that the number n goes to infinity. Many authors have studied in this limit, mostly for nonconserved fields [24, 27, 32-35]. A rather complete discussion for both conserved and nonconserved dynamics in the large- n limit is discussed in ref. [33]. A simple model that has been solved exactly is the one-dimensional Ising model with Glauber dynamics [23]. The last example is the one-dimensional XY model with nonconserved order-parameter which is first given by Newman *et al* [34]. Based upon the scaling hypothesis, theories of phase-ordering dynamics are mainly concerned with two things, i.e. the determination of growth laws and scaling functions. It is interesting that the nonconserved one-dimensional XY model exhibits the “anomalous” growth law, namely $L(t) \sim t^{1/4}$. In the conserved case, there are no exact solution for the model. However, computer simulations give $L(t) \sim t^{1/6}$ [31] instead of the standard growth law $L(t) \sim t^{1/4}$. In this chapter, we will examine phase-ordering dynamics of the coarse-grained 2D XY model below the Kosterlitz-Thouless transition temperature, T_{KT} . An exact solution is possible within the spin-wave theory. We work in the limit $V_0 \rightarrow \infty$, where $|\vec{\phi}|^2 = 1$. Then, the problem are treated as dynamics with phase fluctuations only. This analysis is referred as the zeroth-order theory. Here, the dynamics of the system will be assumed to be nonconserving and purely relaxing. The main purpose of this chapter is to confirm the prediction

by Rutenberg and Bray [20].

This chapter is organised as follows. In the next section, the dynamics of phase variable will be described. We will then perform the calculation for the case of a quench to an arbitrary temperature below T_{KT} . Next, we will calculate the zeroth-order correlation functions. Finally, we will end this chapter by giving a detailed discussion in the scaling regime and asymptotic behaviour.

4.1 Dynamics

The evolution of the phase variable is governed with the equation of evolution, Eq. (3.14),

$$\frac{\partial \theta(\mathbf{x}, t)}{\partial t} = \Gamma_\theta \rho_s \nabla^2 \theta(\mathbf{x}, t) + \xi(\mathbf{x}, t). \quad (4.1)$$

By making the Fourier transformation of Eq. (4.1), the equation of evolution for the Fourier transform of the phase variable, $\theta_{\mathbf{k}}$, can be written as

$$\dot{\theta}_{\mathbf{k}} = -\rho_s \Gamma_\theta k^2 \theta_{\mathbf{k}} + \xi_{\mathbf{k}}, \quad (4.2)$$

where $\theta_{\mathbf{k}}$ and $\xi_{\mathbf{k}}$ are the Fourier transforms of the phase variable and the thermal noise given by

$$\theta_{\mathbf{k}}(t) = \frac{1}{2\pi} \int d^2\mathbf{x} \theta(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}} \quad (4.3)$$

and

$$\xi_{\mathbf{k}}(t) = \frac{1}{2\pi} \int d^2\mathbf{x} \xi(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}}. \quad (4.4)$$

We only keep the component of the thermal noise locally orthogonal to the field $\vec{\phi}$, with

$$\langle \xi_{\mathbf{k}}(t) \xi_{\mathbf{k}'}(t') \rangle = 2\Gamma_\theta k_B T \delta_{\mathbf{k}, -\mathbf{k}'} \delta(t - t'). \quad (4.5)$$

We make $[t]$ dimensionally equivalent to $[l]^2$ while Γ_θ and ρ_s are adsorbed into the time scale for the rest of the chapter. Thus, the equation (4.2) becomes

$$\dot{\theta}_{\mathbf{k}} = -k^2 \theta_{\mathbf{k}} + \xi_{\mathbf{k}}. \quad (4.6)$$

The resultant equation is just the first-order linear ordinary differential equation, which can be solved exactly by the method of integrating factor, and the solution reads

$$\theta_{\mathbf{k}}(t) = \theta_{\mathbf{k}}(0)e^{-k^2 t} + \int_0^t d\tilde{t} e^{-k^2(t-\tilde{t})} \xi_{\mathbf{k}}(\tilde{t}), \quad (4.7)$$

where $t \geq 0$ is measured from the time of the quench. Before going further, we need the initial correlations of the system. Since the system is quenched from at or below T_{KT} , the initial correlations are given by the spin-wave Hamiltonian, Eq. (3.5). The Fourier transformed spin-wave Hamiltonian is given by

$$H = \frac{\rho_s}{2} \sum_{\mathbf{k}} k^2 \theta_{\mathbf{k}}(0) \theta_{-\mathbf{k}}(0). \quad (4.8)$$

Then, the probability distribution reads

$$P[\{\theta_{\mathbf{k}}(0)\}] \propto \exp \left\{ - \sum_{\mathbf{k}} \frac{k^2}{4\pi\eta_i} \theta_{\mathbf{k}}(0) \theta_{-\mathbf{k}}(0) \right\}, \quad (4.9)$$

where η_i and η_f are used to describe the initial and final quench states of our system, respectively. We, thus, can calculate the initial conditions directly, but we will use a short calculation that is to use the equipartition of energy.¹ Then,

$$\rho_s k^2 \langle |\theta_{\mathbf{k}}(0)|^2 \rangle_o = 2 \times \frac{k_B T_i}{2}, \quad (4.10)$$

where T_i is the initial temperature and the factor of 2 accounts for the fact that $\theta_{\mathbf{k}}$ has both real and imaginary parts (i.e. using the fact that $\theta_{\mathbf{k}} = \theta_{-\mathbf{k}}^*$). Hence

$$\langle \theta_{\mathbf{k}}(0) \theta_{-\mathbf{k}}(0) \rangle_o = \frac{2\pi\eta_i}{k^2}. \quad (4.11)$$

4.2 Correlation Functions

In this section, we briefly show the results of calculations for correlation functions. For the details of calculations see Appendix A. Since, the noise and the initial

¹The theorem of the equipartition of energy states that if a degree of freedom makes only a quadratic contribution to the Hamiltonian, then the average energy of the corresponding term in the Hamiltonian is $k_B T/2$ [9].

conditions are Gaussian distributed. The general two-point two-time correlation function is

$$\begin{aligned}
C^\theta(r, t, t') &\equiv \langle \cos[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')] \rangle, \\
&= \text{Re} \left\langle e^{i[\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')]} \right\rangle, \\
&= \exp[-B^\theta(r, t, t')/2],
\end{aligned} \tag{4.12}$$

where $B^\theta(r, t, t') \equiv \langle [\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')]^2 \rangle$ is the phase-difference correlation function. The last equality above is obtained using the Gaussian cumulant expansion. The phase-difference correlation, $B^\theta(r, t, t')$, can be written in terms of the average of the Fourier transforms of the phase variable as

$$\begin{aligned}
B^\theta(r, t, t') &= \int \frac{d^2\mathbf{k}}{(2\pi)^2} [\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t) \rangle + \langle \theta_{\mathbf{k}}(t')\theta_{-\mathbf{k}}(t') \rangle \\
&\quad - 2 \cos(\mathbf{k} \cdot \mathbf{r}) \langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t') \rangle].
\end{aligned} \tag{4.13}$$

The average of the Fourier transforms of the phase variable at general times after a quench at $t = 0$ from a temperature T_i to a temperature T_f , both at or below T_{KT} , can be calculated straight away by using Eq. (4.7),

$$\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t') \rangle = \frac{2\pi}{k^2} [\eta_f e^{-k^2|t-t'|} + (\eta_i - \eta_f) e^{-k^2(t+t')}], \tag{4.14}$$

where the initial phase-phase correlation function, Eq. (4.11), and the following fluctuation-dissipation theorem, Eq. (4.5) have been used. Notice that the first term of Eq. (4.14) is just the equilibrium phase-phase correlation function, which can be obtained from the equilibrium theory, while the last term is the nonequilibrium contribution, which goes to zero as $t \rightarrow \infty$. Substituting Eq. (4.14) into Eq. (4.13), we obtain the $B^\theta(r, t, t')$ in the form

$$B^\theta(r, t, t') = B_{eq}^\theta(r, t, t') + B_{neq}^\theta(r, t, t'), \tag{4.15}$$

where B_{eq}^θ and B_{neq}^θ are the equilibrium and nonequilibrium correlations at the final temperature, respectively. We, then, have

$$B_{eq}^\theta(r, t, t') = \eta_f \{ \gamma + \ln(r^2/4a_0^2) + E_1[r^2/4(a_0^2 + |t - t'|)] \}, \tag{4.16}$$

and

$$B_{neq}^\theta(r, t, t') = (\eta_i - \eta_f) \left\{ \gamma + \ln \left(\frac{r^2}{4\sqrt{(a_0^2 + 2t)(a_0^2 + 2t')}} \right) + E_1[r^2/4(a_0^2 + t + t')] \right\}, \quad (4.17)$$

where $E_1(x) \equiv \int_x^\infty dy e^{-y}/y$ for $x > 0$ and $\gamma \simeq 0.577$ is Euler's constant. A soft ultraviolet cutoff, through a factor of $\exp(-a_0^2 k^2)$ in the integrand of each \mathbf{k} integral, is used in our calculation, where a_0 is of the order of the lattice spacing. Finally, we obtain

$$C^\theta(r, t, t') = C_{eq}^\theta(r, |t - t'|) C_{neq}^\theta(r, t, t'), \quad (4.18)$$

where

$$\begin{aligned} C_{eq}^\theta(r, |t - t'|) &\equiv \exp[-B_{eq}^\theta(r, t, t')/2] \\ &= \exp \left\{ -\frac{\eta_f}{2} \left\{ \gamma + \ln(r^2/4a_0^2) + E_1[r^2/4(a_0^2 + |t - t'|)] \right\} \right\} \end{aligned} \quad (4.19)$$

and

$$\begin{aligned} C_{neq}^\theta(r, t, t') &\equiv \exp[-B_{neq}^\theta(r, t, t')/2] \\ &= \exp \left\{ -\frac{(\eta_i - \eta_f)}{2} \left\{ \gamma + \ln \left(\frac{r^2}{4\sqrt{(a_0^2 + 2t)(a_0^2 + 2t')}} \right) + E_1[r^2/4(a_0^2 + t + t')] \right\} \right\}. \end{aligned} \quad (4.20)$$

4.3 Analytic Results

The late time $t \gg a_0^2$, long-distance $r^2/t \gg 1$ and short-distance $r^2/t \ll 1$ behaviour of the theory are analysed in this section. The asymptotic correlations are evaluated by using the asymptotics of $E_1(x)$:

$$E_1(x) \sim \begin{cases} -\gamma - \ln x, & x \ll 1 \\ e^{-x}/x, & x \gg 1. \end{cases} \quad (4.21)$$

Consider first C_{eq}^θ at equal times $t = t'$. One obtains the asymptotic equilibrium correlations

$$C_{eq}^\theta(r, 0) \sim (r/a_0)^{-\eta_f}, \quad r \gg a_0 \quad (4.22)$$

which reproduces the standard result, Eq. (3.3). The full equal-time pair correlations have the asymptotic behaviour

$$C^\theta(r, t, t) \simeq \begin{cases} (r/a_0)^{-\eta_f} (r/\sqrt{t})^{-(\eta_i - \eta_f)}, & r^2/t \gg 1 \\ (r/a_0)^{-\eta_f}, & r^2/t \ll 1 \end{cases} \quad (4.23)$$

where $r, \sqrt{t} \gg a_0$. We see that both long and short distances have the same equilibrium correlations, but have an additional amplification factor at long distances. The nonequilibrium part are scaled with the single characteristic length $L(t) \sim t^{1/2}$. It is worth noticing the similarities of the single characteristic length scale, $L(t)$, and the nonequilibrium correlation length, ξ , in the 2D XY system. However, these similarities may not occur in the other systems.

Next, the autocorrelation function reads at late times,

$$\begin{aligned} A^\theta(t) &= C^\theta(0, t, 0) \\ &\sim \left(\frac{t}{a_0^2}\right)^{-(\eta_i + \eta_f)/4}, \end{aligned} \quad (4.24)$$

where again we take $t \gg a_0^2$. Using $L(t) \sim t^{1/2}$ and $A^\theta(t) \sim L^{-\lambda}$, Eq. (2.22) we determine the exponent $\lambda = (\eta_i + \eta_f)/2$. We set $\eta_i = \eta_f = \eta$ and find $\lambda_{eq} = \eta$ for the case of the decay of equilibrium correlations.

4.4 Discussion

In this chapter, we have considered phase-ordering dynamics of the coarse-grained 2D XY model below the Kosterlitz-Thouless transition temperature, T_{KT} . Within the spin-wave approximation, the dynamics are treated as phase fluctuations only. The phase dynamics has been taken to be the time-dependent Ginzburg-Landau (TDGL) model or model A in the presence of Gaussian noise. We are able to obtain the growth laws and we can solve explicitly the correlation functions.

From our results of the spin-wave theory, we may say that the prediction given by Rutenberg and Bray is positively supported with our calculations. We will give a brief discussion of the results. The equilibrium part of the correlation function of the 2D XY model decays asymptotically like a power law, Eq. (4.22), with the exponent η_f corresponding to the Kosterlitz-Thouless theory. This result confirms that the Kosterlitz-Thouless phase is critical state. We can see that the equal-time pair correlation function exhibits the scaling form in accordance with Eq. (2.18), with the characteristic length scale $L(t) \sim t^{1/2}$. The system quenched from at or below T_{KT} into below T_{KT} with nonconserved dynamics contain vortex-antivortex pairs and then their approaches to equilibrium which are governed by a power growth law for the single time-dependent length, $L(t) \sim t^{1/2}$ at late times. In contrast, the system quenched from above T_{KT} containing free vortices which give the growth law $L(t) \sim (t/\ln t)^{1/2}$ [36]. We also measure the decay of the autocorrelations which is characterised by an exponent λ through $A^\theta(t) \sim L^{-\lambda}$.

In conclusions, we have found that the equal-time pair correlation function $C^\theta(r, t, t)$ for the 2D XY model following quenches to low-temperature phase satisfy the scaling form,

$$C^\theta(r, t, t) \simeq r^{-\eta} f[r/L(t)], \quad (4.25)$$

where the single time-dependent length $L(t)$ is given by

$$L(t) \sim \begin{cases} t^{1/2}, & T_i \leq T_{KT} \\ (t/\ln t)^{1/2}, & T_i > T_{KT}, \end{cases} \quad (4.26)$$

where T_i denotes the temperature of the initial state.

CHAPTER V

The First-order Correction

As mentioned in Chapter 1, the dynamical evolution of a system in theory of phase-ordering dynamics is a very interesting problem. It is now well established that, at late times, most phase-ordering systems approach a scaling coarsening regime. This means that the equal-time pair correlation function of the order parameter, $C(r, t) = \langle \vec{\phi}(\mathbf{x}, t) \cdot \vec{\phi}(\mathbf{x} + \mathbf{r}, t) \rangle$ can be written in the scaling form as $C(r, t) = f[r/L(t)]$. On the other hand, corrections to scaling which tells us how the scaling coarsening regime is approached, is very important in interpreting experimental results or simulation data correctly. The form of corrections to scaling determines the correct asymptotic scaling exponents and scaling functions [37]. However, there has not been much studied in determining the form of corrections to scaling.

Corrections to scaling in theory of phase-ordering dynamics are arised out of many sources. In phase-ordering systems with topological defects there is, in addition to the characteristic length scale $L(t)$, a second characteristic length scale, the “defect core size” ξ . The corrections to scaling associated with nonzero defect core size are expected to enter as a power of ξ/L . Thermal fluctuations give also corrections to scaling when systems are quenched to a final temperature T_f , where $0 < T_f < T_c$, with T_c the critical temperature [38].

Rapapa and Bray [38] have considered corrections to scaling, associated with deviations of the order-parameter from the scaling morphology in the initial state, for system with $O(n)$ symmetry in phase-ordering dynamics. They supposed that the leading corrections to scaling enter the correlation function in the form

$C(r, t) = f_0(r/L) + L^{-\omega} f_1(r/L)$, where $f_0(x)$ is the “scaling function”, $f_1(x)$ is the “correction-to-scaling function” and ω is the “correction-to-scaling exponent”. While the structure factor is $S(k, t) = L^d g_0(y) + L^{d-\omega} g_1(y)$, where $g_0(y)$ and $g_1(y)$ are the d -dimensional Fourier transforms of $f_0(x)$ and $f_1(x)$ respectively, and $y = kL$. In their work, corrections to scaling are calculated for the nonconserved one-dimensional XY model in the limit $V_0 \rightarrow \infty$ (i.e. $|\vec{\phi}|^2 = 1$), where an exact solution is possible. They found that the correction-to-scaling exponent is $\omega = 2$. While, “memory” of the initial conditions are retained in the correlation function $C(r, t, t)$ even in the long time limit.

In this chapter, we determine corrections to scaling associated with amplitude fluctuations in the nonconserved coarse-grained two-dimensional XY model below the Kosterlitz-Thouless transition temperature T_{KT} . For the time-dependent Ginzburg-Landau (TDGL) model or model A, we quench the system between any two temperatures at or below T_{KT} . In the work here the analysis is extended from the zeroth-order theory to include the first-order correction. We evaluate the first-order correction due to the amplitude-amplitude correlations. We find scaling solution for nonequilibrium equal-time correlations characterised by a single characteristic length $L(t) \sim t^{1/2}$ associated with states with vortex-antivortex pairs. We also measure the first-order correction to autocorrelation and show its asymptotic behaviour.

In the next section, we will describe the dynamical model for the amplitude fluctuations. Next, we will try to evaluate the amplitude-amplitude correlations analytically. In the next section, the analysis results are presented and analysed. Finally, in the last section, the discussion and conclusion are given.

5.1 Dynamics

In this section we work out the first-order correction in details. The results of this section show that the general two-point two-time correlation function $C(r, t, t')$

contains physical properties that we wish to describe. In order to proceed one needs to know the solution of equation of motion, Eq. (3.15),

$$\frac{\partial \rho(\mathbf{x}, t)}{\partial t} = \Gamma_\rho [\nabla^2 \rho(\mathbf{x}, t) - 8V_0 \rho(\mathbf{x}, t)] + \zeta(\mathbf{x}, t). \quad (5.1)$$

In Fourier space, the equation of motion for the amplitude fluctuations becomes

$$\dot{\rho}_{\mathbf{k}} = -\Gamma_\rho (k^2 + 8V_0) \rho_{\mathbf{k}} + \zeta_{\mathbf{k}}, \quad (5.2)$$

where $\rho_{\mathbf{k}}$ and $\zeta_{\mathbf{k}}$ are the Fourier transforms of the amplitude variable and the noise given by

$$\rho_{\mathbf{k}}(t) = \frac{1}{2\pi} \int d^2\mathbf{x} \rho(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}} \quad (5.3)$$

and

$$\zeta_{\mathbf{k}}(t) = \frac{1}{2\pi} \int d^2\mathbf{x} \zeta(\mathbf{x}, t) e^{-i\mathbf{k}\cdot\mathbf{x}}. \quad (5.4)$$

The component of the noise is kept locally orthogonal to the field $\vec{\phi}$, with

$$\langle \zeta_{\mathbf{k}}(t) \zeta_{\mathbf{k}'}(t') \rangle = 2\Gamma_\rho k_B T \delta_{\mathbf{k}, -\mathbf{k}'} \delta(t - t'). \quad (5.5)$$

Similar to the zeroth-order theory, we will absorb Γ_ρ into the time scale, making $[t]$ dimensionally equivalent to $[l]^2$ for the rest of the chapter. The equation of motion, then, becomes

$$\dot{\rho}_{\mathbf{k}} = -(k^2 + 8V_0) \rho_{\mathbf{k}} + \zeta_{\mathbf{k}}. \quad (5.6)$$

By using the method of integrating factor, we obtain the solution for the equation of motion, Eq. (5.6),

$$\rho_{\mathbf{k}}(t) = \rho_{\mathbf{k}}(0) e^{-(k^2 + 8V_0)t} + \int_0^t d\tilde{t} e^{-(k^2 + 8V_0)(t-\tilde{t})} \zeta_{\mathbf{k}}(\tilde{t}), \quad (5.7)$$

where $t \geq 0$ is measured from the time of the quench. Since the system is quenched from at or below T_{KT} , The initial correlations are given by the approximated Hamiltonian Eq. (3.9). First, we make the Fourier transformation of the approximated Hamiltonian. The Hamiltonian for the Fourier transform of the phase, $\theta_{\mathbf{k}}$,

and amplitude, $\rho_{\mathbf{k}}$, variables can be written as

$$\begin{aligned}
H &\approx \int d^2\mathbf{x} \frac{\rho_s}{2} (\nabla\theta)^2 + \int d^2\mathbf{x} \left[\frac{1}{2} (\nabla\rho)^2 + 4V_0\rho^2 \right] \\
&= -\frac{\rho_s}{2} \sum_k \sum_{k'} \theta_{\mathbf{k}}(0)\theta_{\mathbf{k}'}(0)[k_1k'_1 + k_2k'_2] \underbrace{\frac{1}{(2\pi)^2} \int d^2\mathbf{x} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}}_{\delta_{(\mathbf{k}+\mathbf{k}',\mathbf{0})}} \\
&\quad -\frac{1}{2} \sum_k \sum_{k'} \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0)[k_1k'_1 + k_2k'_2] \underbrace{\frac{1}{(2\pi)^2} \int d^2\mathbf{x} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}}_{\delta_{(\mathbf{k}+\mathbf{k}',\mathbf{0})}} \\
&\quad +4V_0 \sum_k \sum_{k'} \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) \underbrace{\frac{1}{(2\pi)^2} \int d^2\mathbf{x} e^{i(\mathbf{k}+\mathbf{k}')\cdot\mathbf{x}}}_{\delta_{(\mathbf{k}+\mathbf{k}',\mathbf{0})}}. \tag{5.8}
\end{aligned}$$

If $\mathbf{k} = -\mathbf{k}'$, we obtain

$$H = \frac{\rho_s}{2} \sum_k k^2 \theta_{\mathbf{k}}(0)\theta_{-\mathbf{k}}(0) + \sum_k \left(\frac{k^2}{2} + 4V_0 \right) \rho_{\mathbf{k}}(0)\rho_{-\mathbf{k}}(0). \tag{5.9}$$

Notice that, in the limit $V_0 \rightarrow \infty$, the Hamiltonian, Eq. (5.9), reduces to the spin-wave Hamiltonian, Eq. (4.8), and the analysis becomes the zeroth-order theory.

Since the variables $\theta_{\mathbf{k}}$ and $\rho_{\mathbf{k}}$ are “statistically independent”, the probability distribution $P[\{\theta_{\mathbf{k}}(0)\}, \{\rho_{\mathbf{k}}(0)\}]$ can then be expressed in terms of the probability distribution $P[\{\theta_{\mathbf{k}}(0)\}]$ and the probability distribution $P[\{\rho_{\mathbf{k}}(0)\}]$:

$$\begin{aligned}
P[\{\theta_{\mathbf{k}}(0)\}, \{\rho_{\mathbf{k}}(0)\}] &= P[\{\theta_{\mathbf{k}}(0)\}]P[\{\rho_{\mathbf{k}}(0)\}] \\
&\propto \exp \left\{ -\sum_k \frac{k^2}{4\pi\eta_i} \theta_{\mathbf{k}}(0)\theta_{-\mathbf{k}}(0) \right\} \\
&\quad \times \exp \left\{ -\sum_k \left(\frac{k^2}{2} + 4V_0 \right) \rho_{\mathbf{k}}(0)\rho_{-\mathbf{k}}(0)/k_B T_i \right\} \tag{5.10}
\end{aligned}$$

Next, we can, now, calculate the initial correlation directly.

$$\langle \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) \rangle_o = \frac{\int_{-\infty}^{\infty} d\rho_{\mathbf{k}_1} d\rho_{\mathbf{k}_2} \dots d\rho_{\mathbf{k}} \dots d\rho_{\mathbf{k}'} \dots e^{-\beta H} \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0)}{\int_{-\infty}^{\infty} d\rho_{\mathbf{k}_1} d\rho_{\mathbf{k}_2} \dots d\rho_{\mathbf{k}} \dots d\rho_{\mathbf{k}'} \dots e^{-\beta H}}, \tag{5.11}$$

where H is given by Eq. (5.9). All the integrals cancel out between the numerator and denominator, except $\rho_{\mathbf{k}}$ and $\rho_{\mathbf{k}'}$. By collecting both real and imaginary parts (i.e. using the fact that $\rho_{\mathbf{k}} = \rho_{-\mathbf{k}}^*$), the correlation, Eq. (5.11), becomes

$$\langle \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) \rangle_o = \frac{\int_{-\infty}^{\infty} d\rho_{\mathbf{k}} d\rho_{\mathbf{k}'} \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) e^{-2(\frac{k^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}}|^2}{k_B T_i}} e^{-2(\frac{k'^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}'}|^2}{k_B T_i}}}{\int_{-\infty}^{\infty} d\rho_{\mathbf{k}} d\rho_{\mathbf{k}'} e^{-2(\frac{k^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}}|^2}{k_B T_i}} e^{-2(\frac{k'^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}'}|^2}{k_B T_i}}}. \tag{5.12}$$

We must now consider in two cases:

(i) $\mathbf{k} \neq \pm\mathbf{k}'$. This means that $\rho_{\mathbf{k}}$ and $\rho_{\mathbf{k}'}$ are distinct. The integrals in Eq. (5.12) factorise, and each of the integrals has the form

$$\int_{-\infty}^{\infty} d\rho_{\mathbf{k}} \rho_{\mathbf{k}}(0) e^{-2(\frac{k^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}}|^2}{k_B T_i}} = 0. \quad (5.13)$$

This yields

$$\langle \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) \rangle_o = 0 \quad |\mathbf{k}| \neq |\mathbf{k}'|. \quad (5.14)$$

(ii) $\mathbf{k} = \pm\mathbf{k}'$. If $\mathbf{k} = \mathbf{k}'$ then we must calculate $\langle \rho_{\mathbf{k}}^2(0) \rangle_o$. We, now, use plane polar coordinates $\rho_{\mathbf{k}} = (|\rho_{\mathbf{k}}|, \theta_{\mathbf{k}})$, for convenience, so

$$d\rho_{\mathbf{k}} = |\rho_{\mathbf{k}}| d|\rho_{\mathbf{k}}| d\theta_{\mathbf{k}}. \quad (5.15)$$

Thus

$$\langle \rho_{\mathbf{k}}^2 \rangle_o \propto \int_0^{2\pi} d\theta_{\mathbf{k}} e^{2i\theta_{\mathbf{k}}} = 0. \quad (5.16)$$

Then, the case $\mathbf{k} = -\mathbf{k}'$ is only non-zero. Since, if $\mathbf{k} = -\mathbf{k}'$, we must calculate $\langle |\rho_{\mathbf{k}}(0)|^2 \rangle_o$. The initial correlation in the Kronecker delta symbol reads

$$\langle \rho_{\mathbf{k}}(0)\rho_{\mathbf{k}'}(0) \rangle_o = \delta_{\mathbf{k}+\mathbf{k}',\mathbf{0}} \langle |\rho_{\mathbf{k}}(0)|^2 \rangle_o. \quad (5.17)$$

After the angular integral over $\theta_{\mathbf{k}}$ in the numerator and denominator are cancelled, we obtain

$$\langle |\rho_{\mathbf{k}}(0)|^2 \rangle_o = \frac{\int_0^{\infty} |\rho_{\mathbf{k}}| d|\rho_{\mathbf{k}}| e^{-2(\frac{k^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}}|^2}{k_B T_i}} |\rho_{\mathbf{k}}|^2}{\int_0^{\infty} |\rho_{\mathbf{k}}| d|\rho_{\mathbf{k}}| e^{-2(\frac{k^2}{2}+4V_0)\frac{|\rho_{\mathbf{k}}|^2}{k_B T_i}}}. \quad (5.18)$$

By defining the dummy variable $z \equiv |\rho_{\mathbf{k}}|$, and using the differential form $zdz = d(z^2/2)$, finally, we obtain

$$\langle \rho_{\mathbf{k}}(0)\rho_{-\mathbf{k}}(0) \rangle_o = \frac{k_B T_i}{k^2 + 8V_0}. \quad (5.19)$$

The amplitude-amplitude correlations at general times after a quench are then calculated straightforwardly from Eq. (5.7)

$$\langle \rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}(t') \rangle = \frac{k_B}{k^2 + 8V_0} [T_f e^{-(k^2+8V_0)|t-t'|} + (T_i - T_f) e^{-(k^2+8V_0)(t+t')}]. \quad (5.20)$$

5.2 Correlation Functions

Corrections due to amplitude fluctuations follow directly from the amplitude correlations. We, now, briefly show the results of calculations (for more details see Appendix B). The amplitude-amplitude correlation is

$$\begin{aligned}
 C^\rho(r, t, t') &\equiv \langle \rho(\mathbf{x}, t) \rho(\mathbf{x} + \mathbf{r}, t') \rangle \\
 &= \int \frac{d^2\mathbf{k}}{(2\pi)^2} \langle \rho_{\mathbf{k}}(t) \rho_{-\mathbf{k}}(t') \rangle e^{i\mathbf{k}\cdot\mathbf{r}} \\
 &= C_{eq}^\rho(r, t, t') + C_{neq}^\rho(r, t, t'), \tag{5.21}
 \end{aligned}$$

where C_{eq}^ρ and C_{neq}^ρ are the equilibrium and nonequilibrium correlations at the final temperature, respectively. In our calculation we use a soft ultraviolet cutoff, through a factor of $\exp(-a_0^2 k^2)$ in the integrand of each \mathbf{k} integral, where a_0 is of the order of the lattice spacing.

To proceed further one must carry out the correlations C_{eq}^ρ and C_{neq}^ρ . Unfortunately, we can not calculate these correlations exactly. However, at late times, the theory simplifies considerably to obtain

$$C_{eq}^\rho(r, t, t') = \frac{k_B T_f}{32\pi V_0} \frac{e^{-8V_0|t-t'| - r^2/4(a_0^2 + |t-t'|)}}{a_0^2 + |t-t'|}, \tag{5.22}$$

and

$$C_{neq}^\rho(r, t, t') = \frac{k_B(T_i - T_f)}{32\pi V_0} \frac{e^{-8V_0(t+t') - r^2/4(a_0^2 + t+t')}}{a_0^2 + t + t'}. \tag{5.23}$$

5.3 Analytic Results

Similar to the zeroth-order theory, we determine the late time $t \gg a_0^2$, long-distance $r^2/t \gg 1$ and short-distance $r^2/t \ll 1$ behaviour of the first-order correction in this section. First, we consider C_{eq}^ρ at equal times $t = t'$. We obtain the asymptotic equilibrium correlations

$$\begin{aligned}
 C_{eq}^\rho(r, t, t) &= \frac{k_B T_f}{32\pi V_0} \frac{e^{-r^2/4a_0^2}}{a_0^2} \\
 &\approx 0, \quad r \gg a_0. \tag{5.24}
 \end{aligned}$$

This means that, at late times, the amplitude-amplitude correlation is uncorrelated as expected. While, the full equal-time correlations after the quench have the asymptotic behaviour

$$C^\rho(r, t, t) \simeq \begin{cases} 0, & r^2/t \gg 1 \\ \frac{k_B(T_i - T_f)}{32\pi V_0} \frac{e^{-16V_0 t - (r/\sqrt{t})^2/8}}{2t}, & r^2/t \ll 1 \end{cases} \quad (5.25)$$

where $r, \sqrt{t} \gg a_0$. We see that $C^\rho(r, t, t)$ has a scaling form, with a length scale of $L \sim t^{1/2}$ characterising the nonequilibrium factor C_{neq}^ρ through Eq. (5.25) at short distances.

Next, we find the asymptotic behaviour of the autocorrelation function at late times

$$\begin{aligned} A^\rho(t) &= C^\rho(0, t, 0) \\ &= \frac{k_B T_i}{32\pi V_0} \frac{e^{-8V_0 t}}{a_0^2 + t} \\ &\sim \frac{k_B T_i}{32\pi V_0} \frac{e^{-8V_0 t}}{t}, \end{aligned} \quad (5.26)$$

where again we take $t \gg a_0^2$. We see that the asymptotic autocorrelation depends only on the initial conditions (through T_i) and decays asymptotically like an exponential.

5.4 Discussion

In this chapter, we extend the analysis from the zeroth-order theory, which treats only the phase fluctuations, to include the amplitude fluctuations, which is referred as the first-order correction. We start this chapter with the dynamical evolution for the amplitude variable and, then, try to work out the amplitude-amplitude correlation function directly but it does not succeed. However, we simplify the theory by considering at long time limit to obtain the two-time correlation function. For the case $t = t'$, we found that the nonequilibrium part of the correlation is scaled with a single characteristic length $L \sim t^{1/2}$ associated with states with

the vortex-antivortex-pair at late times. The scaling form of the nonequilibrium part of the amplitude-amplitude correlations is referred as the corrections to scaling in phase-ordering dynamics of the 2D XY model.

In conclusions, the full equal-time pair correlation function has the modified scaling form of Eq. (2.18), at late times

$$C(r, t, t) \simeq r^{-\eta} \left\{ f_0 \left[\frac{r}{L(t)} \right] + \alpha(t) f_1 \left[\frac{r}{L(t)} \right] \right\}, \quad (5.27)$$

with

$$f_0(x) \simeq \begin{cases} x^{-(\eta_i - \eta_f)}, & x^2 \gg 1 \\ 1, & x^2 \ll 1, \end{cases} \quad (5.28)$$

and

$$f_1(x) \simeq \begin{cases} 0, & x^2 \gg 1 \\ e^{-x^2/8}, & x^2 \ll 1, \end{cases} \quad (5.29)$$

with $L(t) \sim t^{1/2}$ and we take $r, \sqrt{t} \gg a_0$. The coefficient $\alpha(t)$ is of the form

$$\alpha(t) = \frac{k_B(T_i - T_f) e^{-16V_0 t}}{32\pi V_0 2t}. \quad (5.30)$$

We found that our results are similar to the form $C(r, t, t) = f_0(r/L) + L^{-\omega} f_1(r/L)$ which is proposed by Rapapa and Bray [38]. However, it is worth to emphasis that the source of corrections to scaling of our work and of Rapapa and Bray are different.

The full autocorrelation function reads, at late times,

$$A(t) \sim \left(\frac{t}{a_0^2} \right)^{-(\eta_i + \eta_f)/4} \left[1 + \frac{k_B T_i}{32\pi V_0} \frac{e^{-8V_0 t}}{t} \right], \quad (5.31)$$

where we take $t \gg a_0^2$.

CHAPTER VI

Conclusions

In this thesis, we have examined the scaling phenomena and its correction in nonequilibrium statistical mechanics. The problems of interest are the phase-ordering dynamics and nonequilibrium critical dynamics. We will summarise and conclude the study as follows.

The first chapter is an introduction of the thesis. We give a brief historical development of the scaling theory both equilibrium and nonequilibrium phenomena. Basic statements of theories of phase-ordering and nonequilibrium critical dynamics are mentioned. The 2D XY model which is the model of our study are introduced. We give the approximation scheme to obtain the corrections to scaling function. The chapter ends with the outline of this thesis.

In Chapter 2, theories of phase-ordering and nonequilibrium critical dynamics are explained in details. We introduce the dynamical models used in our study. The existence of the dynamical scaling hypothesis and the scaling forms of quantities of interest such as correlation functions, structure factors and autocorrelation functions are explained. The growth law which is the law that governs the evolution of the system in the scaling coarsening regime is stated. We also give some remarks on modelled Hamiltonians.

Chapter 3 and the rest, phase-ordering dynamics of the coarse-grained 2D XY model below the Kosterlitz-Thouless transition temperature, T_{KT} have been studied. In Chapter 3, first, the definition of the coarse-grained 2D XY model is introduced. We employed the spin-wave approximation to investigate the problem in the low-temperature limit, i.e. quenches from at or below T_{KT} to below T_{KT} .

In this limit, the field fluctuates only its phase. The analysis is referred as the zeroth-order theory of the thesis. However, the field, indeed, fluctuates both in its amplitude and phase at the coarse-grained level. In order to solve this problem, we treat the amplitude fluctuations small compared to the phase fluctuations. Then, the dynamics of phase and amplitude fields become decoupled. The dynamics of the amplitude variable is referred as the first-order correction. Next, the dynamics and the initial conditions of the two variables are stated. The dynamical model of the system is a purely relaxational and nonconserved. Finally, the approximated correlations are explained.

In Chapter 4, we have considered the zeroth-theory which gave exact solutions. We start with the equation of motion for the phase variable. By solving the problem analytically, we are able to obtain exact solutions. The results are as follows. We found that the system approaches the scaling coarsening regime at late times, i.e. it exhibits scaling form. The growth laws are given by $L(t) \sim t^{1/2}$, in comparison to the growth laws for quenching from above T_{KT} , $L(t) \sim (t/\ln t)^{1/2}$. This result agrees with the prediction by Rutenberg and Bray [20].

In Chapter 5, we have examined the first-order correction of the problem. Similar to the zeroth-order theory, we first tried to solve the equation of motion for the amplitude variable analytically. We tried to perform exactly analytical calculation for correlations but, however, without any success. Nonetheless, at long time limit, the theory simplifies considerably to obtain the two-time amplitude-amplitude correlations. The results at late times are as follows. We found that the nonequilibrium part of the equal-time amplitude-amplitude correlations exhibits scaling with a single characteristic length $L(t) \sim t^{1/2}$. This means that the system approaches the scaling coarsening regime both in its amplitude and phase with the same growth law. We refer to the scaling form of the nonequilibrium part of the amplitude-amplitude correlations as the corrections to scaling in phase-ordering dynamics of the 2D XY model.

References

- [1] Stanley, H. E. *Introduction to phase transitions and critical phenomena*. Oxford: Clarendon Press, 1971.
- [2] Bray, A. J. Theory of phase-ordering kinetics. *Adv. Phys.* 43 (1994): 357–459.
- [3] Hohenberg, P. C., and Halperin, B. I. Theory of dynamic critical phenomena. *Rev. Mod. Phys.* 49 (1977): 435–478.
- [4] Huang, K. *Statistical mechanics*. New York: John Wiley & Sons, 1987.
- [5] Onuki, A. *Phase transition dynamics*. Cambridge: Cambridge University Press, 2002.
- [6] Kosterlitz, J. M., and Thouless, D. J. Long range order and metastability in two dimensional solids and superfluids. *J. Phys. C: Solid State Phys.* 5 (1972): L124–L126.
- [7] Kosterlitz, J. M., and Thouless, D. J. Ordering, metastability and phase transitions in two-dimensional systems. *J. Phys. C: Solid State Phys.* 6 (1973): 1181–1203.
- [8] Kosterlitz, J. M. The critical properties of the two-dimensional XY model. *J. Phys. C: Solid State Phys.* 7 (1974): 1046–1060.
- [9] Goldenfeld, N. *Lectures on phase transitions and the renormalization group*. New York: Perseus Books, 1992.
- [10] Lifshitz, I. M. Kinetics of ordering during second-order phase transitions. *Sov. Phys. JETP* 15 (1962): 939–942.
- [11] Lifshitz, I. M., and Slyozov, V. V. The kinetics of precipitation from supersaturated solids solutions *J. Phys. Chem. Solids.* 19 (1961): 35–50.

- [12] Wagner, C. *Z. Elektrochem.* 65 (1961): 581.
- [13] Gunton, J. D., San Miguel, M., and Sahni, P. S. In: Domb, C., and Lebowitz, J. L., editors. *Phase transitions and critical phenomena, vol. 8*. New York: Academic Press, 1983. p. 267.
- [14] Binder, K. Theory of first-order phase transitions. *Rep. Prog. Phys.* 50 (1987): 783–859 .
- [15] Furukawa, H. A dynamical scaling assumption for phase separation. *Adv. Phys.* 34 (1985): 703–750.
- [16] Langer, J. S. *An introduction to the kinetics of first-order phase transitions*. In: Godrèche, C., editor. *Solids far from equilibrium*. Cambridge: Cambridge University Press, 1992. p. 297.
- [17] Janssen, H. K., Schaub, B., and Schmittmann, B. New universal short-time scaling behaviour of critical relaxation processes. *Z. Phys. B–Condensed Matter* 73 (1989): 539–549.
- [18] Huse, D. A. Remanent magnetization decay at the spin-glass critical point: A new dynamic critical exponent for nonequilibrium autocorrelations. *Phys. Rev. B* 40 (1989): 304–308.
- [19] Chaikin, P. M., and Lubensky, T. C. *Principles of condensed matter physics*. Cambridge: Cambridge University Press, 1995.
- [20] Rutenberg, A. D., and Bray, A. J. Phase ordering of two-dimensional XY systems below the Kosterlitz–Thouless transition temperature. *Phys. Rev. E* 51 (1995): R1641–R1644.
- [21] Kumar, S., Viñals, J., and Gunton, J. D. Monte Carlo renormalization-group study of the dynamics of the kinetic Ising model. *Phys. Rev. B* 34 (1986): 1908–1917.

- [22] Onuki, A. Dynamics of noninteger derivative models. *Prog. Theor. Phys.* 74 (1985): 1155–1157.
- [23] Bray, A. J. Universal scaling function for domain growth in the Glauber–Ising chain. *J. Phys. A.* 23 (1990): L67–L72.
- [24] Coniglio, A., and Zannetti, M. Multiscaling in growth kinetics. *Europhys. Lett.* 10 (1989): 575–580.
- [25] Oerding, K., and Janssen, H. K. Nonequilibrium critical relaxation with coupling to a conserved density. *J. Phys. A: Math. Gen.* 26 (1993): 3369–3381.
- [26] Oerding, K., and Janssen, H. K. Nonequilibrium critical relaxation with reversible mode coupling. *J. Phys. A: Math. Gen.* 26 (1993): 5295–5304.
- [27] Newman, T. J., and Bray, A. J. Dynamic correlations in domain growth: a $1/n$ expansion. *J. Phys. A: Math. Gen.* 23 (1990): 4491–4507.
- [28] Mermin, N. D., and Wagner, H. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic Heisenberg models. *Phys. Rev. Lett.* 17 (1966): 1133–1136.
- [29] Gupta, R., and Baillie, C. F. Critical behavior of the two-dimensional XY model. *Phys. Rev. B* 45 (1992): 2883–2898.
- [30] Gupta, R., DeLapp, J., Batrouni, G. G., Fox, G. C., Baillie, C. F., and Apostolakis, J. Phase transition in the 2D XY model. *Phys. Rev. Lett.* 61 (1988): 1996–1999.
- [31] Mondello, M., and Goldenfeld, N. Relaxational dynamics after the quench of a conserved system with a continuous symmetry. *Phys. Rev. E* 47 (1993): 2384–2393.
- [32] Mazenko, G. F., and Zannetti, M. Growth of order in a system with continuous symmetry. *Phys. Rev. Lett.* 53 (1984): 2106–2109.

- [33] Coniglio, A., Ruggiero, P., and Zannetti, M. Scaling and crossover in the large- N model for growth kinetics. *Phys. Rev. E* 50 (1994): 1046–1061.
- [34] Newman, T. J., Bray, A. J., and Moore, M. A. Growth of order in vector spin systems and self-organized criticality. *Phys. Rev. B* 42 (1990): 4514–4523.
- [35] Kissner, J. G., and Bray, A. J. Dynamic correlations in phase ordering: the $1/n$ -expansion reconsidered. *J. Phys. A* 26 (1993): 1571–1588.
- [36] Bray, A. J., and Rutenberg, A. D. Growth laws for phase ordering. *Phys. Rev. E* 49 (1994): R27–R30.
- [37] Bray, A. J., Rapapa, N. P., and Cornell, S. J. Corrections to scaling in phase-ordering kinetics. *Phys. Rev. E* 57 (1998): 1370–1376.
- [38] Rapapa, N. P., and Bray, A. J. Corrections to scaling in the phase-ordering dynamics of a vector order parameter. *Phys. Rev. E* 60 (1999): 1181–1188.
- [39] Bellac, M. L. *Quantum and statistical field theory*. Oxford: Clarendon Press, 1991.
- [40] Zheng, B. Monte Carlo simulations of short-time critical dynamics. *Int. J. Mod. Phys. B* 12 (1998): 1419–1484.

APPENDICES



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Appendix A

Determination of $C^\theta(r, t, t')$

We start with the two-point two-time pair correlation function for the phase variable, Eq. (4.12)

$$C^\theta(r, t, t') = \exp[-B^\theta(r, t, t')/2], \quad (\text{A.1})$$

where $B^\theta(r, t, t') \equiv \langle [\theta(\mathbf{x}, t) - \theta(\mathbf{x} + \mathbf{r}, t')]^2 \rangle$ is the phase-difference correlation function and, in terms of the average of the Fourier transforms of the phase variable, the correlation can be written as

$$B^\theta(r, t, t') = \int \frac{d^2\mathbf{k}}{(2\pi)^2} [\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t) \rangle + \langle \theta_{\mathbf{k}}(t')\theta_{-\mathbf{k}}(t') \rangle - 2 \cos(\mathbf{k} \cdot \mathbf{r}) \langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t') \rangle]. \quad (\text{A.2})$$

The phase-phase correlation at general times after a quench at $t = 0$ from a temperature T_i to a temperature T_f , both at or below T_{KT} , is given by Eq. (4.14),

$$\langle \theta_{\mathbf{k}}(t)\theta_{-\mathbf{k}}(t') \rangle = \frac{2\pi}{k^2} [\eta_f e^{-k^2|t-t'|} + (\eta_i - \eta_f) e^{-k^2(t+t')}] . \quad (\text{A.3})$$

The phase-difference correlation function then reads

$$B^\theta(r, t, t') = B_{eq}^\theta(r, t, t') + B_{neq}^\theta(r, t, t'), \quad (\text{A.4})$$

where

$$B_{eq}^\theta(r, t, t') = \frac{\eta_f}{\pi} \int \frac{d^2\mathbf{k}}{k^2} [1 - \cos(\mathbf{k} \cdot \mathbf{r}) e^{-k^2|t-t'|}] \quad (\text{A.5})$$

and

$$B_{neq}^\theta(r, t, t') = \frac{(\eta_i - \eta_f)}{2\pi} \int \frac{d^2\mathbf{k}}{k^2} [e^{-2k^2t} + e^{-2k^2t'} - 2 \cos(\mathbf{k} \cdot \mathbf{r}) e^{-k^2(t+t')}] , \quad (\text{A.6})$$

are the equilibrium and nonequilibrium correlations, respectively.

We first calculate the equilibrium correlation. The technical point is the use of the integral representation

$$\frac{1}{k^2} = \int_0^\infty du \exp(-k^2 u), \quad (\text{A.7})$$

and we use a soft ultraviolet cutoff through a factor of $\exp(-a_0^2 k^2)$. Then, we have

$$\begin{aligned} B_{eq}^\theta(r, t, t') &= \frac{\eta_f}{\pi} \int d^2\mathbf{k} \int_0^\infty du e^{-k^2 u} [1 - \cos(\mathbf{k} \cdot \mathbf{r}) e^{-k^2 |t-t'|}] e^{-a_0^2 k^2} \\ &= \frac{\eta_f}{\pi} \text{Re} \int d^2\mathbf{k} \int_0^\infty du [e^{-k^2(u+a_0^2)} - e^{i\mathbf{k} \cdot \mathbf{r} - k^2(u+a_0^2+|t-t'|)}] \\ &= 2\eta_f \text{Re} \int_0^\infty du \underbrace{\int_0^\infty dk k e^{-k^2(u+a_0^2)}}_{\frac{1}{2(u+a_0^2)}} \\ &\quad - \frac{\eta_f}{\pi} \text{Re} \int_0^\infty du \underbrace{\int d^2\mathbf{k} e^{i\mathbf{k} \cdot \mathbf{r} - k^2(u+a_0^2+|t-t'|)}}_{\frac{\pi}{u+a_1^2} e^{-r^2/4(u+a_1^2)}} \\ &= \eta_f \int_0^\infty du \left[\frac{1}{u+a_0^2} - \frac{e^{-r^2/4(u+a_1^2)}}{u+a_1^2} \right]. \end{aligned} \quad (\text{A.8})$$

For the last two equations, we set $a_1^2 \equiv a_0^2 + |t-t'|$. Let $x = u + a_0^2$ and $x = u + a_1^2$ for the first and the last term, respectively. Then, we have

$$\begin{aligned} B_{eq}^\theta(r, t, t') &= \eta_f \left[\int_{a_0^2}^\infty \frac{dx}{x} - \int_{a_1^2}^\infty dx \frac{e^{-r^2/4x}}{x} \right] \\ &= \eta_f \left[\underbrace{\int_{a_0^2}^{a_1^2} \frac{dx}{x}}_{\ln(a_1^2/a_0^2)} + \int_{a_1^2}^\infty dx \left(\frac{1 - e^{-r^2/4x}}{x} \right) \right]. \end{aligned} \quad (\text{A.9})$$

Let $y = r^2/4x$ for the second integral. By changing the limit of integration, the integral becomes

$$\int_0^{r^2/4a_1^2} dy \left(\frac{1 - e^{-y}}{y} \right). \quad (\text{A.10})$$

By using the formula of the exponential integral $E_1(x)$:

$$E_1(x) = -\gamma - \ln x + \int_0^x dy \left(\frac{1 - e^{-y}}{y} \right), \quad (\text{A.11})$$

where $E_1(x) \equiv \int_x^\infty dy e^{-y}/y$ for $x > 0$ and $\gamma \simeq 0.577$ is Euler's constant. Finally, by substituting $a_1^2 = a_0^2 + |t-t'|$, we obtain

$$B_{eq}^\theta(r, t, t') = \eta_f \{ \gamma + \ln(r^2/4a_0^2) + E_1[r^2/4(a_0^2 + |t-t'|)] \}. \quad (\text{A.12})$$

Next, we calculate the nonequilibrium part of the correlation

$$\begin{aligned}
B_{neq}^\theta(r, t, t') &= \frac{(\eta_i - \eta_f)}{2\pi} \int d^2\mathbf{k} \int_0^\infty du e^{-k^2 u} [e^{-2k^2 t} + e^{-2k^2 t'} \\
&\quad - 2 \cos(\mathbf{k} \cdot \mathbf{r}) e^{-k^2(t+t')}] e^{-a_0^2 k^2} \\
&= \frac{(\eta_i - \eta_f)}{2\pi} \operatorname{Re} \int d^2\mathbf{k} \int_0^\infty du [e^{-k^2(u+a_0^2+2t)} + e^{-k^2(u+a_0^2+2t')} \\
&\quad - 2e^{i\mathbf{k}\cdot\mathbf{r}-k^2(u+a_0^2+t+t')}] \\
&= (\eta_i - \eta_f) \operatorname{Re} \int_0^\infty du \underbrace{\int_0^\infty dk k [e^{-k^2(u+a_0^2+2t)} + e^{-k^2(u+a_0^2+2t')}]}_{\left[\frac{1}{2(u+a_0^2+2t)} + \frac{1}{2(u+a_0^2+2t')} \right]} \\
&\quad - \frac{(\eta_i - \eta_f)}{\pi} \operatorname{Re} \int_0^\infty du \underbrace{\int d^2\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}-k^2(u+a_0^2+t+t')}}_{\frac{\pi}{u+a_1^2} e^{-r^2/4(u+a_1^2)}} \\
&= (\eta_i - \eta_f) \int_0^\infty du \left[\frac{1}{2(u+a_0^2+2t)} + \frac{1}{2(u+a_0^2+2t')} \right. \\
&\quad \left. - \frac{e^{-r^2/4(u+a_1^2)}}{u+a_1^2} \right]. \tag{A.13}
\end{aligned}$$

For the last two equations, we set $a_1^2 \equiv a_0^2 + t + t'$. Let $x = u + a_0^2 + 2t$, $x = u + a_0^2 + 2t'$ and $x = u + a_1^2$ for the first, second and the last term, respectively. Hence

$$\begin{aligned}
B_{neq}^\theta(r, t, t') &= (\eta_i - \eta_f) \left[\int_{a_0^2+2t}^\infty \frac{dx}{2x} + \int_{a_0^2+2t'}^\infty \frac{dx}{2x} - \int_{a_1^2}^\infty dx \frac{e^{-r^2/4x}}{x} \right] \\
&= (\eta_i - \eta_f) \left[\underbrace{\int_{a_0^2+2t}^{a_1^2} \frac{dx}{2x}}_{\ln(a_1/\sqrt{a_0^2+2t})} + \underbrace{\int_{a_0^2+2t'}^{a_1^2} \frac{dx}{2x}}_{\ln(a_1/\sqrt{a_0^2+2t'})} + \int_{a_1^2}^\infty dx \left(\frac{1 - e^{-r^2/4x}}{x} \right) \right]. \tag{A.14}
\end{aligned}$$

Similarly, let $y = r^2/4x$ for the third integral. By changing the limit of integration, using Eq. (A.11) and substituting $a_1^2 = a_0^2 + t + t'$, we obtain

$$\begin{aligned}
B_{neq}^\theta(r, t, t') &= (\eta_i - \eta_f) \left\{ \gamma + \ln \left(\frac{r^2}{4\sqrt{(a_0^2+2t)(a_0^2+2t')}} \right) \right. \\
&\quad \left. + E_1[r^2/4(a_0^2+t+t')] \right\}. \tag{A.15}
\end{aligned}$$

In summary, the two-point two-time pair correlation function for the phase variable, $C^\theta(r, t, t')$, has the form

$$\begin{aligned}
C^\theta(r, t, t') &= \exp[-B^\theta(r, t, t')/2] \\
&= \exp[-B_{eq}^\theta(r, t, t')/2] \exp[-B_{neq}^\theta(r, t, t')/2] \\
&= \exp\left\{-\frac{\eta_f}{2}\{\gamma + \ln(r^2/4a_0^2) + E_1[r^2/4(a_0^2 + |t - t'|)]\}\right\} \\
&\quad \times \exp\left\{-\frac{(\eta_i - \eta_f)}{2}\left\{\gamma + \ln\left(\frac{r^2}{4\sqrt{(a_0^2 + 2t)(a_0^2 + 2t')}}\right)\right.\right. \\
&\quad \left.\left.+ E_1[r^2/4(a_0^2 + t + t')]\right\}\right\}. \tag{A.16}
\end{aligned}$$



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย

Appendix B

Evaluation of $C^\rho(r, t, t')$

For the two-point two-time amplitude correlation function, we start with Eq. (5.21)

$$C^\rho(r, t, t') = C_{eq}^\rho(r, t, t') + C_{neq}^\rho(r, t, t'), \quad (\text{B.1})$$

where C_{eq}^ρ and C_{neq}^ρ are the equilibrium and nonequilibrium correlations at the final temperature, given by the terms proportional to T_f and $T_i - T_f$, respectively, in Eq. (5.20):

$$C_{eq}^\rho(r, t, t') = \frac{k_B T_f}{(2\pi)^2} \int \frac{d^2 \mathbf{k}}{k^2 + 8V_0} e^{-(k^2 + 8V_0)|t-t'| + i\mathbf{k}\cdot\mathbf{r}}, \quad (\text{B.2})$$

and

$$C_{neq}^\rho(r, t, t') = \frac{k_B(T_i - T_f)}{(2\pi)^2} \int \frac{d^2 \mathbf{k}}{k^2 + 8V_0} e^{-(k^2 + 8V_0)(t+t') + i\mathbf{k}\cdot\mathbf{r}}. \quad (\text{B.3})$$

The key technical point in our calculations is the use of the integral representation

$$\frac{1}{(k^2 + 8V_0)} = \int_0^\infty du \exp[-(k^2 + 8V_0)u]. \quad (\text{B.4})$$

We use a soft ultraviolet cutoff through a factor of $\exp(-a_0^2 k^2)$. For the equilibrium correlations, we have

$$\begin{aligned} C_{eq}^\rho(r, t, t') &= \frac{k_B T_f}{(2\pi)^2} \int d^2 \mathbf{k} \int_0^\infty du e^{-(k^2 + 8V_0)u} e^{-(k^2 + 8V_0)|t-t'| + i\mathbf{k}\cdot\mathbf{r}} e^{-a_0^2 k^2} \\ &= \frac{k_B T_f}{(2\pi)^2} e^{-8V_0|t-t'|} \int_0^\infty du e^{-8V_0 u} \underbrace{\int d^2 \mathbf{k} e^{-k^2(u+a_1^2) + i\mathbf{k}\cdot\mathbf{r}}}_{\frac{\pi}{u+a_1^2} e^{-r^2/4(u+a_1^2)}} \\ &= \frac{k_B T_f}{4\pi} e^{-8V_0|t-t'|} \int_0^\infty du \frac{e^{-r^2/4(u+a_1^2) - 8V_0 u}}{u + a_1^2}. \end{aligned} \quad (\text{B.5})$$

For the last two equations, we set $a_1^2 \equiv a_0^2 + |t - t'|$. The integration in Eq. (B.5) cannot be done explicitly. So, we will consider in long time limit. At late time (a_1^2

is very large), the integral becomes

$$\int_0^\infty du \frac{e^{-r^2/4a_1^2 - 8V_0 u}}{a_1^2}. \quad (\text{B.6})$$

The integral becomes

$$\frac{e^{-r^2/4a_1^2}}{8a_1^2 V_0}. \quad (\text{B.7})$$

By substituting $a_1^2 = a_0^2 + |t - t'|$, the equilibrium correlation becomes

$$C_{eq}^\rho(r, t, t') = \frac{k_B T_f}{32\pi V_0} \frac{e^{-8V_0|t-t'| - r^2/4(a_0^2 + |t-t'|)}}{a_0^2 + |t - t'|}. \quad (\text{B.8})$$

Next, we calculate the nonequilibrium correlation

$$\begin{aligned} C_{neq}^\rho(r, t, t') &= \frac{k_B(T_i - T_f)}{(2\pi)^2} \int d^2\mathbf{k} \int_0^\infty du e^{-(k^2 + 8V_0)u} e^{-(k^2 + 8V_0)(t+t') + i\mathbf{k}\cdot\mathbf{r}} e^{-a_0^2 k^2} \\ &= \frac{k_B(T_i - T_f)}{(2\pi)^2} e^{-8V_0(t+t')} \int_0^\infty du e^{-8V_0 u} \underbrace{\int d^2\mathbf{k} e^{-k^2(u+a_1^2) + i\mathbf{k}\cdot\mathbf{r}}}_{\frac{\pi}{u+a_1^2} e^{-r^2/4(u+a_1^2)}} \\ &= \frac{k_B(T_i - T_f)}{4\pi} e^{-8V_0(t+t')} \int_0^\infty du \frac{e^{-r^2/4(u+a_1^2) - 8V_0 u}}{u + a_1^2}. \end{aligned} \quad (\text{B.9})$$

For the last two equations, we set $a_1^2 \equiv a_0^2 + t + t'$. Similar to the equilibrium part, we consider the integral in long time limit and substituting $a_1^2 = a_0^2 + t + t'$ back.

Finally, we obtain

$$C_{neq}^\rho(r, t, t') = \frac{k_B(T_i - T_f)}{32\pi V_0} \frac{e^{-8V_0(t+t') - r^2/4(a_0^2 + t + t')}}{a_0^2 + t + t'}. \quad (\text{B.10})$$

In summary, the two-point two-time pair correlation function for the amplitude variable, $C^\rho(r, t, t')$, has the form

$$\begin{aligned} C^\rho(r, t, t') &= C_{eq}^\rho(r, t, t') + C_{neq}^\rho(r, t, t') \\ &= \frac{k_B T_f}{32\pi V_0} \frac{e^{-8V_0|t-t'| - r^2/4(a_0^2 + |t-t'|)}}{a_0^2 + |t - t'|} \\ &\quad + \frac{k_B(T_i - T_f)}{32\pi V_0} \frac{e^{-8V_0(t+t') - r^2/4(a_0^2 + t + t')}}{a_0^2 + t + t'}. \end{aligned} \quad (\text{B.11})$$

Vitae

Petch Khunpetch was born on November 30, 1983 in Suratthani, Thailand. He received Bachelor's Degree of Science in Physics (2nd class honour) from Prince of Songkla University in 2006.



ศูนย์วิทยทรัพยากร
จุฬาลงกรณ์มหาวิทยาลัย