Topological defects in cosmology

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Abstract

In this dissertation I study topological defects by performing numerical simulations of classical scalar field theories in one spatial dimension. I devise three methods of counting defect densities and run multiple simulations to find out how different counting methods compare. I discover a difference that might help in the interpretation of future simulations of topological defects. I also run multiple simulations with varying parameters to see how the density of topological defects changes under different conditions. With this data I observe that a low rate of energy damping will have interesting and surprising effects on the defect density.
Introduction

The standard theory of beginning of the Universe is the so called Hot Big Bang model. This theory stipulates that all matter and space was at the beginning of time compressed to an extremely small and extremely hot point and that this point started to expand and cool. In the very early state of the Universe, the energy density was so enormous that all interactions were indistinguishable from each other. Approximately $10^{-38}$ seconds after the Big Bang a phase transition occurred, triggered by the dilution of the energy density, causing gravity to separate from rest of the interactions. The Universe kept expanding and cooling and $10^{-36}$ seconds after the Big Bang the strong interactions separated from the electroweak interactions and phenomenon known as cosmic inflation happened. This phase transition separating the strong interaction from the electroweak interaction should have created a large number of magnetic monopoles and anti-monopoles. Because monopoles/anti-monopoles can only be destroyed through annihilation and have quite large mass it would have caused Universe to collapse back in to single point. To dilute the gravitational effect of monopoles/anti-monopoles it is necessary to introduce cosmological inflation to the model. There are other motivations for adding cosmological inflation to the Hot Big Bang model aside for the magnetic monopoles. For example the curvature of space seemed to be very close to zero (known as the flatness problem) and different regions in the Universe that should not be able to interact with each other have the same temperature and other physical properties (known as the horizon problem). A Big Bang model with inflation does not have these problems [1]. As it took place, the volume of the Universe grew at least a factor of $10^{26}$ while particles were constrained to propagate only at the speed of light. After inflation, the volume of the Universe continued to grow but at a slower rate. $10^{-12}$ seconds after the Big Bang electromagnetism and weak interactions became separate forces. At this point the four interactions as we know them had come to be and the Universe was filled with a quark-gluon plasma. $10^{-6}$ seconds after the Big Bang the Universe had cooled enough to allow hadrons to be formed. Hadron/anti-hadron pairs kept forming until 1 second after the Big Bang leaving a net density of hadrons. Similarly lepton/anti-leptons kept forming until 10 seconds after the Big Bang leaving a net density of leptons. During the next 380,000
years the Universe would go from energy-dominated to matter-dominated as first nuclei would start to form and later atoms. The last moments of this last epoch of the Big Bang can still be seen as the Cosmic Microwave Background. This was followed by a radiation-dominated and later matter-dominated Universe in which stars and galaxies started to form (possibly by influence cosmic strings) and finally the epoch in which we still find ourselves. The exact number and nature of the phase transitions that happened during the Big Bang is not certain but most likely they were second-order in nature. There might have been numerous other transitions that had no inflationary or topological effects.

The latest major change to the narrative of the beginning of the Universe is the cosmological inflation which is needed among many things to counter the gravitational effects of monopoles/anti-monopoles. What causes monopoles/anti-monopoles to be created is the Kibble-Zurek mechanism (KZM) formulated by T. W. B. Kibble [2] and further refined by W. H. Zurek [3]. In essence the KZM means that when a system experiences spontaneous symmetry break topological defects will be formed and such defects have been observed in experiments done with supercondutors, superfluids and liquid crystals. I will describe the KZM in greater detail in section after this introduction.

In addition to magnetic monopoles/anti-monopoles there are a number of possible topological defects that KZM can create: cosmic strings, domain walls, solitons, Skyrmions and textures. These defects might have had significant effect in the evolution of the early Universe and formation of large cosmic structures. Cosmic strings are the only topological defects that are expected to be found in astronomical observations. Magnetic monopoles are so small and so rare that it will be virtually impossible to find in the Universe outside, possibly, accelerator experiments. Domain walls can not have persisted beyond the recombination because they would create unacceptable gravitational effects. Textures are not localized similarly to other defects and are unstable and unlikely to be ever found. Solitons have been found and Skyrmions have been reported in some experiments done in laboratories but none in experiments regarding cosmology or in particle accelerators.

A cosmic string is a one dimensional structure that is extremely thin, less than a trillion times smaller than the radius of a hydrogen atom and yet 10 km length of one such string will weigh as much as the Earth itself. They are "infinitely" long or form closed loops meaning that cosmic strings cannot end. Given that cosmic strings may have formed very early in the history of the Universe, they may have been the initial seed for the formation of large structures in cosmology and possibly could be the answer for the horizon problem. Cosmic strings are the defects that seem to be easiest to detect because their enormous density should produce gravitational lensing. However, there are expected to be very few cosmic strings in the observable Universe, one per Hubble volume [4], making the task very difficult indeed.
In this dissertation I use a one dimensional classical lattice field simulations to find the density of topological defects in a generic symmetry breaking phase transition. The usual method for counting defects, which I shall refer as "propagator" method, is to assume that the field is Gaussian and zeros in the field represent defects and derive from this the density of defects [5, 6]. The problem with this approach is that defects are non-linear objects and their presence makes the field non-Gaussian, invalidating the original assumption. Numerical simulations confirm this [7]. Instead of the propagator method I will use a method that uses the field correlator to find the density of defects in the simulations and two other methods that simply go through the data produced by the simulations and count each defect individually. Having multiple methods of finding defect density allows me to compare them and find any possible discrepancies in the results they give. This information could be useful in simulations in which it is not possible or feasible to count each defect separately such as quantum mechanical simulations or very large simulations. Usefulness of finding the topological density itself lies in that it seems to be a universal constant regardless of system [8] including our Universe. Since cosmic strings could have such a significant impact on the evolution of the Universe this number could be useful constraint when creating future models for the Universe.

In the first chapter I go through of all textbook theory regarding one dimensional field and defects needed to understand the model I am simulating, the model itself being a 1+1 dimensional scalar field theory with O(N) symmetry. In the second chapter I derive three methods for finding defects in the simulation data. In the third chapter I describe the simulations themselves and go through the immediate results. In the fourth chapter I discuss the results of the simulations and suggest future simulations in order to study this subject further. In the Appendix are exact results of simulations, more detailed derivation of certain equations and the simulation code written in pseudo-code.

**Kibble-Zurek mechanism**

According to Kibble [2], if the Hot Big-Bang model of the Universe is true, a number of finite temperature symmetry breaking phase transitions may have taken place. Because of causality and the finite speed of light, a domain structure can be expected to have arisen as a result. Depending on symmetry that has been broken, these domains may subsequently evolve into domain walls (2-dimensional defects in 3 spatial dimensions), cosmic strings (1-dimensional), monopoles (0-dimensional) or textures (not localised in space).

In the context of condensed matter experiments Zurek [3] developed a general model for the topological defect formation and later applied this to
Cosmology. According to his model the characteristic correlation length $\hat{\xi}$ should be order of

$$\hat{\xi} = \left(\frac{2\Delta M_{PL}}{T_c}\right)^{1/3} \cdot \frac{1}{\beta^{1/3} T_c}$$

where $T_c$ is the critical temperature at which the second-order phase transition happens, $M_{PL}$ is the Planck mass, $\beta$ is the coupling coefficient from a Landau-Ginzburg model

$$V(\phi) = \alpha (T - T_c)|\phi|^2 + \frac{1}{2} \beta |\phi|^4$$

and $\Delta$ depends on the effective number of different spin states $s$ of relativistic particles $\Delta = 1/(4\pi) \sqrt{45/(\pi s)}$. Here I can use quench time\(^*\) $\tau_Q$ since it obeys following relation $\tau_Q = 2\Delta M_{PL}/T_c^2$ which gives me

$$\hat{\xi} = \frac{1}{\beta^{1/3} T_c^{2/3}} \cdot \tau_Q^{1/3}.$$

Because there is a link between the correlation length and the density of defects a similar power law relation will apply to the density of defects also. A more detailed derivation for the characteristic correlation length can be found in Appendix B.

The fact that in a symmetry breaking transition topological defects will form in combination with a qualitative predicting power regarding the density of defects, constitutes the Kibble-Zurek mechanism. In addition to assuring the formation of defects it predicts that the density of topological defects will obey a power law

$$n \propto \tau_Q^{-\sigma}$$

where $n$ is the density of defects, $\tau_Q$ is the quench time and $\sigma$ is a universal constant. A lot of work has gone to try to pin down $\sigma$, but what happens is that theoretical approaches give (depending on the model) $\sigma = 1/3$ or $1/4$ while numerical simulations give $\sim 0.3$.

\(^*\)See Chapter 1 for better definition of the quench time.
Chapter 1

Topological defects

Although topological defects can have multiple dimensions for the sake of simplicity I will only be interested in one dimensional simulations of domain walls. As seen in figures 1.2 and 1.4 domain wall is a defect that separates two different regions with different vacua. This kind of one dimensional defect is stable but may be annihilated if it encounters a defect with opposite configuration (see figure 1.1 for visual example).

I start by normalizing constants as $\hbar = c = k_B = 1$ which means that mass $\mu$ and momentum $k$ are in units of $[\text{energy}]$, time $t$ and space $x$ are units of $[\text{energy}]^{-1}$, coupling constant $\lambda$ and potential fields $V_{\text{ini}}$ and $V$ are in units of $[\text{energy}]^2$ and the action $S$, field $\phi_a$ and correlator $G$ are dimensionless. However, in chapter 2 I Fourier transforming the correlator from position space ($G = \langle \phi^2(x) \rangle$) to momentum space ($G = \langle \phi^2(k) \rangle$) which changes the correlator from being dimensionless to being in units of $[\text{energy}]^{-1}$. In order to find a mathematical model for domain wall I consider a classical theory of $N$ real scalar fields $\phi_a$ with $a \in \{0, ..., N-1\}$ in 1+1 dimensions. With $V(\phi_a)$ as potential I get the O(N) symmetric continuum action

$$S = \int dx dt \left( \frac{1}{2} \partial_\mu \phi_a(x,t) \partial^\mu \phi_a(x,t) - V(\phi_a(x,t)) \right). \tag{1.1}$$

To investigate dynamics of the system I have a simple setup in which the potential varies with time. Initially, it corresponds to free field with mass $\mu$,

$$V_{\text{ini}}(\phi_a) = \frac{1}{2} \mu^2 \phi_a \phi_a, \tag{1.2}$$

and at the moment $t = 0$ this changes to

$$V(\phi_a) = -\frac{1}{2} \mu^2 \phi_a \phi_a + \frac{\lambda}{24N} (\phi_a \phi_b)(\phi_b \phi_a). \tag{1.3}$$

This instantaneous change triggers a symmetry break transition. In practice, the simulations start at $t = 0$, with initial conditions mimicking a quantum vacuum in the pre-quench potential (1.2), i.e. around $|\phi| = 0$. 


I need to add a small damping term $\Gamma \partial_t \phi$ to the equation of motion giving

$$\partial_t^2 \phi_a(x, t) + \Gamma \partial_t \phi_a(x, t) - \partial_x^2 \phi_a(x, t) - \mu^2 \phi_a(x, t) + \frac{\lambda}{6N} (\phi_b \phi_b) \phi_a(x, t) = 0. \quad (1.4)$$

Adding of a constant damping term ensures the freeze-in of defects and prevents finite-temperature restoration of symmetry (without damping, energy is conserved). It also ensures that the system will eventually reach zero temperature state. The importance of damping in defect formation can be clearly seen in figure 3.1 depicting evolution of similar simulations that I will use. This importance also makes the damping term a useful parameter to manipulate when running simulations. This will be shown in chapter 3.

I will concentrate on the case $N = 1$, for which the minima of the potential are

$$\phi_0(\pm \infty) = \pm v = \pm \mu \sqrt{\frac{6}{\lambda}}. \quad (1.5)$$

Assuming that $\phi_0(-\infty) = -v$ and $\phi_0(\infty) = v$ then a hyperbolic tangent satisfies the equation of motion for $\Gamma = 0$ and describe the one dimensional defect

$$\phi_{\text{defect}}(x) = v \tanh \frac{x}{d} \quad (1.6)$$

where $d = \sqrt{2}/\mu$ is the width of defect.

Special attention should be paid toward the mass term $\mu$ and the quench time $\tau_Q$ because in my simulations $\mu$ changes depending on $\tau_Q$ as time passes. The quench time is defined by time $t$, temperature $T$ and critical temperature $T_c$ as $\tau_Q = t \cdot T_c / (T - T_c)$. It is a relaxation time for the potential field $\phi$ and it determines the moment when the shape the field $\phi$ has reached its degenerate minimum form "W" (see figure 1.3) from its non-minimum "U". The quench time affects the mass term as follows:

$$\mu^2(t) = \mu^2(1 - 2t/\tau_Q), \quad t < \tau_Q$$
$$\mu^2(t) = -\mu^2, \quad t > \tau_Q. \quad (1.7)$$

Essentially what it means is that as time passes $\mu$ gets smaller and eventually changes sign and goes to $-\mu^2$ at $t = \tau_Q$. After that it stays at $\mu^2(t) = -\mu^2$.

*See appendix B for more detailed derivation.*
Figure 1.1: Here is a visualization of a annihilation of a topological defect. Time passes from top to bottom.
Figure 1.2: This graph depicts a one dimensional defect in \((\phi,x)\)-coordinates. It has width \(d\) and it goes from \(-v\) to \(+v\). This particular defect is a domain wall.

Figure 1.3: This graph depicts the potential. The two degenerate minima \(+v\) and \(-v\) are clear and separate as in figure 1.2. Depending on the quench time \(\tau_Q\) the potential wall between the minima can grow at different rates allowing \(\phi_a\) to change from one minima to the other at different rates. This makes the quench time very useful parameter to manipulate when studying formation of defects in simulations along with the damping term \(\Gamma\).
Figure 1.4: This graph combines perspectives of the two previous graphs giving a three dimensional\([(V(\phi), \phi, x)]\) depiction of potential field in its degenerate minimum. In addition to the potential \(V(\phi)\), the field \(\phi\) is depicted to have different values along the \(x\)-axis and forming a defect in the middle where it crosses from one minimum to the other.
Chapter 2

Methods for finding defects

Because my simulations are fully classical it will be easy to find defects in the field \( \phi_a \). One could simply examine the results of the simulations and count every time \( \phi_0 \) changes its value from \(-v\) to \(+v\) or vice versa or compare two adjacent points of \( \phi_0 \) and count a defect if their values differ too much from each other. Incidentally this is one of the methods that I will use with the results of my simulations, but the main method of counting defects will be based on the use of two-point correlator \( G_{ab}(x,y,t,t') = \langle \phi_a(x,t)\phi_b(y,t') \rangle \) which corresponds to an average over the whole system. In this correlator is encoded all information of the system and once I know what kind of effects topological defects has on the correlator I can calculate, as averaging over an ensemble of defects, the quantity of defects in the system. I shall refer to this method of counting defects as "correlator" method.

2.1 Looking for defects in the correlator

A common method (i.e. the propagator method) to find the density of defects in the field \( \phi_a \) is to assume it as a Gaussian field [5, 9, 10, 11]. Then the density of defects \( n_0 \) would be

\[
   n_0 = \frac{1}{\pi} \sqrt{-\frac{G''(0,t,t)}{G(0,t,t)}}
\]

where \( G = \langle \phi(0)\phi(x)' \rangle \) is a symmetric correlation function. This is known as Halperin's formula [6]. It expresses the density of zeros of a Gaussian field distribution in terms of its two-point function. The problem with this method is that the Gaussian estimation is exact only in early regime after which it becomes unreliable [5]. It also seems that the Gaussian approximation is most valid when number of dimensions approaches infinity [11]. Instead of using this method I shall use method devised by Anders Tranberg and Arttu Rajantie [7].
I assume that there is a one-dimensional lattice field with spacing \( a \) and each point in this field can only have values \( +v \) or \( -v \). I shall further assume there are infinitesimally thin defects, points where value of the field goes from \( +v \) to \( -v \) or vice versa, in the field with density \( n \). This means that within a length of space \( a \) the probability of defect is \( na \). I choose the field to be positive at point \( x \) which gives me

\[
G(0) = (+v) \cdot (+v) = (+v)^2. \tag{2.2}
\]

The probability that there is a defect between points \( x \) and \( x + a \) is \( na \). In this case I get

\[
G(a) = (+v) \cdot (-v) = (-v)^2 \tag{2.3}
\]

and the probability that there is no defect is \( (1 - an) \) gives me

\[
G(a) = (+v) \cdot (+v) = (+v)^2. \tag{2.4}
\]

In order to know what happens between points \( x \) and \( x + a \) I must add up all events with their probabilities giving me

\[
G(a) = na \cdot (-v^2) + (1 - na) \cdot v^2 = (1 - 2na)v^2. \tag{2.5}
\]

In the case of defects between points \( x \) and \( x + 2a \) there is a possibility of having two defects, one defect and no defects at all. In the case of two defects I get

\[
an \cdot an \cdot v^2 = (an)^2 v^2, \tag{2.6}
\]

in the case of one defect being within either of the two \( a \)’s gives

\[
an \cdot (1 - an) \cdot (-v^2) + (1 - an) \cdot an \cdot (-v^2) = -2na(1 - na)v^2, \tag{2.7}
\]

and in the case of no defects at all gives

\[
(1 - an) \cdot (1 - an) \cdot v^2 = (1 - an)^2 v^2. \tag{2.8}
\]

Similarly to the first case (2.5) I must add these up

\[
G(2a) = [(an)^2 - 2na(1 - na) + (1 - an)^2] \cdot v^2. \tag{2.9}
\]

This can be also done with distance of \( 3a \). In that case the combined equation will be

\[
G(3a) = [-(an)^3 + 3(an)^2(1 - an) - 3(an)(1 - an)^2 + (1 - an)^3] \cdot v^2. \tag{2.10}
\]

I notice that this is a binomial series and can be generalized as

\[
G(Ma,t,t) = v^2 \sum_{k=0}^{M} (-1)^k (na)^k (1-na)^{M-k} \frac{M!}{(M-k)!k!} = v^2(1-2na)^M. \tag{2.11}
\]
This equation can be changed into exponential form by choosing $Ma = |x-y|$ and letting $M$ grow to infinity

$$v^2(1 - 2na)^M = v^2 \left(1 - \frac{2n|x-y|}{M}\right)^M \xrightarrow{M \to \infty} v^2 e^{-2n|x-y|}$$  \hspace{1cm} (2.12)

and now it can be Fourier transformed from position space to momentum space

$$v^2 e^{-2n|x-y|} \to G(k, t, t) = \frac{4n}{4n^2 + k^2} v^2.$$  \hspace{1cm} (2.13)

This form of the correlator is potentially problematic. Firstly, it has similar form as the correlator of weakly coupled scalar field in thermal equilibrium

$$G_{rm}(k, t, t) = \frac{T}{k^2 + m^2}.$$  \hspace{1cm} (2.14)

Secondly, the correlator (2.13) is based on a step function and defects in my simulations are not step functions, they are hyperbolic tangent functions as shown in (1.6). To correct this I must divide out the step function and add hyperbolic tangent function.

The step function can have values of $+v$ or $-v$ and therefore it has form $v(2\theta(x-x_0) - 1)$. By Fourier transforming this I find out what it is in the Fourier transformed correlator

$$\int_{-\infty}^{\infty} dx (2\theta(x-x_0) - 1)e^{-ikx} = \frac{2}{ik}.$$  \hspace{1cm} (2.15)

Since this is the correlator and the correlator is $\langle \phi_k^{\dagger} \phi_k \rangle$ I must multiply it with its complex conjugate

$$\rightarrow \left| \frac{2}{ik} \right|^2 = \frac{4}{k^2}.$$  \hspace{1cm} (2.16)

Now I can divide out the step function defect (2.16) from the correlator (2.13) and replace it with the actual defect width $|\phi_{\text{defect}}(k)|^2$

$$G(k, t, t) = \frac{4n}{4n^2 + k^2} \frac{k^2}{4} |\phi_{\text{defect}}(k)|^2.$$  \hspace{1cm} (2.17)

Now I need to find the Fourier transformed form of the hyperbolic tangent function of equation (1.25). To describe the defect more accurately I replace $x$ with $x-x_0$ where $x_0$ is the center of the defect

$$\int_{-\infty}^{\infty} dx \tanh \frac{x-x_0}{d} e^{-ikx}.$$  \hspace{1cm} (2.18)
In order to ease calculation I replace $x - x_0$ with $y$

$$y = x - x_0 \Rightarrow \int_{-\infty}^{\infty} dy \tanh \frac{y}{d} e^{-i k y} e^{-i k x_0} = -e^{-i k x_0} \frac{1}{i k \sinh \frac{1}{2} \pi k d} \frac{1}{\sinh \frac{1}{2} \pi k d}.$$

(2.19)

Now I only have to Fourier transform this and I get

$$\phi_{\text{defect}}(k) = v \frac{2}{i k \sinh \frac{1}{2} \pi k d}.$$

(2.20)

With this I get the actual correlator

$$G(k, t, t) = 4 n^4 + k^2 \left( \frac{\frac{1}{2} \pi k d}{\sinh \frac{1}{2} \pi k d} \right)^2 v^2.$$

(2.21)

Since $d = \sqrt{2}/\mu$ and $v = \mu \cdot \sqrt{6}/\lambda$ are known, this equation has the density of defects $n$ as only free parameter.

While I am in momentum space I can take a new look at the function (2.1). $G(x, y)$ being a homogeneous function I can do following

$$G(x, y) = G(x - y, 0) = \int_k dk G(k) e^{i k (x - y)}$$

(2.22)

which in turn changes $G''$ into

$$G'' = (\partial_x)^2 \int_k dk G(k) e^{i k (x - y)} = \int_k dk G(k) \partial_x^2 e^{i k (x - y)} = -\int_k dk k^2 G(k) e^{i k (x - y)}.$$

(2.23)

Now with (2.22) and (2.23) I can make similar calculation as with (2.1)

$$n_0 = \frac{1}{\pi} \sqrt{\frac{\int d k k^2 G(k)}{\int d k G(k)}} \approx \frac{2}{\pi} \frac{\sqrt{n}}{3d}.$$

(2.24)

This shows a clear difference in the expected defect densities with mathematical model that assumes defects to be step function and one that does not (see figure 2.1). If I calculate (2.1) using (2.21) I get $n_0 \propto \sqrt{n}$ instead of $n_0 \propto n$. Therefore (2.1) cannot be correct!

To see how this method works in practice one needs to look at figures 2.2 and 2.3. Figure 2.2 is a graph of the potential field $\phi$ of a small simulation in its end phase. It shows that defects have clearly formed. Figure 2.3 shows a graph that has been generated by Fourier transforming the same data. To find the number of defects I simply have to fit the correlator (2.21) as best as I can to the given data and because $n$ is the only variable I should be able to find it after a couple of iterations.

In figure 2.3 one can clearly see that there is a hump in the beginning and it is followed by a slope. Since y-axis is logarithmic the slope gradient must be a negative exponent of some function. In other words $G$ obeys negative power of $k$ during the slope.
2.2 Other methods for counting defects

The previous method could be summarized as finding defects in the correlator or as correlator method. Since I use a fully classical model in my simulations I can also count the defects by simply examining the configuration of the potential field $\phi$ and count everything that looks like a defect. I shall refer to these kind of methods as "mechanical" methods from now on. Since actually counting the defects by hand would be slow and tedious I added a subroutine to the simulation to count them for me.

I have two kinds of methods counting defects mechanically. In the first method the subroutine counts something to be a defect when ever $\phi_0$ went from within 10% of $-v$ to within 10% $+v$ or vice versa. This is very effective especially in the final stages of the simulation as domains walls become very distinct (see figures 2.2 and 3.1). In the second method the subroutine compares two adjacent lattice points of $\phi_0$. This is done simply calculating $|\phi(x) - \phi(x+1)|$ and if the result is large enough it is reasonable to consider that there is a defect.
Figure 2.2: This is what a simulation looks at the end. The defects can clearly seen and easily counted.

Figure 2.3: This graph was generated by Fourier transforming the data that was used to plot figure 2.2. Now the density of defects can be measured by how it affects the gradient of slope. $G$ in $\log G$ is the correlator (2.21)
Chapter 3

Simulations and results

3.1 About the field evolution in the simulations

The simulations I use are one dimensional fully classical field simulations. Using one dimensional simulations has the advantage of being faster and easier to run and the results will be easier to comprehend. Since the density of topological defects should to an extent be universal regardless of the system [8] my simulations should be even more relevant. One dimension does have the disadvantage of making methods that assume field $\phi$ to be Gaussian most inaccurate when trying to find the density of defects [11].

The simulations consist of a 40960 point lattice$^*$ where each point can have any field value, but typically between $+v$ and $-v$. Time in the simulations starts from 0 and ends at 20000. Time advances in single time steps $\delta t$ and I have set it to be 0.05. Ending at moment 20000 ensures that defects have been formed when the simulations ends.

For each simulation I have to choose a quench time $\tau_Q$ and constants that are in equation of motion (1.4): a damping term $\Gamma$, a mass term $\mu$ and a coupling constant $\lambda$. The quench time $\tau_Q$ determines the moment in time when potential wall between two minima has reached its maximum, as shown in figures 1.3 and 1.4. It also affects the mass term $\mu$ as described by equation (1.7). The mass term $\mu$ determines the mass of the field fluctuations through

$$m = \sqrt{2}\mu. \quad (3.1)$$

It also determines the width of the defects through relation $d = \sqrt{2}/\mu$. The damping term $\Gamma$ removes energy from the system ensuring that the system will eventually go to zero-temperature state and guaranteeing formation and preservation of defects.

In addition to these constants I had to choose two parameters for the simulations $nI$ and $nR$. $nR$ is how many times simulations run and adds

$^*$Although size of the lattice should not change the density of defects, too small lattice might skew results. Fortunately, lattice size in my simulations is way above such numbers.
up results meaning that in end I have average over nR results. Averaging
over multiple results will give more consistent and reliable results. nI is
how many data batches the simulations handle simultaneously. This simply
makes the simulations run faster if set correctly (or slower if set incorrectly).
I set nR to be 40 and nI to be 10.

To calculate the density of defects from the simulation data I use at least
one of these methods:

1. The correlator method: In the correlator method I plot the simulation
in its final moment as $(\sqrt{k^2}, \log G)$ ($\sqrt{k^2}$ ensures that the x-axis gets
positive results). Since I use $\log G$ as the y-axis I must take logarithm
of equation (2.21) in order to get a fit. This gives

$$
\log G = \log(v^2) + \log \left( \frac{4n}{4n^2 + k^2} \left( \frac{\frac{1}{2} \pi kd}{\sinh \frac{1}{2} \pi kd} \right)^2 \right). \quad (3.2)
$$

I set $\log(v^2)$ as constant $C$ leaving the latter part of the equation (3.1)
only dependent on the density of defects $n$ in the simulation. Then I
numerically fit $\log G$ to the plot and after a few iterations get value
for $n$.

2. Mechanical methods:

(a) First mechanical method: Compare $\phi(x)$ and $\phi(x + 1)$ by sub-
tracting them from each other. Two possible outcomes are of
interest:

i) $\phi(x + 1) - \phi(x) > \mu \sqrt{\frac{6}{\lambda}}/3d = \mu^2/\sqrt{3\lambda}$

ii) $\phi(x + 1) - \phi(x) < -\mu \sqrt{\frac{6}{\lambda}}/3d = -\mu^2/\sqrt{3\lambda}$

where $d$ is width of a defect $\sqrt{2}/\mu$. Every time ii) happens after
i) or correspondingly i) happens after ii) a kink is counted.

(b) Second mechanical method: Count a defect every time when $\phi$
had value within 10% of 0 and divide result by $d = \sqrt{2}/\mu$ to
ensure that counting same defect multiple times would not skew
results.
Figure 3.1: This is an example how my simulations evolve. The top graph is earliest and further down graphs are later in the evolution. In the beginning each point of the lattice is given random initial condition. As the simulation starts to evolve points on the lattice start to choose their minima. Usually preferring same minimum at adjacent points but this depends how the constants ($\tau_Q, \Gamma, \mu, \lambda$) in the simulations have been set. As time passes more points have made their choice. As the amount of energy is constantly being reduced it becomes harder for any point to change their minima and when the quench happens, it becomes next to impossible. In the final moments energy is reduced next to nothing and defects are clearly to see.
3.2 Comparing different defect counting methods by varying the damping term $\Gamma$

The goal of these simulations is to find out possible discrepancies of my three defect counting methods I derived in chapter 2. The quench time $\tau_Q$ is set to 0 meaning that the simulation starts with the two minima already divided by the maximum potential wall. The mass term $\mu$ is set to 0.1 and the coupling constant $\lambda$ is set to 0.6. In each simulation the damping term $\Gamma$ is different. It has eleven different values beginning from 0.0003125 doubling in every subsequent simulation reaching 0.32. This will give result that can be plotted logarithmically showing possible differences more clearly than a linear plot would.

The exact results of the simulation can be seen in the appendix A table A.1 and I have plotted them in figure 3.2. In the plot clear differences between the mechanical methods and the correlator method can be seen but the mechanical methods give nearly identical results. This tells me that for some reason using the correlator method tends to detect up to 2% more defects than the mechanical methods. Now it could be that both the mechanical methods are wrong but given that they do give such similar results makes that unlikely.

The reason for the correlator method for giving different results could be that the density of defects is so high that the defects are too close to each other and no longer have the hyperbolic tangential profile assumed in the derivation of the method. Hidden assumption made during derivation of the correlator method is that distance between defects is larger than the width $d$ of defects. If this is not the case erroneous results are bound to occur.
Figure 3.2: This graph shows clear difference between the methods. It also shows how similar results the mechanical methods gave. $\mu = 0.1$, $\lambda = 0.6$, $\tau_Q = 0$ and $\Gamma$ has values 0.0003125, 0.000625, 0.00125, 0.0025, 0.005, 0.01, 0.02, 0.04, 0.08, 0.16, 0.32.
3.3 Varying the quench time \( \tau_Q \) and the damping term \( \Gamma \)

The goal of these simulations is to study how varying the quench time \( \tau_Q \) and the damping term \( \Gamma \) affects the density of defects \( n \). According to the KZM, the results of these simulations should follow the power law \( n \sim \tau_Q^\sigma \) where \( n \) is the density of defects, \( \tau_Q \) is the quench time, \( \sigma \) is the constant exponent that should be same regardless of number of dimensions [12] (or even the type of system that is being observed).

The mass term \( \mu \) is set to 0.7 and the coupling constant \( \lambda \) is set to 0.1. The damping term \( \Gamma \) and the quench time \( \tau_Q \) differ in each simulation. The damping term has seven values starting from 0.001 and doubling until it reaches 0.064 and quench time has values 5, 10, 20, 40, 80, 160, 320, 500, 1000, 1500, 2000, 2500. I expect that at higher values of quench time something more interesting would happen requiring more data points to understand.

The exact results of the simulation can be seen in the appendix A table A.2 and I have plotted them in figure 3.3. What I discover is that it is not possible to derive any kind of sensible power law at least with my configurations. It seems that the KZM does not apply when the damping term is very low. Only when a certain "tipping point" has been reached the KZM starts to apply. This kind of results are seldom seen [6].

When considering the results one should keep in mind that the damping effects mostly after the transition. The damping is effective for time \( t \), so that \( \Gamma t > 1 \). The anomalous curve can be explained by very small damping term. As the simulation has lots of energy the defects have time to unwind themselves (or annihilate). This is why the density of defects goes down at fixed quench time as damping decreases. As the damping term gets bigger it will damp initial fluctuations away before the symmetry breaking takes place. This is why the density of defects goes up when the quench time is large and the damping is decreased. As a general rule, when the symmetry breaking slows down, the density of defects goes down, exception being with very small damping terms it seem to go up.

An interesting side result can be seen if one plots logarithmically every value of the damping term with respect to the defect density (\( \log \Gamma, n \)). Clear pattern can be seen in figure 3.4. This implies that there is some kind of function \( f(x) = a + b \log \Gamma \) that can predict the limits where the KZM applies.
Figure 3.3: This graph shows clear differences in the defect densities when the damping term is varied over different quench times. $\mu = 0.7$, $\lambda = 0.1$ and $\tau_Q$ has values 5, 10, 20, 40, 80, 160, 320, 500, 1000, 1500, 2000, 2500.

Figure 3.4: Here on red is plotted $(\log \Gamma, n)$ where $n$ is the highest density of defects for that damping term. Green graph is made with equation $f(x) = a + b \log \Gamma$ where $a = 0.0325596$ and $b = 0.002914$. Values for $a$ and $b$ were gained by numerical iteration. For values for defect density see table A.2 in appendix A.
Chapter 4

Conclusions

In the third chapter I ran two series of one dimensional simulations with slightly different constants (mass term $\mu$, coupling constant $\lambda$) and significantly differing constants (damping term $\Gamma$, quench time $\tau_Q$). The results of the first series of simulations show that the correlator method is a really good approximation with errors of a few percent. Results of the second series of simulations shows possible limitations for the KZM. Anyone who wishes to study topological defects formation and density should take these results into consideration.

The first series of simulations shows that for some reason using the correlator for counting the density of defects gives results that are bigger than the two mechanical counting methods give, up to 2%. This was not expected. One possible reason for this discrepancy is the hidden assumption that each defect has width $d$. If there were multiple defects within space of a single $d$ it would count only as a single defects. This hypothesis is supported by the fact that discrepancy between the methods grew as number of defects grew.

The second series of simulations produced surprising results which seem to contradict the Kibble-Zurek power law $n \sim \tau_Q^\rho$ predicted by the KZM or at least put some constraints where it can be applied. For very small damping terms the defect density seemed to peak at some point and only after that point the power law seemed to work. As a side result plotting these peaks for each damping term gave a simple equation for predicting limits for the KZM. To find out how mass or the coupling constant affects this possible limit for the KZM further simulations are needed. However, these constraints might not have significant effect for cosmological observations or condensed matter experiments if the real world parameters never go outside range where the KZM still works.

It would be simple to improve and expand the results of this thesis. With more simulations the errors caused by using the correlator method could be confirmed and mapped and if the errors would prove to be systematic then additional simulations could be used to calibrate it. Additional simulations
would be also useful for mapping possible limitations for the KZM with different mass terms and coupling constants. Indeed, detailed study of possibly limits of the KZM could discover significant limits in its applicability. In any case, from now on people should be wary when relying simply to the correlator for finding the density of defects.
Appendix A

The simulation data

<table>
<thead>
<tr>
<th>$\Gamma$</th>
<th>$n_1$</th>
<th>$n_2$</th>
<th>$n_3$</th>
</tr>
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<td>0.000623411</td>
<td>946</td>
<td>9.567155e+02</td>
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<td>2799</td>
<td>2.821710e+03</td>
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</tr>
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Table A.1: These are the results for the simulation where I measured the number of defects with different methods. In this simulation $\tau_Q = 0$, $\mu = 0.1$ and $\lambda = 0.6$. Note that $n_1$ is the density of defects where as $n_2$ and $n_3$ are the actual number of defects. In order to get the density of defects for $n_2$ and $n_3$ one must divide with $40*40960$ where 40960 is size of lattice and 40 is number of data batches that have been added together. (See 3.1 or appendix C for further details.)
Table A.2: Here are the defect density results for the simulations where the quench time $\tau_Q$ and the damping term $\Gamma$ were given varied values. The results marked with asterisk are the highest value the density of defects has (These are used in figure 3.3). In this simulation $\mu = 0.7$ and $\lambda = 0.1$. The result for when $\Gamma = 0.016$ and $\tau_Q = 320$ has been lost and could not be recovered.

<table>
<thead>
<tr>
<th>$\tau_Q$</th>
<th>$\Gamma = 0.001$</th>
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<th>$\Gamma = 0.004$</th>
<th>$\Gamma = 0.008$</th>
<th>$\Gamma = 0.016$</th>
<th>$\Gamma = 0.032$</th>
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## Appendix B

### Derivations of certain equations

#### B.1 Zurek’s derivations for correlation lengths

In order to find the characteristic correlation length $\hat{\xi}$ I need to find the correlation length $\xi$ at moment $\hat{t}$ when the phase transition happens i.e. when $T = T_c$ where $T$ is the temperature of the system and $T_c$ is the critical temperature. This is because in the cosmological unit system ($\hbar = c = k_B = 1$) the correlation length and the relaxation time $\tau$ have same value, 

$$\tau(t) = \xi(t) = \frac{1}{\sqrt{\abs{\alpha}}} \left( \sim \frac{1}{\sqrt{\epsilon}} \right) \Rightarrow \hat{\xi} = \tau(\hat{t}) = \hat{t} \quad \text{(B.1)}$$

where $\epsilon$ is the relative temperature $\epsilon = (T - T_c)/T_c$ and $\alpha$ is the coefficient in Landau-Ginzburg model (see page 4.). The relaxation time can be expressed as $\tau = \tau_0/\sqrt{\abs{\epsilon}}$ and the quench time as $\tau_Q = t/\epsilon$. This gives

$$\hat{t} = \tau(\hat{t}) = \tau_0/\sqrt{\abs{\epsilon}} = \tau_0/\sqrt{\hat{t}/\epsilon} \Rightarrow \hat{t} = \tau_0^{2/3} \tau_Q^{1/3}. \quad \text{(B.2)}$$

Since the equation of state for the early Universe is dominated by radiation, the rate of phase transition is determined by the relation

$$T\hat{t}^2 = \Delta M_{PL} \quad \text{(B.3)}$$

where $t$ is time since ”big bang”, $M_{PL}$ is the Planck mass and $\Delta$ depends on the effective number of different spin states $s$ of relativistic particles

$$\Delta = 1/(4\pi) \cdot \sqrt{45/(\pi s)}. \quad \text{(B.4)}$$
With (B.2) I can determine value for $\tau_Q$

$$\frac{1}{\tau_Q} = \epsilon \Rightarrow \frac{de}{dt} \frac{dT}{dt} \frac{1}{T_c} = \frac{d}{dt} \sqrt{\frac{\Delta M_{PL}}{T_c}} \frac{1}{T_c} = -\frac{1}{2} \sqrt{\Delta M_{PL} t^{-3/2}} \frac{1}{T_c}$$  \hspace{1cm} (B.5)

$$= -\frac{1}{2} \sqrt{\Delta M_{PL}} \left( \frac{\Delta M_{PL}}{T_c^2} \right)^{-3/2} \frac{1}{T_c} = -\frac{1}{2} \frac{T_c^2}{\Delta M_{PL}} \Rightarrow \frac{(\Delta M_{PL})}{T_c^2} = \tau_Q.\$$

$\tau_0$ can be evaluated with approximation $\alpha/\epsilon \approx \beta T_c^2$ as

$$\tau = \frac{1}{\sqrt{|\alpha|}} = \frac{\tau_0}{|\epsilon|} \Rightarrow \tau_0 = \sqrt{\frac{\epsilon}{\alpha}} \approx \frac{1}{\sqrt{\beta T_c^2}} = \frac{1}{\sqrt{\beta T_c}}.  \hspace{1cm} (B.6)$$

Now I can simply insert $\tau_Q$ and $\tau_0$ to equation (B.2) and get $\xi$

$$\dot{\xi} = \frac{1}{(\beta^{1/2} T_c)^{2/3}} \frac{1}{T_c^{1/3}} \left( \frac{2 \Delta M_{PL}}{T_c} \right)^{1/3} = \frac{1}{\beta^{1/3} T_c} \left( \frac{2 \Delta M_{PL}}{T_c} \right)^{1/3} = \xi. \hspace{1cm} (B.7)$$

### B.2 Derivation of equation of motion (1.4)

From (1.1) I get one dimensional action

$$S = \int dx dt \left( \frac{1}{2} (\partial_t \phi_a)^2 - \frac{1}{2} (\partial_x \phi_a)^2 - V(\phi_a) \right). \hspace{1cm} (B.8)$$

With small variations this turns in to

$$\delta S = \int dx dt \left( \frac{1}{2} 2 \partial_t \phi_a \partial_t (\delta \phi_a) - \frac{1}{2} 2 \partial_x \phi_a \partial_x (\delta \phi_a) - V'(\phi_a) \delta (\phi_a) \right) = 0. \hspace{1cm} (B.9)$$

With partial integration I can get the partial derivatives out of the integral

$$\int dt \partial_t \phi_a \partial_t (\delta \phi_a) = -\int dt \partial_t^2 \phi_a (\delta \phi_a) + \partial_t \phi_a (\delta \phi_a). \hspace{1cm} (B.10)$$

I assume that $\delta \phi_a$ outside integral is very small and thus I can simplify the equation to

$$\int dt \partial_t \phi_a \partial_t (\delta \phi_a) = -\int dt \partial_t^2 \phi_a (\delta \phi_a). \hspace{1cm} (B.11)$$

This applies to the partial derivatives of $x$ giving me

$$\delta S = \int dx dt \left( -\partial_t^2 \phi_a (\delta \phi_a) + \partial_x^2 \phi_a (\delta \phi_a) - V'(\phi_a) \delta (\phi_a) \right) = 0. \hspace{1cm} (B.12)$$

To find out what $V'(\phi_a)$ is I take (1.3) and derive it with $\phi_a$

$$V'(\phi_a) = -\frac{1}{2} \mu^2 2 \phi_a (\delta \phi_a) + \frac{\lambda}{24} (\phi_a \phi_b) \phi_a (\delta \phi_a). \hspace{1cm} (B.13)$$

When this is inserted back to (B.12) I get

$$-\partial_t^2 \phi_a + \partial_x^2 \phi_a + \mu^2 \phi_a - \frac{\lambda}{6N} (\phi_b \phi_b) \phi_a = 0. \hspace{1cm} (B.14)$$

All that needs to be done is change the signs and add the damping term $\Gamma \partial_t \phi$ and I get the equation of motion (1.4).
B.3 Derivation of shape of defect (1.6)

I start with the equation (B.14) assuming that $-\partial_t^2 \phi_a = 0$ and with rearranging it gives me

$$\partial_x^2 \phi_a(x, t) = -\mu^2 \phi_a(x, t) + \frac{\lambda}{6N} (\phi_b \phi_b) \phi_a(x, t)$$

(B.15)

$$\Rightarrow \phi_a''(x) = \left( -\mu^2 + \frac{\lambda}{6N} \phi_a^2(x) \right) \phi_a(x)$$

(B.16)

If I denote

$$g(y) = \sqrt{\frac{\lambda}{6N\mu^2} \phi_a(x)}$$

(B.17)

and

$$x = \frac{1}{\mu} y \Rightarrow \frac{\partial^2}{\partial x^2} = \mu^2 \frac{\partial^2}{\partial y^2}$$

(B.18)

and apply these to (B.16) gives me

$$\mu^2 \frac{\partial^2}{\partial y^2} g(y) \sqrt{\frac{6N\mu^2}{\lambda}} = \left( -\mu^2 + \frac{\lambda}{6N} \frac{6N\mu^2}{\lambda} g^2(y) \right) g(y) \sqrt{\frac{6N\mu^2}{\lambda}}$$

(B.19)

$$\Rightarrow g''(y) + \left( 1 - g^2(y) \right) g(y) = 0.$$  

(B.20)

Now I guess that the field $\phi_a$ behaves like a hyperbolic tangent and try to solve (B.20) with ansatz $g(y) = A \tanh(By^\alpha)$. This gives me

$$ABy^{-2+\alpha} \alpha (-1 + \alpha) \frac{1}{\cosh^2(By^\alpha)}$$

(B.21)

$$-2AB^2 y^{-2+2\alpha} \alpha^2 \frac{1}{\cosh^2(By^\alpha)} \tanh(By^\alpha)$$

$$+ \left( 1 - (A \tanh(By^\alpha))^2 \right) A \tanh(By^\alpha) = 0.$$  

(B.22)

I choose $\alpha = 1$ and this simplifies the equation to

$$2AB^2 \frac{\tanh(By)}{\cosh^2(By)} = \left( 1 - (A \tanh(By))^2 \right) A \tanh(By).$$

(B.23)

I divide with $A \tanh(By)$ and use the identity $1 - \tanh^2 x = 1/\cosh^2 x$ and get

$$2B^2 \left( 1 - \tanh^2(By) \right) = \left( 1 - (A \tanh(By))^2 \right).$$

(B.24)

This means that $B = 1/\sqrt{2}$ and $A = 1$. Inserting these back to the ansatz and (B.17) gives me

$$\sqrt{\frac{\lambda}{6N\mu^2}} \phi_a(x) = g(y) = g(x/\mu) = \tanh \frac{x}{\sqrt{2}\mu}$$

(B.24)
\[ \Rightarrow \phi_a(x) = \tanh \left( \frac{x}{d} \right) \sqrt{\frac{6N\mu^2}{\lambda}} \]  
\[ \text{where } d = \sqrt{2}/\mu \text{ is width of defect. } N=1 \text{ and } \tanh(\pm \infty) = \pm 1 \text{ and highest and lowest value field } \phi_0 \text{ can have are } \pm v \text{ thus I get} \]
\[ \phi_0(\pm \infty) = \pm v = \pm \sqrt{\frac{6}{\lambda}} \mu. \]

\section*{B.4 Derivation of classical thermal equilibrium}

I start with following field
\[ \phi_k = \frac{(a_k e^{-i\omega_k t} + a_k^\dagger e^{i\omega_k t})}{\sqrt{2\omega_k}} \]  
\[ \text{where } a_k \text{ and } a_k^\dagger \text{ are creation/annihilation operators, } \omega_k = \sqrt{k^2 + \mu^2}, \mu \text{ is the mass and } k \text{ is the momentum. This gives me correlator} \]
\[ \langle \phi_k^\dagger \phi_k \rangle = \frac{n_k + 1}{\omega_k}. \]

Here \( a_k^\dagger a_k = n_k, a_k a_k^\dagger = n_k + 1 \) and \( n_k \) is occupation number. Since I’m using classical equations I can drop 1/2 and get
\[ \langle \phi_k^\dagger \phi_k \rangle = \frac{n_k}{\omega_k}. \]

Bose-Einstein gives me for energy states
\[ n_k = \frac{1}{e^{\frac{\omega_k}{T}} - 1} \]
and since I am using classical theory I let the temperature \( T \) got to infinity and then approximate
\[ \frac{1}{e^{\frac{\omega_k}{T}} - 1} \approx \frac{1}{(1 + \frac{\omega_k}{T}) - 1} = \frac{T}{\omega_k}. \]

Inserting this to the equation (B.29) I get
\[ \langle \phi_k^\dagger \phi_k \rangle = \frac{n_k}{\omega_k} = \frac{T}{\omega_k^2} = \frac{T}{k^2 + m^2} = G_{rm}(k, t, t) \]

Which is the classical thermal equilibrium.
Appendix C

Simulation code

Here is description of the computer code used in the simulations of this thesis. It is written in C and its original author is Anders Tranberg. I made certain minor modifications to code he wrote and one major one which is the subroutine that counts defects while simulation is running.

I will use a pseudo-code to describe the actual code. This will make following description easier and makes it easier for reader to implement same program on programming language of her or his choosing. Structure of program following:

1. start of the simulation and [α] for(nR)-loop

In the beginning of the simulation certain variables must be defined or loaded from an external configuration file. These variables are the initial conditions per batch $nI$, the number of batches $nR$, size of the simulation lattice $nx^*$, the mass $\mu$, the coupling constant $\lambda$, the damping term $\Gamma$, the quench time $\tau_Q$, seed for the pseudo-random generator† $\text{theseed}$, the time step $\delta t$ and the

*It is important to note that in my pseudo-code $nx$ does not mean $n \cdot x$ but simply means the lattice size variable 'nx'.

†Pseudo-random generator I used was Mersenne twister (http://en.wikipedia.org/wiki/Mersenne_twister)
moment when simulation ends \( t_{\text{stop}} \). In addition to these two special plan-
variables \( \text{planen} \) and \( \text{planen}_2 \) are needed for fast Fourier transformation\(^*\).

Simulation also needs two output files and certain arrays. Output files are \textit{corrfile} and \textit{kinkfile} which function and content will be explained later. Arrays are four \textit{fftw} complex type \( \text{ar1}[nx] \), \( \text{ar2}[nx] \), \( \text{ar3}[nx] \) and \( \text{ar4}[nx] \), arrays for the field \( \phi(x) \), \( F[nI][nx] \), and its time derivative \( \dot{\phi}(x) \), \( P[nI][nx] \), and arrays \( \text{cor}_\text{sum}[nx] \) and \( \text{cor}_\text{sum2}[nx] \) that are needed for \textit{get_correlator} subroutine.

After defining or loading the variables from configuration files the sim-
ulation creates pseudo random number and enters for(\( nR \))-loop (\( \beta \)). This
loop will be executed \( nR \)-times and it is only time the variable \( nR \) will be
used.

In the second step the simulation time \( t \) and the counter for making data
dump are set (back) to zero and the field \( \phi(x) \) and its time derivative \( \dot{\phi}(x) \)
are (re)initialized.

**[2] initial\_conditions subroutine**

Every element of arrays \( \text{ar1}[nx] \) and \( \text{ar2}[nx] \) are set to \( 0+i0 \) and go through
every point of the field \( \phi(x) \) (except when \( x = 0 \) and \( x = nx/2 \)). If \( 2 - 2\cos(2\pi \cdot x/nx) < \mu^2 \), then

\[
\begin{align*}
\text{ar1}[x].re &= \sqrt{-2\log n_1 \sin(2\pi n_2) / \sqrt{\omega/4}} \\
\text{ar1}[x].im &= \sqrt{-2\log n_1 \cos(2\pi n_2) / \sqrt{\omega/4}} \\
\text{ar2}[x].re &= \sqrt{-2\log n_3 \sin(2\pi n_4) / \sqrt{\omega/4}} \\
\text{ar2}[x].im &= \sqrt{-2\log n_3 \cos(2\pi n_4) / \sqrt{\omega/4}}
\end{align*}
\]

where \( \omega = \sqrt{2 - 2\cos(2\pi \cdot x/nx) + 0.5(\sqrt{2}\mu)^2} \) and \( n_1 \), \( n_2 \), \( n_3 \) and \( n_4 \) are random numbers so that \( n_1 \neq n_2 \) and \( n_3 \neq n_4 \). In the case when \( x = 0 \) or \( x = nx/2 \) then

\[
\begin{align*}
\text{ar1}[x].im &= \text{ar2}[x].im = 0 \\
\text{ar1}[x].re &= \sqrt{2} \cdot \text{ar1}[x].re \\
\text{ar2}[x].re &= \sqrt{2} \cdot \text{ar2}[x].re
\end{align*}
\]

This is followed of flipping arrays \( \text{ar1} \) and \( \text{ar2} \) around (Here mod is modulo operator.):

\[
\begin{align*}
\text{ar1}[(nx - x) \mod nx].re &= \text{ar1}[x].re \\
\text{ar1}[(nx - x) \mod nx].im &= -\text{ar1}[x].im \\
\text{ar2}[(nx - x) \mod nx].re &= \text{ar2}[x].re \\
\text{ar2}[(nx - x) \mod nx].im &= -\text{ar2}[x].im
\end{align*}
\]

\(^*\)I use FFTW package in my Fourier transformations(http://www.fftw.org/). Planen is a data structure containing all the information that FFTW needs in order to compute the 1D Fourier transform. FFTW also needs one dimensional \textit{fftw} complex type arrays where each element has real and imaginary part, \textit{ar}[\text{nx}]=\textit{ar}[\text{nx}].re+\textit{ar}[\text{nx}].im.
Fourier transforming these arrays will give initial values for $\phi(x)$ and $\dot{\phi}(x)$.

$$\phi(x) = ar3/\sqrt{n}\times = \int_{-\infty}^{\infty} ar1[x]e^{2\pi i x k}/\sqrt{n}\times$$
$$\dot{\phi}(x) = ar4/\sqrt{n}\times = \int_{-\infty}^{\infty} ar2[x]e^{2\pi i x k}/\sqrt{n}\times$$

[β] do while -loop

Then begins do-while loop where the time $t$ advances from 0 to $t_{stop}$ in time step $\delta t$ increments. In beginning of this loop the field $\phi(x)$ is iterated by iterate subroutine and one is added to the dstep counter. If $dstep = if\_dump$ then get_correlator and kink_counts subroutines are triggered and dsteps is returned to 0.

[3] iterate subroutine

First, to every point of $\phi(x)$ will be added $\delta t \cdot \dot{\phi}(x)$ then every point of $\dot{\phi}(x)$ will be changed as follows:

$$\dot{\phi} := \frac{1.0}{1.0 + \Gamma \delta t} \left( \dot{\phi} - \left( \delta t (2.0 + \mu_r) + \delta t \frac{\lambda}{6.0} \right) \phi + \delta t \left( \phi(x+1) + \phi(x-1) \right) \right)$$

(C.1)

where if $\tau_Q > 0.0$ then $\mu_r$ will be $0.5 \cdot (\sqrt{2})^2 \mu^2 \cdot (1-t/\tau_Q)$. If $\tau_Q \leq 0.0$ or $t > 2\tau_Q$ then $\mu_r = -0.5\mu^2$. $\phi(x)$ is considered to be circular so that the last and the first point of the field $\phi(x)$ are adjacent of each other.

[4] get_correlator subroutine

Subroutine starts by searching for corr_file and if it finds one it loads values for ksqu[x], ksqu2[x], cor_sum[x], cor_sum2[x] from it. If corr_file is not found every element of arrays cor_sum[x] and cor_sum2[x] are set to zero. What follows will happen for both cases of previous corr_file existing and not. Difference being that if previous corr_file exist the data will be added to it.

After finding/not finding corr_file array ar1[x] will be set to ar1[x].re:=F[x] and ar1[x].im=0. After this it ar1[x] will be Fourier transformed:

$$\phi(x) = ar2[x]/\sqrt{n}\times = \int_{-\infty}^{\infty} ar1[x]e^{-2\pi i x k}/\sqrt{n}\times.$$

With this Fourier transformed array ar2[x] arrays cor_sum[x] and cor_sum2[x] are given values

$$cor\_sum[x] = (ar2[x].re)^2 + (ar2[x].im)^2$$
$$cor\_sum2[x] = ((ar2[x].re)^2 + (ar2[x].im)^2)^2$$

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and ksqu\[x\] and ksqu2\[x\] are given values:

\[
ksqu[x] = 2 - 2 \cos(2\pi \cdot x/nx)
\]

\[
ksqu2[x] = (2\pi \cdot x/nx)^2.
\]

After this ksqu\[x\], ksqu2\[x\], cor_sum\[x\] and cor_sum2\[x\] will be written to corr file output file. Name of the file will be corr[t].dat where [t] is current value of time t.

[4]kink_counts subroutine

This subroutine goes through \(\phi(x)\) looking for kinks in two different manners. In first method two adjacent points of \(\phi(x)\) are compared by simply subtracting from each other. Two possible outcomes are interest to me:

a) \(\phi(x + 1) - \phi(x) > \mu \sqrt{2/3}d = \mu^2/\sqrt{3}\lambda\)

b) \(\phi(x + 1) - \phi(x) < -\mu \sqrt{2/3}d = \mu^2/\sqrt{3}\lambda\)

where \(d\) width of kink \(\sqrt{2}/\mu\). Every time b) happens after a) and correspondingly a) happens after b) kink is counted. In second method it is considered as kink when \(|\phi(x)| < 0.1\). Number of kinks must be divided by \(0.2 \cdot \sqrt{2}/\mu\) which is average width of kink. This prevents same kink to be counted multiple times. These results will be printed in kink file. All results of these measurements are printed in to the same file.

[5]after t_stop

This section only prints out status reports.

[6]program ends

Here the program closes all files and prints out final report and the program ends.
Bibliography