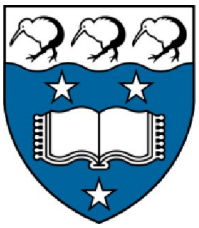
Kibble - Zurek Mechanism



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Abstract

This project tries to offer a systematic development of the Kibble-Zurek mechanism (KZM). A continuous phase transition leads to the formation of a non-conserved order due to spontaneous symmetry breaking. Such a phase transition, driven at a finite rate results in the formation of topological defects. The general theory which describes what happens during this crossover is given by the Kibble-Zurek mechanism. The mechanism exploits the critical slowing down in the neighbourhood of the critical point, this is, the divergence of the relaxation time of the system. KZM predicts the typical size of the domains in the broken symmetry phase to be fixed and generally applies to spontaneous symmetry breaking scenarios where a global symmetry is broken. In this dissertation, we start from a statistical field theory point of view and develop a mathematical relation for the so called correlation length and relaxation time. Then we use this to show that at a continuous phase transition, finite size domains should form in the underlying system and the boundaries where these different domains meet should develop defects. We show that KZM predicts a power-law behavior for this defect density as the function of the quench rate. At the end, we also investigate KZM in thin magnetic films with the help of computer simulations.

Acknowledgment

I would like to thank my supervisor A.Prof. Malcolm Grimson for all his guidance and suggestions during my work as well as his valuable feedback when writing this dissertation. Thanks for being so easy to reach and cooperative!

Contents

Introduction

We all are well familiar with the phenomena of phase transition from the different phases of water. But to precisely define the term phase transition we would first have to define what we mean by a phase.

The phase of a system is characterized by the symmetry the system possesses. For example, in going from a liquid to a solid phase the underlying system loses some symmetry (namely the rotational symmetry) and this symmetry is said to be broken. The modern representation of phase transition isn't limited to just the three phases of matter but instead have become a very general concept appearing nearly everywhere in physics where the concept of symmetry breaking applies.

The focus of this project is on continuous phase transitions leading to the formation of non-conserved order due to spontaneous symmetry breaking. This order can be characterized by some parameter called order parameter. The most important period during this transition is when the system crosses its critical point. The general theory which describes what happens during this crossover at a finite rate is given by the Kibble-Zurek mechanism. Kibble first studied spontaneously broken gauge symmetry in the context of the early universe [Kibble, 1976][Bunkov and Godfrin, 2012]. His idea was, that when a system approaches its critical point, then due to the critical slowing down of dynamics of the system, the causal horizon - the maximum distance over which one part of a system can communicate with the other - is finite and hence a global order cannot be established. Different regions acquire a different value of this order parameter and the junction where these different domains meet lead to the formation of defects like domain walls, string, and monopoles. Zurek extended this theory further to general condensed matter systems [Zurek, 1985][Zurek, 1996]. This was possible due to the universal nature of phase transitions.

The Kibble-Zurek theory provides quantitative predictions for the defect number scaling with the quench speed [Del Campo and Zurek, 2014]. This is experimentally measurable and therefore is particularly intriguing since it represents a practical way to test the universality of phase transitions.

This dissertation is organized as follows

- Chapter 1, motivates a shift of paradigm from a particles based approach, which is usually used in elementary statistical mechanics, to a field based one by introducing the idea of coarse graining. We also constructs the of form Landau-Ginzburg Hamiltonian and develop a theory of correlation length and shows that it diverges at the critical point.
- Chapter 2, discusses out-of-equilibrium dynamics using the Time-dependent Ginzburg-Landau theory, deriving it using the Langevin equation. It ends with the conclusion that the so called relaxation time should also diverge at the critical point.
- Chapter 3, is a slight detour and discusses about defects in superfluid and superconductors.

- Chapter 4, finally introduces the Kibble-Zurek mechanism (KZM) and discusses some of its achievements.
- In chapter 5, we envisage KZM in thin magnetic films with the help of computer simulations and present some Python generated pictures.

Chapter 1

Landau Ginzburg Equation

In principle, all thermodynamic properties of a system can be extracted from the partition function obtained by summing over all degrees of freedom, written as

$$Z(T) = \mathrm{tr}\left[e^{-\beta \mathcal{H}_{\mathrm{mic}}}\right], \quad \text{with} \quad \beta = \frac{1}{k_{\mathrm{B}} T} \tag{1.1}$$

Unfortunately, this simplicity comes with a cost. This partition function becomes too complicated even to deal with tiny macroscopic systems if one tries to write down the microscopic Hamiltonian for the system by tracking all the available degrees of freedom. Below we will see that "sometimes" we can give up on some of the details of this $Z(T)$ by taking a *mesoscopic approach* and still get the right result. These details turn out to be unnecessary for our purpose and hence ignoring them doesn't affect our analysis but leads to simplification.

1.1 From Particles to Fields

In this section, we introduce a shift of methodology from a particle-based approach (which is usually introduced first in elementary statistical mechanics) to a field-based one.

Let's consider the thermodynamics of matter at very low temperatures ($T \to 0$). From here we would conclude that at such low temperature only long wavelength collective excitations dominate the dynamics of a macro system.

Consider a homogeneous and isotropic lattice at temperature $T \sim 0$. Small fluctuations of the lattice constituents about their ideal positions can be written as $\vec{q}_{\vec{r}} = \vec{q}^{*}_{\vec{r}} + \vec{u}(\vec{r})$ where $\vec{q}_{\vec{r}}$ is the position at T = 0. The potential energy of such a low-temperature system is

$$\mathcal{V} = \mathcal{V}^{*} + \frac{1}{2} \sum_{\vec{r},\vec{r}'} \frac{\partial^2 \mathcal{V}}{\partial q_{\vec{r}} \partial q_{\vec{r}'}} u(\vec{r}) u\left(\vec{r}'\right) + O\left(u^3\right) \tag{1.2}$$

One can think of these tiny vibrations about the ideal position as disturbance caused due to the motion of a complex sound wave through the system. Consider the sound to be of low intensity so we can terminate the potential expansion at the quadratic order.

Following the above line of thought, let's now frame our theory in terms of the normal modes of vibrations (called phonons). The amplitude $\vec{u}(\vec{r})$ can be written in terms of Fourier modes of the sound wave that created the disturbance,

This chapter is heavily based on Chapter 1 and 2 of [Kardar, 2007]

$$u(\vec{r}) = \sum_{\vec{k}'} \mathrm{e}^{i\vec{k}\cdot\vec{r}} u(\vec{k}) \tag{1.3}$$

Since the lattice is uniform hence the same form of $\vec{u}(\vec{r})$ should hold for different locations. Now we see that the dynamics of our system is explicitly a function of $\vec{k}$.

Since as $T \to 0$, only modes with $\hbar\omega(k) < k_{\mathrm{B}}T$ should be excited and hence only small values of $\vec{k}$ should mainly contribute to the dynamics of our system. These small $\vec{k}'s$ implies long wavelength modes! Hence only long wavelength phonons generated due to collective excitations are present.

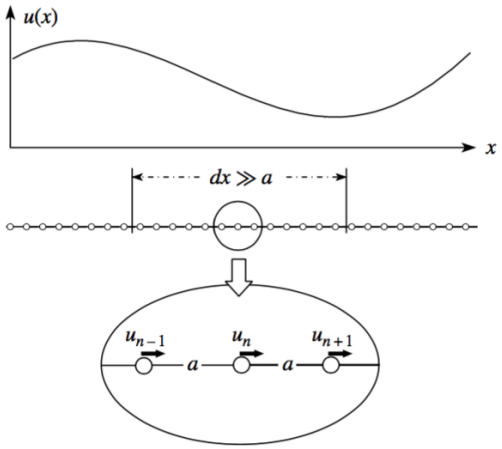


Figure 1.1: A one-dimensional string of particles. Here u_n is the displacements from mean and $u(x)$ is the coarse-grained field

So if the fluctuations at shorter wavelengths aren't important, then we can average over them in a region dx (Figure 1.1) and define a new continuously varying function $\vec{u}(x)$ at each location x separated dx distance apart. This averaging process is called coarse-graining and rest on the assumption that the tiny microscopic details become unimportant and so can be ignored.

1.2 Landau Ginzburg Hamiltonian

Our goal here is to develop a theory, not at $T \sim 0$ but instead at $T \sim T_c$ (the phase transition temperature). Fortunately these two regimes show very similar behavior and now we would like to explicitly show that.

Consider the familiar example of "Critical Opalescence". This phenomenon occurs when a liquid-gas system is close to criticality, where, the otherwise transparent system suddenly becomes milky and opaque. This phenomena, as well as similar observations of fluctuations via scattering experiments in other systems when they are close to their T_c, suggest that their behavior is also similarly dominated by collective fluctuations of many particles over long wavelengths. Hence field theory should be the right approach to study them.

We shall initially frame our theory of phase transition in terms of magnetic systems and later on generalize it.

Let's consider a magnet with some magnetization field $\vec{m}(\mathbf{x})$ defined on it. This $\vec{m}(\mathbf{x})$ represents the average value of the elemental spins of the magnet in the vicinity of some point $\mathbf{x}$. Now define a new partition function *over the field*

$$Z(T) = \mathrm{tr}\left[\mathrm{e}^{-\beta\mathcal{H}_{\mathrm{mic}}}\right] \equiv \int \mathcal{D}\vec{m}(\mathbf{x})\mathrm{e}^{-\beta\mathcal{H}[\vec{m}(\mathbf{x})]} \tag{1.4}$$

The symbol $\mathcal{D}\vec{m}(\mathbf{x})$ means integrating over all available configurations of the field. The different configurations of the field are weighted with a probability $P = \mathrm{e}^{-\beta\mathcal{H}[\vec{m}(\mathbf{x})]}$ where $\beta\mathcal{H}[\vec{m}(\mathbf{x})]$ is now called effective Hamiltonian (more correctly, effective Hamiltonian density) since it is a coarse-grained version of our original Hamiltonian.

The theory to be developed below is valid for many different systems with different types of $\vec{m}(\mathbf{x})$ hence we can generalize the problem if needed by considering a n-component field, existing in a d-dimensional space,

$$\mathbf{x} \equiv (x_1, x_2, \ldots, x_d) \in \Re^d \quad , \quad \vec{m} \equiv (m_1, m_2, \ldots, m_n) \in \Re^n$$

Obtaining the exact form of $\beta\mathcal{H}$ is still very difficult, but it turns out that it can be described in terms of some phenomenological parameters. The principles, very briefly are as follows:

- **Locality and uniformity:** The properties of our system can be derived by summing over the properties of its individual parts from each location

$$\beta\mathcal{H} = \int \mathrm{d}^d\mathbf{x}\Phi[\vec{m}(\mathbf{x}), \mathbf{x}] \tag{1.5}$$

  Here Φ is the energy density. Since our system in uniform hence Φ shouldn't depend on the position $\mathbf{x}$ where it's being calculated. To consider the interaction between different parts of the system, we also have to include gradients of the field($\nabla\vec{m}$).We assume only short-range interactions hence a good description can be obtained by including only a few derivatives.

$$\beta\mathcal{H} = \int \mathrm{d}^d\mathbf{x}\Phi\left[\vec{m}(\mathbf{x}), \nabla\vec{m}, \nabla^2\vec{m}, \cdots\right] \tag{1.6}$$

- **Analyticity:** Φ can be written as a Taylor expansion in powers of $\vec{m}(\mathbf{x})$ and its gradients, $\nabla\vec{m}, \nabla^2\vec{m}$.

- **Symmetries:** Since all orientations of $\vec{m}(\mathbf{x})$ are equally valid for an isolated isotropic system, hence Φ can't have a direct dependence of $\vec{m}(\mathbf{x})$ and $\nabla\vec{m}$ because that would break the degeneracy but Φ can depend on the squares of those quantities.

  To describe magnetic systems, and most other systems close to critical transition, only the leading terms prove to be sufficient. Hence in this way, we arrive at the **Landau–Ginzburg Hamiltonian**

$$\beta\mathcal{H} = \int d^d\mathbf{x}\left[\frac{t}{2}m^2(x) + um^4(x) + \frac{K}{2}(\nabla m)^2 + \cdots - \vec{h}\cdot\vec{m}(x)\right] \tag{1.7}$$

  In the above equation, only those terms are listed which can cause non-analyticities at the phase transition point. For example, the contributions to $\beta\mathcal{H}$ from the phonon degree of freedom are ignored. Also $\vec{h}$ represents the externally applied field.

- **Stability:** The coefficient of the highest order power of $\vec{m}$ i.e. the parameter u, should be positive.

1.3 Saddlepoint Approximation

It's still not easy to evaluate $Z(T)$, so we take the simplest approach. Replace the value of the integrand by the most probable configuration of the field $\vec{m}(\mathbf{x})$. This approximation is called saddle point approximation.

$$Z_{\text{sp}} = \int \mathrm{d}\vec{m} \exp\left[-V\left(\frac{t}{2}m^2 + um^4 + \cdots - \vec{h}.\vec{m}\right)\right] \tag{1.8}$$

The corresponding saddle point free energy is

$$\beta F_{\text{sp}} = -\ln Z_{\text{sp}} \approx V \min\{\Psi(\vec{m})\}_{\vec{m}} \tag{1.9}$$

Where

$$\Psi(\vec{m}) \equiv \frac{t}{2}\vec{m}^2 + u\left(\vec{m}^2\right)^2 + \cdots - \vec{h}.\vec{m} \tag{1.10}$$

and most likely value of magnetization is

$$\Psi'(\vec{m}) = t\vec{m} + 4u\vec{m}^3 + \cdots - \vec{h} = 0 \tag{1.11}$$

The behavior of $\vec{m}$ strongly depends on the sign of the parameter t. If we consider an isolated magnet ($\vec{h} = 0$), then on solving the above equation we get

$$|m(h=0)| = \begin{cases} 0 & t > 0 \\ \sqrt{\frac{-t}{4u}} = \sqrt{\frac{a}{4u}}\,(T_c - T)^{1/2} & t < 0 \end{cases} \tag{1.12}$$

So we see, that the system spontaneously develops a magnetization(i.e. order) when $t < 0$, as shown in the figure below.

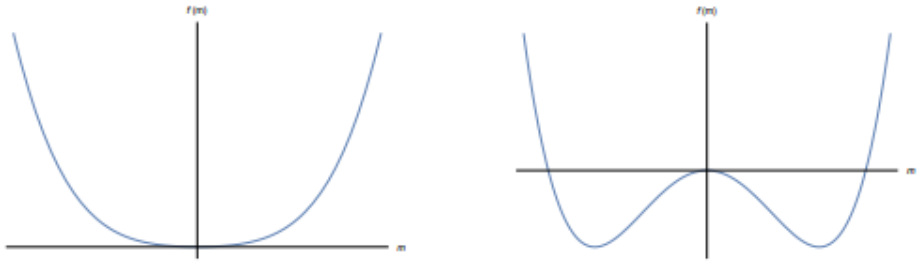


Figure 1.2: Free energy as a function of magnetization, when $t > 0$ and $t < 0$

It should be noted that the $|m|$ defined above is only the magnitude of $\vec{m}(\mathbf{x})$ and the parameters $(t, u, K, ..)$ are considered as analytic functions of temperature and hence can be Taylor expanded around $T = T_c$. For example, above we assume

$$t = a\,(T - T_c) + \quad . \quad . \quad , \qquad \text{with} \qquad (a, u, K) > 0 \tag{1.13}$$

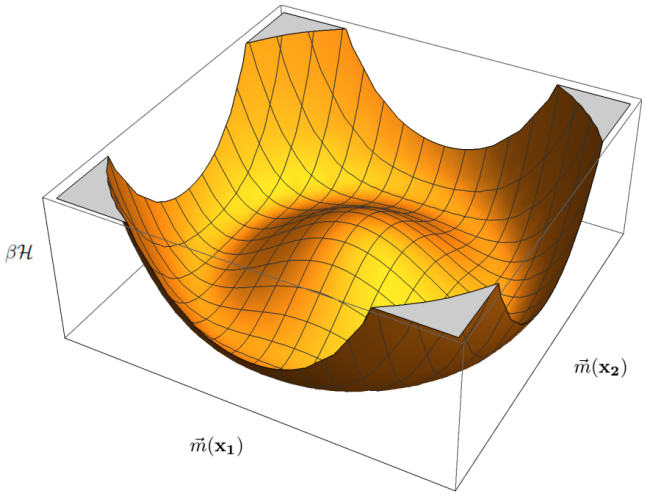


Figure 1.3: Image showing the minima of free energy (the ring shape at the bottom) for a continuous symmetry breaking phase transition. Here $\vec{m}(\mathbf{x})$ is a 2-dimensional field and can acquire any of the values lying on the 1 dimensional manifold of minima

Since all directions in our system are equivalent in the absence of an external field, hence there is an equally likely chance for $\vec{m}(\mathbf{x})$ to choose any direction in the d dimensional space. For $T < T_c$ the average of $\vec{m}(\mathbf{x})$ over the entire system would be $|m|$ ($\langle\vec{m}(\mathbf{x})\rangle = |m|$) but it's reasonable to assume that at least locally the system can fluctuate from this value. So let's consider, that around some point $\mathbf{x}$,

$$\vec{m}(\mathbf{x}) = [\,|m| + \phi_\ell(\mathbf{x})]\,\hat{e}_\ell + \phi_t(\mathbf{x})\hat{e}_t \tag{1.14}$$

Here we assume $\vec{m}(\mathbf{x})$ to be a 2-dimensional field for simplicity and hence ϕ_ℓ representing the small fluctuations in the longitudinal direction and ϕ_t in the transverse direction of $\vec{m}(\mathbf{x})$. Referring to Fig (1.3), these longitudinal fluctuations would point in the uphill direction while the transverse fluctuations would point along circular minima located at the bottom of the potential. On substituting this new value of $\vec{m}(\mathbf{x})$ in our earlier equation

$$\mathcal{P}[\vec{m}(\mathbf{x})] \propto \exp\{-\beta\mathcal{H}\}\,,$$

then we get

$$\mathcal{P}[\vec{m}(\mathbf{x})] \propto \exp\left\{-\int \mathrm{d}^2\mathbf{x}\left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + um^4\right]\right\} \tag{1.15}$$

$$\begin{aligned}\Rightarrow -\ln\mathcal{P} = \beta\mathcal{H} = V\left(\frac{t}{2}|m|^2 + u|m|^4\right) + \int d^d\mathbf{x}\left[\frac{K}{2}\left(\nabla\phi_\ell\right)^2 + \frac{t+12u|m|^2}{2}\phi_\ell^2\right] \\ + \int \mathrm{d}^d\mathbf{x}\left[\frac{K}{2}\left(\nabla\phi_t\right)^2 + \frac{t+4u|m|^2}{2}\phi_t^2\right] + \mathcal{O}\left(\phi_t^3, \phi_t^3\right)\end{aligned} \tag{1.16}$$

For reasons to become apparent shortly, in the above equation we define

$$\frac{K}{\xi_\ell^2} \equiv t + 12u|m|^2 = \left.\frac{\partial^2\Psi(m)}{\partial\phi_\ell^2}\right|_{|m|} = \begin{cases} t & \text{for } t > 0 \\ -2t & \text{for } t < 0 \end{cases} \tag{1.17}$$

and

$$\frac{K}{\xi_t^2} \equiv t + 4u|m|^2 = \left.\frac{\partial^2 \Psi(m)}{\partial \phi_t^2}\right|_{|m|} = \begin{cases} t & \text{for } t > 0 \\ 0 & \text{for } t < 0 \end{cases} \tag{1.18}$$

where $\frac{K}{\xi_\ell^2}$ and $\frac{K}{\xi_t^2}$ can be seen as stiffness constants of the restoring force for displacements ϕ_ℓ and ϕ_t and K is a constant. Thus we see that when $t < 0$, there is no restoring force for the *transverse fluctuations*. That means, that $\xi_t \to \infty$ as $t \to 0$. But what's the physical significance of this statement?

Let's now switch to momentum space as things get more transparent for our field description there. In this space, we see $\phi(\vec{x})$ as

$$\phi(\vec{x}) = \sum_{\mathbf{q}} \phi_{\mathbf{q}} \mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}}/\sqrt{V} \tag{1.19}$$

The probability of every fluctuation mode is obtained by Fourier transforming Eq. (1.15) and gives

$$\mathcal{P}\left[\{\phi_{\ell,\mathbf{q}}; \phi_{t,q}\}\right] \propto \prod_{\mathbf{q}} \exp\left\{-\frac{K}{2}\left(q^2 + \xi_\ell^{-2}\right)|\phi_{\ell,\mathbf{q}}|^2\right\} . \exp\left\{-\frac{K}{2}\left(q^2 + \xi_t^{-2}\right)|\phi_{t,q}|^2\right\} \tag{1.20}$$

We see that each mode of fluctuation behaves as a Gaussian random variable with zero mean and different modes are linearly independent. It turns out that the behavior of $\phi_{t,q}$ is particularly interesting. When $t \to 0$,

$$\mathcal{P}\left[\{\phi_{t,q}\}\right] \propto \prod_{\mathbf{q}} \exp\left\{\frac{-Kq^2}{2}\right\} \tag{1.21}$$

Therefore $\phi_{t,q}$ with very small $\mathbf{q}$ have a higher probability ($\mathcal{P}\left[\{\phi_{t,q}\}\right]$) of occurrence. These modes for small values of $\mathbf{q}$ are called *Goldstone modes* and it takes essentially no energy to excite them. But smaller $\mathbf{q}$ means longer wavelength (λ), so as $T \to T_c$, we should find that mainly *long wavelength fluctuations should dominate* the system. This is the confirmation of what we initially assumed at the start of this section!

Interestingly we see that $\xi_{t,q}$ and λ show very similar behavior near criticality. $\xi_{t,q}$ is called the correlation length of the transverse fluctuations and our theory predicts its divergence at the critical point ($T = T_c$) [Kardar, 2007].

Chapter 2

Time-Dependent Ginzburg Landau Equation

In the last chapter, our focus was only on the equilibrium behavior of the underlying system. Now we would like to study the behavior of this system, when it's off equilibrium. For motivation, we first examine the behavior of a Brownian particle while coming into thermal equilibrium with a liquid and in the subsequent section extend this line of thought to describe a continuous field dynamics.

2.1 Dissipative Particle Dynamics: The Langevin Equation

Consider a dust particle suspended in a liquid. This dust particle wouldn't stay stationary but instead move in a very zig-zag motion known as the Brownian motion. The displacement $\vec{x}(t)$ of the particle can be described by the equation

$$m\ddot{\vec{x}} = -\frac{\dot{\vec{x}}}{\mu} - \frac{\partial \mathcal{V}}{\partial \vec{x}} + \vec{f}_{\text{random}}(t) \tag{2.1}$$

The three forces acting on the particle as listed on the RHS of the above equation are:

- $\frac{\dot{\vec{x}}}{\mu}$ is the frictional force due to the viscosity of the liquid, where μ called the mobility and $\overline{\eta}$ is the specific viscosity.
- $\mathcal{V}(\vec{x})$ is the force due to some external potential
- $\vec{f}_{\text{random}}(t)$ is the force due to random impacts from the liquid particles. Since this force is a random variable hence from the central limit theorem, it should be Gaussian distributed with zero mean.

If the viscous force dominates the inertial one (due to $\mathcal{V}(\vec{x})$) then the particle hardly accelerates and our equation reduces to what is known as the Langevin equation,

$$\dot{\vec{x}} = \vec{v}(\vec{x}) + \vec{\eta}(t) \tag{2.2}$$

Here $\vec{v}(\vec{x}) = -\mu\partial\mathcal{V}/\partial\vec{x}$ is the deterministic velocity and $\vec{\eta}(t) = \mu\vec{f}_{\text{random}}(t)$ is the stochastic velocity which has zero mean,

$$\langle\vec{\eta}(t)\rangle = 0 \tag{2.3}$$

This chapter is heavily based on Chapter 9 of [Kardar, 2007]

The Langevin equation defined here, does a good job in describing the dynamics of a single particle but on the other hand we usually deal with not one but a multitude of such particles. The next section provides an efficient way of dealing with such a situation.

2.2 Dynamics of a Dissipative Field

The Langevin equation on the last page was limited to a single particle dynamics, now we will generalize it for a collection of degrees of freedom, described by a continuous field $\vec{\Phi}(\mathbf{x}, t)$. (From here on, the symbol for the field has been changed from $\vec{m}(\mathbf{x})$ to $\vec{\Phi}(\mathbf{x}, t)$, to show that the description is valid for any general field).

Let's consider a field $\vec{\Phi}(\mathbf{x}, t)$. From chapter 1, the equilibrium effective Landau Ginzburg Hamiltonian is

$$\mathcal{H}[\vec{\Phi}] = \int \mathrm{d}^d\mathbf{x} \left[\frac{\varepsilon}{2}\Phi^2 + u\Phi^4 + \frac{K}{2}(\nabla\Phi)^2 + \cdots \right] \tag{2.4}$$

Above, we replaced the coefficient of Φ^2 from t to ε because now we are dealing with dynamics and therefore reserve t for time. To construct a Langevin equation governing the dynamics of $\vec{\Phi}(\mathbf{x}, t)$, we first calculate the analogous force on each field component from the variations of $\mathcal{H}[\vec{\Phi}]$. The functional derivative of Eq. (2.4) yields,

$$F_i(\mathbf{x}) = -\frac{\delta\mathcal{H}[\vec{\Phi}]}{\delta\Phi_i(\mathbf{x})} = -\varepsilon\Phi_i - 4u\Phi_i|\vec{\Phi}|^2 + K\nabla^2\Phi_i \tag{2.5}$$

Taking analogy from the Langevin equation for the Brownian particle, we get

$$\frac{\partial\Phi_i(\mathbf{x}, t)}{\partial t} = \mu F_i(\mathbf{x}) + \eta_i(\mathbf{x}, t) \tag{2.6}$$

The resulting Langevin equation for our field is known as the *time-dependent* Ginzburg-Landau equation (TDGL).

$$\frac{\partial\vec{\Phi}(\mathbf{x}, t)}{\partial t} = -\mu\varepsilon\vec{\Phi} - 4\mu u\Phi^2\vec{\Phi} + \mu K\nabla^2\vec{\Phi} + \vec{\eta}(\mathbf{x}, t) \tag{2.7}$$

This is essentially non-linear due to the $4\mu u\Phi^2\vec{\Phi}$ term, but luckily our interest is in the disordered phase (symmetric phase) where $\langle\vec{\Phi}\rangle$ is negligible and hence we can ignore the coefficient of the quartic term in the TDGL equation. The resulting equation is linear and can be solved by transforming the components to the Fourier space as

$$\vec{\Phi}(\mathbf{q}, t) = \int \mathrm{d}^d\mathbf{x}\mathrm{e}^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}}\vec{\Phi}(\mathbf{x}, t) \tag{2.8}$$

which, after taking the Fourier transform of Eq. (2.6), evolve as

$$\frac{\partial\vec{\Phi}(\mathbf{q}, t)}{\partial t} = -\mu\left(\varepsilon + Kq^2\right)\vec{\Phi}(\mathbf{q}, t) + \vec{\eta}(\mathbf{q}, t) \tag{2.9}$$

Lets calls the coefficient of $\vec{\Phi}(\mathbf{q}, t)$ as $\frac{1}{\tau(\mathbf{q})}$

$$\mu\left(\varepsilon + Kq^2\right) = \frac{1}{\tau(\mathbf{q})} \tag{2.10}$$

These modes $\vec{\Phi}(\mathbf{q},t)$ are linearly independent and form a basis of the Fourier space. On integrating (2.7), we find that each mode evolves independently at time t as

$$\vec{\Phi}(\mathbf{q},t) = \vec{\Phi}(\mathbf{q},0)\mathrm{e}^{-\frac{1}{\tau(\mathbf{q})}} + \int_0^t \mathrm{d}\tau\, \mathrm{e}^{-\frac{(t-\tau)}{\tau(\mathbf{q})}}\vec{\eta}(\mathbf{q},t) \tag{2.11}$$

Also the Fourier noise has zero mean, $\langle \eta_i(\mathbf{q},t)\rangle = 0$, hence the average of each Fourier component becomes

$$\langle\vec{\Phi}(\mathbf{q},t)\rangle = \vec{\Phi}(\mathbf{q},0)\exp[-t/\tau(\mathbf{q})] \tag{2.12}$$

Where we notice that the $\tau(\mathbf{q})$ defined earlier, turns out to be the relaxation time for the decay of Fluctuations in each mode $\vec{\Phi}(\mathbf{q},t)$. Therefore

$$\tau(\mathbf{q}) = \frac{1}{\mu\,(\varepsilon + Kq^2)} \tag{2.13}$$

and hence for a very small $\mathbf{q}$, i.e. very long wavelength modes,

$$\tau(\mathbf{q}) \approx \frac{1}{\mu\varepsilon} \tag{2.14}$$

Hence as $\varepsilon \to 0$, $\tau_{max} \to \infty$. Therefore on approaching $\varepsilon = 0$, the time required for our system to equilibrate diverges. This phenomenon is known as *critical slowing down* as the time now required for the system to attain equilibrium is essentially infinite.

Also, from last chapter we know that

$$\xi^2 = \frac{K}{\varepsilon + 4u|\Phi|^2}$$

and since $\varepsilon > 0$ hence, $|\Phi| = 0$, therefore the order parameter in this Gaussian model is correlated over the length

$$\xi(\varepsilon) = \sqrt{\frac{K}{\varepsilon}} \tag{2.15}$$

More generally,

$$\xi(\varepsilon) = \frac{\xi_0}{|\varepsilon|^v} \tag{2.16}$$

where the constant ξ_0 depends on the microscopic qualities of the system. Also the exponent $v = 1/2$ for our case, but a better approximation for v comes from the Scaling and Renormalization theory which predicts $v = 2/3$ [Hohenberg and Halperin, 1977].

Just like $\tau_(\mathbf{q})$, ξ also diverges at $\varepsilon = 0$. Thus the critical point is characterized by diverging time and length scales! For our above model ξ and τ are related through the relation [Kardar, 2007]

$$\tau(\varepsilon) = \frac{\xi^z(\varepsilon)}{\mu K} \tag{2.17}$$

again more generally,

$$\tau(\varepsilon) = \frac{\tau_0}{|\varepsilon|^{zv}} \tag{2.18}$$

where $z = 2$ for our case, but a better approximation for z is $z = 3/2$, τ_0 is also a system depended constant [Hohenberg and Halperin, 1977][Chandran et al., 2012].

The z and v are called dynamical critical exponents and depend on the underlying universality class of the model under consideration. What's fascinating, is that system with the same set of critical exponents show similar behavior close to their critical point.

Chapter 3

Defects in Superfluids and Superconductors

In this chapter, we will consider a class of defects, called topological defects, in systems with broken *continuous symmetry* and show how they could arise in different systems like superfluids and superconductors. To achieve this goal, we would first need some background regarding the phenomena of superfluidity and superconductivity and the next section is devoted to that.

3.1 Superfluids Introduction

While most other quantum effects only appear in the atomic regime, superfluids and superconductors show quantum mechanical phenomena even on a macroscopic scale.

The most well-known example of a superfluid is liquid Helium. The reason that He^4 is a superfluid while other fluids like Neon, Argon etc aren't is that at low enough temperatures He^4 atoms have a de Broglie wavelength which is larger than the average separation between their neighboring pairs. Since He^4 is a Bose particle, hence this leads to a constructive superposition of the wavefunctions of all atomic He^4 into a single coherent state [Annett, 2004][Schmitt, 2015].

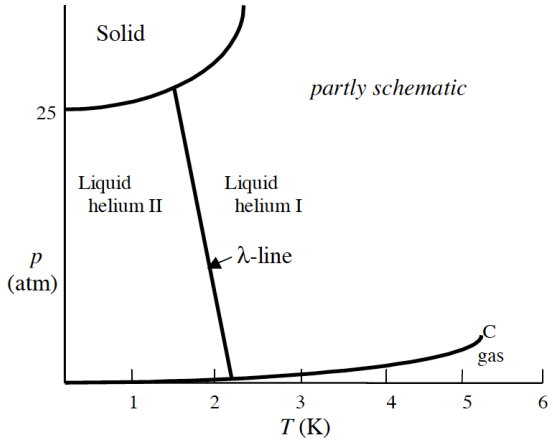


Figure 3.1: Helium-4 Phase Diagram.

The figure above shows, that for pressures below 25 atm, there is no solid phase of He^4 at any temperature, and it remains a liquid even down to absolute zero. As shown in Fig (3.1), liquid He^4 has two distinct liquid phases, He^4 I and He^4 II. He^4 I is a normal

fluid, characterized by fairly standard liquid state properties. But He^4 II is a superfluid, characterized by the properties like fluid-flow with zero viscosity and infinite thermal conductivity.

3.2 The Macroscopic Wavefunction

The unusual properties of liquid helium can be understood if we imagine that the state of the He^4 can be characterized by a local wave function $\Phi(r)$ at every point in space.

$$\Phi(r) = \sqrt{n(r)}\exp\left(i\theta(r)\right) \tag{3.1}$$

The wave function corresponds to a condensate of a macroscopic number of particles. This wavefunction could be normalized so that the density of particles in the condensate is given by

$$n = |\Phi^2(r)| \tag{3.2}$$

But is it justified to call n the density of the condensate, when we know from the Born interpretation that $|\Phi^2(r)|$ represents the probability density for finding a particle and not a physical density in space?

It's correct that $\Phi(r)$ represents the probability amplitude of a particle's wavefunction. But what if there are an enormous number of particles present in exactly the same state, all of them having exactly the same wavefunction? Then chances of finding any one particle at a certain location are still given by $|\Phi^2(r)|$but since there are so many, that even if we look in a tiny volume, it's very likely that we would find some particle there. Hence on making a measurement in some volume dv, we will generally find a particle number close to $|\Phi^2(r)|dv$ and therefore it would be reasonable to assume $|\Phi^2(r)|$ as the number density of particles [Feynman, 1965].

That's exactly the case for our condensate wavefunction $\Phi(r)$ where an enormous number of particles are occupying the same state. Hence a new physical interpretation of the wave function is possible here.

We postulate that the phase transition temperature T_c, is the point where the wavefunction's phase first becomes ordered throughout the fluid and hence $\Phi(r)$ (a complex scalar field) serves as the order parameter for our superfluid phase transition.

The $\theta(r)$ in our expression (3.1) is some angle that describes the orientation of the unit vector $n(r)$ in space.

$$n(r) = (n_x, n_y) = (\cos\theta, \sin\theta) \tag{3.3}$$

For He^4 I, $n(r)$ takes on random spatial directions but for He^4 II we observe an order in $n(r)$. This transition from disorder to order, in the choice of $n(r)$, is very similar to what we observed for the case of a magnetic phase transition.

In analogy with the probability current density of a particle's wavefunction from quantum mechanics, we can postulate the current density of particle flow as

$$\mathbf{j} = \frac{\hbar}{2mi}\left[\Phi^*(\mathbf{r})\nabla\Phi(\mathbf{r}) - \Phi(\mathbf{r})\nabla\Phi^*(\mathbf{r})\right] \tag{3.4}$$

where

$$\nabla\Phi(\mathbf{r}) = e^{i\theta}\nabla\sqrt{n} + i\sqrt{n}e^{i\theta}\nabla\theta,$$

and it's complex conjugate is

$$\nabla\Phi^*(\mathbf{r}) = e^{-i\theta}\nabla\sqrt{n} - i\sqrt{n}e^{-i\theta}\nabla\theta.$$

Substituting these into Eq. (3.4) we get [Annett, 2004]

$$\mathbf{j} = \frac{\hbar}{m}n\nabla\theta \tag{3.5}$$

and dividing $\mathbf{j}$ by n, results in the expression for the superfluid velocity of flow,

$$\mathbf{v}_s = \frac{\hbar}{m}\nabla\theta \tag{3.6}$$

3.3 Vortices and Flow quantization

Taking the curl of the superflow velocity $\mathbf{v}_s$ defined above gives

$$\nabla \times \mathbf{v}_s = 0 \tag{3.7}$$

So the flow is irrotational.

But what if we put the superfluid in a closed tube and generate a circulation? We can define this circulation as κ

$$\kappa = \oint \mathbf{v}_s \cdot d\mathbf{r} \tag{3.8}$$

The irrotational property $\nabla \times \mathbf{v}_s = 0$ implies that integral around a closed loop shouldn't depend on the path taken, as long as the endpoints are the same. Substituting Eq. (3.6) into Eq. (3.8) results in,

$$\kappa = \frac{\hbar}{m}\oint \nabla\theta \cdot d\mathbf{r} = \frac{\hbar}{m}\Delta\theta \tag{3.9}$$

Here, $\Delta\theta$ is the change in the phase angle θ as the fluid completes a full cycle around the tube. But since the macroscopic wave function would be unchanged by a full cycle, therefore we must have

$$\Phi(\mathbf{r}) = \Phi(\mathbf{r})e^{i\Delta\theta} \tag{3.10}$$

which implies

$$\Delta\theta = 2\pi n_w \tag{3.11}$$

where n_w is an integer. The consequence of the quantization of circulation of superflow means, that no circulation could exist until we reach a quantum of circulation, $\frac{\hbar}{m}$. Subsequent increase in the flow velocity would also occur in jumps of units $\frac{\hbar}{m}$[Annett, 2004].

The quantum number n_w, also called the topological winding number, is the number of times θ winds through an angle of 2π as the fluid goes around the closed path.

But now what if we put the fluid in a cylinder instead of a tube and then set it rotating? Then it should be impossible to have any form of circulation due to the condition $\nabla \times \mathbf{v}_s = 0$. But we do find the fluid to rotate, how is this possible?

The irrotational flow would imply

$$\oint \mathbf{v}_s \cdot d\mathbf{r} = 0 \tag{3.12}$$

Hence a rotation is only possible if the fluid has vortices (See Fig (3.2)).

A vortex is a circulating flow which satisfies the condition $\nabla \times \mathbf{v}_s = 0$ except at its core and still allows a net rotation of the fluid.

This tells us that the flow velocity around the vortex must be

$$\mathbf{v}_s = \frac{\kappa}{2\pi r}\mathbf{e}_\phi \tag{3.13}$$

The flow velocity is inversely proportional to r and should increase as the center of the vortex is approached. Also, the $\mathbf{e}_\phi$ unit vector means that the velocity points in the $\hat{\phi}$ direction in spherical polar coordinates. The core region of the vortex isn't a superfluid, forming a narrow line of normal fluid. Vortex lines can be found in two different configurations, the lines, and rings. A line cannot suddenly end in the middle of the fluid but must extend from one boundary of the fluid to another (Fig (3.2)). Another possibility is that vortex can bend and join up with its other end, forming a ring structure[Williams, 1992].

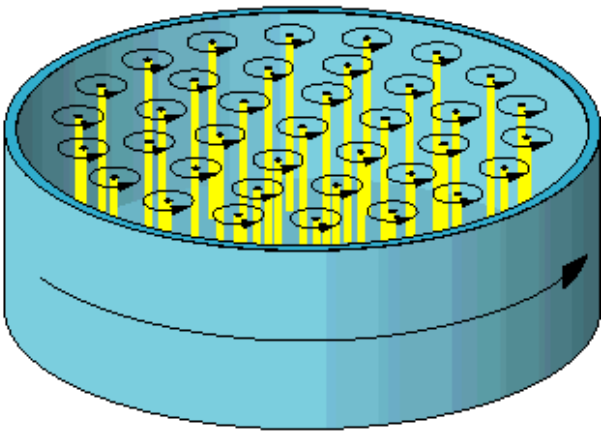


Figure 3.2: The circular flow pattern of liquid around vortex lines when the object containing the liquid is set into rotation

Rotating the superfluid isn't the only possible way to generate vortices. Kosterlitz and Thouless deduced, that raising the temperature of a thin (nearly 2D) layer of superfluid should also lead to the generation of many pairs of vortices, with each vortex having an opposite flow to that of its corresponding pair (Fig (3.3)). At low temperature, these vortices are tightly bound to each other. As such they do not have much effect on the superfluid because the fluid flow from each vortex cancels that of its pair, except in the tiny region directly between the vortex and anti-vortex pair where the flow combines to produce a strong current. But as we raise the temperature, the average separation

between these pairs increases and also more such pairs are continually introduced. The tiny region where the flow was reinforced, now grows and this flow orients itself in such a way so as to cancel the superflow. Hence the generation of these vortices causes an abrupt decrease in the density of the superfluid. Inversely, we can say that on cooling the liquid a multitude of the vortices bind together and can no longer affect the superflow and the system behaves like a superfluid. This binding-unbinding of vortices appears as if they can create and annihilate each other in pairs. So the conclusion is, that at a superfluid phase transition, vortices arise naturally and play a key role in deciding the phase of a fluid [**?**]. We would very soon see that some vortices can't be annihilated at the phase transition point and subsequently leads to defects in the geometry of the system.

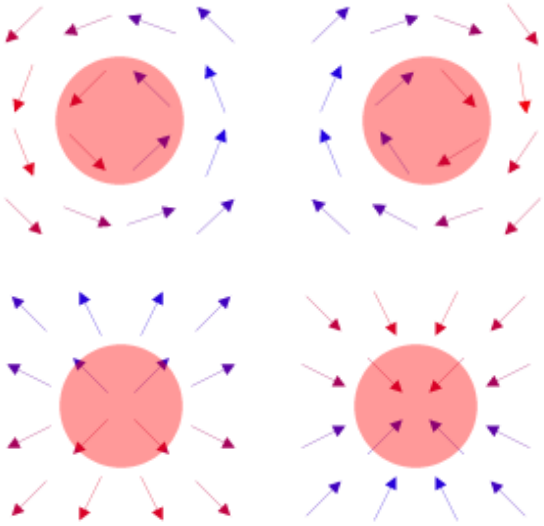


Figure 3.3: Two pair of vortices in a two-dimensional array of spins. These are the vortex and anti-vortex pairs with winding number $n_w = \pm 1$ which were briefly introduced above in the case of Kosterlitz-Thouless theory.

3.4 Superconductors

We can develop the theory of superconductivity in close analogy to superfluidity. Superconductivity is characterized by frictionless flow of electron in a metal below a certain temperature. Due to the interactions of the electrons with the vibrations of the atoms in the lattice, crudely speaking, there is a small net effective attraction between the electrons in the metal. This results in the electrons forming a loosely bound pair. An electron is a fermi particle but two electrons together as a pair can behave like a bose particle. Many such pairs now behaving like bosons would prefer to co-exist in a single wavefunction state and hence form a condensate very similar to the He^4 case. The resulting electron fluid flows like a superfluid and has analogous properties.

Vortex structures can exist in superconductors as well, where the paired electrons flow in patterns similar to the vortex flow in He^4. Let's discuss that in a bit more detail. Take a piece of a metal in its symmetric phase and leave it in a magnetic field. Then slowly lower the temperature until the CP is crossed. Once the CP is crossed, the field from the inside of the metal is expelled due to Miessner effect as the metal undergoes a superconductive phase transition. Our metal achieves this task by inducing a vortex flow of paired electron current in such a way that the resulting magnetic field cancels

the externally applied one. But what would happen if we now suddenly switch off the external field? The charge flow would keep on going and the piece of metal would be left with vortices. Because the vortex flow is due to a charged fluid, hence there would be a resultant magnetic field at the core of the vortex. It turns out that similar to the quantization of circulation of the liquid He^4 vortices, the current circulation in this piece of metal is also quantized. This ultimately means that the strength of the induced magnetic field at the core should also be so. This quantized magnetic field looks like a tube at the core of a vortex and hence known as a flux tube [Feynman, 1965][**?**].

3.5 Topological Defects

The structures like vortex lines and flux tubes are defects in the otherwise uniform topology of our system. The vortex lines lying at the core of the vortices in a superfluid consist of normal fluid while the flux tube at the core of the vortices in a type-II superconductor consists of ordinary metal.

These defects cannot be made to disappear by any continuous deformations of the order parameter. They are, therefore, called topological defects [Chaikin et al., 1995].

In a 2-dimensional system, pairs of vortices with opposite winding number (often called opposite charge) can annihilate each other. Thus, the state with a vortex-antivortex pair is topologically equivalent to a uniform state. Whereas a single vortex is topologically protected and represents a permanent defect in the geometry of the underlying system. Vortex flow has significance far beyond superfluid and superconductors. They show up in some systems of magnetic spins, in fluid turbulence and perhaps even in the early cosmic phase transitions. This brings us to our next question. How such defects can occur in the cosmic phase transitions and is the theory of continuous phase transition we developed above, applicable to the cosmos?

Here we focus only on continuous symmetry breaking cosmic phase transition. The standard mechanism for breaking symmetry for cosmic phase transitions involves the hypothetical Higgs field that pervades all space. As the universe cools, the Higgs field can adopt different ground/vacuum states. In a symmetric phase ground state (i.e. before the transition), the Higgs field is zero everywhere. Symmetry breaks when the Higgs field spontaneously takes on a finite value[Bunkov and Godfrin, 2012][Gangui, 2001].

Kibble saw the possibility of defect formation when he realized that in a cooling universe the evolution of the order in a system after a phase transition can proceed only at a finite rate. This rate is determined by the speed at which one part of the system could communicate with the other. In an expanding universe, widely separated regions in space do not have enough time to communicate amongst themselves and are therefore not correlated, due to a lack of causal contact. It is therefore natural to suppose that different regions would end up having arbitrary orientations of the Higgs field and that, when they merge together, it would be hard for domains with very different orientations of the Higg's field to adjust themselves. Therefore the formation of uncorrelated domains which subsequently merge, leave behind relics in the form of defects at their interface. This general feature of the existence of these uncorrelated domains is now known as the Kibble mechanism [Gangui, 2001].

One such defect that could have occurred in the early universe is called cosmic strings. They are linear defects, analogous to the defects discussed above and result from the symmetry breaking of a complex scalar field. They might have been formed at a grand unification transition, or, conceivably, much later, at the electroweak transition, or somewhere in between[Kibble, 1976][Hindmarsh and Kibble, 1995]. They exist in the vacuum

background and are yet to be detected. We will learn more about such defects in the next chapter.

Chapter 4

Kibble-Zurek Mechanism

The divergence of τ_{eq} implies that at the critical point no part of the system can ever come to an equilibrium in a finite amount of time as fluctuations would heavily dominate the system. We know that there are statistical fluctuations present in a system and when the system approaches T_c, the correlation length scale of such fluctuations become infinite[Kardar, 2007]. This divergence of correlation length reflects the fact that as the system crosses the critical point, the order parameter should acquire a finite non-zero value in the entire system.

In chapter 2, we saw that the dynamics of a field $\vec{\Phi}$ critically slows down when the system approaches T_c from above. This chapter shows the implications of this phenomenon when an initially out of equilibrium system crosses its critical point at a finite rate. This transformation of our system can be carried out by the variation of some thermodynamic variable, called control parameter.

4.1 The Mechanism

The essence of KZM can be seen in the steps below:

- Choose a system of interest, which is initially in equilibrium in the symmetric phase and significantly far away from the critical point.
- Pick a thermodynamic control parameter, $g(t)$, that we wish to slowly vary in order to make the system fall toward the the critical point, characterized by g_c. Here t stands for time and is scaled to zero at g_c, i.e. $g(0) = g_c$.
- Let the initial value of this parameter be g_0. In the beginning $g_0 > g_c$, but now we slowly anneal the system toward g_c. We focus on linear quenches

$$g(t) = g_c(0)\left(1 - \frac{t}{\tau_Q}\right) \tag{4.1}$$

Let's choose the starting point as $g_0 = g\left(t = -\tau_Q\right) = 2g_c$ where τ_Q is the time for which the quench is performed. Far from g_c the equilibrium relaxation time, τ_{eq}, is barely larger than the microscopic time (average time over which a particle experiences collision). Thus, for small annealing rate, i.e., very long τ_Q, the system evolves adiabatically and remains in equilibrium as we change $g(t)$. However, this regime must inevitably break down since τ_{eq} diverges at the critical point[Biroli et al., 2010][Del Campo and Zurek, 2014].

KZM claims that the end of the adiabatic regime occurs when the time, t, required for the system to reach g_c becomes smaller than $\hat{\tau_{eq}}$, the time it requires at the freeze-out instant, $\hat{t}$, to reach equilibrium. This is certainly a lower bound on the value of t. The system maintains its adiabatic nature only if it has sufficient time to equilibrate inside the interval over which $g(t)$ changes from one value to another. But once $\hat{t}$ is reached, even the particular configuration of the system at $\hat{t}$ won't be able to equilibrate even in the total remaining time.

Since after crossing $\hat{t}$ the system fails to attain equilibrium, hence the order parameter would cease to evolve over larger regions and different domains with a different independent value of the order parameter would be locked in place. The regime below $\hat{t}$ is called impulsive regime and the time, $\hat{t}$, separating these two regimes is called freeze-out time.

4.2 Some Quantitative results of KZM

In chapter 2, we showed that a second order phase transition is characterized by the power-law divergence of the correlation length, ξ, and relaxation time, τ, at the critical point, defined as

$$\xi(\varepsilon) = \frac{\xi_0}{|\varepsilon|^v} \tag{4.2}$$

and

$$\tau(\varepsilon) = \frac{\tau_0}{|\varepsilon|^{zv}} \tag{4.3}$$

Here v and z are the dynamic critical exponents, which depend only on the universality class of the transition, while ξ_0 and τ_0 are constants determined by the microscopic properties of the specific system. From these quantities, one can estimate the characteristic speed of perturbations of the order parameter in the system as

$$v = \frac{\xi}{\tau_{eq}} = \frac{\xi_0}{\tau_0}|\varepsilon|^{v(z-1)} \tag{4.4}$$

For a linear quench in time, substituting the reduced temperature,

$$\varepsilon = \frac{g_c - g}{g_c} \tag{4.5}$$

in Eq. (4.1) and assuming the control parameter $g(t)$, to be temperature, we get

$$\varepsilon(t) = \frac{t}{\tau_Q} \tag{4.6}$$

and

$$\frac{\Delta\varepsilon}{\Delta t} = \frac{\varepsilon}{t} = \dot{\varepsilon}$$

The quench parameter $\dot{\varepsilon}$ defines the rate at which a phase is crossed and is called the quench rate. Substituting for ε from Eq. (4.6) into the above equation gives,

$$\dot{\varepsilon} = \frac{1}{\tau_Q} \tag{4.7}$$

Hence the rate at which the temperature of our system changes ($\dot{\varepsilon}$) is characterized by τ_Q. Freeze-out happens when

$$\tau(\hat{t}) = \hat{t} \tag{4.8}$$

and on comparing Eq (4.6) and Eq. (4.7), we get

$$\tau(\hat{t}) \sim \left| \frac{\varepsilon(\hat{t})}{\dot{\varepsilon}(\hat{t})} \right| \tag{4.9}$$

The relaxation time at the freeze-out can be expressed as

$$\hat{\tau} = \tau(\hat{\varepsilon}) = \frac{\tau_0}{|\hat{\varepsilon}|^{vz}} = \frac{\tau_0 \tau_Q^{vz}}{|\hat{\mathrm{t}}|^{vz}} \tag{4.10}$$

From our earlier definition $\tau(\hat{t}) = \hat{t}$, hence $\hat{t}$ should also depend on the parameters like v, z, t, τ_0 introduced above. In fact, if we substitute $\hat{t}$ for $\hat{\tau}$ in the above equation, then we find that

$$\hat{t} \sim \left(\tau_0 \tau_Q^{zv}\right)^{\frac{1}{1+zv}} \tag{4.11}$$

Since $\hat{t}$ determines the freeze-out time, hence the dynamics of our system should be frozen in the region $-\hat{t} < t < \hat{t}$ and should restart once the $t = -\hat{t}$ is crossed.

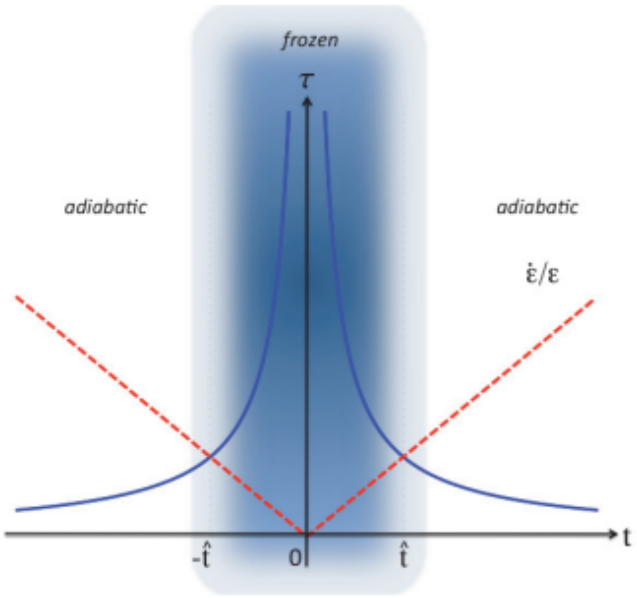


Figure 4.1: Picture shows relaxation time as a function of quench time. The transition from the adiabatic to impulsive regime corresponds to the instant when the straight line $\hat{\tau} = \hat{t}$ (red), intersects the blue curve. Due to the divergence of the equilibrium relaxation time, in the interval around the critical point $[-\hat{t}, \hat{t}]$ where the dynamics is frozen, the order parameter of the system ceases to follow the equilibrium expectation value and enters an impulse stage.

KZM predicts that the average domain size at the freeze-out is limited to the length of $\xi(\hat{\varepsilon})$ and explicitly given by

$$\xi = \xi(\hat{\varepsilon}) = \frac{\xi_0}{|\varepsilon|^v} = \xi_0 \left(\frac{\tau_Q}{\tau_0}\right)^{\frac{v}{1+zv}} \tag{4.12}$$

The density of defects n created in the system is given by

$$n \sim \frac{\xi^d}{\hat{\xi}^D} \tag{4.13}$$

where D is the dimension of our system and d is the dimension of the defect created. KZM predicts that n would scale with the quench time τ_Q as a power law,

$$n \sim \frac{1}{\xi_0^{D-d}} \left(\frac{\tau_0}{\tau_Q}\right)^{(D-d)\frac{v}{1+zv}} \tag{4.14}$$

$$\implies n \sim \left(\frac{\tau_0^{(D-d)\frac{v}{1+zv}}}{\xi_0^{D-d}}\right) {\tau_Q}^{-(D-d)\frac{v}{1+zv}} \tag{4.15}$$

More generally KZM predicts that for every continuous phase transition the defect density should scale as

$$n \propto \tau_Q^{-\alpha} \tag{4.16}$$

where α is another critical exponent, depending on the universality class of the underlying system[Zurek, 1996][Del Campo and Zurek, 2014]. The figure below demonstrates this relation of defect density on the quench rate.

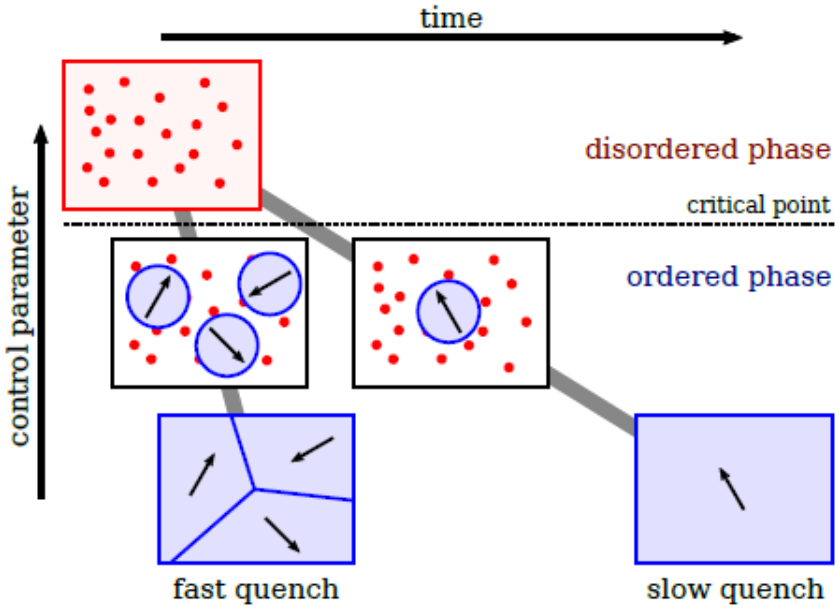


Figure 4.2: In this picture, an initially symmetric system, experiences a continuous phase transition when a control parameter is reduced below its critical value. Due to the finite speed of causality, different independent domains choose random orientation of the order parameter, represented with arrows. The size of the domains is a function of the quench rate.

Chapter 5

Software Implementation Results

5.1 Some Final Comments

We studied in the last chapter that a finite quench leads to the formation of topological defects in our system once the transition temperature is crossed. In essence some defects can decay over time but not all. In this chapter, we would like to see qualitatively, how such a quench could lead to the formation of vortices. This would be analogous to the vortex lines and flux tubes studied earlier. It's also believed that this should also be true for a cosmic phase transition leading to the formation of cosmic strings which are defects in the vacuum. To demonstrate this we take the help of computer simulations.

Topological defects have been observed in the lab as well. Experimental results also reproduce a similar power-law dependence of the defect density on the quench rate. For more information: [Hendry et al., 1994][Kibble, 2007][Dodd et al., 1998][Hendry et al., 2000].

5.2 Simulations

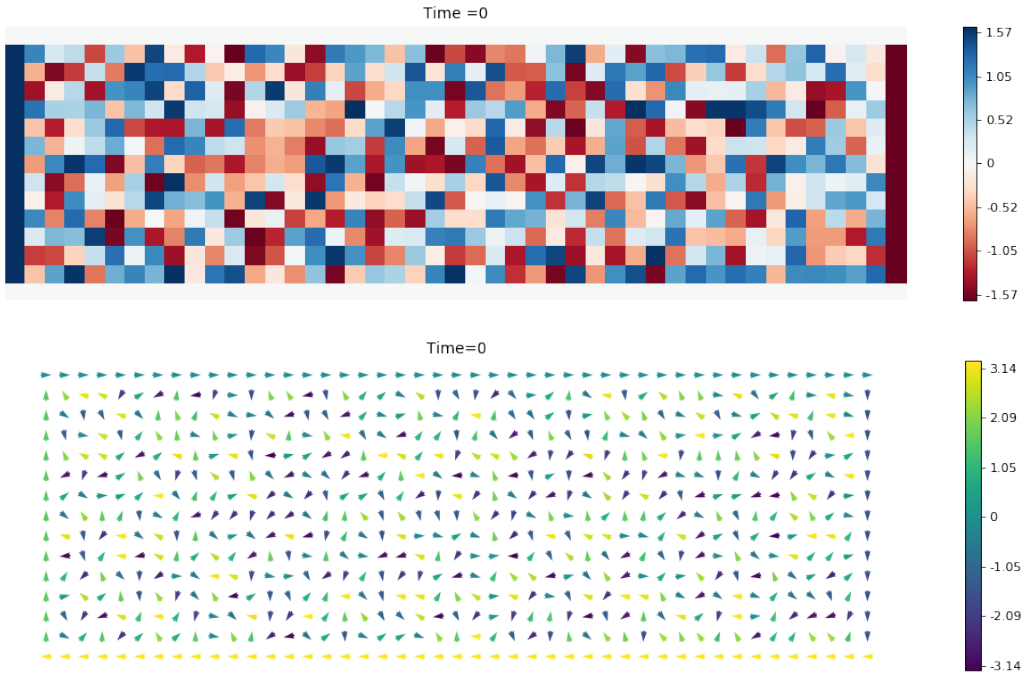
Here we envisage KZM in thin (2D) films. In these calculations, we simulate a system of magnetic spins on a 2D lattice which is one dimension lower than a 3D lattice. In short-range interacting systems, two dimension is the lower critical dimension where continuous symmetry breaking is not able to occur, as stated by the Mermin Wagner theorem [Nui et al., 2018]. However, it is the marginal dimension where one can still observe topological changes [Yates and Zurek, 1998]. In addition, 3D magnetic systems are known to have phase transition properties identical to those of the superfluid/superconductor transition. This analogy is justified since they fall in the same universality class of 3D XY model. So studying defects in one system of this universality class (here a magnetic system), could reveal the behavior of defects in the others.

These simulations we carried out on a $45*15$ rectangular and a $25*25$ square lattice using Metropolis algorithm [Murthy, 2004]. Here each cell on the lattice represents a magnetic spin. We start in the symmetric phase (above the phase transition point) and perform moves as required by the Metropolis algorithm. This tiny lattice mimics what happens at the boundaries during a phase transition, where different domains with different values of order parameter meet. We fix the order parameter on the boundaries of the lattice and let the system free to evolve on the inside. Different boundary condition leads to the formation of defects in our system as shown below

In these figures, we select one spin on the lattice randomly and change its angle θ (with respect to the x-axis) to any new random value. We accept the new orientation of the

spin if it satisfies the Metropolis condition, else reject it. This entire two-step process of selecting and changing the orientation of a random spin and then either accepting or rejecting it, constitute one Monte Carlo Step (MCS). In a single MCS, the system switches from the current state to a next state. A consecutive set of V numbers of MCS constitutes one Monte Carlo Step per Spin (MCSS) also called Monte Carlo Sweep. The time on the top of the images corresponds to the number of MCSS of the lattice performed by the algorithm. Each sweep consist of $45 * 45$ MCS on a rectangular lattice and $25 * 25$ MCS on a square lattice. After performing a sufficient amount of sweeps, we observe the emergence of vortex like structure in the lattice under consideration. The numbers on the color bar on the right-hand side of the images corresponds to angle θ (in radians) of the spins on the lattice.

Similar dynamics carried out using Creutz algorithm as well as some animation showing the spin dynamics in action (using both Metropolis and Creutz Algorithm) can be found here[1] . The main difference between Metropolis and Creutz algorithm lies in the fact that Metropolis treats the lattice as a canonical ensemble, assuming that the system is in contact with some heat-bath and hence maintains a constant temperature while Creutz algorithm assumes the lattice as a micro-canonical ensemble, where the system is considered isolated from its surrounding and hence maintains a fixed value for its energy [Creutz, 1983].



[1] The code used to generate the below pictures is also available here: https://drive.google.com/drive/folders/1fXbw0OcP-y1dDzazXz3vsRjvWkbidutv?usp=sharing

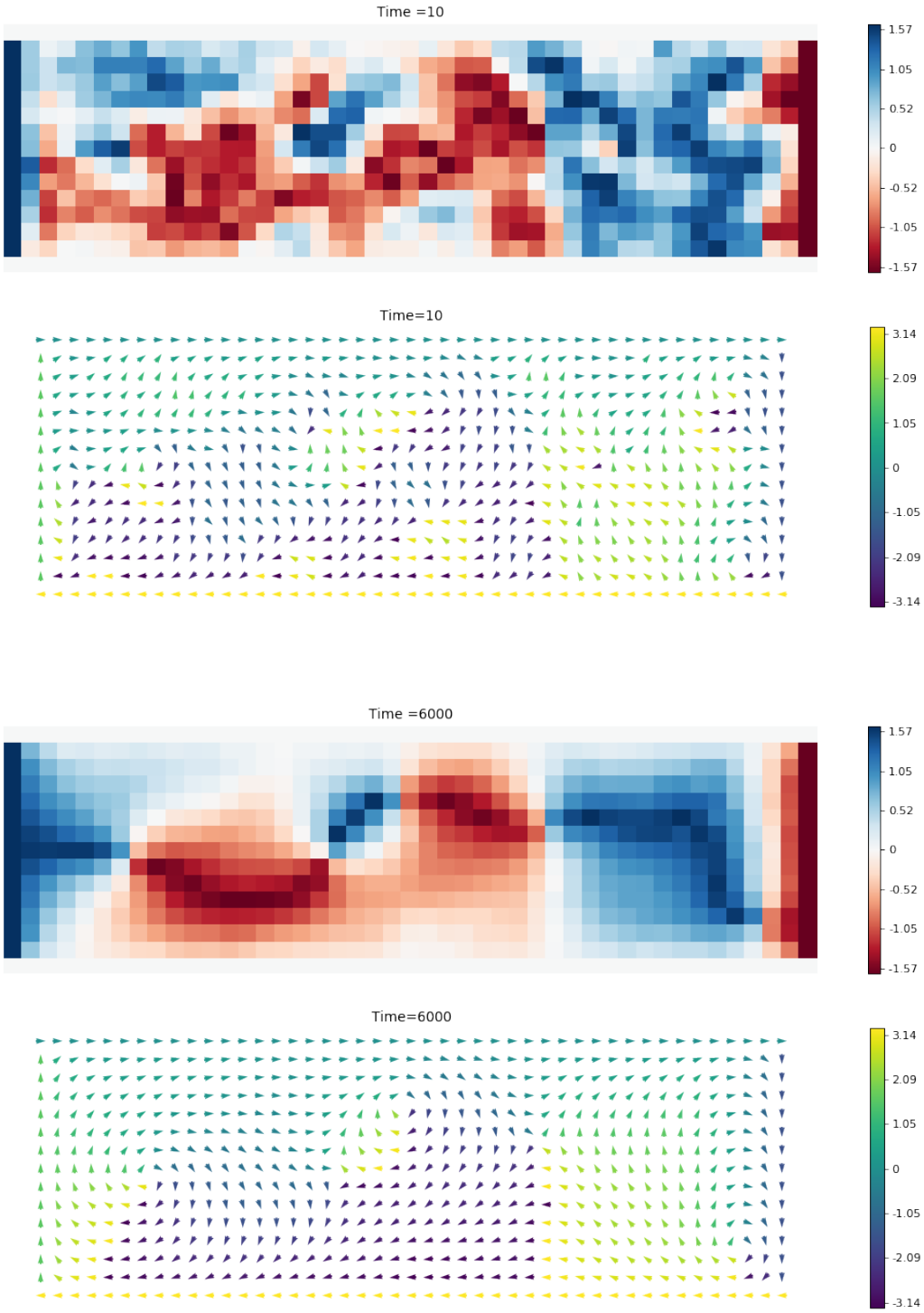
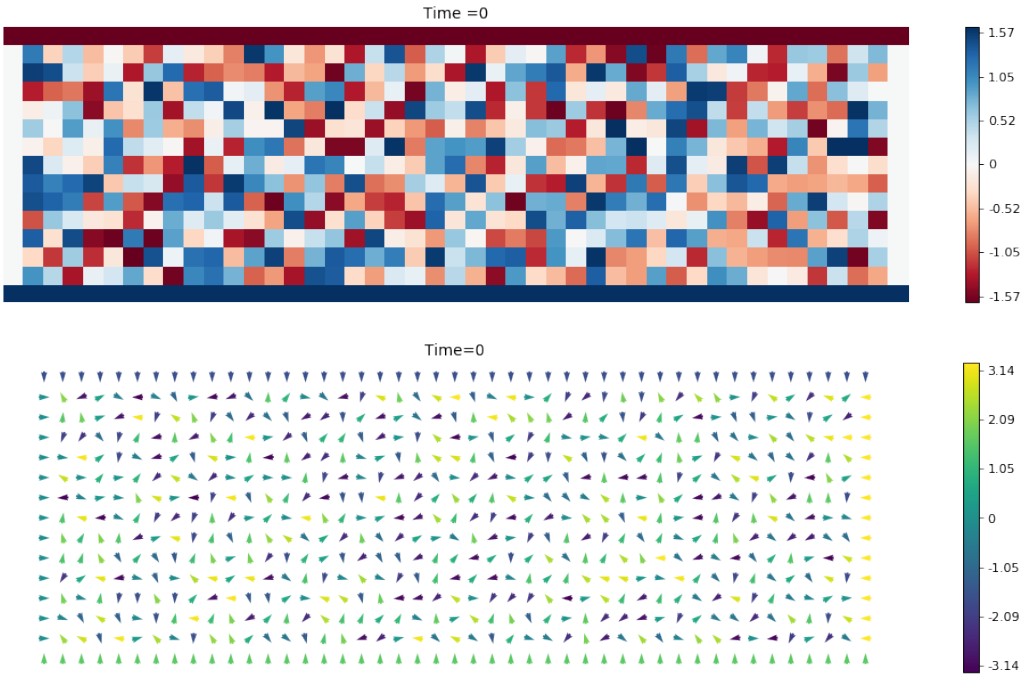


Figure 5.1: Above three figures show the dynamics of magnetic spins on a 2D lattice for a *clockwise boundary condition*. Initially, at time = 0, the spin configuration on the inside of the lattice is random. This could be thought as the system being in its symmetric phase, yet to undergo a phase transition. Now if the domains on the boundaries of this lattice acquire some fixed spin orientation (clockwise in this case) then the inner spins start to orient themselves with their nearest boundaries. This eventually leads to the formation defects (vortices with $n_w = 1$) since the boundary conditions on different sides are different.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0.52
0
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-1.57
Time=0
3.14
2.09
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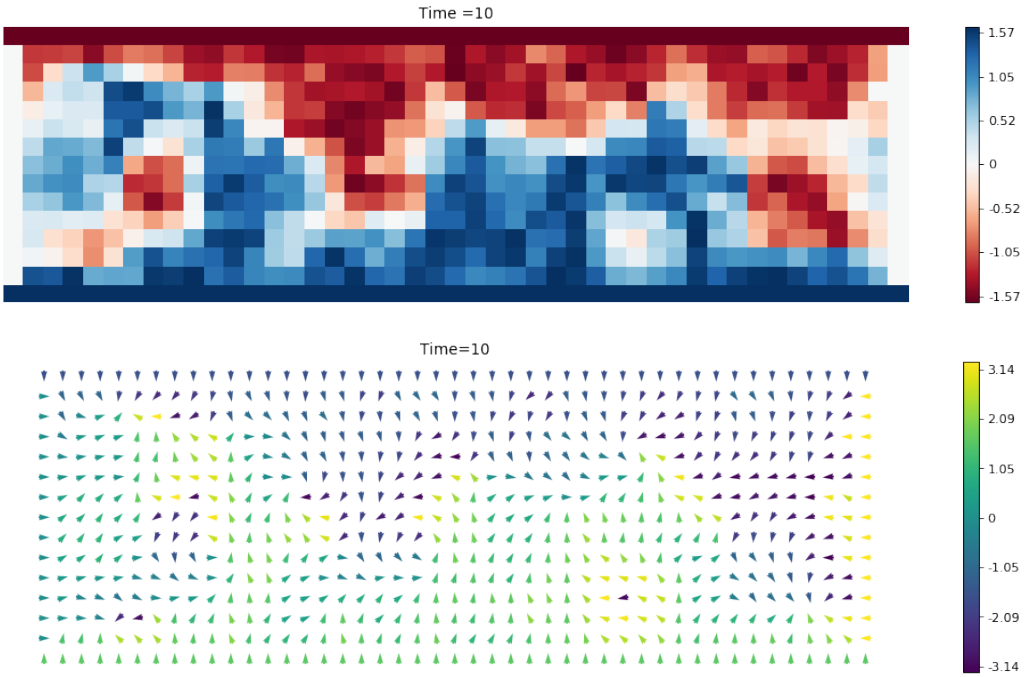
-2.09
-3.14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-2.09
-3.14

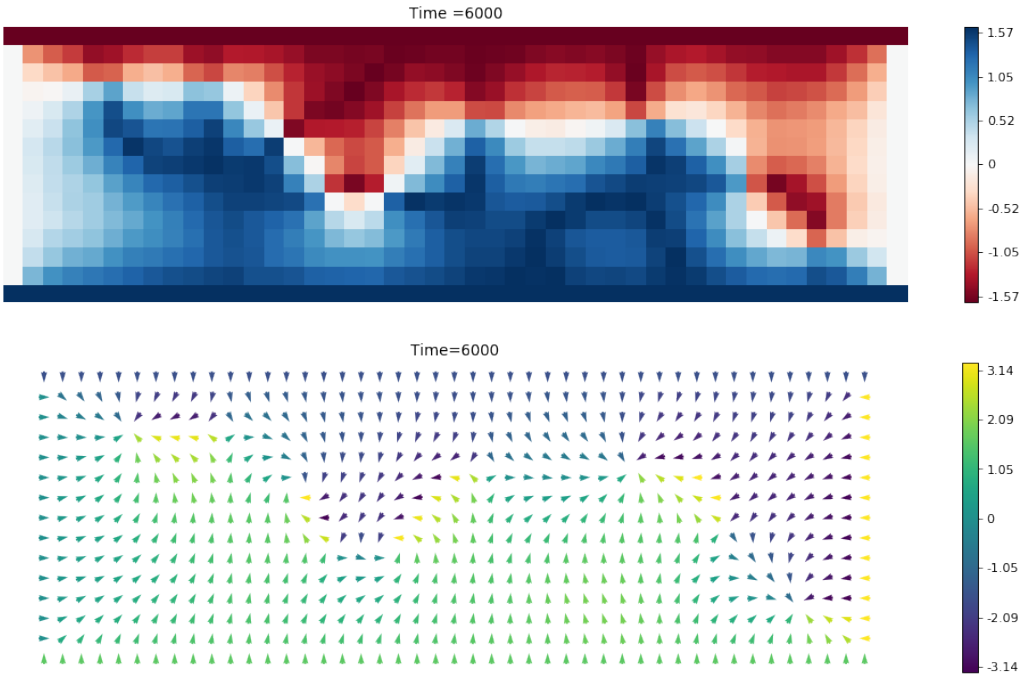
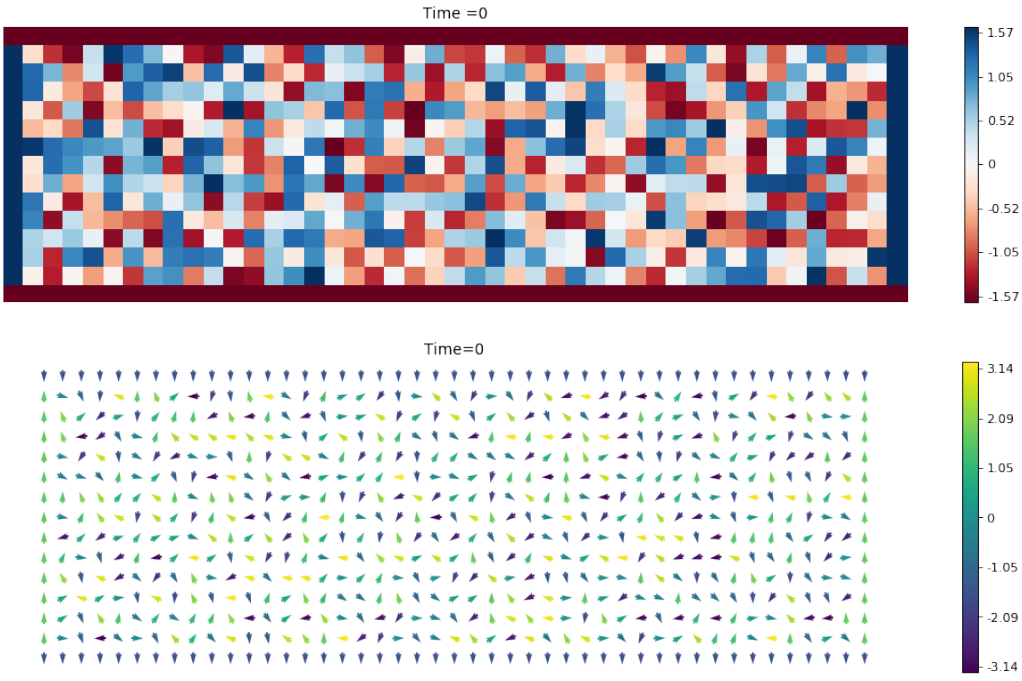


Figure 5.2: The above three figures show the spins behavior for an *inflowing boundary condition*. Again the inner spins orient themselves with their nearest boundaries and the place where these differently oriented spins meet lead to the formation of defects (vortices with $n_w = -1$).



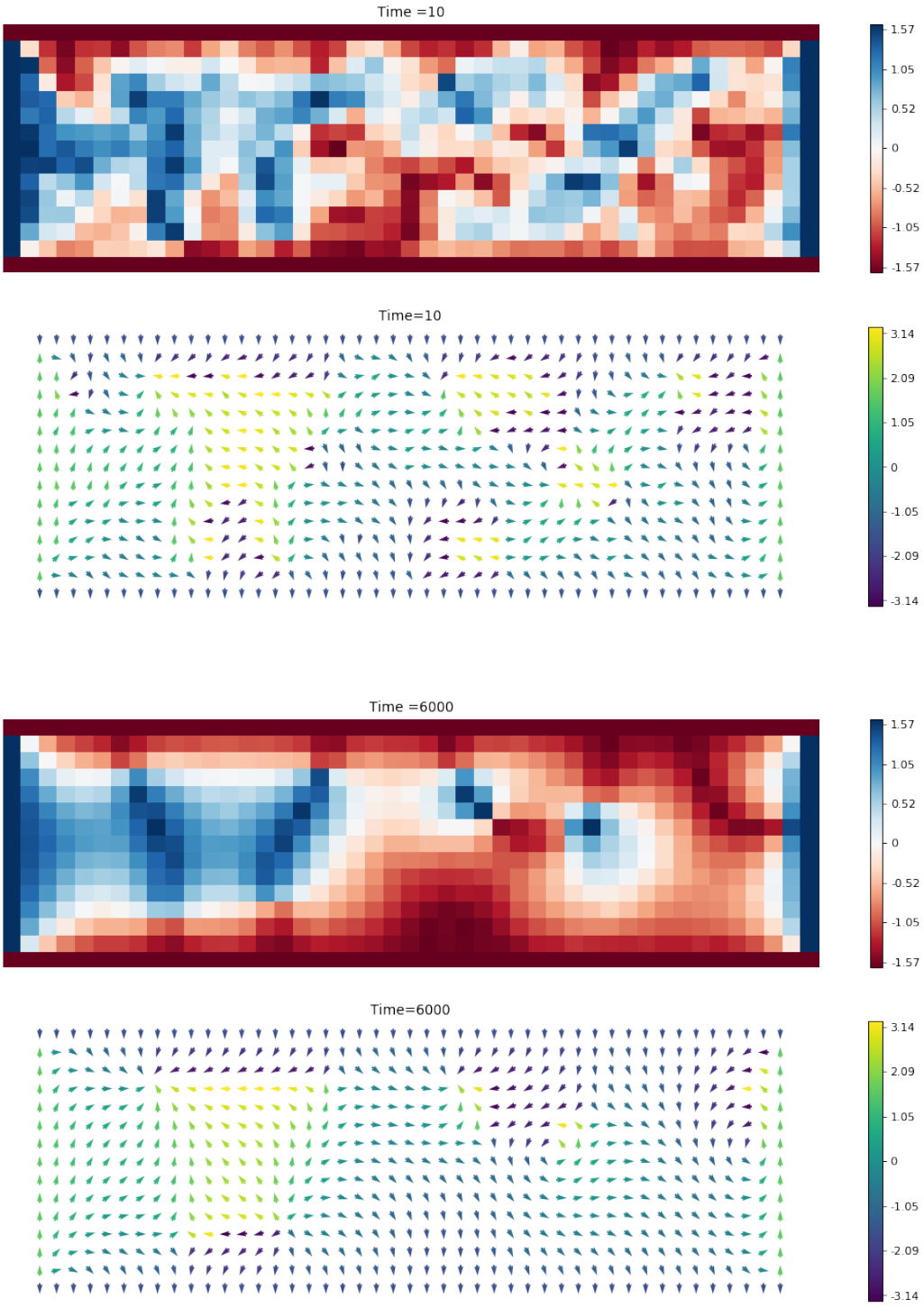
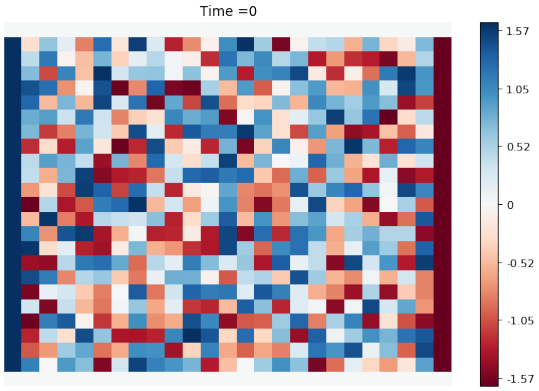


Figure 5.3: The above three figures show the spins behavior for a *Periodic boundary condition*. Again the inner spins orient themselves with their nearest boundaries and the place where these differently oriented spins meet lead to the formation of defects (vortices with $n_w = \pm 1$).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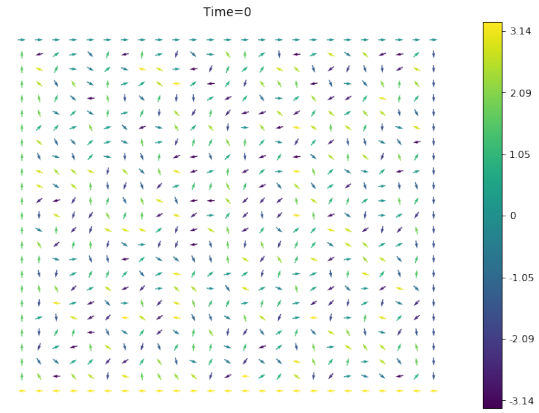
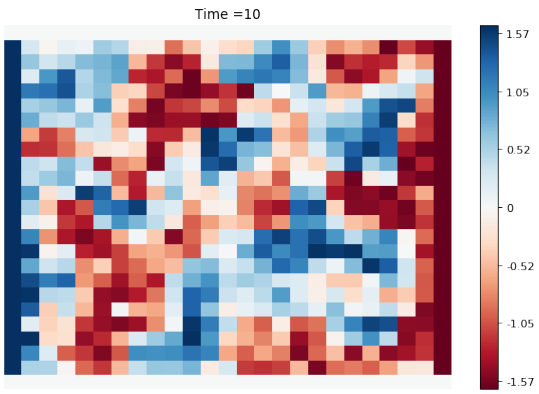
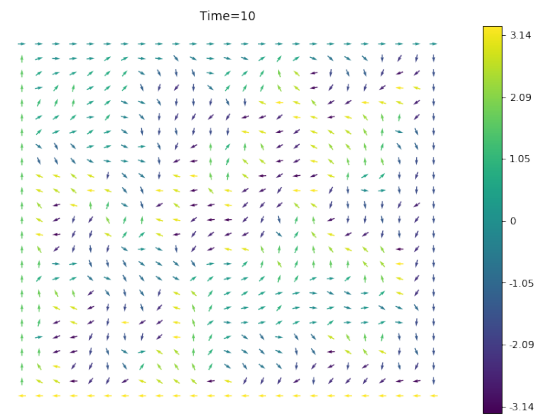
1.57
1.05
0.52
0
-0.52
-1.05
-1.57


Time=0
3.14
2.09
1.05
0
-1.05
-2.09
-3.14


Time =10
1.57
1.05
0.52
0
-0.52
-1.05
-1.57


Time=10
3.14
2.09
1.05
0
-1.05
-2.09
-3.14

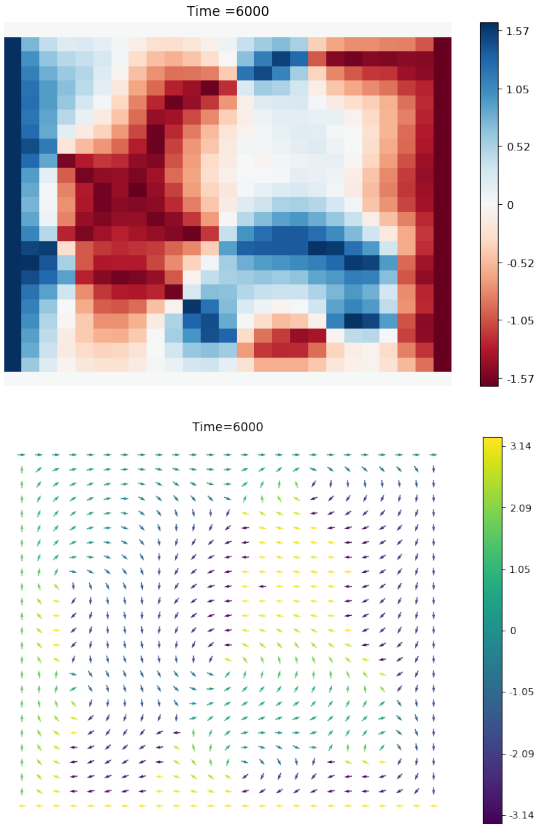
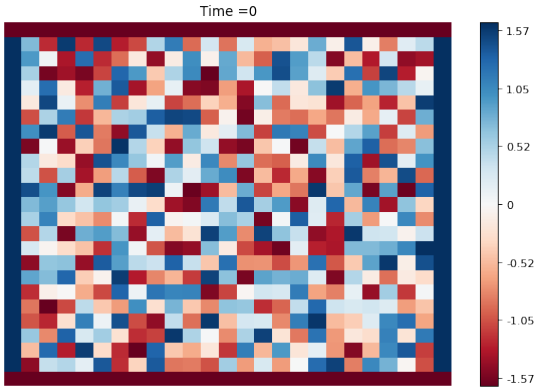
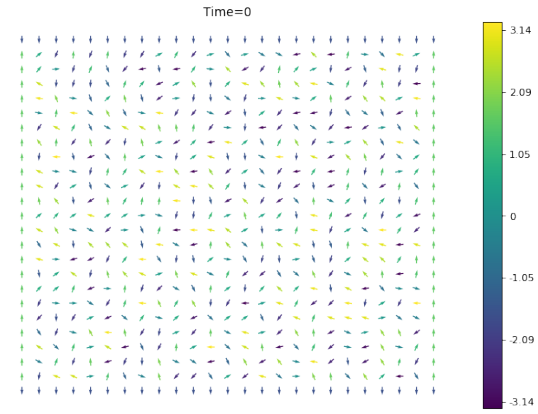
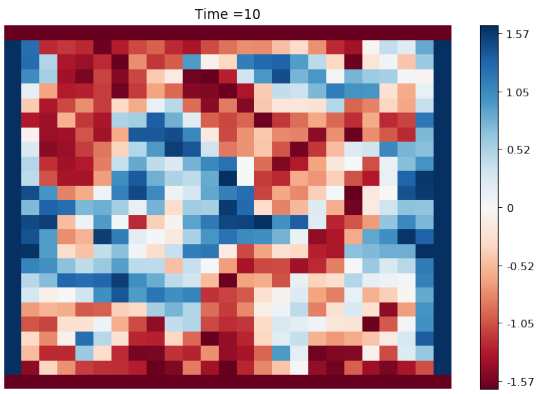
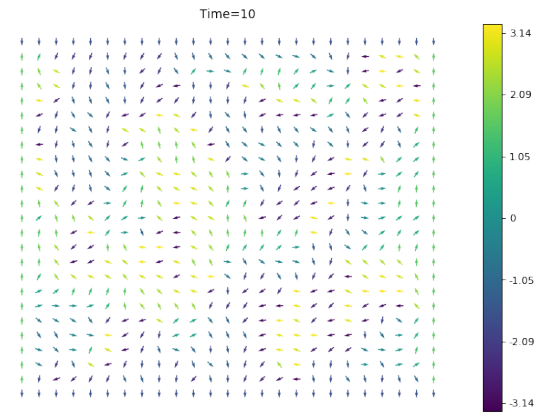


Figure 5.4: The above three figures show the spins behavior for a *Clockwise boundary condition* but now on a square lattice. Once again the inner spins orient themselves with their nearest boundaries and the place where these differently oriented spins meet lead to the formation of defects. Here we can find vortices with both $n_w = 1$ and $n_w = -1$. It is believed that if we wait for a sufficiently long time then the vortex-antivortex pair would annihilate each other and ultimately only vortices with $n_w = 1$ would be left.


Time =0
1.57
1.05
0.52
0
-0.52
-1.05
-1.57


Time=0
3.14
2.09
1.05
0
-1.05
-2.09
-3.14


Time =10
1.57
1.05
0.52
0
-0.52
-1.05
-1.57


Time=10
3.14
2.09
1.05
0
-1.05
-2.09
-3.14

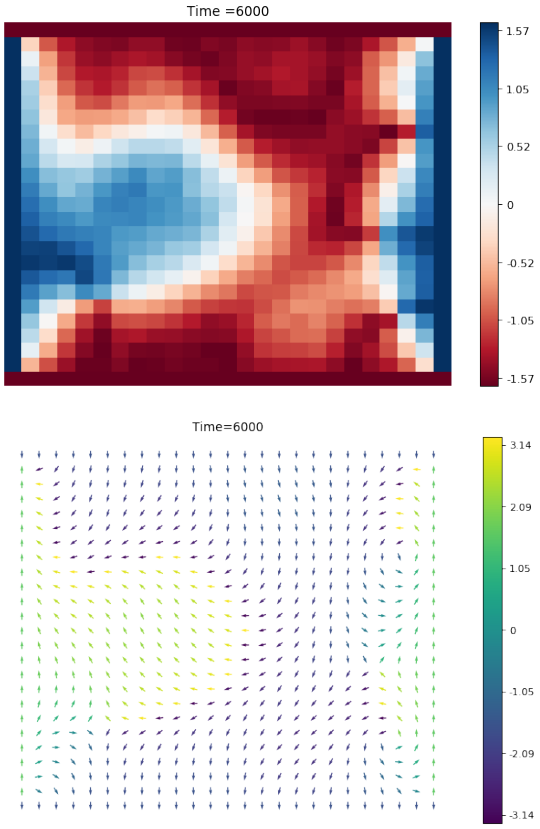


Figure 5.5: The above three figures show the spins behavior for a *Periodic boundary condition* on a square lattice. Here we see vortices with $n_w = \pm 1$.

5.3 Conclusion

In this dissertation, we discussed the Kibble-Zurek mechanism essentially from a condensed matter viewpoint. It was shown that isolated systems undergoing a continuous phase transition would experience a spontaneous symmetry breaking which would lead to an emergence of order. We described the non-equilibrium dynamics of a system and derived the phenomenon of critical slowing down in the vicinity of the critical point due to the divergence of the relaxation time. The consequence was that our system formed different independent domains with different order. This lead to the formation of defects at the boundaries where these different domains meet. We showed that KZM predicts the typical size of domains in the broken symmetry phase to be fixed and the defect density follows have a power law dependence on the quench rate. Finally, we investigated KZM in thin magnetic films and saw how different boundary condition could lead to the formation of defects (vortices) in these 2D magnetic spin systems.

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